A Microscopic Study of the Quantum Critical Behavior of the Spin-$\frac{1}{2}$ Anisotropic Heisenberg Models

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ABSTRACT

We extend our own previous applications of the microscopic coupled-cluster method (CCM) to quantum antiferromagnets. In particular, we carry out a systematic calculation involving high-order multispin correlations for the spin-$\frac{1}{2}$ anisotropic Heisenberg models on the one-dimensional chain and the two-dimensional square lattice. Their ground-state properties are obtained as functions of the anisotropy parameter. Our CCM analysis not only produces accurate results for such physical quantities as the ground-state energy which are comparable to the best results from other techniques, but it also enables us to study the quantum phase transitions of the spin models in a systematic and unbiased manner.

1. Introduction

The microscopic coupled-cluster method (CCM) was developed some 35 years ago to deal with many-body correlations in atomic nuclei [1]. Somewhat later, it was independently formulated for calculations of the electronic correlation energy in atoms and molecules [2], and, thereafter, the method quickly became one of the most popular techniques in theoretical quantum chemistry. Nowadays, the CCM is widely applied by chemists as a method of first choice for dealing with electronic correlations, due to both its power and versatility, and great accuracy attainable from it within practical levels of implementation [3].

In physics, the number of applications of the CCM is also enormous [4]. The last few years, in particular, have witnessed considerable progress in applications of the CCM to various lattice Hamiltonian systems. These include quantum spin-lattice systems [5–8], lattice gauge field theory [9, 10], and electronic Hubbard models [11, 12], etc. In particular, several systematic approximation schemes specially tailored for lattice systems have been developed by us [6, 8]. The efficiency of these approximation schemes has been well tested in all of our previous applications [6, 8, 9].

In this article, we extend our earlier work [6, 8]

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for the spin-$\frac{1}{2}$ anisotropic Heisenberg models on the one-dimensional (1D) chain and the two-dimensional (2D) square lattice. We can now include multispin correlations of a very high order by employing computer-algebraic techniques to derive the resulting sets of coupled equations for the cluster correlation coefficients. We note that the 1D spin-$\frac{1}{2}$ model is exactly solvable by the Bethe *ansatz* [13] and therefore provides a stringent test for our CCM analysis. Despite the fact that all our calculations have been done on a microcomputer, the numerical results that we obtain are already very impressive indeed when compared with the best of the Monte Carlo calculations [14–16] and the results from series expansion techniques [17], both of which are very much more computationally intensive. A further advantage of our CCM analysis lies in the fact that the coupled sets of many-body equations are derived and solved as explicit functions of the anisotropy parameter. This enables us to study, in a very systematic and unbiased manner, the possibility of quantum phase transitions which are usually revealed by the appearance of singular behavior in the anisotropic susceptibility (i.e., the second-order derivative of the ground-state energy with respect to the anisotropy parameter).

The remainder of this article is organized as follows: In Section 2, we outline our CCM analysis for the spin-lattice models. We then first discuss in Section 3 two particular truncation schemes, namely, the so-called SUBn scheme and a further subapproximation to it, namely, the SUBn-m scheme. These schemes are particularly useful for motivating the later introduction in Section 4 of the systematic local approximation, namely, the LSUBm scheme, which we employ to obtain with high accuracy the ground-state properties as functions of the anisotropy parameter. The critical behavior is investigated by calculating the anisotropic susceptibility as a function of the anisotropy parameter, using the same extrapolation rules previously determined heuristically in the SUB2-m scheme. We conclude this article by a discussion in Section 5.

2. The CCM Formalism for Spin-Lattice Models

Since the details of our CCM analysis for the spin-lattice models have been published earlier [6, 8], we only briefly discuss our approach in this section. We study the following anisotropic Heisenberg Hamiltonian (which is also referred to as the XXZ model in the literature):

$$H = \frac{1}{2}\sum_{l=1}^{N}\sum_{\rho=1}^{z}\left[\Delta s_l^z s_{l+\rho}^z + \tfrac{1}{2}(s_l^+ s_{l+\rho}^- + s_l^- s_{l+\rho}^+)\right]; \quad s = \tfrac{1}{2}, \tag{2.1}$$

on a bipartite lattice, where the index l runs over all N ($\to \infty$) lattice sites with the usual periodic boundary condition imposed; the index ρ runs over all z nearest-neighbor sites ($z = 2$ and 4 for the 1D and 2D models, respectively); the operators s_l^z and $s_l^\pm$ ($\equiv s_l^x \pm i s_l^y$) are spin operators obeying the usual angular momentum commutation relations; and Δ is the anisotropy parameter. In the special cases, $\Delta = 0, 1, \infty$, the corresponding Hamiltonians of Eq. (2.1) are referred to as the planar XY model, the isotropic Heisenberg model, and the Ising model, respectively.

