Systematic Inclusion of High-Order Multispin Correlations for the Spin-$\frac{1}{2}$ XXZ Models

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We apply the microscopic coupled-cluster method (CCM) to the spin-$\frac{1}{2}$ XXZ models on both the one-dimensional chain and the two-dimensional square lattice. Based on a systematic approximation scheme of the CCM developed by us previously, we carry out high-order *ab initio* calculations using computer-algebraic techniques. The ground-state properties of the models are obtained with high accuracy as functions of the anisotropy parameter. Furthermore, our CCM analysis enables us to study their quantum critical behavior in a systematic and unbiased manner.

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Over the last few years the microscopic coupled-cluster method (CCM) [1] has successfully been applied to many lattice Hamiltonian systems [2–5], producing the best or among the best results in terms of accuracy and power. For example, in the so-called SUB2 approximation discussed below, the exact analytic solution of the corresponding CCM equations often exhibits a terminating point. This is clearly demonstrated [3] to correspond to a physical critical point of the system by the behavior within the same approximation of such calculated quantities as the order parameter, correlation functions, and the gap in the excitation spectrum. Recently we have developed several efficient, systematic approximation schemes of the CCM specifically tailored for use with lattice systems [3,4].

In this Letter, we report our new results from an *ab initio* high-order calculation for the spin-$\frac{1}{2}$ XXZ model on both the one-dimensional chain (1DC) and the two-dimensional square lattice (2DSL). In particular, we have obtained with high accuracy the ground-state energy, the anisotropic susceptibility (i.e., the second-order energy derivative with respect to the anisotropy parameter), and the staggered magnetization, as functions of the anisotropy parameter. Furthermore, since these physical quantities are obtained as functions of the anisotropy parameter, we are able to study the possible quantum phase transitions of the anisotropic models in a systematic, unbiased manner. This is in contrast to the series expansion technique [6], in which one has to make a Padé approximation or to assume a particular critical behavior (from the spin-wave theory of Anderson [7], for example) for those physical quantities from the outset.

Since the details of our CCM analysis have been published elsewhere [3], we only outline the specific approximation schemes employed here. The spin system under consideration is the so-called spin-$\frac{1}{2}$ XXZ model described by the following Hamiltonian:

$$H = \frac{1}{2}\sum_{l=1}^{N}\sum_{\rho=1}^{z}\left[\Delta s_l^z s_{l+\rho}^z + \frac{1}{2}(s_l^+ s_{l+\rho}^- + s_l^- s_{l+\rho}^+)\right], \quad (1)$$

where the index l runs over all N ($\rightarrow \infty$) lattice sites with the usual periodic boundary condition imposed, the index ρ runs over all z nearest-neighbor sites, the operators s_l^z and $s_l^{\pm}$ ($\equiv s_l^x \pm i s_l^y$) are spin operators, and Δ is the anisotropy parameter. The special case $\Delta = 1$ gives the isotropic Heisenberg model, which, with spin $s = \frac{1}{2}$ on the 2DSL, has been under intensive study over the last six years or so [8].

We first consider the case of $\Delta \rightarrow \infty$. Equation (1) then reduces to the Ising model with a classical ground state (i.e., the Néel state) given by two alternating sublattices, one with all spins down, the other with all spins up. For clarity, we use the index $\{i\}$ exclusively for the spin-down sublattice and the index $\{j\}$ exclusively for the spin-up sublattice. Naturally, we choose the Néel state as the model state $|\Phi\rangle$ in our CCM analysis and incorporate the quantum correlation effects by considering the excitations with respect to this model state. The elementary operators of these excitations are clearly given by the spin-raising operators s_i^+ on the i sublattice and the spin-lowering operators s_j^- on the j sublattice. The CCM ansatz for the ground ket state is therefore given by

$$|\Psi_g\rangle = e^S|\Phi\rangle, \quad S \equiv \sum_{n=1}^{N/2} S_{2n}, \quad (2)$$

