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ACCURATE COUPLED CLUSTER CALCULATIONS OF GENERAL QUANTUM ANTIFERROMAGNETS: AN EXAMPLE ON A FRUSTRATED LATTICE

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1. INTRODUCTION

In recent years there has been a great deal of interest, both theoretical and experimental, and in a wide variety of physical contexts, in studying the properties of quantum-mechanical systems described by a Hamiltonian defined on an extended regular spatial lattice. Examples include: (i) spin-lattice systems such as the solid phases of ^3He , thin layers of ^3He adsorbed on graphite, and various models exhibiting antiferromagnetism and other magnetic phases; (ii) models of strongly-interacting electrons on lattices, such as the Hubbard or t - J models; and (iii) lattice field theories such as the Abelian $U(1)$ and non-Abelian $SU(3)$ gauge models of quantum electrodynamics and quantum chromodynamics respectively, and a latticised $O(4)$ version of the nonlinear sigma model as a chiral meson field theory of pion dynamics.

Until relatively recently most of the available theoretical results for such spin lattice systems have come from large-scale quantum Monte Carlo (QMC) simulations, extrapolations from exact diagonalisations on small finite lattices, or other semi-microscopic techniques such as those based on attempts to extend into the physical domain the perturbative results obtained in the weak- and/or strong-coupling limits using Padé and similar analyses. The latter techniques have been difficult to systematise and often suffer from unknown sources of error in the extrapolations.

On the other hand, although the QMC results can also be prone to systematic errors (which typically arise from the choice of a trial wave function for use in the importance sampling part of the procedure), they usually give accurate benchmark results where they can be performed. Nevertheless, their availability is dramatically curtailed when the system under study cannot be mapped onto an equivalent bosonic system, and hence where the well-known "minus-sign problem" thereby cannot be avoided. In the case of spin-lattice problems, for example, the ground states of simple Heisenberg-like antiferromagnetic Hamiltonians on bipartite lattices can often be readily attacked using QMC techniques, due to the existence for such lattices of

the Marshall-Peierls sign rule [1], which provides a means to eliminate the minus-sign problem by providing full information about the nodal surface structure of the wave function. By contrast, the same antiferromagnetic models on geometrically frustrated lattices such as the triangular lattice, have no such known sign rules for the ground-state wave function, and QMC techniques have proven to be much more difficult and less accurate to implement in these cases.

For these reasons powerful, general-purpose techniques of microscopic quantum many-body theory have, in the last few years, increasingly been modified and applied to extended lattice Hamiltonian systems. One of the present authors has presented a recent overview [2], which illustrates these new applications of such well-established techniques as the coupled cluster method (CCM) and the method of correlated basis functions. In the present work we describe specifically how the CCM has now been developed into a rather powerful, general-purpose tool for applications to spin-lattice problems. We note that it is now capable of being systematically implemented within a very general framework to increasingly high orders of approximation; that it is already capable of giving numerical results which are fully competitive with those from QMC simulations in those cases where no minus-sign problems arise, usually at a fraction of the computational cost; and, furthermore, that the CCM techniques are equally applicable to frustrated systems at no essential increase in the computational effort.

The remainder of this paper is organised as follows. After the general CCM methodology for the spin-lattice models has been described in Sec. 2, we outline in Sec. 3 its application to a specific two-dimensional (2D), spin-half, anisotropic antiferromagnetic model on the frustrated triangular lattice, for which the isotropic point is just the usual nearest-neighbour Heisenberg model. Results of the CCM calculations are given in Sec. 4, and we conclude in Sec. 5 with a general discussion of their quality and with a brief outline of possible extensions of the work.

2. THE CCM FORMALISM FOR QUANTUM SPIN LATTICES

Detailed descriptions of both the general CCM formalism [2-11] and its application to specific spin-lattice models [12-18] have been given elsewhere. Nevertheless, we highlight here such of the essential ingredients as are required for present purposes. Our aim in this Section is to be as general as possible.

In the so-called single-reference version of the normal (as opposed to the extended [7,9]) variant of the CCM, to which we restrict ourselves here, we first need to choose a suitable single model or reference state $|\Phi\rangle$, in terms of which a quantitative and systematic description of the many-body (i.e., in the present case, multi-spin) correlations or fluctuations may be given. We defer till later the important question of how to choose $|\Phi\rangle$ in practice, but state now that it is required only to be a cyclic vector with respect to two well-defined Abelian subalgebras of multi-configurational creation operators $\{C_I^+\}$ and their Hermitian-adjoint destruction counterparts $\{C_I^- \equiv (C_I^+)^{\dagger}\}$. Thus, $|\Phi\rangle$ plays the role of a vacuum state with respect to a suitable set of (mutually commuting) many-body creation operators $\{C_I^+\}$,

$$C_I^- |\Phi\rangle = 0 \quad , \quad \forall I \neq 0 \quad , \quad (1)$$

with $C_0^- \equiv I$, the identity operator. These operators are also complete in the many-body Hilbert (or Fock) space,

$$I = |\Phi\rangle\langle\Phi| + \sum_{I \neq 0} C_I^+ |\Phi\rangle\langle\Phi| C_I^- . \quad (2)$$