For the XY model ($\Delta = 0$), the spins align in the xy plane. However, in the limit $\Delta \to \infty$ (the Ising model), the Hamiltonian has two degenerate ground states, each of which is given by two alternating sublattices, one with all spins down (i.e., along the $-z$-axis) and the other with all spins up (i.e., along the $+z$-axis). Either one of these two states is referred to as the Néel state. We study the Hamiltonian of Eq. (2.1) from the large-Δ side. Therefore, we choose one Néel state as our model state $|\Phi\rangle$, and the quantum correlation effects are incorporated by considering the multi-spin-flip excitations with respect to this model state. For clarity, we use the vector indices $\{i\}$ exclusively to label the sites of the spin-down sublattice and the vector indices $\{j\}$ exclusively for the sites of the spin-up sublattice. The CCM *ansatz* for the ground ket state is therefore given by

$$|\Psi_g\rangle = e^S|\Phi\rangle; \qquad S \equiv \sum_{n=1}^{N/2} S_{2n}, \tag{2.2}$$

with the correlation operators S_{2n} defined by

$$S_{2n} = \frac{(-1)^n}{(n!)^2}\sum_{i_1,i_2,\ldots,i_n}\sum_{j_1,j_2,\ldots,j_n} \mathcal{S}_{i_1 i_2 \ldots i_n, j_1 j_2 \ldots j_n} \times s_{i_1}^+ s_{i_2}^+ \cdots s_{i_n}^+ s_{j_1}^- s_{j_2}^- \cdots s_{j_n}^-, \tag{2.3}$$

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

The ground bra state $\langle\tilde{\Psi}_g|$ within the CCM is correspondingly written as

$$\langle\tilde{\Psi}_g| = \langle\Phi|\tilde{S}e^{-S}; \qquad \tilde{S} \equiv 1 + \sum_{n=1}^{N/2} \tilde{S}_{2n}, \quad (2.4)$$

with

$$\tilde{S}_{2n} = \frac{(-1)^n}{(n!)^2} \sum_{i_1, i_2, \ldots, i_n} \sum_{j_1, j_2, \ldots, j_n} \tilde{\mathscr{S}}_{i_1 i_2 \ldots i_n, j_1 j_2 \ldots j_n} \times s_{i_1}^- s_{i_2}^- \cdots s_{i_n}^- s_{j_1}^+ s_{j_2}^+ \cdots s_{j_n}^+. \quad (2.5)$$

By definition, it is easy to see that we have the explicit normalization

$$\langle\tilde{\Psi}_g \mid \Psi_g\rangle = \langle\Phi \mid \Psi_g\rangle = \langle\Phi \mid \Phi\rangle = 1. \quad (2.6)$$

The c-number coefficients $\{\mathscr{S}_{i_1 \ldots i_n, j_1 \ldots j_n}, \tilde{\mathscr{S}}_{i_1 \ldots i_n, j_1 \ldots j_n}\}$ of Eqs. (2.3) and (2.5) are determined by the usual variational principle, namely,

$$\frac{\delta\langle H\rangle}{\delta\tilde{\mathscr{S}}_{i_1 \ldots i_n, j_1 \ldots j_n}} = 0; \qquad \frac{\delta\langle H\rangle}{\delta\mathscr{S}_{i_1 \ldots i_n, j_1 \ldots j_n}} = 0, \qquad \forall n, \quad (2.7)$$

where the symbol $\langle \ldots \rangle$ denotes the expectation value taken with respect to the ket state $|\Psi_g\rangle$ and the bra state $\langle\tilde{\Psi}_g|$. Each of the above equations always involves the Hamiltonian in the similarity-transformed form, namely,

$$\bar{H} \equiv e^{-S} H e^{S} = H + [H, S] + \frac{1}{2!}[[H, S], S] + \cdots, \quad (2.8)$$

where the expansion series actually terminates at the fourth-order term [6] for the Hamiltonian of Eq. (2.1). Furthermore, Eq. (2.7) can be written more explicitly as

$$\langle\Phi|s_{i_1}^- s_{i_2}^- \cdots s_{i_n}^- s_{j_1}^+ s_{j_2}^+ \cdots s_{j_n}^+ \bar{H}|\Phi\rangle = 0; \qquad \forall n, \quad (2.9)$$

for the ket-state coefficients $\{\mathscr{S}_{i_1 \ldots i_n, j_1 \ldots j_n}\}$, and

$$\langle\Phi|\tilde{S}\left[\bar{H}, s_{i_1}^+ s_{i_2}^+ \cdots s_{i_n}^+ s_{j_1}^- s_{j_2}^- \cdots s_{j_n}^-\right]|\Phi\rangle = 0; \qquad \forall n, \quad (2.10)$$

for the bra-state coefficients $\{\tilde{\mathscr{S}}_{i_1 \ldots i_n, j_1 \ldots j_n}\}$ with the ket-state coefficients as known input.

