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A COHERENT MICROSCOPIC APPROACH TO QUANTUM CRITICALITY: APPLICATIONS TO ANTIFERROMAGNETS ON SQUARE AND TRIANGULAR LATTICES

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1. INTRODUCTION

The techniques now available in the field of *ab initio* microscopic quantum many-body theory have become increasingly refined over the last decade or so. This is particularly true for what are nowadays recognized as the two most powerful modern techniques, namely the coupled cluster method (CCM) [1–11] and the method of correlated basis functions (CBF) [12–18]. Both methods have by now been deeply and thoroughly tested, and both have been found to give extremely accurate results for a wide variety of physical systems. In many cases the results obtained from these fully microscopic techniques are found to be completely competitive with those obtained from the much more computationally intensive quantum Monte Carlo (QMC) simulations, in those situations where the latter can be applied.

However, QMC simulations remain unavailable for many systems of current interest, typically those where the infamous "fermion minus sign problem" cannot be circumvented. In view of the proven applicability of the *ab initio* techniques, it therefore now seems timely to apply them to those problems where QMC results are unavailable, and especially to that most interesting class of topical systems characterized by novel ground states, and which display *quantum order* in some region of the relevant parameter space. Examples of such systems include heavy fermions, high-temperature superconductors, the fractional quantum Hall effect, new quantum states in the condensed phases of helium, and antiferromagnetic materials.

In this context particular interest centres on whether any of the modern microscopic formulations of quantum many-body theory can provide an *unbiased* microscopic description of the quantum order. One is particularly interested in whether any of the techniques which have been developed for conventional systems can detect the position of the critical value of the relevant parameter driving the quantum phase

transition, and, if so, evaluate the corresponding critical exponents of the associated singularities in the order parameter and other physical quantities. The aim of the present paper is to show that at least one method, namely the CCM, does indeed have this capability, at least so far as our preliminary investigations indicate for applications involving one important class of systems exhibiting quantum order, namely antiferromagnets.

Over the last few years the CCM has been applied rather successfully to various lattice Hamiltonian systems, including spin-lattice models [19–23], lattice gauge models [24–27], and such models of strongly interacting electrons as the Hubbard model [28–31]. In the present paper we extend the earlier calculations on the spin-lattice models, and in particular make the first application to a frustrated lattice, namely the two-dimensional (2D) triangular lattice. By explicit applications to various anisotropic antiferromagnetic model Hamiltonians on both bipartite (unfrustrated) and frustrated lattices, we show how the CCM enables us to study the quantum phase transitions, including the detailed critical behaviour, of these systems in a very systematic and unbiased manner [32,33].

2. THE CCM FORMALISM FOR SPIN-LATTICE MODELS

2.1 Basic Ingredients

Detailed descriptions of the basic CCM formalism have been given many times [1–11], and therefore we only review the essential ingredients here. The exact ket and bra ground-state energy eigenvectors, $|\Psi_0\rangle$ and $\langle\tilde{\Psi}_0|$, of a many-body system described by a Hamiltonian H,

$$H|\Psi_0\rangle = E_g|\Psi_0\rangle \;\; ; \quad \langle\tilde{\Psi}_0|H = E_g\langle\tilde{\Psi}_0| \;\; , \tag{1}$$

are parametrized within the CCM as follows,

$$|\Psi_0\rangle = \mathrm{e}^S|\Phi\rangle \;\; ; \quad S = \sum_{I\neq 0} s_I C_I^+ \;\; , \tag{2a}$$

$$\langle\tilde{\Psi}_0| = \langle\Phi|\tilde{S}\mathrm{e}^{-S} \;\; ; \quad \tilde{S} = 1 + \sum_{I\neq 0} \tilde{s}_I C_I^- \;\; . \tag{2b}$$

A fundamental role is thus played by the model or reference state $|\Phi\rangle$, which is required to have the property of being a cyclic vector with respect to two well-defined Abelian subalgebras of multiconfigurational creation operators $\{C_I^+\}$ and their Hermitian-adjoint destruction counterparts $\left\{C_I^- \equiv \left(C_I^+\right)^\dagger\right\}$. Thus, $|\Phi\rangle$ plays the role of a vacuum state with respect to a suitable set of (mutually commuting) many-body creation operators $\{C_I^+\}$,

$$C_I^-|\Phi\rangle = 0 \;\; , \quad I \neq 0 \;\; , \tag{3}$$

where $C_0^- \equiv 1$, the identity operator. These operators are complete in the many-body Hilbert (or Fock) space $\mathcal{H}$,

$$1 = |\Phi\rangle\langle\Phi| + \sum_{I\neq 0} C_I^+|\Phi\rangle\langle\Phi|C_I^- \;\; . \tag{4}$$