The choice of the operators $\{C_I^+\}$ clearly depends on the choice of $|\Phi\rangle$, but for spin-lattice problems C_I^+ will usually involve products of the basic $SU(2)$ spin operators $\{s_k^+, s_k^-, s_k^z\}$ on different lattice sites k , which obey the fundamental commutation relations,

$$[s_k^z, s_l^\pm] = \pm s_k^\pm \delta_{kl} ; \quad [s_k^+, s_l^-] = 2s_k^z \delta_{kl} , \quad (3)$$

where $s_k^\pm \equiv s_k^x \pm i s_k^y$. The set-index I will thus generally incorporate the indices for a set of lattice sites. We discuss particular choices of $\{|\Phi\rangle, C_I^+\}$ in more detail below in the context of a specific example.

The exact ground-state energy eigenket and eigenbra vectors, $|\Psi\rangle$ and $\langle\tilde{\Psi}|$ respectively, of a many-body system described by a Hamiltonian H , satisfy the Schrödinger equations,

$$H|\Psi\rangle = E_g|\Psi\rangle ; \quad \langle\tilde{\Psi}|H = E_g\langle\tilde{\Psi}| . \quad (4)$$

We have introduced the tilde notation on the bra state, $\langle\tilde{\Psi}|$, to remind ourselves of the fact that although the *exact* $\langle\tilde{\Psi}|$ is self-evidently related to $|\Psi\rangle$ by Hermiticity, the CCM parametrisations of $|\Psi\rangle$ and $\langle\tilde{\Psi}|$ do not manifestly preserve this Hermiticity, as explained below. Furthermore, the tilde notation also serves to recall that even if the exact Hermiticity holds, $\langle\tilde{\Psi}|$ differs from $(|\Psi\rangle)^\dagger$ by a normalisation constant, as discussed below.

The ket and bra states are now specified within the single-reference normal CCM as,

$$|\Psi\rangle = e^S |\Phi\rangle ; \quad S = \sum_{I \neq 0} S_I C_I^+ ,$$

$$\langle\tilde{\Psi}| = \langle\Phi| \tilde{S} e^{-S} ; \quad \tilde{S} = 1 + \sum_{I \neq 0} \tilde{S}_I C_I^- , \quad (5)$$

where the tilde notation on the operator $\tilde{S}$ is not intended to convey any direct mathematical relationship between $\tilde{S}$ and S . Rather, Eq. (5) *defines* the operators S and $\tilde{S}$. We note that the correlation operator S is decomposed entirely in terms of the multiconfigurational creation operators $\{C_I^+\}$, and similarly for $\tilde{S}$ in terms of the destruction operators $\{C_I^-\}$. We further note that although the manifest Hermiticity, $(\langle\tilde{\Psi}|)^\dagger = |\Psi\rangle/\langle\tilde{\Psi}|\Psi\rangle$, is lost, the intermediate normalisation condition, $\langle\tilde{\Psi}|\Psi\rangle = \langle\Phi|\Psi\rangle = \langle\Phi|\Phi\rangle \equiv 1$ is imposed. Furthermore, the cluster correlation coefficients $\{S_I, \tilde{S}_I\}$ are regarded as being independent variables, even though formally we have the relation,

$$\langle\Phi|\tilde{S} = \frac{\langle\Phi|e^{S^\dagger}e^S}{\langle\Phi|e^{S^\dagger}e^S|\Phi\rangle} . \quad (6)$$

In particular, the full set of coefficients $\{S_I, \tilde{S}_I\}$ provides a complete CCM description of the many-body ground state. For example, an arbitrary operator A has a ground-state expectation value,

$$\bar{A} \equiv \langle \tilde{\Psi} | A | \Psi \rangle = \langle \Phi | \tilde{S} e^{-S} A e^S | \Phi \rangle = \bar{A}(\{S_I, \tilde{S}_I\}) . \quad (7)$$

We note that the specific parametrisation of Eq. (5) for $\langle \tilde{\Psi} |$ is consistent with the Hellmann-Feynman theorem [7], even though it does not manifestly preserve the Hermiticity relation with $|\Psi\rangle$. Furthermore, and very importantly, this parametrisation for $\langle \tilde{\Psi} |$ is actually derivable from the Hellmann-Feynman theorem if one chooses the specific functional form for the energy, $E_g = \langle \Phi | e^{-S} H e^S | \Phi \rangle$, which immediately follows from Eqs. (4) and (5).