with the correlation operators S_{2n} defined by

$$S_{2n} = \frac{(-1)^n}{(n!)^2}\sum_{i_1,i_2,\ldots,i_n}\sum_{j_1,j_2,\ldots,j_n} S_{i_1 i_2 \ldots i_n, j_1 j_2 \ldots j_n} \times s_{i_1}^+ s_{i_2}^+ \cdots s_{i_n}^+ s_{j_1}^- s_{j_2}^- \cdots s_{j_n}^-, \quad (3)$$

where we have restricted ourselves to the conserved sector of zero z component of total spin, s_{total}^z ($\equiv \sum_{l=1}^{N} s_l^z$), by including only those configurations with equal numbers of spin flips on both sublattices.

The ground-state energy and the c-number coefficients $\{S_{i_1 \ldots i_n, j_1 \ldots j_n}\}$ of Eq. (3) are determined by taking the inner products of the Schrödinger equation in the form $e^{-S}He^S|\Phi\rangle = E_g|\Phi\rangle$, first with the model state itself and second with the states constructed by acting on $|\Phi\rangle$ with

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the corresponding correlation operators in S_{2n}. We thus find, respectively, the ground-state energy E_g,

$$E_g = \langle\Phi|e^{-S}He^{S}|\Phi\rangle, \tag{4}$$

and the coupled set of equations for $\{S_{i_1\ldots i_n,j_1\ldots j_n}\}$,

$$\langle\Phi|s^-_{i_1}s^-_{i_2}\cdots s^-_{i_n}s^+_{j_1}s^+_{j_2}\cdots s^+_{j_n}e^{-S}He^{S}|\Phi\rangle = 0, \tag{5}$$

with $n = 1,2,\ldots,N/2$.

Each of the above equations always involves the Hamiltonian in a similarity-transformed form, namely,

$$e^{-S}He^{S} = H + [H,S] + \frac{1}{2!}[[H,S],S] + \cdots, \tag{6}$$

where the expansion series terminates at the fourth order [3]. Therefore, once an approximation for S is chosen, no further approximation is necessary in order to obtain and solve the coupled set of Eqs. (5). For the spin-$\frac{1}{2}$ XXZ model of Eq. (1), it is easy to derive the following exact equation for the ground-state energy per spin:

$$\frac{E_g}{N} = -\frac{z}{8}(\Delta + 2b_1), \tag{7}$$

where $b_1 \equiv S_{i,i+\rho}$ is the nearest-neighbor pair correlation coefficient, and $z = 2,4$ for the 1DC and 2DSL models, respectively. We note that b_1 is independent of both the index i and index ρ by the lattice symmetries.

We clearly need an approximation method to truncate S for any practical calculation. The three most commonly used truncation methods are the SUBn scheme, in which all correlations involving only n or fewer spins are retained; the simpler SUBn-m subapproximation scheme, where only SUBn correlations spanning a range of no more than m adjacent lattice sites are included, and finally the systematic local LSUBm scheme, which includes all possible multispin correlations over a specified locale on the lattice, where m is the nominal index that characterizes the size of the given locale. In each case, the remaining correlation coefficients are set to zero. For example, the LSUB4 scheme for the 1D spin-$\frac{1}{2}$ model retains three independent configurations, represented by b_1, b_3, and g_4, respectively [3]. In particular, b_1 corresponds to the nearest-neighbor two-spin-flip configuration mentioned before, b_3 to the third-nearest-neighbor two-spin-flip configuration, and g_4 to the spin-flip configuration of four adjacent spins. The corresponding LSUB4 coupled equations are given by [3]

$$1 - 2\Delta b_1 - 3b_1^2 + 2b_1b_3 + 2b_3^2 + 2g_4 = 0, \tag{8}$$

$$b_1^2 - 4\Delta b_3 - 4b_1b_3 + g_4 = 0, \tag{9}$$

$$-\Delta(b_1^2 + 2b_1b_3) + g_4(\Delta + 4b_1 + b_3) + 2b_1b_3^2 = 0. \tag{10}$$

After solving these coupled equations, we obtain the ground-state energy by substituting b_1 into Eq. (7).