Once the ground states are determined, the ground-state energy E_g is obtained as a function of these ground-state coefficients, namely,

$$E_g = \langle H\rangle = \langle\Phi|\bar{H}|\Phi\rangle, \quad (2.11)$$

where in the second equality we have used Eq. (2.9). Hence, one sees that the determination of E_g involves the ket-state coefficients only. For the spin-$\frac{1}{2}$ models of Eq. (2.1), it is easy to derive the following exact energy equation:

$$\frac{E_g}{N} = -\frac{z}{8}(\Delta + 2b_1), \quad (2.12)$$

where $b_1 \equiv \mathscr{S}_{i, i+\rho}$ is the nearest-neighbor pair correlation coefficient, and $z = 2$ and 4 for the 1D chain and the 2D square lattice, respectively. We note that b_1 is independent of both index i by translational invariance and index ρ by the lattice symmetries under rotations and reflections. The equation for b_1, which is obtained from Eq. (2.9) with $n = 2$, couples to the four-spin-flip coefficients $\{\mathscr{S}_{ii', jj'}\}$. The equations for these four-spin-flip coefficients then couple to the six-spin-flip coefficients $\{\mathscr{S}_{ii'i'', jj'j''}\}$, and so on. There are a number of practical approximation schemes available that truncate this otherwise infinite hierarchy. We discuss some of them in the following sections.

3. The SUBn Scheme

The most common truncation scheme for the correlation operators S and $\tilde{S}$ of the CCM is perhaps the SUBn scheme which includes all correlations involving n or fewer multispin flips with respect to the Néel model state and which sets to zero those coefficients in Eqs. (2.3) and (2.5) involving more than n spin flips. We take the SUB2 scheme as an example. One writes the two-body coefficients as $\mathscr{S}_{i,j} \equiv b_{\mathbf{r}}$, where $\mathbf{r} \equiv \mathbf{r}_j - \mathbf{r}_i$, by making use of the lattice symmetries, and where $\mathbf{r}_i$ and $\mathbf{r}_j$ are the position vectors of lattice sites i and j,

respectively. The corresponding equation for $b_{\mathbf{r}}$ is derived from Eq. (2.9) with $n = 2$ as

$$\sum_{\rho=1}^{z}\left[(1 + 2\Delta b_1 + 2b_1^2)\delta_{\mathbf{r},\mathbf{r}_\rho} - \frac{1}{2}(\Delta + 2b_1)b_{\mathbf{r}} + \sum_{\mathbf{r}'} b_{\mathbf{r}'}b_{\mathbf{r}-\mathbf{r}'-\mathbf{r}_\rho}\right] = 0, \quad (3.1)$$

where $\mathbf{r}_\rho$ is a lattice vector joining nearest-neighbor sites. Equation (3.1) has a physical analytical solution, found by sublattice Fourier transformation [6], given by

$$b_{\mathbf{r}} = K\int_{-\pi}^{\pi}\frac{d\mathbf{q}}{(2\pi)^d}\frac{e^{-i\mathbf{r}\cdot\mathbf{q}}}{\gamma_{\mathbf{q}}}\left(1 - \sqrt{1 - k^2\gamma_{\mathbf{q}}^2}\right), \quad (3.2)$$

where d is the dimensionality of the lattice system and

$$K \equiv \Delta + 2b_1,$$
$$k^2 \equiv \frac{1 + 2\Delta b_1 + 2b_1^2}{K^2},$$
$$\gamma_{\mathbf{q}} \equiv \frac{1}{z}\sum_{\rho=1}^{z} e^{i\mathbf{r}_\rho\cdot\mathbf{q}}. \quad (3.3)$$

In Eq. (3.2), one obtains a self-consistency equation for b_1 by setting $\mathbf{r} = \mathbf{r}_\rho$, any one of the nearest-neighbor lattice vectors. Substituting this value for b_1 into the energy equation (2.12), one obtains the ground-state energy as a function of Δ. We note that, in Eq. (3.2), $k = 1$ is a physical terminating point because there is no real solution when $k > 1$. This point determines the critical anisotropy Δ_c, which was positively identified by us [6] as corresponding to the SUB2 approximation to the phase transition point between the Ising-like and planar XY-like phases, from a calculation of the spin-wave spectrum, staggered magnetization, and spin–spin correlation function within the same SUB2 scheme.