The exponentiated form of the ground-state eigenket parametrisation of Eq. (5) ensures the proper counting of the *independent* fluctuations of excited multi-spin configurations (described by the set-index I) with respect to $|\Phi\rangle$, which are present in the exact ground state $|\Psi\rangle$, as well as the exact incorporation of the linked cluster theorem of Goldstone. The latter, in turn, guarantees the size-extensivity of all relevant physical quantities, and thus allows us to work in the CCM directly in the thermodynamic limit, $N \rightarrow \infty$, where N is the number of lattice spins.

By taking appropriate projections of the ground-state bra and ket Schrödinger equations (i.e., with states $C_I^+ |\Phi\rangle$ and $\langle \Phi | C_I^-$, respectively), we obtain coupled sets of equations which may be solved to obtain the coefficients $\{S_I\}$ and $\{\tilde{S}_I\}$. Completely equivalently, the cluster correlation coefficients $\{S_I, \tilde{S}_I\}$ may be determined variationally by requiring that the ground-state energy functional $\bar{H}(\{S_I, \tilde{S}_I\})$, defined as in Eq. (7), is stationary with respect to variations in each of the (independent) variables of the full set. The following coupled sets of equations are thereby easily derived,

$$\delta \bar{H} / \delta \tilde{S}_I = 0 \Rightarrow \langle \Phi | C_I^- e^{-S} H e^S | \Phi \rangle = 0 , \quad \forall I \neq 0 ; \quad (8)$$

$$\delta \bar{H} / \delta S_I = 0 \Rightarrow \langle \Phi | \tilde{S} e^{-S} [H, C_I^+] e^S | \Phi \rangle = 0 , \quad \forall I \neq 0 . \quad (9)$$

Equation (8) also ensures that the ground-state energy at the stationary point has the simple form

$$E_g = E_g(\{S_I\}) = \langle \Phi | e^{-S} H e^S | \Phi \rangle , \quad (10)$$

which also follows simply by projecting the ground-state ket equation (4) with $\langle \Phi | e^{-S}$. We note that this bi-variational formulation does *not*, however, lead to an upper bound for E_g when the summations over configurations $\{I\}$ in Eq. (5) for S and $\tilde{S}$ are truncated in specific approximations, since the exact Hermiticity between $|\Psi\rangle$ and $\langle \tilde{\Psi} |$ will thereby be lost. On the other hand, it is important to note that the Hellmann-Feynman theorem *is* preserved in all such approximations, and for many purposes this may be of greater usefulness than the variational bound on the energy.

Equation (8) clearly represents a coupled set of nonlinear multinomial equations for the c -number correlation coefficients $\{S_I\}$. The well-known nested commutator expansion for the similarity-transformed Hamiltonian,

$$\hat{H} \equiv e^{-S} H e^S = H + [H, S] + \frac{1}{2!} [[H, S], S] + \dots , \quad (11)$$

and the fact that all of the individual components of S in the sum in Eq. (5) commute with one another, together imply that each element of S in Eq. (5) is directly linked to the Hamiltonian in each of the non-vanishing terms in Eq. (11). Each of the coupled set of equations (8) is hence of linked cluster type. What is more, each of these equations is also of finite length when expanded using Eq. (11), since this otherwise infinite series will actually terminate at a finite order here, provided only that each term in the Hamiltonian H contains a finite number of single-site spin operators, as is usually the case. The CCM parametrisation thus leads in a very natural way to a workable scheme, which can also be efficiently implemented as described in more detail below. It is also important to realize that the similarity transformation lies at the heart of the CCM and is one of its most vital ingredients. It may be contrasted with its unitary transformation counterpart in a standard variational formulation in which the bra state $\langle \tilde{\Psi} |$ is manifestly taken as being proportional to the Hermitian adjoint of $|\Psi\rangle$, as in Eq. (6).

We turn now to the choice of $|\Phi\rangle$ and the operators $\{C_I^+\}$ for spin-lattice problems. To be specific we restrict ourselves henceforth to spin- $\frac{1}{2}$ quantum antiferromagnets in regions where the corresponding classical limit is described by a generalised Néel ordering in which all spins on each sublattice are separately aligned in the co-ordinates of a global spin quantisation axis and corresponding global spin axes. In such cases it is a simple matter (and see Sec. 3 for specific details in the case considered here) to introduce a different local quantisation axis and spin coordinates on each sublattice, by a suitable rotation in spin space, so that the corresponding Néel-like state becomes a fully aligned ("ferromagnetic") state in the local axes. This "ferromagnetic" state is chosen as the uncorrelated CCM model state, $|\Phi\rangle$, in which all spins point, say, along the respective negative z -axes of the corresponding local frames,

$$|\Phi\rangle = \bigotimes_{i=1}^N |\downarrow\rangle_i ; \quad \text{in the local quantisation axes.} \quad (12)$$

Thus, in the local spin coordinates,

$$s_k^z |\Phi\rangle = -\frac{1}{2} |\Phi\rangle , \quad (13)$$

for any arbitrary site k .