For the higher-order approximations the derivation of the coupled equations becomes very tedious. We have developed our own software using C++ and FORTRAN to automate this process. Also, we have used standard computer algebra packages to check our results independently. For the LSUBm schemes, we have derived and solved the coupled equations up to $m = 10$ for the 1DC case and up to $m = 6$ for the 2DSL case. It should be noted that all of our calculations were done on microcomputers. The numbers of independent spin-flip configuration coefficients retained in the these two cases are 81 and 72, respectively.

Some of our results for the 1DC model have already been published [3]. In particular, we have shown that for a given value of m the LSUBm scheme reproduces exactly the corresponding $2m$th order of large-Δ perturbation theory and that the LSUBm scheme also gives good results in the planar region ($|\Delta| < 1$) where perturbation theory is not valid. The new high-order calculations further push the numerical results closer to their exact counterparts obtained by the Bethe ansatz [9], over a wide range of Δ ($0 < \Delta < \infty$). In particular, at the isotropic point ($\Delta = 1$), the LSUB10 scheme yields -0.4420 for the ground-state energy per particle. We have made a naive attempt to extrapolate our results for the LSUBm scheme with $m = 4,6,8,10$, and find that a $1/m^2$ rule seems to fit them very well. The ground-state energy per particle after this extrapolation yields -0.4431 ± 0.0001 from a least-squares fit, while the exact result by the Bethe ansatz [9] is -0.4432 to the accuracy of four significant figures.

In Fig. 1 we show some of our results for the ground-state energies of the 2DSL model, together with a

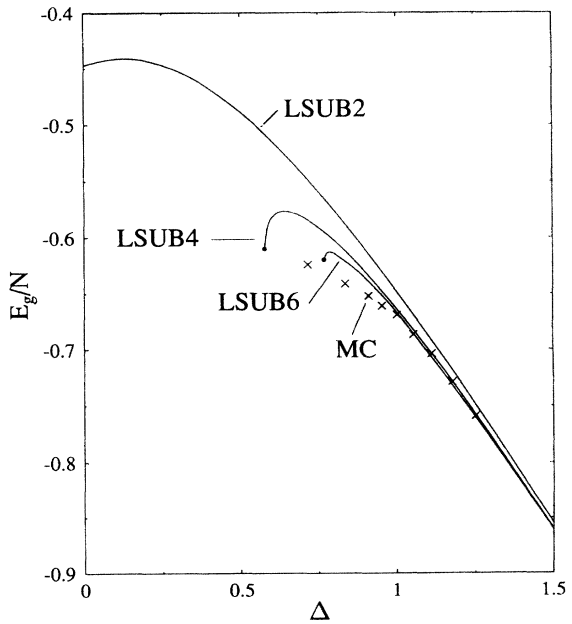

FIG. 1. Ground-state energy per spin as a function of Δ for the spin-$\frac{1}{2}$ XXZ model on the 2DSL. Shown are the numerical results of the LSUBm scheme with $m = 2,4,6$ and of a Monte Carlo calculation of Ref. [10].

Monte Carlo calculation [10] on an 8×8 lattice for comparison. One sees that the results for our high-order calculations are in excellent agreement with the Monte Carlo calculations over a wide range. At the isotropic point ($\Delta = 1$), our best numerical results for the ground-state energy of the 2DSL model, obtained from the LSUB6 scheme, is -0.6670. We find that the $1/m^2$ rule also fits our 2D LSUBm data well. The extrapolated result is -0.6691 ± 0.0003. This number compares well with the values $-0.669\,34 \pm 0.000\,04$ from a large-scale Monte Carlo calculation by Runge [11] and -0.6694 ± 0.0001 from the series expansion techniques [6].

