Ab initio simulation of the nodal surfaces of Heisenberg antiferromagnets

R. F. Bishop
Department of Physics, University of Manchester Institute of Science and Technology (UMIST), P.O. Box 88, Manchester M60 1QD, United Kingdom

D. J. J. Farnell
Institut für Theoretische Physik, Universität zu Köln, Zülpicher Strasse, 50937 Köln, Germany

Chen Zeng
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855
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The spin-half Heisenberg antiferromagnet (HAF) on the square and triangular lattices is studied using the coupled-cluster-method (CCM) technique of quantum many-body theory. The phase relations between different expansion coefficients of the ground-state wave function in an Ising basis for the square lattice HAF is exactly known via the Marshall-Peierls sign rule, although no equivalent sign rule has yet been obtained for the triangular-lattice HAF. Here the CCM is used to give accurate estimates for the Ising-expansion coefficients for these systems, and CCM results are noted to be fully consistent with the Marshall-Peierls sign rule for the square-lattice case. For the triangular-lattice HAF, a heuristic rule is presented which fits our CCM results for the Ising-expansion coefficients of states which correspond to two-body excitations with respect to the reference state. It is also seen that Ising-expansion coefficients which describe localized, *m*-body excitations with respect to the reference state are found to be highly converged, and from this result we infer that the nodal surface of the triangular lattice HAF is being accurately modeled. Using these results, we are able to make suggestions regarding possible extensions of existing quantum Monte Carlo simulations for the triangular-lattice HAF. [S0163-1829(99)09901-4]

I. INTRODUCTION

The coupled-cluster method[1–9] (CCM) has been previously applied[10–25] to a number of unfrustrated and frustrated lattice quantum spin systems with a great deal of success. Recently, it has been shown[24] for a CCM calculation, within the so-called SUB2 approximation which contains *all* two-body correlations, that the ket-state correlation coefficients can be related to the Marshall-Peierls sign rule[26] for the square-lattice Heisenberg antiferromagnet (HAF). Furthermore, it was shown in this treatment[24] that the CCM ket-state correlation coefficients for the Heisenberg model on the triangular lattice also demonstrate a seemingly regular pattern. This relationship between the Marshall-Peierls sign rule and the CCM ket-state correlation coefficients was further investigated[25] and clarified for a spin model with both nearest-neighbor and next-nearest-neighbor exchange, namely, the J_1-J_2 model, on the linear chain and square lattices. The Marshall-Peierls sign rule at the Heisenberg point on the square lattice was found to be preserved by *all* of the Ising-expansion coefficients within a localized approximation scheme, as well as within the SUB2 scheme. No assumption was made other than the choice of an initial reference state with respect to which the ground-state wave function was approximately constructed in the infinite lattice limit using the CCM formalism. It was also possible to obtain a quantitative value for the point at which the sign rule breaks down with increasing antiferromagnetic next-nearest-neighbor exchange for the square-lattice case. This quantitative value was found to be in good agreement with exact diagonalization calculations.[27]

The Marshall-Peierls sign rule for Heisenberg antiferromagnets on bipartite lattices is an exact statement for the phase relations between the expansion coefficients of the ground-state wave function in an Ising basis. This statement is of intrinsic interest because it provides exact information regarding the ground-state wave function in cases (e.g., the square lattice HAF) for which no general exact solution has yet been determined. It is also of interest because by using this rule one implicitly has full knowledge of the ''nodal surface'' of the ground-state wave function within this basis. (Note that whenever the words ''nodal surface'' are referred to in this article, this is taken to mean the magnitudes and signs of these expansion coefficients.) Of course, for the square lattice HAF the signs are exactly known via the Marshall-Peierls sign rule, although the magnitudes are known only via exact or approximate calculation. Quantum Monte Carlo (QMC) calculations for fermionic and spin systems demonstrate the infamous ''sign problem,'' and so such information regarding the signs of the expansion coefficients is of importance in these calculations.

For nonbipartite lattices (e.g., the triangular-lattice HAF) or for other models containing frustration (e.g., the J_1-J_2 model on the square lattice) corresponding exact sign-rule theorems are generally not known. Hence, various approximate ways of simulating the nodal surface have been developed for use, for example, in fixed-node quantum Monte Carlo calculations. However, one is always limited in such simulations by not knowing how close is the trial wave function or guiding wave function that one uses to the true ground-state wave function. It is therefore of considerable

interest to develop theories which simulate the nodal surface from an *ab initio* stand point, such as is done here via the CCM. In this way, one might be able to utilize this CCM information concerning the nodal surface in a QMC calculation, or at least suggest possible extensions of previous QMC calculations. It is also conceivable that one might observe patterns in the expansion coefficients obtained via the CCM and so infer rules concerning these coefficients or subclasses of them which relate to specific types of excitation.