The correlation operator S of Eq. (5) may now be decomposed wholly in terms of sums of products of single spin-raising operators, s_k^+ , again defined with respect to the local quantisation axes. Thus, we may write,

$$\begin{aligned} S &= \sum_{i_1} S_{i_1} s_{i_1}^+ + \sum_{i_1, i_2} S_{i_1 i_2} s_{i_1}^+ s_{i_2}^+ + \cdots \\ &= \sum_{n=1}^N \sum_{i_1 \cdots i_n} S_{i_1 \cdots i_n} s_{i_1}^+ \cdots s_{i_n}^+ , \end{aligned} \quad (14a)$$

where $S_{i_1 i_2 \cdots i_n}$ are the corresponding (fully symmetric) spin-correlation coefficients specified by the sets of site indices $\{i_1, i_2, \cdots, i_n\}$ on the regular lattice under consid-

eration. The corresponding expansion for the operator $\tilde{S}$ of Eq. (5) is given by

$$\tilde{S} = 1 + \sum_{n=1}^N \sum_{i_1 \dots i_n} \tilde{S}_{i_1 \dots i_n} s_{i_1}^- \dots s_{i_n}^- . \quad (14b)$$

The coefficients $\{\tilde{S}_{i_1 \dots i_n}, \tilde{S}_{i_1 \dots i_n}; n = 1, 2, \dots, N\}$ are thus what we denoted generically by the set $\{\tilde{S}_I, \tilde{S}_I\}$ previously. Equation (8) thus yields the specific set of coupled nonlinear CCM equations,

$$\langle \Phi | s_{i_1}^- s_{i_2}^- \dots s_{i_n}^- e^{-S} H e^S | \Phi \rangle = 0 , \quad (15)$$

to determine the correlation coefficients $\{\tilde{S}_{i_1 \dots i_n}\}$.

We note that we may map the sets of coefficients $\{\tilde{S}_{i_1 \dots i_n}\}$ and $\{\tilde{S}_{i_1 \dots i_n}\}$ onto sets $\{\mathcal{X}_r\}$ and $\{\tilde{\mathcal{X}}_r\}$ respectively, where r labels the *independent* or fundamental configurations, i.e., only those that are inequivalent under the lattice symmetries (namely, translations, rotations, and reflections) of the Hamiltonian and under permutations of the indices. The sets $\{\mathcal{X}_r\}$ and $\{\tilde{\mathcal{X}}_r\}$ are thus defined to count the independent correlation coefficients associated with each fundamental configuration once and once only. Generally speaking there will be $N\nu_r(n_r)!$ equivalent configurations on the lattice associated with each fundamental configuration, where n_r is the number of sites in the r th configuration and $(n_r)!$ is the combinatoric factor associated with permutations of the n_r indices, the factor N arises from the translations, and the factor ν_r is the replication factor of the r th configuration associated with the point symmetry group (or sub-group) of transformations on the lattice which preserve the Hamiltonian. In particular, we need only to consider one of the $N\nu_r(n_r)!$ equivalent sets of equations (15) associated with each independent coefficient $\mathcal{X}_r$.

At this point we need to consider approximation schemes whereby the expansions of S and $\tilde{S}$ in Eq. (14a,b) may be truncated to some finite or infinite subset of the full set of independent (fundamental) multi-spin configurations. The three most commonly employed schemes have been: (1) the SUB n 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 SUB n - m sub-approximation, in which all SUB n correlations spanning a range of no more than m adjacent lattice sites are retained; and (3) the localised LSUB m scheme, which retains all multi-spin correlations over all possible distinct locales on the lattice defined by m or fewer contiguous sites. For the results reported below we adopt only the LSUB m scheme here.