The more interesting feature from our 2DSL LSUBm calculations is the appearance of terminating points in the real solutions of the LSUBm equations for $m > 2$, as indicated in Fig. 1, beyond which the solution becomes complex. This behavior is totally different from that observed in the 1DC model where, unlike in the SUB2 scheme discussed above which retains two-spin correlations of arbitrarily long range, there is no evidence of such terminating points in the localized LSUBm scheme at any value $m \leq 10$. Since we have derived the corresponding coupled equations for a given LSUBm scheme as closed analytical forms with Δ as a parameter, we can straightforwardly study the terminating points by taking the derivatives on both sides of the coupled set of equations [e.g., Eqs. (8)–(10)] with respect to Δ and solving directly for the derivatives of the coefficients. From Eq. (7), we define the second-order derivative of the ground-state energy as the anisotropic susceptibility χ_a,

$$\chi_a \equiv -\frac{\partial^2(E_g/N)}{\partial\Delta^2} = \frac{z}{4}\frac{\partial^2 b_1}{\partial\Delta^2}. \tag{11}$$

The numerical results for χ_a as a function of Δ are shown in Fig. 2 for the 1DC and 2DSL models, respectively. It is clear from the figure that there is no singular behavior for the 1DC model. By comparison, the exact calculation [9] gives an essential singularity at $\Delta = 1$, with the result that any finite order of derivative with respect to Δ is indeed continuous. However, the anisotropic susceptibility for the 2DSL model clearly shows a singular behavior (except for the low-order LSUB2 scheme). Furthermore, although the values of the terminating points Δ_m are different for the LSUB4 and LSUB6 cases, both schemes yield similar critical behavior, namely,

$$\chi_a \rightarrow \text{const} \times (1 - x^2)^{-\lambda}, \quad x \rightarrow 1, \tag{12}$$

with $\lambda = 3/2$, and $x \equiv \Delta_m/\Delta$. This clearly suggests that E_g/N for the 2DSL model within the LSUBm approximation has the following expansion near the terminating point:

$$\frac{E_g}{N} \rightarrow A_m + B_m(1 - x^2)^{1/2} + C_m(1 - x^2) + D_m(1 - x^2)^{3/2} + \cdots, \tag{13}$$

where $x \equiv \Delta_m/\Delta$.

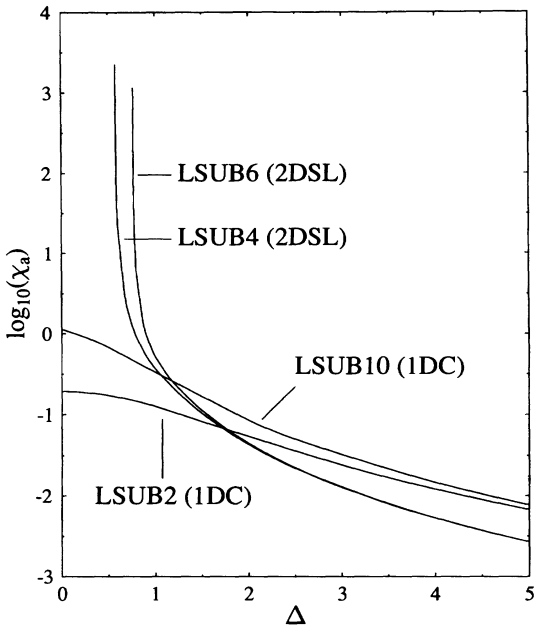

FIG. 2. The second-order derivative of the ground-state energy per spin with respect to Δ for the 1DC and 2DSL models as functions of Δ. Shown are the results of several LSUBm schemes.

We note that the spin-wave theory of Anderson [7] gives the exponent $\lambda = 1/2$. It is not difficult to show that our full SUB2 scheme also yields the same value [3], whereas from the above we see that the LSUBm schemes yield $\lambda = 3/2$. In order to understand this difference, we consider the SUB2-m scheme of the 2DSL model with $m \leq 14$. We observe that the SUB2-m scheme also has the singular behavior described by Eq. (13), yielding $\lambda = 3/2$. However, the coefficient $B_m \rightarrow 0$ as $m \rightarrow \infty$. Therefore, the fourth term in Eq. (13) is the dominant singular term, yielding $\lambda = 1/2$ for the full SUB2 scheme (i.e., the SUB2-∞ scheme). Furthermore, we notice that the coefficients B_m also seem to decay by a $1/m^2$ rule as m increases in the SUB2-m scheme. It seems likely that, in the LSUBm scheme, the B_m coefficients also decrease as m increases, and the first singular term has the coefficient D_m as $m \rightarrow \infty$, so that $\lambda = 1/2$ is recovered. Although we only have the LSUB4 and LSUB6 schemes for consideration, the results confirm that the value of B_m in the LSUB6 scheme is much smaller than that of the LSUB4 scheme. Therefore, we expect that the exact result, namely the LSUBm scheme with $m \rightarrow \infty$, has the value of $\lambda = 1/2$. We will present the details of the expansion Eq. (13) for our various approximation schemes elsewhere.