In this article, we briefly introduce the CCM formalism for the lattice quantum spin systems and also make an explicit link between the expansion coefficients of the ground-state wave function and the CCM ket-state correlation coefficients. This link is investigated for the square and triangle-lattice HAF's, and the Ising-expansion coefficients corresponding to states which correspond to two-body excitations with respect to a reference state are determined within well-defined approximation schemes. These coefficients are seen to be well-converged using a *localized* approximation scheme. For the triangular-lattice HAF, a heuristic rule is presented which fits our CCM results for the Ising-expansion coefficients of states which correspond to two-body excitations with respect to the reference state. The Ising-expansion coefficients of states which correspond to *m*-body excitations are also shown, within this same localized approximation scheme, to be well converged. Patterns are also seen in the Ising-expansion coefficients which correspond to these *m*-body excitations for the triangular-lattice HAF, although no generic sign rule for them is formulated. Finally, suggestions are made regarding possible extensions of existing quantum Monte Carlo simulations for the triangular-lattice HAF.

II. THE SPIN MODEL AND THE CCM FORMALISM

A. The Heisenberg model

In this paper we consider the zero-temperature $(T=0)$ properties of the spin-half Heisenberg antiferromagnet (HAF) quantum spin system, which is described by the Hamiltonian

$$H=\sum_{\langle i,j\rangle}\mathbf{s}_i\cdot\mathbf{s}_j\,, \tag{1}$$

where the index i runs over all N lattice sites on the square and triangular lattices with periodic boundary conditions, and the index j runs over all nearest-neighbor sites to i. The angular brackets indicate that each nearest-neighbor bond (or link) is counted once and once only.

The Heisenberg model on the square lattice has not been solved exactly up till now, although it been extensively studied using various approximate methods.[28–31] Runge[31] has performed the most accurate Monte Carlo simulation to date for the square-lattice isotropic HAF. He finds a value for the ground-state energy per spin of $E_g/N=-0.66934(4)$, and a value for the sublattice magnetization which is 61.5% $\pm 0.5\%$ of the classical value. Extensive CCM calculations have also been carried out for this model[23] giving a value for the ground-state energy per spin of $E_g/N=-0.66968$, and a value for the sublattice magnetization which is 62% of the classical value. In comparison, linear spin-wave theory (LSWT) (Ref. 28) gives a value of $E_g/N=-0.658$ for the ground-state energy, and a value for the sublattice magnetization which is 60.6% of the classical value.

Again, no exact solution exists for the Heisenberg model on the triangular lattice, although many approximate calculations have been carried out.[23,32–37] Exact series expansion[33] calculations obtain a value for the ground-state energy per spin of this model of $E_g/N=-0.551$. Similarly, spin-wave theory (SWT) (Ref. 34) gives a value of $E_g/N=-0.5388$, and a fixed-node quantum Monte Carlo (FNQMC) (Ref. 35) calculation gives a value of $E_g/N=-0.5431\pm 0.0001$. Exact diagonalizations of finite-sized clusters of spins[36] which have been extrapolated to the infinite lattice limit give a value for the ground-state energy per spin of $E_g/N=-0.5445$. In comparison, a recent coupled-cluster-method calculation[23] predicts a value for the energy of $E_g/N=-0.5505$, which is fully consistent with the best of the other results obtained for this system so far.

Classically, this system orders as a Néel state on the triangular lattice such that each nearest-neighbor pair of spins makes an angle of 120° to each other. The results of approximate theories for the amount of this ordering that remains in the quantum limit, i.e., the sublattice magnetization, are typically[23,34,36] that 50% of the classical ordering remains in the quantum limit. The FNQMC calculation of Ref. 35 places this value at 60%, which is probably still too high. A notable exception to all of these results quoted above is the result of exact series expansion calculations[33] which predicts that as little as 20% of the classical ordering remains.