The practical implementation of the CCM thus now consists of first enumerating all distinct multi-spin correlation configurations retained in the selected approximation, and then generating the corresponding set of CCM equations. The first stage is essentially a problem in graph theory, whereas Eq. (15) shows that the second stage involves two distinct computational aspects in the calculation of all possible nonzero contributions to the matrix element on the left-hand side of this equation. Thus, the first step is to calculate the similarity-transformed Hamiltonian, $\tilde{H} = e^{-S} H e^S$, and hence $\tilde{H}|\Phi\rangle$; while the second is to select those terms of $\tilde{H}|\Phi\rangle$ which match exactly the string of spin-lowering operators represented by the set of site indices $\{i_1, i_2, \dots, i_n\}$.

and which hence give a nonzero overlap. Clearly, the former problem is intrinsically related to the noncommutative nature of quantum spin operators, and relies only on the algebraic relations of Eq. (3); while the latter problem is intrinsically related to the geometric properties of the spatial lattice under consideration, and is essentially a problem of pattern-matching. We have shown elsewhere [18] how each of the above stages may very efficiently be implemented computationally to very high orders, to yield a set of coupled CCM ket-state equations which may then be solved by standard Newton-Raphson techniques. The bra-state equations are also handled in an analogous fashion.

In the following Section the power of the CCM is illustrated by application to a spin-half anisotropic Heisenberg model on an infinite 2D triangular lattice.

3. SPIN-HALF TRIANGULAR LATTICE ANTIFERROMAGNET

3.1 Historical Perspective

Both classical and quantum antiferromagnets are typically characterised by some semblance of Néel ordering [19], in which a small number (which depends essentially on the geometric structure of the crystal lattice) of ferromagnetic sublattices are arranged in such a way as to make the total magnetic moment or magnetisation vanish. In the classical limit the Néel order is usually envisaged to be perfect at zero temperature ($T = 0$), but the effect of quantum mechanics is to diminish the order by quantum fluctuations. The important question thus arises as to whether the quantum fluctuations, possibly in combination with such other effects as geometric frustration, will or will not completely destroy the underlying Néel-like magnetic long-range order (LRO). Naturally, thermal fluctuations will also tend to destroy the LRO beyond some critical temperature. In the latter regard we also recall the Mermin-Wagner theorem [20], which asserts that any Néel order present at $T = 0$ will be destroyed by thermal fluctuations in two or fewer spatial dimensions at vanishingly small temperatures, and we shall hence be concerned here only with the $T = 0$ case.

About 70 years ago Heisenberg [21] proposed the effective Hamiltonian which nowadays bears his name,

$$H = J \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j, \quad (16)$$

to describe the magnetic properties of quasi-localised fermions, where $\vec{s}_i$ denotes the vector spin operator at site i on the lattice. The sum in Eq. (16) on $\langle i, j \rangle$ runs over all nearest-neighbour pairs and counts each pair once; and J is the exchange constant. When $J > 0$ the Heisenberg interaction favours anti-aligned nearest-neighbour pairs and hence antiferromagnetism, and in the rest of this paper we put $J = 1$.

As shown by Thouless [22], the Heisenberg Hamiltonian of Eq. (16) should be interpreted as the leading term of an effective Hamiltonian which describes the tunneling of fermions between lattice sites. He showed how the overall antisymmetry of the fermionic wave function may be used to map the spatial exchange onto exchange in the spin variables, and he hence arrived at an effective multi-spin exchange

Hamiltonian,

$$H = \sum_{\{p\}} (-1)^p J_{\{p\}} P_{\{p\}} , \quad (17)$$

where $P_{\{p\}}$ is a permutation operator for a cycle $\{p\}$ of p spins on the lattice, and where $J_{\{p\}} (> 0)$ is equal to one-half of the tunneling frequency of the associated p -spin exchange cycle. The summation on $\{p\}$ runs over all permutations of p -spin cycles on the lattice, and the signature factor $(-1)^p$ in Eq. (17) arises from the antisymmetry. Considerations of both kinetic and potential energy lead to the expected outcome that tunneling associated with short symmetric cycles is most probable. Hence, one generally expects that the summation in Eq. (17) can be truncated on physical grounds to a few terms.

The Heisenberg form of Eq. (16) includes only the nearest-neighbour two-cycle, and we note from its above derivation that $J > 0$. In the case of spin- $\frac{1}{2}$ particles, the properties of the Pauli operators may readily be used to reduce the effective Hamiltonian of Eq. (17) to sums of products of terms proportioned to $(\vec{s}_{i_1} \cdot \vec{s}_{j_1}) \cdots (\vec{s}_{i_n} \cdot \vec{s}_{j_n})$ with $n = [p/2]$, and in which all of the $2n$ spins in the product are distinct. In particular, both the terms involving two and three nearest-neighbour spin-exchange cycles reduce to a nearest-neighbour Heisenberg term of the form in Eq. (16), but with an effective coefficient, $J_{\text{eff}} = J_2 - 2J_3$. Thus, 3-body exchange tends to promote ferromagnetism, and if Eq. (17) cannot be truncated at the lowest (Heisenberg) level, the Pauli exclusion principle itself thus tends to frustrate the antiferromagnetic Néel order. In the present paper, however, we shall deal with antiferromagnetic Hamiltonians containing only nearest-neighbour exchange, although we shall introduce an additional anisotropy into Eq. (16) as discussed below in Sec. 3.2.