For example, we obtained $\Delta_c = 0.3728$ and 0.7975 at this SUB2 level for the 1D and 2D models, respectively. We note that for the 1D case the exact analysis [13] shows a phase transition at $\Delta = 1$, whereas no analytical results are known for the corresponding 2D model. We now focus on the behavior near the critical point Δ_c for the 2D case. It is easy to show that the ground-state energy behaves in the SUB2 scheme as

$$\frac{E_g}{N} \propto (1 - x^2)^{3/2}, \qquad x \to 1, \quad (3.4)$$

where $x \equiv \Delta_c/\Delta$. Therefore, the anisotropic susceptibility χ_a, which is defined by

$$\chi_a \equiv -\frac{\partial^2(E_g/N)}{\partial\Delta^2} = \frac{z}{4}\frac{\partial^2 b_1}{\partial\Delta^2}, \quad (3.5)$$

clearly shows a singular behavior at Δ_c, namely, $\chi_a \propto (1 - x^2)^{-\lambda}$, with the critical exponent $\lambda = 1/2$. This critical behavior agrees with the prediction of spin-wave theory [18]. This is not surprising because both the SUB2 scheme of the CCM and spin-wave theory include only two-body correlations.

In general, it is difficult to obtain analytical solutions beyond the SUB2 scheme discussed above. To include the effects of higher-order multispin correlations (i.e., four-spin and six-spin correlations, etc.), we developed a different local truncation approximation which efficiently includes the most important multispin-flip configurations. This local approximation is to be discussed in the following section. Here, as a first step and as guidance to the later discussion, we consider a local two-body approximation, the so-called SUB2-m scheme, in which one includes only the two-body correlations spanning a range of no more than m adjacent lattice sites. We may then investigate by making an extrapolation from the results of the SUB2-m scheme to estimate the full SUB2 results. The analytical solution of the full SUB2 scheme thereby provides a stringent test for the extrapolation rules which will play an important role in the ensuing local approximations.

By definition, the SUB2-2 scheme in all dimensionalities retains only a single coefficient, b_1, and the SUB2-4 scheme retains two coefficients on the 1D chain but three coefficients on the 2D square lattice. We again focus on the 2D model. The three 2D SUB2-4 configurations are illustrated in Figure 1. The corresponding equations are

$$1 - 6\Delta b_1 - 5b_1^2 + 4(b_3^a)^2 + 14(b_3^b)^2 + 2b_1b_3^a + 12b_1b_3^b + 8b_3^ab_3^b = 0, \quad (3.6)$$

$$-8\Delta b_3^a + b_1^2 + 8(b_3^b)^2 - 8b_1b_3^a + 8b_1b_3^b = 0, \quad (3.7)$$

$$-8\Delta b_3^b + 3b_1^2 + 6(b_3^b)^2 - 4b_1b_3^a - 2b_1b_3^b + 8b_3^ab_3^b = 0. \quad (3.8)$$

In a similar fashion, we derived the SUB2-m equations for the 2D model with $m \leq 14$. The SUB2-14 scheme, for example, contains 28 independent two-spin-flip configurations. More generally, the

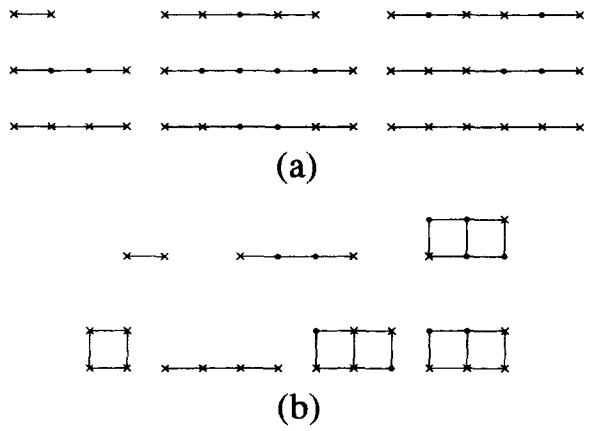

FIGURE 1. (a) *The nine independent configurations* retained in the 1D LSUB6 scheme. The first column constitutes the 1D LSUB4 scheme. (b) The seven independent configurations retained in the 2D LSUB4 scheme. The three configurations in the first row represent the coefficients b_1, b_3^a, and b_3^b of the SUB2-4 scheme. The crosses indicate the positions of the spins which are flipped with respect to the Néel model state.