B. The CCM formalism

The CCM formalism[1–9] is now briefly considered, although the reader should note that more detailed descriptions of the CCM applied to spin systems are given in Refs. 10–25. To calculate the ground state wave function $|\Psi\rangle$ of a spin system we start with a model state $|\Phi\rangle$ and a correlation operator S such that

$$|\Psi\rangle=e^S|\Phi\rangle, \tag{2}$$

where the ket-state correlation operator S may be written as

$$S=\sum_{I\neq 0}\mathcal{S}_I C_I^+\,. \tag{3}$$

The correlation operator S is formed from a linear combination of multiconfigurational creation operators $\{C_I^+\}$ (which themselves are formed from products of spin raising operators) multiplied with the relevant ket-state correlation coefficients $\{\mathcal{S}_I\}$. In addition, we define a set of destruction operators $\{C_I^-\}$ which are the Hermitian adjoints of $\{C_I^+\}$.

For the square lattice case, the model state is chosen to be the classical Néel state. The lattice is divided into two sublattices and one sublattice is populated with ''up'' spins and the other with ''down'' spins. In order to treat the spins equivalently the local spin axes of the ''up'' spins are rotated by 180° about the y axis, which is mathematically written as

$$s^x\rightarrow -s^x,\quad s^y\rightarrow s^y,\quad s^z\rightarrow -s^z. \tag{4}$$

The Hamiltonian may now be written, with the introduction of an anisotropy coefficient x on the off-diagonal elements of H, as

$$H=-\sum_{\langle i,j\rangle}\left\{s_i^z s_j^z+\frac{x}{2}(s_i^+ s_j^+ + s_i^- s_j^-)\right\}, \tag{5}$$

where the sum on $\langle i,j\rangle$ runs over all nearest-neighbor pairs and counts each pair once only, and where $x=1$ corresponds to the isotropic Heisenberg Hamiltonian of Eq. (1). The Marshall-Peierls sign rule for the original Hamiltonian of Eq. (1), in terms of rotated spin coordinates, now differs from the original sign rule.[26] For the ground-state wave function, $|\Psi\rangle=\Sigma_I \Psi_I |I\rangle$, the Ising-expansion coefficients $\{\Psi_I\}$ must now all be greater than (or equal to) zero with respect to a complete set of Ising basis states $\{|I\rangle\}$ in the rotated spin coordinates.

For the triangular lattice case, we choose $|\Phi\rangle$ to again be the classical Néel state, and we start the CCM calculation by dividing the lattice into three sublattices, denoted $\{A,B,C\}$. 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 HAF to include an Ising-like anisotropy first introduced by Singh and Huse[33] and to make a suitable choice of the CCM model state, we perform the following spin-rotation transformations. Specifically, we leave the spin axes on sublattice A unchanged, and we rotate about the y axis the spin axes on sublattices B and C by $-120°$ and $+120°$, respectively,

$$\begin{aligned} s_B^x &\rightarrow -\frac{1}{2}s_B^x-\frac{\sqrt{3}}{2}s_B^z, \quad s_C^x \rightarrow -\frac{1}{2}s_C^x+\frac{\sqrt{3}}{2}s_C^z, \\ s_B^y &\rightarrow s_B^y, \quad s_C^y \rightarrow s_C^y, \\ s_B^z &\rightarrow \frac{\sqrt{3}}{2}s_B^x-\frac{1}{2}s_B^z, \quad s_C^z \rightarrow -\frac{\sqrt{3}}{2}s_C^x-\frac{1}{2}s_C^z. \end{aligned} \tag{6}$$

We may rewrite Eq. (1) in terms of spins defined in these local quantization axes for the triangular lattice with a further introduction of an anisotropy parameter λ for the non-Ising-like pieces

$$H=\sum_{\langle i\rightarrow j\rangle}\left\{-\frac{1}{2}s_i^z s_j^z+\frac{\sqrt{3}\lambda}{4}(s_i^z s_j^+ + s_i^z s_j^- - s_i^+ s_j^z - s_i^- s_j^z) + \frac{\lambda}{8}(s_i^+ s_j^- + s_i^- s_j^+) - \frac{3\lambda}{8}(s_i^+ s_j^+ + s_i^- s_j^-)\right\}, \tag{7}$$

where $\lambda=1$ corresponds to the isotropic Heisenberg Hamiltonian of Eq. (1). We note that the summation in Eq. (7) again runs over nearest-neighbor bonds, but now also with a *directionality* indicated by $\langle i\rightarrow j\rangle$, which goes from A to B, B to C, and C to A. We note that no exact sign rule has yet been proven for the Hamiltonian of Eq. (7). When $\lambda=0$, the Hamiltonian in Eq. (7) describes the usual classical Ising system with a unique ground state which is simply the fully aligned (''ferromagnetic'') configuration in the local spin coordinates described above.