Very soon after Néel [19] proposed his essentially classical description of antiferromagnetism, Landau and Görtner raised the very serious objection that such an $SU(2)$ symmetry-breaking state cannot possibly be the true ground state of the Heisenberg Hamiltonian of Eq. (16). It was not until some 20 years later that Anderson [23] proposed his semi-classical (linear or lowest-order) spin-wave theory (SWT) of the excitations on this now quasi-classical Néel state. In very broad terms he described how one can overcome the objections of Landau and Görtner if, in the thermodynamic limit, a large number of eigenfunctions of Eq. (16) collapse to the ground state, thereby permitting a spontaneous breaking of the $SU(2)$ and spatial symmetries. These quasi-degenerate joint states, the so-called tower of states, form the quantum-mechanical counterpart of the classical Néel state. This analysis, first sketched by Anderson [23], has very recently been demonstrated in great detail by Lhuillier and her co-workers [24-26]. They have demonstrated strong numerical evidence in the case of the triangular Heisenberg antiferromagnet (HAF) for a large set of such low-lying levels for an N -spin lattice, each of which collapses to the ground state as $N \rightarrow \infty$.

The triangular HAF is interesting because the two-dimensional triangular lattice is the simplest lattice exhibiting geometric frustration. Thus, in a classical description, if we attempt to couple three spins on a triangular plaquette antiferromagnetically, we find that it is impossible to anti-align all three pairs. This simple fact seems to imply a certain inherent instability of the ground state compared with that on a corresponding bipartite (e.g., square) lattice. The theoretical study of the triangular

HAF was begun by Anderson and Fazekas [27], who suggested that on the triangular lattice a combination of the geometric frustration and quantum fluctuations might be strong enough to destroy the LRO associated with the classical Néel state comprising three ferromagnetic sublattices with spins aligned at 120° to each other. In particular, their own resonating valence bond (RVB) type of variational wave function for this system implied a disordered spin-liquid state with an $S = 0$ ground state which exhibits no magnetic LRO at $T = 0$.

Since the pioneering work of Anderson and Fazekas [27] the spin-half triangular HAF has been studied by many authors [24-26, 28-36], some of whom have supported the ground state being a spin-liquid state and some of whom have been led to the opposite conclusion that the Néel-like magnetic LRO survives. For example, some variational calculations [28] have also exhibited a disordered ground state, while others [29,30] have exhibited LRO. In the latter class, Huse and Elser [30] used a correlated Néel trial wave function with two-spin correlations of arbitrary range and nearest-neighbour three-spin correlations, and obtained an ordered ground state with a sublattice magnetisation $M^+ \simeq 0.68$ (in units where $M^+ = 1$ is the classical Néel value), and with a considerably lower energy per spin, $E_g/N \simeq -0.537$, (in units where $J = 1$) than the value, $E_g/N \simeq -0.47$ obtained using the RVB trial variational wave function of Anderson [27]. Nevertheless, firm conclusions on the presence or absence of LRO based on variational calculations are impossible to draw, and one must look to other methods. For example, very recently a fixed-node Green function Monte Carlo calculation [31] has been performed using lattices of up to 324 sites, yielding an extrapolated upper bound for the ground-state energy per spin in the infinite lattice of $E_g/N \simeq -0.5431 \pm 0.0001$ and a sublattice magnetisation of $M^+ \simeq 0.60$. We note that there is still a considerable systematic uncertainty in these fixed-node GFMC results due to the trial wave function containing only two- and three-spin correlations.

Anderson's spin-wave theory (SWT) [23] has also been applied to the spin-half triangular HAF [32,33]. SWT calculations have shown that the quantum fluctuations and geometric frustration are insufficient to destabilise the three-sublattice Néel LRO, but give a sublattice magnetisation reduced to about 50% of its classical value. For example, Jolicoeur and Le Guillou [32] quote a value $M^+ \simeq 0.478$ from a first-order SWT calculation. By contrast, series expansion calculations of Singh and Huse [34], utilising up to 11th-order terms in an Ising-like anisotropy parameter that we describe in Sec. 3.2 and use in our own calculations here, suggested that the spin-half triangular HAF may either be precisely at or very close to the critical point of losing LRO, with a sublattice magnetisation either exactly zero or with an extrapolated value $M^+ \simeq 0.20$, respectively. We return to a further discussion of these results in Sec. 4.2.