We note that although the manifest Hermiticity, $(\langle\tilde{\Psi}_0|)^\dagger = |\Psi_0\rangle$, is lost, the intermediate normalization condition $\langle\tilde{\Psi}_0|\Psi_0\rangle = \langle\Phi|\Psi_0\rangle = \langle\Phi|\Phi\rangle \equiv 1$ is explicitly imposed. The cluster correlation coefficients $\{s_I, \tilde{s}_I\}$ are regarded as being independent parameters, even though formally we have the relation,

$$\langle\Phi|\tilde{S} = \frac{\langle\Phi|e^{S^\dagger}e^S}{\langle\Phi|e^{S^\dagger}e^S|\Phi\rangle} \quad . \tag{5}$$

The full set $\{s_I, \tilde{s}_I\}$ provide a complete description of the ground state. For example, an arbitrary operator A has a ground-state expectation value given as,

$$\bar{A} \equiv \langle\tilde{\Psi}_0|A|\Psi_0\rangle = \langle\Phi|\tilde{S}e^{-S}Ae^S|\Phi\rangle = \bar{A}[s_I, \tilde{s}_I] \quad . \tag{6}$$

We note that the exponentiated form of the ground-state CCM parametrization of Eq. (2) ensures the correct counting of the *independent* fluctuations of excited correlated many-body clusters with respect to $|\Phi\rangle$ which are present in the exact ground state $|\Psi_0\rangle$. It also ensures the exact incorporation of the Goldstone linked cluster theorem, which itself guarantees the size-extensivity of all relevant extensive physical variables.

The coefficients $\{s_I, \tilde{s}_I\}$ are themselves determined by taking appropriate projections onto the ground-state Schrödinger equations (1). Equivalently, they may be determined variationally by requiring the ground-state energy expectation functional $\bar{H}[s_I, \tilde{s}_I]$, defined as in Eq. (6), to be stationary with respect to variations in each of the (independent) parameters of the full set. We thereby easily derive the coupled sets of equations,

$$\delta\bar{H}/\delta\tilde{s}_I = 0 \;\Rightarrow\; \langle\Phi|C_I^-e^{-S}He^S|\Phi\rangle = 0, \quad I \neq 0 \quad , \tag{7}$$

$$\delta\bar{H}/\delta s_I = 0 \;\Rightarrow\; \langle\Phi|\tilde{S}e^{-S}[H, C_I^+]e^S|\Phi\rangle = 0, \quad I \neq 0 \quad . \tag{8}$$

Equation (7) also shows that the ground-state energy at the stationary point has the simple form

$$E_g = E_g[s_I] = \langle\Phi|e^{-S}He^S|\Phi\rangle = \langle\Phi|He^S|\Phi\rangle \quad . \tag{9}$$

It is important to realize that this (bi-)variational formulation does *not* lead to an upper bound for E_g when the summations for S and $\tilde{S}$ in Eq. (2) are truncated, due to the lack of Hermiticity when such approximations are made. However, it is clear that the important Hellman-Feynman theorem *is* preserved in all such approximations.

We also note that Eq. (7) represents a coupled set of nonlinear equations for the c-number cluster correlation coefficients $\{s_I\}$. The nested commutator expansion,

$$e^{-S}He^S = H + [H, S] + \frac{1}{2!}[[H, S], S] + \cdots \quad , \tag{10}$$

together with the fact that all of the individual components of S in the sum in Eq. (2) commute with one another, imply that each element of S in Eq. (2) is linked directly to the Hamiltonian in each of the terms in Eq. (10). Thus, each of the coupled equations (7) is of linked cluster type. Furthermore, each of these equations is of finite length when expanded, since the otherwise infinite series of Eq. (10) will always

terminate at a finite order, provided (as is usually the case) that each term in the second-quantized form of the Hamiltonian H contains a finite number of single-body destruction operators, defined with respect to $|\Phi\rangle$. It is important to note that this is in sharp contrast with the unitary transformation equivalent of the fundamental similarity transformation that lies at the heart of the CCM, which would arise in a standard variational formulation in which the bra state $\langle\tilde{\Psi}_0|$ is simply taken as the explicit Hermitian adjoint of $|\Psi_0\rangle$.