From the Schrödinger equation $H|\Psi\rangle=E|\Psi\rangle$ we obtain an expression for the ground state energy which is given by

$$E=\langle\Phi|e^{-S}He^{S}|\Phi\rangle. \tag{8}$$

This equation illustrates one of the key aspects of CCM, which is named the similarity transform—here of the Hamiltonian. The similarity transform of any operator may be expanded as a series of nested commutators such that an exact expression for the ground-state energy in terms of the ket-state correlation coefficients $\{\mathcal{S}_I\}$ which is already determined in the infinite lattice limit $N\rightarrow\infty$, can often be found for whatever (nontrivial) approximations are made for S. The approximation in S means that we obtain approximate values for ket-state coefficients $\{\mathcal{S}_I\}$ and so the ground-state energy is approximately determined, although, as stated above, the equation for the ground-state energy is an exact expression of one or more of these coefficients. To determine the CCM ket-state coefficients we operate on the Schrödinger equation with $\exp(-S)$ and then by $\langle\Phi|C_I^-$, for a given cluster configuration indicated by the index I. An explanation of how the CCM equations may be derived and then solved is presented in Refs. 10–25.

The three most commonly employed approximation schemes are (1) the SUBn scheme, in which all correlations involving only n or fewer spins are retained, but no further restriction is made concerning their spatial separation on the lattice, (2) the SUBn-m sub-approximation, in which all SUBn correlations spanning a range of no more than m adjacent lattice sites are retained, and (3) the localized LSUBm scheme, which retains all multispin correlations over distinct locales on the lattice defined by m or fewer contiguous sites. In order to clarify the physical significance of the approximation schemes outlined above, we note that since the SUBn scheme contains all n-body (and lower-order) correlations, the SUBn approximation contains both *long-ranged* and *short-ranged* n-body (and lower-order) correlations. In contrast, the SUBn-m scheme contains only those *short-ranged* n-body (and lower-order) correlations within a locale defined by m, although it is noted that results of the SUBn-m scheme converge to those of the SUBn scheme in the limit $m\rightarrow\infty$. Similarly, the LSUBm scheme contains only those *short-ranged* m-body (and lower-order) correlations in a locale also defined by m. (For specific examples of the application of such schemes to lattice spin models the reader is referred to Refs. 10–25.) Note that all 30 cluster configurations which are used in the LSUB4 approximation for the triangular lattice antiferromagnet, and which are independent under the six-point symmetry group inherent in the Hamiltonian of Eq. (7), are listed in Fig. 1.

We now consider an expansion of the ground-state wave function in a complete Ising basis $\{|I\rangle\}$ (in terms of the *local* coordinates after rotation). This may be again written as $|\Psi\rangle=\Sigma_I \Psi_I |I\rangle$, where the sums over I go over all 2^N Ising states, and we find that this expression naturally leads from Eq. (2) (also see Ref. 25) to an exact mapping of the CCM correlation coefficients $\{\mathcal{S}_I\}$ to the Ising-expansion coefficients $\{\Psi_I\}$, which is given by

$$\Psi_I=\langle\Phi|C_I^- e^{S}|\Phi\rangle \equiv \langle\Phi|s_{i_1}^- s_{i_2}^- \cdots s_{i_l}^- e^{S}|\Phi\rangle . \tag{9}$$

It is possible to match the terms in the exponential to the ''target'' configuration of C_I^- in Eq. (9), and so obtain a numerical value for the $\{\Psi_I\}$ coefficients once the CCM ket-state equations have been derived and solved for a given value of the anisotropy. As the target configuration is formed