Essentially all other results on the spin-half triangular HAF have come from the exact diagonalisation of finite clusters of up to 36 spins [24-26,35,36]. However, the extrapolation of these results to the thermodynamic limit of an infinite lattice by different authors has also led to conflicting conclusions. Lhuillier and her co-workers [24-26] have stressed that both the proper quantum-mechanical definition of an order parameter for a finite cluster and the subsequent consistent extrapolation of the finite-size data to the thermodynamic limit are extremely subtle points. Both steps require a proper understanding of the nature of the symmetry breaking caused by

the quasi-degenerate joint states (or tower of states) discussed above, both for its microscopic quantum features and for the large-scale (i.e., long-wavelength) asymptotic behaviour. Thus, the quasi-degenerate joint states are lower in energy than the softest magnons, with the former collapsing to the intensive ground-state energy per spin parameter, E_g/N , as N^{-2} , whereas the latter collapse as $N^{-3/2}$. Lhuillier and her co-workers have argued convincingly [25] that an incorrect treatment of either one or both of the above points has led other authors [35,36] to the incorrect conclusion that the three-sublattice Néel magnetic LRO does not exist in the spin-half triangular HAF, whereas their own careful treatment gives a sublattice magnetisation of $M^+ \simeq 0.50$.

In view of the considerable uncertainty which has surrounded this system, it is our intention in the remainder of this paper to demonstrate the power of the CCM by applying our general formalism to it. We note that whereas previous CCM calculations [15] of the spin-half triangular HAF have been done in the SUB2 approximation which includes only two-spin correlations (albeit of arbitrarily long range), we concentrate here on the localised LSUB m scheme of approximations discussed in Sec. 2 in which localised correlations among up to m spins are incorporated. The results in Sec. 4 are presented for $m \leq 6$.

3.2 Anisotropic Heisenberg Hamiltonian and CCM Model State

The spin-half triangular HAF is described by the antiferromagnetic-coupling Hamiltonian of Eq. (16) with $J > 0$, and where we henceforth put $J = 1$. The vector operator $\vec{s}_i$ is thus given in terms of the three spin-half Pauli operators at site i on the infinite triangular lattice. We note that the spin operators in Eq. (16) are defined in terms of some global spin quantisation 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) quantisation axes for each of the three sublattices (A, B, and C) of the triangular lattice. The classical ground state of Eq. (16) is the Néel state where all spins on each sublattice are separately aligned (all in the xz -plane, say). The spins on sublattice A are oriented along the negative z -axis, and spins on sublattices B and C are oriented at $+120^\circ$ and -120° , respectively, with respect to the spins on sublattice A. In order to facilitate the extension of the isotropic HAF to include an Ising-like anisotropy first introduced by Singh and Huse [34], and in order 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 $+120^\circ$ respectively,

$$\begin{aligned} s_B^x &\rightarrow -\frac{1}{2}s_B^x - \frac{\sqrt{3}}{2}s_B^z, \quad s_B^y \rightarrow s_B^y, \quad s_B^z \rightarrow \frac{\sqrt{3}}{2}s_B^x - \frac{1}{2}s_B^z; \\ s_C^x &\rightarrow -\frac{1}{2}s_C^x + \frac{\sqrt{3}}{2}s_C^z, \quad s_C^y \rightarrow s_C^y, \quad s_C^z \rightarrow -\frac{\sqrt{3}}{2}s_C^x - \frac{1}{2}s_C^z. \end{aligned} \quad (18)$$

We may rewrite Eq. (16) in terms of spins defined in these local quantisation axes for the triangular lattice with a further introduction of an anisotropy parameter

λ for the non-Ising-like pieces,

$$H = \sum_{\langle i \rightarrow j \rangle} \left\{ -\frac{1}{2} s_i^z s_j^z + \frac{\sqrt{3}\lambda}{4} \left(s_i^z s_j^+ + s_i^z s_j^- - s_i^+ s_j^z - s_i^- s_j^z \right) \right. \\ \left. + \frac{\lambda}{8} \left(s_i^+ s_j^- + s_i^- s_j^+ \right) - \frac{3\lambda}{8} \left(s_i^+ s_j^+ + s_i^- s_j^- \right) \right\}, \quad (19)$$

where $\lambda = 1$ corresponds to the isotropic Heisenberg Hamiltonian of Eq. (16) with $J=1$. We note that the summation in Eq. (19) again runs over nearest-neighbour 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. When $\lambda = 0$, the Hamiltonian in Eq. (19) 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. We choose this state as the uncorrelated CCM model state $|\Phi\rangle$ which is, of course, precisely given by Eq. (12).