Although we shall not be concerned here with excited states, for reasons of space, we note that excited states also have a similar CCM parametrization. The interested reader is referred to the literature [5, 8–11] for details.

2.2 Applications to Spin-Lattice Models

The general CCM formalism described above is now specialized to the specific case of spin-$\frac{1}{2}$ anisotropic Heisenberg models defined on two-dimensional (2D) lattices. We consider both the non-frustrated bipartite square lattice and the frustrated non-bipartite triangular lattice. We shall choose different models of the anisotropic terms for the two lattices, for reasons described below. However, we note that both reduce at the isotropic point to the usual nearest-neighbour Heisenberg model. This is described by the antiferromagnetic-coupling Hamiltonian,

$$H = \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \quad , \tag{11}$$

where $\mathbf{s}_i$ are the spin-$\frac{1}{2}$ operators at site i on the lattice, defined as $\mathbf{s}_i \equiv \frac{1}{2}\vec{\sigma}_i$ in terms of the usual Pauli spin operators $\vec{\sigma}_i$. The sum in Eq. (11) runs over nearest-neighbour lattice bonds. We note that the operators in Eq. (11) are defined in terms of some global spin quantization axes referring to all spins, whereas henceforth we shall consistently employ a notation in which the spin operators are described in terms of local (Néel-like) quantization axes defined separately below for each sublattice of the lattice under consideration.

For the bipartite square lattice we refer the local coordinates to a perfect classical Néel state. Thus, on (only) one of the two equivalent sublattices we perform the up-down transformation in which the Pauli matrices on the rotated sublattice undergo the canonical transformation: $\sigma^x \rightarrow -\sigma^x$, $\sigma^y \rightarrow \sigma^y$, $\sigma^z \rightarrow -\sigma^z$. Such a transformation not only makes transparent the physical meaning of the correlation operator S, but it also facilitates later discussions on the Marshall-Peierls sign theorem. In these local quantization axes referred to the Néel state, the anisotropic Heisenberg or XXZ model Hamiltonian is specified as

$$H_1 = \frac{1}{4} \sum_{\langle ij \rangle} \left[-\sigma_i^z \sigma_j^z - \frac{\lambda}{2} \left(\sigma_i^+ \sigma_j^+ + \sigma_i^- \sigma_j^- \right) \right] \quad , \tag{12}$$

where $\sigma^{\pm} \equiv \sigma^x \pm i\sigma^y$ are the corresponding spin creation and destruction operators in the local coordinates, and λ denotes the anisotropy parameter.

When $\lambda = 0$, the Hamiltonian H_1 describes the usual Ising antiferromagnet with a perfect Néel-ordered ground state. This is simply the fully aligned ("ferromagnetic") configuration in the local spin coordinates described above. A natural choice

for the CCM model state $|\Phi\rangle$ is thus the Néel state, where in the local axes all spins point along the respective negative z-axes,

$$|\Phi\rangle = \bigotimes_{i=1}^{N} |\downarrow\rangle_i \;\; ; \quad \text{in local quantization axes,} \tag{13}$$

where $N \to \infty$ is the number of lattice sites. Finally, when $\lambda = 1$, Eq. (12) reverts to the usual antiferromagnetic Heisenberg Hamiltonian, expressed in global coordinates in Eq. (11).