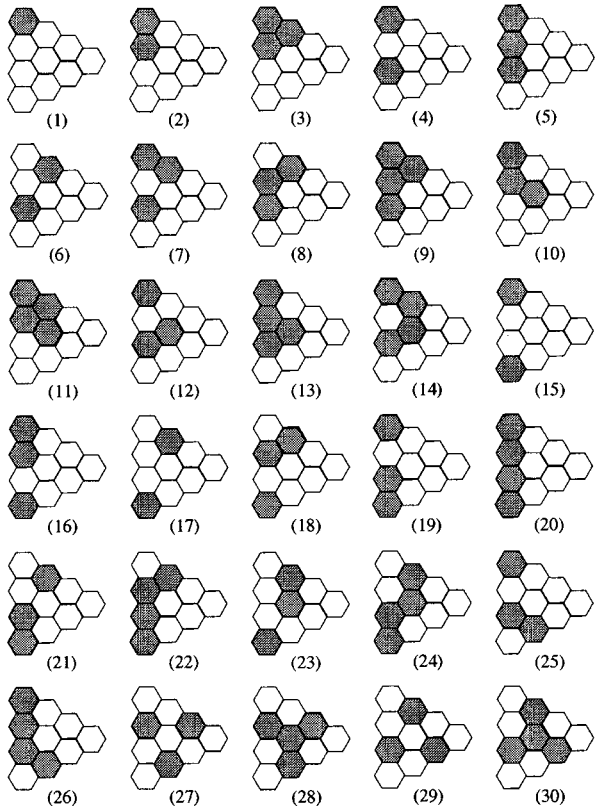

FIG. 1. Excitation cluster configurations for the triangular-lattice antiferromagnet within the LSUB4 approximation. Each hexagon marks the lattice position of a spin raising operator applied to the model state at a given point on the triangular lattice.

from a finite number of spin lowering operators, there is a cutoff point in the Taylors series expansion of the exponential above which no contribution to Ψ_I in Eq. (9) can possibly occur. This matching may be achieved[25] in two ways: analytically at the SUB2 level of approximation or at small LSUB*m* levels of approximation; or by using computational-algebraic techniques. We note that we use, for the sake of consistency, the same configurations for the 'target' configurations in C_I^- in Eq. (9) as are used in the ket-state correlation operator S for the approximation schemes define above. We also note that, although this is an approximate calculation, we are already dealing with the infinite lattice limit, $N \rightarrow \infty$. The next section describes our results for the set of $\{\Psi_I\}$ coefficients for the spin-half Heisenberg model on the square and triangular lattices using the CCM formalism, and discuss possible rules that can be inferred from these results.

III. RESULTS

A. The two-body excitations

The results for the Ising-expansion coefficients $\{\Psi_I\}$ corresponding to two-body excitations with respect to the model state for the spin-half square-lattice HAF ($x=1$) are shown in Fig. 2. (Note that the solution to the CCM equations is tracked from $x=0$, at which point we know that all of the ket-state correlation coefficients $\{\mathcal{S}_I\}$ are zero, to the isotropic Heisenberg point.) The results for the two-body $\{\Psi_I\}$ coefficients are then determined and it is found that these coefficients are *all* positive for the LSUB*m* approximation

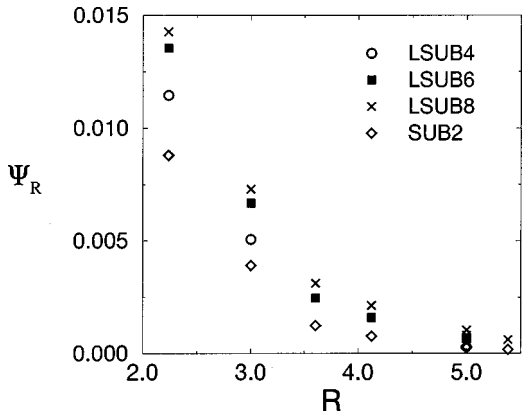

FIG. 2. Results for the Ising-expansion coefficients, plotted as a function of the lattice distance R, corresponding to two-body excitations with respect to the model state for the spin-half, square-lattice HAF ($x=1$) obtained via the LSUB*m* approximation scheme (with $m=\{4,6,8\}$) and the SUB2 approximation.

scheme (with $m \leqslant 8$) and within the SUB2 approximation. (This result for the SUB2 case was previously seen in Ref. 25.) This is an expression of the Marshall-Peierls sign rule[26] which provides an exact relation between the $\{\Psi_I\}$ expansion coefficients. However, we note that the CCM predicts such behavior with no recourse to exact proofs, and this prediction is a natural result of the CCM calculations. Furthermore, the convergence of the LSUB*m* series of results compared to SUB2 calculation can clearly be seen in Fig. 2. For short lattice distance, we believe that the LSUB*m* results are much better model of the ''nodal surface'' of states corresponding to two-body excitations than those of the SUB2 calculation.