2D SUB2-m approximation retains $m(m+2)/8$ independent spin-flip configurations with respect to the Néel model state. By taking the derivatives with respect to Δ in the corresponding coupled set of equations [cf., Eqs. (3.6)–(3.8) in the case of $m = 4$], one can easily solve for $\partial^2 b_1/\partial\Delta^2$, which yields the values of χ_a as a function of Δ by Eq. (3.5). We find that for each value of $m \geq 4$ in the SUB2-m scheme the corresponding χ_a shows a critical behavior at a different value of the anisotropy, $\Delta = \Delta_m$, but always with the same value of the critical exponent, namely, $\lambda = 3/2$. This suggests the following expansion series for the ground-state energy in the SUB2-m scheme ($m \geq 4$) near the corresponding critical point:

$$\frac{E_g}{N} \to A_m + B_m(1-x^2)^{1/2} + C_m(1-x^2) + D_m(1-x^2)^{3/2} + \cdots, \qquad x \to 1, \quad (3.9)$$

where A_m, B_m, C_m, D_m, ..., are all constants, and $x \equiv \Delta_m/\Delta$. Furthermore, our numerical results clearly show that as m increases the constants B_m decrease rapidly in the asymptotic form $B_m \propto 1/m^2$ as $m \to \infty$. We therefore conclude that $B_m \to 0$ as $m \to \infty$ and the critical term in the series Eq. (3.9) is determined by the fourth term with the constant D_m. Hence, the result $\lambda = 1/2$ of the full SUB2 scheme is recovered. We also find that the values Δ_m of the SUB2-m scheme seem to fit a simple asymptotic $1/m^2$ rule very well, namely, $\Delta_m \to \Delta_\infty + a/m^2$ as $m \to \infty$, with the parameter a as a constant. Using this rule and the SUB2-m values with $m \leq 14$, we obtain a least-squares fit $\Delta_\infty = 0.798 \pm 0.002$, which agrees well with the exact value 0.7985 of the analytical result of the full SUB2 scheme mentioned earlier. It should be pointed out that the numerical results of the ground-state energy in the SUB2-m scheme are also well fitted by a similar asymptotic $1/m^2$ rule.

We next discuss the behavior of the order parameter, namely, the staggered magnetization, within the SUB2 and SUB2-m schemes. The staggered magnetization is defined as

$$M^z \equiv \frac{|\langle s_l \rangle|}{s}, \qquad \forall l, \qquad (3.10)$$

where M^z is independent of the lattice index l due to the lattice translational invariance and where the expectation value is taken with respect to ground ket and bra states. One clearly now needs to calculate the bra state also. The bra ground state in the CCM is parametrized by Eqs. (2.4) and (2.5), and the corresponding bra-state coefficients $\{\tilde{\mathscr{S}}_{i_1 \ldots i_n, j_1 \ldots j_n}\}$, within the same approximation scheme as for the ket-state coefficients $\{\mathscr{S}_{i_1 \ldots i_n, j_1 \ldots j_n}\}$, are determined by a similarly truncated coupled set of Eqs. (2.10), taking the ket-state coefficients as the known input. In the full SUB2 scheme, we obtained $M^z = 0$ and 0.682 for the 1D and the 2D models, respectively, at their corresponding critical points Δ_c [6]. (The exact 1D result [13] yields $M^z = 0$ at the critical point.) We again extrapolate the results for M^z in the 2D SUB2-m scheme. We find that the SUB2-m results for M^z now follow an asymptotic $1/m$ rule, by comparison with the corresponding $1/m^2$ rule mentioned above for the critical anisotropy Δ_m and for the ground-state energy. Using this same $1/m$ rule, we obtain a least-squares fit $M^z = 0.688 \pm 0.006$ for the large-m asymptotic value of the 2D model at the critical point, using the SUB2-m values with $m \leq 14$, which again agrees well with the analytical full 2D SUB2 solution.

One sees that the above extrapolation rules for the local SUB2-m scheme provide an efficient and reliable means to obtain the full SUB2 (i.e., SUB2-∞) results, even including results for the critical properties. In the following section, we discuss a systematic local approximation scheme involving high-order multispin correlations, using similar extrapolation rules.

4. The LSUBm Scheme

A. GROUND-STATE ENERGY

The LSUBm scheme was developed by us for particular use with lattice models containing only short-range interactions, such as the spin-lattice models under discussion [6]. In the LSUBm scheme, one includes all possible many-body correlations over a specified locale on the lattice, with m, the nominal index, characterizing the maximum size of the locale retained at this particular order. Thus, for spin-$\frac{1}{2}$ systems, the LSUBm scheme retains only k-spin-flip configurations for S and $\tilde{S}$ with respect to the Néel model state with $k \leq m$ and, furthermore, where all retained configurations extend over no more than m contiguous sites on the lattice. For example, the LSUB4 and LSUB6 schemes for the spin-$\frac{1}{2}$ 1D model retain three and nine independent configurations, respectively, as shown in Figure 1(a). We derived a general formula for the number of independent coefficients of a given LSUBm scheme in the 1D case [6]. For the 2D spin-$\frac{1}{2}$ case, the number of independent configurations within the same LSUBm scheme is obviously much larger than is the corresponding 1D case. In Figure 1(b), we show the seven configurations of the LSUB4 scheme on the 2D square lattice. It should be pointed out that the LSUBm scheme is also strongly motivated by the expectation that in the Ising limit ($\Delta \to \infty$) it reproduces the large-Δ perturbation series for the ground-state energy out to terms of $(2m)$th order. This expectation has been explicitly proven for the 1D LSUBm scheme [6].