The triangular lattice has three equivalent sublattices, again defined so that no two sites on the same sublattice are nearest neighbours on the original lattice. The *classical* ground state of Eq. (11) is now the Néel-like state where all spins on each sublattice are separately aligned (all in the xz-plane, say), and where, say, the spins on sublattice A are oriented along the negative z-axis, and spins on sublattices B and C are oriented at $+120°$ and $-120°$, respectively, with respect to the spins on sublattice A. In order both to facilitate the extension of the isotropic Heisenberg antiferromagnet to include an Ising-like anisotropy and to make the choice of CCM model state the same as in Eq. (13), we again perform the requisite spin-rotation transformations on each sublattice. Specifically, we leave the spins on sublattice A unchanged, and we rotate about the y-axis the spins on sublattices B and C by $-120°$ and $+120°$ respectively,

$$\begin{aligned} \sigma_B^x \to -\frac{1}{2}\sigma_B^x - \frac{\sqrt{3}}{2}\sigma_B^z; \quad \sigma_C^x \to -\frac{1}{2}\sigma_C^x + \frac{\sqrt{3}}{2}\sigma_C^z \;\; , \\ \sigma_B^y \to \sigma_B^y; \quad \sigma_C^y \to \sigma_C^y \;\; , \\ \sigma_B^z \to \frac{\sqrt{3}}{2}\sigma_B^x - \frac{1}{2}\sigma_B^z; \quad \sigma_C^z \to -\frac{\sqrt{3}}{2}\sigma_C^x - \frac{1}{2}\sigma_C^z \;\; . \end{aligned} \tag{14}$$

We may thus rewrite Eq. (11) in terms of spins defined in these local quantization axes for the triangular lattice. With the further introduction of a comparable anisotropy parameter λ for the non-Ising-like piece which thus results, we obtain

$$H_2 = \frac{1}{4}\sum_{\langle i \to j \rangle} \left\{ -\frac{1}{2}\sigma_i^z\sigma_j^z + \frac{\sqrt{3}\lambda}{4}\left(\sigma_i^z\sigma_j^+ + \sigma_i^z\sigma_j^- - \sigma_i^+\sigma_j^z - \sigma_i^-\sigma_j^z\right) \right.$$

$$\left. + \frac{\lambda}{8}\left(\sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+\right) - \frac{3\lambda}{8}\left(\sigma_i^+\sigma_j^+ + \sigma_i^-\sigma_j^-\right) \right\} \;\; , \tag{15}$$

where $\lambda = 1$ again corresponds to the isotropic Heisenberg Hamiltonian of Eq. (11). We note that the summation in Eq. (15) again runs over all nearest-neighbour bonds, as in Eq. (12), but now also with a directionality indicated by $i \to j$, which goes from A to B, B to C, and C to A. As already indicated, in these specified local spin coordinates the CCM model state is again chosen to be that specified in Eq. (13).

With the above choice of model state $|\Phi\rangle$ for both H_1 and H_2, the CCM operators $\{C_I^+\}$ now simply become products of single spin-raising operators $\{\sigma_i^+\}$. The multiconfigurational indices $\{I\}$ thus label a set of lattice sites, and in principle one

should include all distinct multi-spin configurations allowed by the symmetries of the lattice and the Hamiltonian. For example, since the Hamiltonian H_1 on the square lattice commutes with the total z-component of spin (in global coordinates), the configurations $\{I\}$ for the Néel choice of model state need only include those in which an equal number of sites are chosen on the two sublattices.

To effect the CCM in practice we clearly need a well-defined hierarchical approximation scheme in which the expansions of the correlation operators S and $\tilde{S}$ in Eq. (2) can be truncated to some finite or infinite subset of the full set of multi-spin configurations $\{I\}$. The implementation of the CCM thus amounts to the two distinct problems of enumerating the set of independent configurations $\{I\}$ to be retained at a given order, and then evaluating the corresponding sets of (finite-order) equations (7) and (8). We note that both steps can be enormously aided by the use of computer-algebraic techniques. This is vital for the implementation of the higher orders of the truncation schemes reported below. Once the resulting equations for the retained coefficients $\{s_I, \tilde{s}_I\}$ have been solved, the calculation of arbitrary ground-state quantities in the corresponding approximation is then effected via the enumeration of Eq. (6).

We have investigated three main approximation schemes, namely: (i) the SUBn scheme, in which all correlations involving only n or fewer spins are retained, however far separated on the lattice; (ii) the simpler SUBn-m subapproximation, where only SUBn correlations spanning a range of no more than m adjacent lattice sites are retained; and (iii) the systematic local LSUBm ($\equiv$ SUBm-m) scheme, in which all multi-spin correlations over all possible distinct locales on the lattice defined by m or fewer adjacent lattice sites are retained.