For the spin-half triangular-lattice HAF ($\lambda=1$), the results for the Ising-expansion coefficients $\{\Psi_I\}$ corresponding to two-body excitations with respect to the model are shown in Fig. 3 and in Table I. (Note again that the solution to the CCM equations is tracked from $\lambda=0$, at which point again we know that all of the ket-state correlation coefficients $\{\mathcal{S}_I\}$ are zero, to the isotropic Heisenberg point.) A rule that fits

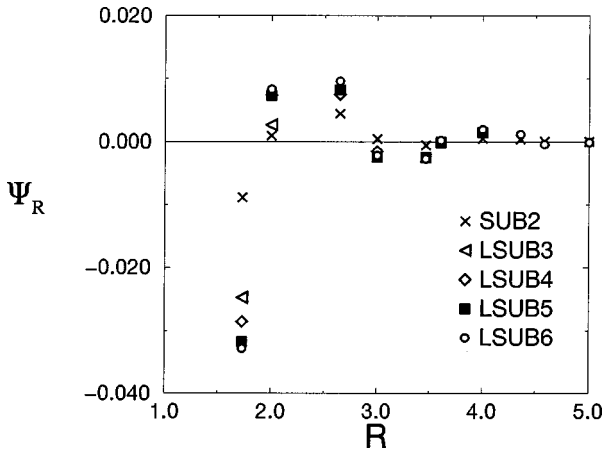

FIG. 3. Results for the Ising-expansion coefficients, plotted as a function of the lattice distance R, corresponding to two-body excitations with respect to the model state for the spin-half triangular-lattice HAF ($\lambda=1$) obtained via the LSUB*m* approximation scheme (with $m=\{3,4,5,6\}$) and the SUB2 approximation.

TABLE I. Expansion coefficients $\{\Psi_I\}$ for the spin-half triangular-lattice HAF ($\lambda=1$) for the clusters given in Fig. 1 within LSUBm (with $m=\{3,4,5,6\}$) approximation scheme and the SUB2 approximation. For the sake of consistency, the only clusters expansion coefficients $\{\Psi_I\}$ that have been determined are those which are also used within the given approximation.

Cluster	SUB2	LSUB3	LSUB4	LSUB5	LSUB6
1	0.000000	0.000000	0.000000	0.000000	0.000000
2	0.114444	0.128096	0.141570	0.145502	0.149245
3		0.000000	0.000000	0.000000	0.000000
4	0.000941	0.002642	0.007384	0.007310	0.008302
5		0.000000	0.000000	0.000000	0.000000
6	−0.008838	−0.024744	−0.028535	−0.031743	−0.032843
7			0.004098	0.004380	0.004694
8		−0.029600	−0.039855	−0.044560	−0.047332
9			0.020290	0.021182	0.022933
10		0.029600	0.039855	0.044560	0.047332
11			0.055163	0.060557	0.065889
12			−0.004098	−0.004380	−0.004694
13			0.020290	0.021182	0.022933
14			0.014343	0.013776	0.014106
15	0.000428		−0.001568	−0.002414	−0.002185
16			0.000133	0.000437	0.000409
17	0.004417		0.007473	0.008187	0.009555
18			−0.001828	−0.002663	−0.002865
19			−0.000133	−0.000437	−0.000409
20			0.019778	0.020721	0.022046
21			0.005219	0.006398	0.007213
22			0.025031	0.027608	0.029788
23			−0.005219	−0.006398	−0.007213
24			0.013840	0.012139	0.012059
25			0.001828	0.002663	0.002865
26			0.025031	0.027608	0.029788
27			0.004266	0.006421	0.007184
28			0.000679	0.004521	0.006052
29			−0.004266	−0.006421	−0.007184
30			0.000679	0.004521	0.006052

the behavior seen in Fig. 3 can now be stated as ''the coefficients are found to be positive if the lattice vector of between the two spin-raising operators in S connects sites on different sublattices; conversely, the $\{\Psi_I\}$ coefficients are found to be negative if the lattice vector connects sites on the same sublattice.'' It is again seen that the LSUBm series is clearly well converged for small lattice distance R. This series of LSUBm results also clearly present a much better representation of the ''nodal surface'' for the two-body excitations, for small lattice distance than the corresponding $\{\Psi_I\}$ coefficients within the SUB2 approximation.[24]

B. The m-body excitations

For the Ising-expansion coefficients $\{\Psi_I\}$ corresponding to m-body excitations for the square lattice HAF ($x=1$), it has previously been noticed[25] that the CCM calculation outlined above predicts that they are *all* positive. This is an indication that the CCM results are (once more) fully consistent with the exact Marshall-Peierls sign rule for this model. It should be again noted that the only assumption made is the initial model state, and that the rest follows naturally on from the CCM calculation.