It is obvious that for higher-order approximations the manual derivation of these coupled sets of equations is very tedious indeed. Fortunately, this labor can easily be automated by the use of computer-algebraic techniques. To this end, we developed our own software using the language C++. Also, we applied standard computer algebra systems to check our results independently. The computer-algebraic techniques have enabled us to carry out calculations to quite high orders. For example, we derived the CCM equations in the full SUB6 scheme for the spin-$\frac{1}{2}$ anisotropic Heisenberg model on a general bipartite lattice. (The full SUB4 equations were published earlier by us [6].) We also remark that Harris [7] recently derived, for the 2D isotropic model ($\Delta = 1$), both the full SUB4 equations and also the corresponding equations involving a subset of the six-spin-flip configurations, although he applied a different truncation scheme to that employed here.* For the LSUBm schemes, we derived and solved the coupled equations as functions of Δ for $m \leq 10$ for the 1D model and for $m \leq 6$ for the 2D model. The numbers of independent spin-flip configuration coefficients retained in the 1D LSUB10 and 2D LSUB6 schemes are 81 and 72, respectively.

We show some of our numerical results for the ground-state energies for the 1D model in Table I and for the 2D model in Table II and Figure 2. One sees that the results from our high-order calculations are in excellent agreement with the exact results from the Bethe *ansatz* [13] in the 1D case and with the much more computationally intensive results of Monte Carlo calculations [16] in the 2D case. In particular, after using the asymptotic $1/m^2$ rule which fits our LSUBm results well, we obtain the value -0.4431 ± 0.0001 for the ground-state energy per spin of the isotropic ($\Delta = 1$) 1D model, using the results from the LSUBm schemes with $m = 4, 6, 8, 10$ to perform a least-squares fit to this simple asymptotic form. By comparison, the exact value from the Bethe *ansatz* is -0.4432 to an accuracy of four significant figures. For the isotropic 2D model, our similarly extrapolated result is -0.6691 ± 0.0003, which is in excellent agreement both with Monte Carlo calculations yielding -0.6692 ± 0.0002 [14] and -0.66934 ± 0.00004 [15] and with the value -0.6694 ± 0.0001 from the series expansion techniques [17].

B. ANISOTROPIC SUSCEPTIBILITY

As mentioned earlier, we studied the quantum critical behavior of the spin systems by calculating the anisotropic susceptibility χ_a, defined by Eq. (3.5). Since the coupled sets of equations in a truncation scheme of the CCM, such as the LSUBm scheme, are always derived explicitly in terms of finite-order multinomials of the multispin-flip con-

*We have been unable to reproduce precisely Harris' results [7] involving four-spin-flips. Indeed, we performed two independent calculations, using different computer-algebraic techniques, for the same approximation used by Harris for the truncated SUB4 scheme. We obtain results which agree precisely with each other, but which do not precisely agree with those quoted by Harris. Furthermore, his results including terms involving six-spin-flip configurations are based upon a further uncontrolled approximation in his corresponding six-body equations. For these reasons, we do not compare his results with ours.

TABLE I

Ground-state energy per spin for several values of Δ for the 1D model in the LSUBm scheme and the extrapolated value ("LSUB∞") using the LSUBm results with $m = 4, 6, 8, 10$; the exact results by Bethe *ansatz* are also shown for comparison.

	Δ					
	0.0	0.5	1.0	1.5	2.0	5.0
LSUB2	−0.2887	−0.3421	−0.4167	−0.5069	−0.6076	−1.2986
LSUB4	−0.3193	−0.3692	−0.4363	−0.5195	−0.6155	−1.2995
LSUB6	−0.3198	−0.3730	−0.4400	−0.5218	−0.6167	−1.2995
LSUB8	−0.3196	−0.3741	−0.4414	−0.5226	−0.6170	−1.2995
LSUB10	−0.3196	−0.3745	−0.4420	−0.5230	−0.6171	−1.2995
"LSUB∞"	—	—	−0.4431	−0.5236	−0.6171	−1.2995
Exact	−0.3183	−0.3750	−0.4432	−0.5234	−0.6172	−1.2995