While our CCM analysis seems to agree with spin-wave theory [7] for the critical exponent λ, there does seem to be a real difference in the corresponding predictions for the value of the critical point Δ_c. We first consider

the SUB2-m scheme. As given previously [3], the terminating point is $\Delta_\infty = 0.7984$. The terminating point in the SUB2-m scheme rapidly approaches this value as m increases. Interestingly, the $1/m^2$ rule also seems to fit well. We attempt to apply the $1/m^2$ rule for the LSUBm scheme also. We thus obtain the predicted critical point as $\Delta_c \approx 0.92 \pm 0.01$. Although this is clearly smaller than the value 1 predicted by spin-wave theory [7], the quoted error is merely that of least-squares fit at this level, and we cannot yet preclude agreement when higher-order corrections in the LSUBm scheme (i.e., $m > 6$) are included in the extrapolation.

Finally, we calculate the staggered (sublattice) magnetization $M^z \equiv \langle s_j^z \rangle / s$ for the XXZ models, where the expectation value is taken with respect to the ground ket and bra states within the same CCM approximation schemes [3]. Our results show, as expected, that there is clearly a difference between the 1DC and 2DSL models. For the 1DC case, the staggered magnetization shows no singular behavior at all, even for the LSUB10 scheme. However, for the 2DSL model, the singular behavior is clearly seen for all high-order schemes beyond the LSUB2 scheme. For the 2DSL model, at the isotropic point, $M^z = 0.8514, 0.7648, 0.7278$ in the LSUB2, LSUB4, and LSUB6 schemes, respectively. From these numbers we obtain $M^z = 0.68 \pm 0.01$ by extrapolation, using a $1/m$ rule (which was found to work well for the SUB2-m scheme). This value is somewhat bigger than the corresponding values 0.606 from spin-wave theory [7] and 0.62 ± 0.02 from series expansion techniques [6], although it agrees well with the best of the corresponding Monte Carlo results, which vary between 0.68 ± 0.02 and 0.62 ± 0.04 [11].

In conclusion, our high-order CCM analyses not only produce with high accuracy the ground-state properties for the spin-$\frac{1}{2}$ XXZ models, but they also enable us to study the the quantum phase transitions in a systematic, unbiased manner. They clearly show that the LSUBm approximations themselves represent a natural extension of perturbation theory. In effect, they comprise a well-defined analytical continuation or resummation of the perturbation theory results within the context of a natural and consistent hierarchy of approximations. More significantly, this hierarchy is capable of predicting a possible quantum phase transition. Another calculation under consideration is the energy gap of the excited states near the critical point in the LSUBm scheme. Our result [3] for the energy gap in the SUB2 scheme is quite similar to that of spin-wave theory, but higher-order multispin correlations have been proved to be significant [6,12].

Finally, we note that the combination of the CCM as a theoretical framework and the use of computer algebraic techniques to implement it at high orders of approximation has resulted in a formalism which is capable for the 2D spin-lattice models of attaining numerical results with a precision comparable to those from the much more computationally intensive state-of-the-art Monte Carlo simulations. It will be of great interest to apply our techniques to similar electron-lattice problems of interest in high-temperature superconductivity which involve vacancies on the lattice (e.g., the Hubbard model), where Monte Carlo algorithms are not easily applicable, due to the infamous fermion sign problem.

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