Table I indicates the $\{\Psi_I\}$ expansion coefficients for the triangular lattice HAF ($\lambda=1$) states corresponding to localized, m-body (with $m\leqslant 4$) configurations (i.e., those also used within the LSUB4 approximation) with respect to the model state. One should note however that these $\{\Psi_I\}$ expansion coefficients are determined within the SUB2 and LSUBm (with $m=\{3,4,5,6\}$) approximations. It is again seen in Table I that all of the expansion coefficients are well converged for the LSUB5 and LSUB6 levels of approximation. Note, however, that within the LSUB5 and LSUB6 approximation many other $\{\Psi_I\}$ coefficients have been determined, within the ''consistency'' assumption explained above.

Patterns in the $\{\Psi_I\}$ expansion coefficients for the triangular lattice HAF ($\lambda=1$) for states corresponding to m-body excitations (with $m\geqslant 1$) have also been observed. It was seen that, with m odd, all of the coefficients for excitation clusters which are equivalent under both the symmetries of the lattice

(a point group of order twelve) and the Hamiltonian (a point group of order 6), were found to have both CCM correlation coefficients and Ising-expansion coefficients which are zero at all levels of approximation; e.g., configurations (1), (3), and (5) in Fig. 1 and in Table I. In contrast, those $\{\Psi_I\}$ coefficients corresponding to configurations with *odd* numbers of spins which are equivalent under the symmetries of the lattice but are *not* equivalent under the symmetries of the Hamiltonian were found to have equal magnitudes but opposite signs. That is, there exists pairs $(12/6=2)$ of coefficients, for the odd-number spin-excitation clusters, which differ with respect to each other only by a phase factor of -1; e.g., those pairs (7,12), (8,10), (16,19), (18,25), (21,23), and (27,29) in Fig. 1 and in Table I. In contrast, for the Ising-expansion coefficients $\{\Psi_I\}$ corresponding to m-body excitations, with m even, we find that those $\{\Psi_I\}$ coefficients corresponding to configurations which are equivalent under symmetries of the lattice but are *not* equivalent under the symmetries of the Hamiltonian are exactly the same. That is, there exist pairs $(12/6=2)$ of coefficients, for the even-number spin-excitation clusters, which have a phase factor with respect to each other of unity; e.g., pairs (9,13), (22,26), and (28,30) in Fig. 1 and in Table I.

We note that these simple relations were obtained with no assumption other than the model state, which is of course the classical ground state of this system. This is in contrast to variational calculations,[32] spin-wave theory,[37] and FNQMC (Ref. 35) which assume that the classical phase relations are correct phase relations for their quantum mechanical counterparts. It has been shown[19] that in a case in which the Hamiltonian shares some symmetry of the model state then the values of the CCM correlation coefficients in the ground state, for configurations which are equivalent under these symmetries, must be completely identical. We believe that the ''rules'' presented above for the m-body expansion coefficients for the triangular lattice HAF are therefore a reflection of the symmetries inherent in the Hamiltonian and lattice. Furthermore, it remains an open question as to the solution of *all* branches of coupled, nonlinear, ket-state CCM equations for high-order calculations. One should note that it might be possible to obtain another solution branch which might *not* demonstrate the full symmetries of the lattice and Hamiltonian, as has been seen for other systems treated by CCM before. A full treatment of this subject would form the contents of another article.

Apart from these simple observations, we cannot infer a more general rule as to the behavior of the expansion coefficients for m-body excitations with $m>2$. However, we do have results for the signs of all of the expansion coefficients within the LSUBm approximation scheme, as is illustrated in Table I, and hence the CCM is simulating, from an *a priori* viewpoint, the nodal surface of this model. From the amount of convergence of the results of the expansion coefficients within the LSUBm scheme described above, we therefore also believe that we have an accurate simulation of the nodal surface of this model using the LSUBm approximation scheme.