figuration coefficients, one can straightforwardly take the derivatives analytically with respect to the anisotropy parameter Δ on both sides of the equations (again using computer-algebraic techniques), and one can thus solve directly for $\partial^2 b_1/\partial\Delta^2$. We show the computed behavior of χ_a as a function of Δ in Figures 3 and 4 for the 1D and 2D cases, respectively. It is clear that there is no observed singular behavior for the 1D model. This is not surprising because the exact results by the Bethe *ansatz* give an essential singularity at $\Delta = 1$ for which every finite order of the derivative is continuous [13]. However, for the 2D model, the LSUB4 and LSUB6 results clearly show a singular behavior. Interestingly, as in the SUB2-m scheme, both LSUB4 and LSUB6 schemes yield the same exponent $\lambda = 3/2$, although their critical values Δ_m are quite different, with $\Delta_4 \approx 0.577$, $\Delta_6 \approx 0.766$. This suggests the expansion series for the energy when $\Delta \to \Delta_c$ is the same as in Eq. (3.9). Again, as in the SUB2-m scheme, the constant B_6 in the LSUB6 scheme is much smaller than is the corresponding B_4 of the LSUB4 scheme. From the analysis of the SUB2-m scheme discussed in Section 3, we conclude that $B_m \to 0$ as $m \to \infty$. Similarly, the critical exponent $\lambda = 1/2$ is also expected for the LSUBm scheme with $m \to \infty$. We determine the critical anisotropy Δ_c using the same assumed $1/m^2$ asymptotic rule. Using the critical values Δ_4 and Δ_6 from the LSUB4 and LSUB6 schemes, respectively, we obtain $\Delta_c \approx 0.92$, which is smaller than the value of 1 from spin-wave theory [18]. Clearly, it is now of great interest to perform calculations involving higher-order multispin correlations (e.g., LSUBm calculations with $m > 6$) in order to confirm this difference.

C. STAGGERED MAGNETIZATION

To calculate the staggered magnetization, defined by Eq. (3.10), we need to determine also the bra-state coefficients in the LSUBm scheme. We carried out such calculations in the LSUBm scheme, again using computer-algebraic techniques for both the 1D and 2D models. As expected, the exact

TABLE II

Ground-state energy per spin for several values of Δ for the 2D model in the LSUBm scheme; also included are the results from the extrapolation ("LSUB∞").

	Δ					
	0.9	1.0	1.5	2.0	3.0	5.0
LSUB2	−0.6111	−0.6483	−0.8550	−1.0806	−1.5547	−2.5332
LSUB4	−0.6310	−0.6637	−0.8604	−1.0831	−1.5555	−2.5333
LSUB6	−0.6364	−0.6670	−0.8610	−1.0833	−1.5555	−2.5333
"LSUB∞"	−0.6388	−0.6691	−0.8619	−1.0835	−1.5555	−2.5333

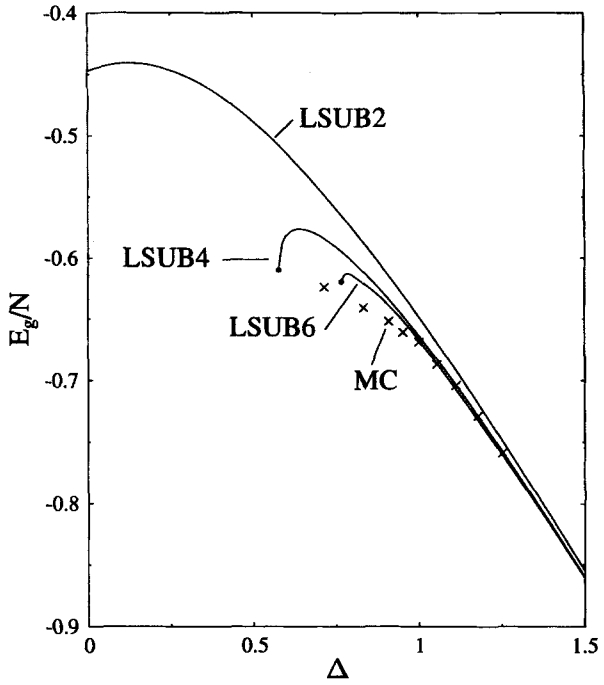

FIGURE 2. Ground-state energy per spin as a function of Δ for the 2D model. Shown are the numerical results of the LSUBm scheme and of a Monte Carlo calculation [16].