3. RESULTS FROM THE SUB2 APPROXIMATION SCHEME

3.1 Square Lattice Results

In the case of the square lattice the SUB2 approximation for the correlation operators S and $\tilde{S}$ becomes

$$S \rightarrow S_2 = \sum_{\mathbf{r},\mathbf{r}'} B_{\mathbf{r}\mathbf{r}'} \sigma_{\mathbf{r}}^{+} \sigma_{\mathbf{r}'}^{+} \quad ; \quad \tilde{S} \rightarrow \tilde{S}_2 = \sum_{\mathbf{r},\mathbf{r}'} \tilde{B}_{\mathbf{r}\mathbf{r}'} \sigma_{\mathbf{r}}^{-} \sigma_{\mathbf{r}'}^{-} \quad , \tag{16}$$

where the coefficients $B_{\mathbf{r}\mathbf{r}'}$ and $\tilde{B}_{\mathbf{r}\mathbf{r}'}$ depend only on the difference of their lattice vector indices, i.e., $B_{\mathbf{r}\mathbf{r}'} = B_{\mathbf{r}-\mathbf{r}'}$, $\tilde{B}_{\mathbf{r}\mathbf{r}'} = \tilde{B}_{\mathbf{r}-\mathbf{r}'}$, due to the lattice translational symmetries. The summations run over all lattice sites $\mathbf{r}$ and $\mathbf{r}'$ such that the vector $\mathbf{r} - \mathbf{r}'$ connects sites on different sublattices, i.e., $(\mathbf{r} - \mathbf{r}') \in \mathcal{A}$, where $\mathcal{A}$ is the set of distinct *sublattice* vectors.

Evaluation of Eq. (9) yields the exact result for the ground-state energy of the Hamiltonian H_1 on the square lattice,

$$\frac{E_g}{N} = -\frac{1}{2}(1 + 16\lambda B_1) \quad , \tag{17}$$

where B_1 denotes the correlation coefficient for a pair of nearest-neighbour spins. Similarly, the set of equations (7), with $C_I^- \rightarrow \sigma_{\mathbf{r}}^- \sigma_{\mathbf{r}'}^-$, can be evaluated to yield the

SUB2 approximation for the coefficients $B_{\mathbf{r}-\mathbf{r}'}$. These may be further decoupled by performing a sublattice Fourier transform with respect to $(\mathbf{r}-\mathbf{r}') \in \mathcal{A}$,

$$B_{\mathbf{q}} \equiv \sum_{\mathbf{r}\in\mathcal{A}} e^{i\mathbf{q}\cdot\mathbf{r}} B_{\mathbf{r}} \Leftrightarrow B_{\mathbf{r}} = \frac{2}{N} \sum_{\mathbf{q}\in\mathcal{M}} e^{-i\mathbf{q}\cdot\mathbf{r}} B_{\mathbf{q}} \ , \tag{18}$$

where $\mathcal{M}$ is the first *sublattice* (or magnetic) Brillouin zone (in the limit $N \to \infty$). We find,

$$\left(\frac{\lambda}{64} + \frac{B_1}{4} + 2\lambda B_1^2\right)\gamma_{\mathbf{q}} - \left(\frac{1}{4} + 4\lambda B_1\right) B_{\mathbf{q}} + \lambda\gamma_{\mathbf{q}} B_{\mathbf{q}}^2 = 0 \ , \tag{19}$$

$$\gamma_{\mathbf{q}} \equiv \frac{1}{4}\sum_{\rho=1}^{4} \exp(i\mathbf{q}\cdot\mathbf{r}_\rho) \ , \tag{20}$$

where the index ρ runs over the four nearest-neighbour lattice vectors on the square lattice. The (physical) solution to the quadratic equation (19) is easily obtained for $B_{\mathbf{q}}$, and thence we may evaluate E_g/N from Eq. (18) using the result,

$$B_1 = \frac{2}{N}\sum_{\mathbf{q}\in\mathcal{M}} \exp(i\mathbf{q}\cdot\mathbf{r}_\rho) B_{\mathbf{q}} = \frac{2}{N}\sum_{\mathbf{q}\in\mathcal{M}} \gamma_{\mathbf{q}} B_{\mathbf{q}} \ . \tag{21}$$

We note that Eqs. (19) and (21) impose a quantitative self-consistency condition on the solution. This may be contrasted with the conventional SWT [34], where the consistency of the assumption of an ordered phase can only be qualitatively ascertained.