C. Relevance to QMC calculations

For the triangular lattice HAF, a ''naive'' picture of how important each excitation configuration can be found by looking at the magnitude of its corresponding Ψ_I coefficient, illustrated in Table I. In this manner, we find that the two-body, nearest-neighbor configuration [configuration (2) in Fig. 1] is the most important correlation for this model. By this rationale, the next most important configurations are a ''diamond-shaped,'' four-body configuration [configuration (11) in Fig. 1] and a ''dog-leg,'' three-body configuration [configurations (8) and (10) in Fig. 1]. A previous FNQMC calculation[35] contains all two-body correlations and this particular three-body correlation, and so a straightforward extension of this calculation would be to include this four-body configuration. However, from this ''naive'' interpretation of our results it appears that, as well as the two-body configurations and the two configurations mentioned above, many other *localized* three-body and four-body configurations are also very important. (These configurations are localized in the same sense of those configurations contained in the LSUBm approximation.) Hence, to attempt an accurate simulation of this model one probably needs to find a way of also including many, if not all, of these localized, higher-order correlations. One way of achieving this would therefore be to use the nodal surface predicted by the CCM in a FNQMC calculation.

IV. CONCLUSIONS

In this article it has been shown that the expansion coefficients of the ground-state wave function in the infinite lattice limit may be approximately determined via CCM calculations. The two-body expansion coefficients have thereby been obtained as a function of lattice distance. For the triangular-lattice HAF, a Heuristic rule which fits CCM results for the coefficients corresponding to two-body excitations with respect to the model state was also obtained. Certain patterns, for the triangular-lattice HAF, were also seen for coefficients corresponding to higher-order excitations, although no complete Heuristic rule for all Ising states could be inferred. For the square lattice HAF, it has once more been noted that *all* of these expansion coefficients obey the Marshall-Peierls sign rule for the LSUBm and SUB2 approximations with no other assumption other than the model state. The convergence of the Ising-expansion coefficients for the LSUBm series of results was also seen for small lattice distance for both lattices. In this manner, the LSUBm results are believed to provide an accurate simulation of the true nodal surface of these models at small lattice separation.

In the above context it is evident that a knowledge of the precision of the calculations presented here is essential in order to ascertain the certainty of the derived sign rule information. The errors involved are both numerical and systematic. In the first place we note that the numerical errors are completely under control. Thus, the calculations to find the $\{\Psi_I\}$ coefficients for the infinite $(N\rightarrow\infty)$ lattice are essentially exact *within a given* LSUBm *approximation for S*. This is because the process of matching the configurations $\{I\}$ and the corresponding multiconfigurational creation operators $\{C_I^+\}$ to the spin-raising operators in the exponential CCM ket-state operator e^S always terminates at a finite order, and because the (finite) truncated CCM equations themselves can easily be solved numerically to (arbitrarily) high accuracy. For these reasons we have not put error bars on the coeffi-

cients $\{\Psi_I\}$ in Table I or Figs. 2 and 3, since to the accuracy displayed the results are exact for each level of approximation shown.

The only remaining source of error thus arises from the systematic ''errors'' between the exact results and the results at a particular level of approximation. This is completely analogous to the systematic errors involved in the difference between the essentially exact results for finite-sized systems (e.g., by exact diagonalizations or by QMC techniques) and the unknown results for the infinite systems. In both cases one needs to extrapolate: to the limit $m\rightarrow\infty$ for the CCM results in the LSUBm approximation scheme, and to the limit $N\rightarrow\infty$ for the finite-size calculations. Whereas finite-size scaling typically provides a guide to the correct $N\rightarrow\infty$ extrapolation rule for macroscopic parameters such as the ground-state energy and staggered magnetization for the finite-sized results, no such exact $m\rightarrow\infty$ extrapolation rules are known for the LSUBm CCM results, particularly for the CCM correlation coefficients. Although simple Heuristic rules for the extrapolation of CCM results for such global quantities as the ground-state energy and staggered magnetization have been very effective in previous calculations[23,25] no such simple rules have yet been found for the coefficients $\{\mathcal{S}_I\}$ or $\{\Psi_I\}$. Furthermore, for the higher-order coefficients shown in Figs. 2 and 3 we only have relatively few points, and it is not yet technically feasible to perform a credible quantitative extrapolation. Nevertheless, the results (and see Table I) clearly demonstrate excellent qualitative convergence, particularly since for present purposes we are primarily interested only in the signs of the coefficients.

Finally, suggestions were made with respect to further QMC calculations for the triangular-lattice HAF. The first was the inclusion of a ''diamond-shaped'' cluster in a FN-QMC calculation, which we believe to be the most important cluster not yet used in such a calculation. However, we also infer from our results that many three- and four-body clusters are important in order to accurately simulate this model. One method of including these correlations in a QMC calculation would be to use the nodal surface predicted by CCM calculations, thereby overcoming the infamous ''sign problem'' which is the main present stumbling block in performing QMC calculations of arbitrary accuracy, within statistical errors controlled only by the length of the run.

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