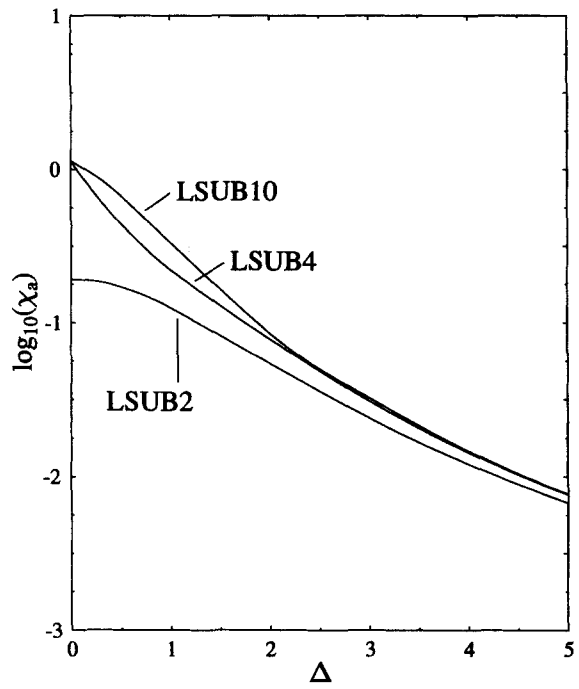

FIGURE 3. Anisotropic susceptibility of the 1D model as a function of Δ. Shown are the results of the LSUBm scheme.

essential singularity [13] for M^z at $\Delta = 1$ in the 1D model is not reproduced by our LSUBm scheme, even with values of m as high as 10. For the 2D model, our results for M^z from the LSUBm scheme show a nonzero value even at the corresponding critical points, in agreement with other calculations [14, 17, 18]. In particular, at the isotropic point $\Delta = 1$, we obtain values $M^z = 0.8514, 0.7648$, and 0.7278 from the LSUB2, LSUB4, and LSUB6 schemes, respectively. Using our heuristically determined $1/m$ rule for extrapolation, we find a least-squares best estimate $M^z = 0.68 \pm 0.01$ at $\Delta = 1$. This value is again in good agreement with the corresponding values 0.606 from spin-wave theory [18] and 0.62 ± 0.02 from series expansion techniques [17]. The best of the corresponding Monte Carlo results [14] vary between 0.68 ± 0.02 and 0.62 ± 0.04.

5. Conclusions

In this article, we performed a systematic series of CCM calculations involving high-order multispin

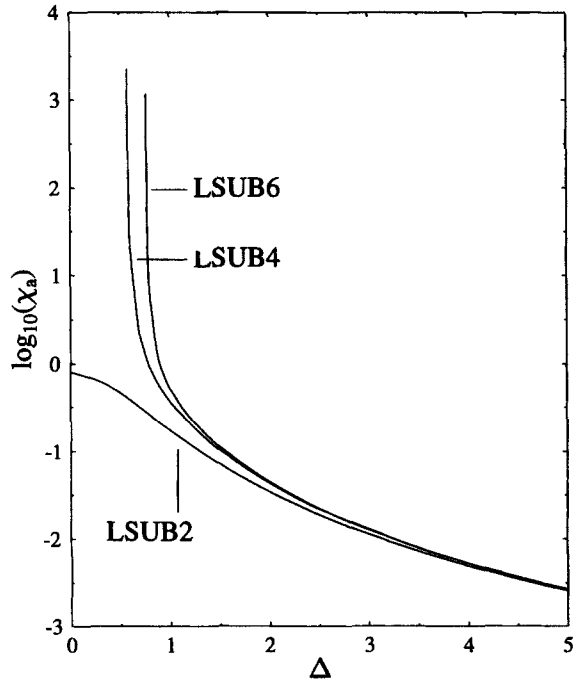

FIGURE 4. Anisotropic susceptibility of the 2D model as a function of Δ. Shown are the results of the LSUBm scheme.

correlations for the spin-$\frac{1}{2}$ anisotropic Heisenberg models on the 1D chain and the 2D square lattice. The ground-state energy of the 1D model from our CCM calculations agrees very well with the exact results of Bethe [13]. The ground-state properties of the 2D model are also in excellent agreement with other state-of-the-art calculations [14, 15, 17]. Furthermore, our CCM analyses provide a systematic means to study the critical behavior of the spin systems. It particularly allows us to calculate directly the important anisotropic susceptibility.

As is well known, the CCM also provides a formalism for the calculation of excited states. Our earlier SUB2 calculation [6] for the anisotropic Heisenberg models produced similar spin-wave excitation spectra to those of spin-wave theory [18]. We are currently investigating the effects of high-order multispin correlations for the excitation energy gap.

Finally, we note that the isotropic Heisenberg model on the 2D square lattice is itself a limiting form of the electronic Hubbard model at half-filling. It will be of great interest to apply our techniques to study high-temperature superconductivity via the Hubbard models at less than half-filling [12], where Monte Carlo techniques encounter the well-known difficulty of the fermion sign problem.

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