At the Heisenberg point ($\lambda = 1$) the SUB2 scheme gives a ground-state energy per spin, $E_g/N \approx -0.6508$. This may be compared with the corresponding classical result of -0.5, and the results of -0.6580 from lowest-order SWT [34] and approximately -0.6693 from QMC simulations [35]. The corresponding result for the SUB2 Heisenberg sublattice magnetization M^z is about 83% of the classical value, compared with an SWT value of 60.6% and with the best of the QMC results which vary between $68 \pm 2\%$ and $62 \pm 4\%$.

The most interesting aspect of the SUB2 approximation, however, is the existence of a terminating point at $\lambda_c \approx 1.252$, beyond which no physical solution exists. Although the CCM based on the Néel model state is sure to break down in that region of the anisotropy parameter space where the true ground-state wave function has a different symmetry from that of the Néel ordering, we have clearly demonstrated [19] that this terminating point corresponds, at this level of approximation, to a true critical point of a phase transition. The nature of the critical point can be examined in more detail by studying the singular behaviour of various physical quantities. We find, for example, by analytic evaluation, that in the full SUB2 approximation we obtain,

$$M^z \underset{\lambda\to\lambda_c^-}{\longrightarrow} M_c^z + \kappa(\lambda_c - \lambda)^{1/2} \ , \quad \text{SUB2} \ , \tag{22}$$

$$\frac{\partial^2(E_g/N)}{\partial\lambda^2} \underset{\lambda\to\lambda_c^-}{\longrightarrow} \mu(\lambda_c - \lambda)^{-1/2} \ ; \quad \text{SUB2} \ , \tag{23}$$

where M_c^z, κ, and μ are constants.

These critical exponents agree with those from SWT, which is perhaps not surprising since both the CCM SUB2 scheme and SWT include only two-body correlations, although, in both cases, of arbitrarily long range. It is interesting to note that in the truncated SUB2-n approximation, we find

$$\frac{\partial^2(E_g/N)}{\partial\lambda^2} \underset{\lambda\to\lambda_c^-}{\longrightarrow} \nu_n(\lambda_c^n-\lambda)^{-3/2}+\mu_n(\lambda_c^n-\lambda)^{-1/2} \quad ; \quad \text{SUB2}-n \quad , \qquad (24)$$

where ν_n and μ_n are constants, and where λ_c^n is the critical anisotropy, at the given SUB2-n level of approximation. We find heuristically, however, that $\nu_n \to 0$ ($\propto n^{-2}$), and $\mu_n \to \mu$ as $n \to \infty$.

3.2 Triangular Lattice Results

The corresponding SUB2 approximation for the triangular lattice is now more complicated than in the previous case. We have now $S \to S_1+S_2$, $\tilde{S} \to \tilde{S}_1+\tilde{S}_2$, where the two-spin correlation operators have the same form as in Eq. (16), except that the vector $\mathbf{r}-\mathbf{r}'$ can now connect sites on the same sublattice since the reference state is no longer an eigenstate of the z-component of total spin. For the same reason, the single spin-flip operators S_1 and $\tilde{S}_1$ are no longer automatically excluded. The analogues of Eq. (19) are now also considerably more complicated. For present purposes, although the full SUB2 equations may have other solutions, we restrict ourselves henceforth to the so-called symmetric and coplanar solution. This has $S_1 = 0 = \tilde{S}_1$, and the two-spin correlation coefficients $B_{\mathbf{r}\mathbf{r}'}$ and $\bar{B}_{\mathbf{r}\mathbf{r}'}$ for a given lattice separation $\mathbf{r}-\mathbf{r}'$ depend only on whether the two spins are on the same or different triangular sublattices A, B, or C.

The analogues of Eq. (19) for the coupled sets of nonlinear equations for the two-body correlations in the first magnetic Brillouin zone $\mathcal{M}$ can no longer be solved analytically for the triangular lattice. Instead, we use a large number N_k of points to discretize $\mathcal{M}$. Typically, we have used up to 600×600 points to obtain accurate numerical estimates. Such large numbers of points are typically required only for high accuracy near the critical point.

At the isotropic Heisenberg point ($\lambda = 1$) we find $E_g/N \approx -0.504$, compared with a classical value of -0.375 and a value of -0.5525 ± 0.0025 extrapolated from a series expansion about the Ising point ($\lambda = 0$) [36]. The fact that the SUB2 ground-state energy captures only about 70% of the quantum corrections to the classical energy, compared with a corresponding figure of about 90% for the square lattice, essentially reflects the importance in the triangular case of the neglected three-spin correlations which are strictly absent for the square lattice.

As for the Hamiltonian H_1 on the square lattice, so for H_2 on the triangular lattice we also find a terminating point, namely at $\lambda_c \approx 1.33525$. We also find that in SUB2 approximation the power-law singularities for the triangular model H_2 are the same as in Eqs. (22) and (23). This provides rather strong evidence that both transitions belong to the same universality class. It also strongly supports the existence of nonzero three-sublattice ordering in the frustrated triangular antiferromagnet. This is quite consistent with the result that the sublattice magnetization computed within the SUB2 approximation is nonzero. In fact, at the isotropic Heisenberg point ($\lambda = 1$), we calculate a value of about 85% of the classical value.

3.3 Comparison of Ground-State Wave Functions

It is of great interest to compare and contrast the structure of the ground-state ket wave functions obtained for both of the above models at the SUB2 level of approximation. This is of particular relevance for a discussion of the possibility of performing QMC simulations for the triangular lattice. In this context, the essential ingredient for the unfrustrated antiferromagnets is provided by the Marshall-Peierls sign theorem [37]. This addresses the phase relations of the projection coefficients of the true ground-state wave function onto a complete set of multi-spin configurations. When applied to the Hamiltonian H_1 on the square lattice, the theorem asserts that all of the coefficients, when expressed in the local spin-quantization coordinates introduced here, are positive. The ground-state wave function thus has only one nodal region, a connected region via the Hamiltonian in the spin configuration space where the wave function always has the same sign. It is this feature which lies at the heart of straightforward applications of QMC simulations [35].

A direct expansion of the exponential operator in the CCM parametrization of Eq. (2) shows immediately that each two-spin correlation coefficient $B_{\mathbf{rr}'}$ is a projection of the ground-state wave function onto the corresponding elementary excitation configuration which flips two spins with respect to the model Néel state $|\Phi\rangle$. Although it is by no means clear *a priori* that the CCM SUB2 approximation will satisfy the Marshall-Peierls sign theorem for the Hamiltonian H_1 on the square lattice, explicit solution shows that it is obeyed. By contrast, the corresponding coefficients for the Hamiltonian H_2 on the triangular lattice are found to have an intriguing oscillatory behaviour in their signs as a function of relative lattice separation.

We note that there has been some recent work [38] which suggests that the Marshall-Peierls sign theorem might survive the onset of weak frustration in certain models. Our present findings, however, point to its breakdown for the triangular Heisenberg antiferromagnet. More interestingly, perhaps, we also note that the fixed-node Monte Carlo method [39] and its extension to deal with both lattice and continuum fermion problems [40] require a reliable trial wave function in terms of which the true wave function is well approximated, especially for its nodal surface structure. It is our hope that the oscillatory behaviour observed in the SUB2 scheme for the frustrated triangular Heisenberg antiferromagnet might represent a sufficiently accurate description of the nodal structure of the exact wave function as to permit a successful implementation of a fixed-node Monte Carlo approach for this system for the first time. We expect that this will be true so long as corrections from correlations between three and more spins are not too large.

4. RESULTS FROM LSUBn APPROXIMATIONS

In order to go beyond the essentially mean-field-like SUB2 approximation, we have also performed some LSUBm calculations for $m > 2$. We report here only on results for the Hamiltonian H_1 on the square lattice, for which one may show that the number of independent configurations $\{I\}$ retained, after the lattice symmetries have been taken into account, are 1, 7, and 72 in the LSUBm schemes with $m = 2, 4$, and 6, respectively. At the isotropic Heisenberg point ($\lambda = 1$), for example, the LSUB6 approximation yields $E_g/N \approx -0.6670$ and $M^z \approx 0.728$. We find heuristically that

for both the 1D chain (for which exact results are known via the Bethe *ansatz* method) and the 2D square lattice our LSUBm results for E_g/N and M^z approach the exact asymptotic ($m \to \infty$) limits as m^{-2} and m^{-1}, respectively. Our best extrapolated values at the Heisenberg point for the square lattice are $E_g/N \approx -0.6691 \pm 0.0003$ and $M^z \approx 0.68 \pm 0.01$, based on LSUB$m$ results with $m = 2, 4, 6$. Both values are in excellent agreement with the best available QMC results [35].

Interestingly, the LSUBm calculations with $m > 2$ also show corresponding critical points λ_c^m; $\lambda_c^4 \approx 1.733, \lambda_c^6 \approx 1.253$. The corresponding SUB2-m results for λ_c^m appear to approach the full SUB2 value for λ_c as m^{-2}. A naive assumption of the same extrapolation law for the LSUBm results gives a corresponding prediction for the extrapolated critical point at $\lambda_c \equiv \lambda_c^\infty \approx 0.87$. It will be of great interest to perform higher-order LSUBm calculations with $m > 6$ in order to sharpen this still relatively crude estimate of the critical anisotropy.

The critical index for the singular term in E_g/N as $\lambda \to \lambda_c^-$ may also be obtained from an analysis of the LSUBm results. An especially interesting possibility in this regard is to employ a variant of the so-called coherent anomaly method of Suzuki [41]. One of the great advantages of the CCM is that since at any level of approximation we have analytic expressions for the coupled sets of equations that determine the multi-spin correlation coefficients, we may take their derivatives analytically also. In this way, for example, we may *directly* evaluate the anisotropy susceptibility, $\chi_a \equiv -\partial^2(E_g/N)/\partial\lambda^2$. A numerical analysis for the LSUBm approximants, χ_a^m, with $m > 2$, yields

$$\chi_a^m(\lambda) \to \bar{\chi}_a^m \, (\lambda_c^m - \lambda)^{-\alpha_0} \quad ; \quad \lambda \to \lambda_c^m \quad , \tag{25}$$

with an exponent $\alpha_0 \approx 1.50$. This behaviour appears to be identical to that of the SUB2-m subapproximants with finite values of m, for which $\alpha_0 = 3/2$, as in Eq. (24).

However, we have also seen from Eq. (23) that in the full SUB2 approximation $\alpha_0 = 1/2$. Indeed, just as for the SUB2-m series, the LSUBm results can be fitted with a prefactor $\bar{\chi}_a^m$ of the so-called coherent anomaly form,

$$\bar{\chi}_a^m \to K \, (\lambda_c^m - \lambda_c^\infty)^\nu \quad ; \quad \lambda \to \lambda_c^\infty \quad , \tag{26}$$

where K is a constant. Thus, as explained by Suzuki [41], one may expect the asymptotic form,

$$\chi_a(\lambda) \sim (\lambda_c^\infty - \lambda)^{-\alpha_0 + \nu} \quad ; \quad \lambda \to \lambda_c^\infty \quad . \tag{27}$$

A CAM analysis along these lines of our LSUBm results for $m = 4, 6$ yields an exponent $\nu \approx 1.25 \pm 0.2$, and hence a singular term in E_g/N near λ_c with a critical exponent $2 - \alpha_0 + \nu \approx 1.75 \pm 0.2$. This may be compared with the corresponding value of 3/2 from both the mean-field-like CCM SUB2 and SWT approximations. Doubtless it will be of considerable interest to extend our LSUBm results to values $m > 6$ in order to refine the above analysis and to sharpen our predictions for the critical indices.

Similar LSUBm results can also, in principle, be obtained for the triangular-lattice Hamiltonian H_2, and we intend to report on such calculations elsewhere.

5. DISCUSSION AND CONCLUSIONS

The results presented here clearly show that the combination of the theoretical framework of the CCM and the use of computer algebra to implement it at high orders of approximation, results in a powerful formalism for dealing with both unfrustrated and frustrated spin-lattice problems. We have been able both to obtain predictions for ground-state properties which are competitive with the best available alternative calculations, and also to study quantitatively the critical properties of the quantum phase transitions exhibited by these models. Based on this success, it will be of considerable interest to extend the applications to include similarly high-order calculations of electron-lattice models of interest to high-temperature superconductivity, where, as in the case of the triangular lattice, QMC results are not readily available due to the infamous fermion sign problem.

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