3.3 Fundamental Cluster Correlation Configurations

We note from the outset that in enumerating the symmetry-distinct CCM cluster configurations we must be careful to remember that not all of the lattice point-group symmetries leave the lattice-spin Hamiltonian invariant. The Hamiltonian of Eq. (19) (or the CCM model state) explicitly breaks some of the lattice symmetries because of the presence of bond-directionality in the Hamiltonian. Thus only 6 (instead of the full 12) point-group symmetries should be used in the symmetry reduction. These are, specifically, three rotational operations (0° , 120° , and 240°) together with three reflections about the lattice axes (i.e., lines that coincide with the edges of the triangular lattice). For the purpose of illustration, let us consider the connected configurations of size 6. If all 12 point-group symmetries were used, we would have obtained 82 symmetry-inequivalent configurations as shown in Fig. 1, which are further classified into two groups: 17 in group A and 65 in group B. The configurations in group A are of higher symmetries than those in group B, and thus do not lead to new symmetry-inequivalent configurations when only 6 point-group symmetries must be used in the symmetry reduction as discussed above. Each configuration in group B, however, results in one other new symmetry-inequivalent configuration. Therefore, the total number of symmetry-inequivalent connected configurations of size 6 is 147 for the present spin-Hamiltonian problem. The set of symmetry-inequivalent configurations (connected and disconnected) thereby forms the set of fundamental configurations. We tabulate the number, N_F , of fundamental configurations up to the LSUB7 level of approximation in Table 1. Note, however, that CCM computations only up to the LSUB6 level of approximation are actually carried out in this article. We also note that we explicitly include the single spin-flip (LSUB1) configuration in N_F , despite the fact that the corresponding coefficients $\tilde{S}_i$ and $\tilde{S}_i^*$ in Eqs. (14a,b) are identically zero in each of our LSUB m solutions.

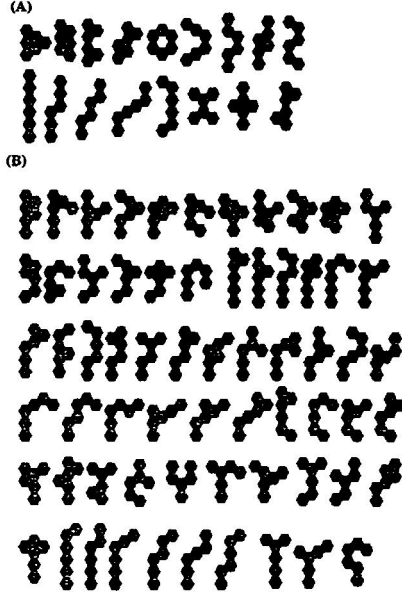


Figure 1. All 82 lattice animals of size 6 on a triangular lattice after symmetry reduction by translational and 12 point-group symmetry operations (see text for details). The centres of the hexagons mark the relative positions of the sites of the triangular lattice on which the spins are flipped with respect to the model state. See text for a discussion of group A and group B diagrams.

3.4 CCM Equations

In order to evaluate the CCM ket-state equations (15), we first require the similarity-transformed Hamiltonian, $\hat{H}$, defined as in Eq. (11). By making use of the fundamental $SU(2)$ commutation relations of Eq. (3) it is straightforward to show that after letting $\hat{H}$ act on $|\Phi\rangle$, as needed in Eq. (15), we have

$$\hat{H}|\Phi\rangle \equiv e^{-S} H e^S |\Phi\rangle = (\hat{H}_1 + \hat{H}_2 + \hat{H}_3)|\Phi\rangle, \quad (20)$$

where

$$\begin{aligned} \hat{H}_1 = & \frac{1}{4} \sum_{k\rho} \left\{ -2(G_{km} + F_k F_m) - \frac{3\lambda}{2} + \sqrt{3}\lambda(F_k - F_m)(1 + 2G_{km} + F_k F_m) \right\} s_k^+ s_m^+ \\ & + \frac{1}{4} \sum_{k\rho} \left\{ -\frac{\lambda}{2}(F_m^2 + F_k^2) - 3\lambda G_{km}^2 - 6\lambda G_{km} F_k F_m - \frac{3\lambda}{2} F_k^2 F_m^2 \right\} s_k^+ s_m^+, \quad (21) \end{aligned}$$

$$\begin{aligned}\hat{H}_2 = \frac{1}{4} \sum_{k\rho} \left\{ \left[F_m - \frac{\sqrt{3}\lambda}{2}(1 - F_m^2) + \frac{\lambda}{2}F_k \right] s_m^+ + \left[F_k + \frac{\sqrt{3}\lambda}{2}(1 - F_k^2) + \frac{\lambda}{2}F_m \right] s_k^+ \right\} \\ + \frac{\sqrt{3}\lambda}{4} \sum_{k\rho} (G_{km} + F_k F_m) (s_k^+ - s_m^+) \\ + \frac{3\lambda}{8} \sum_{k\rho} (2G_{km} + F_k F_m) (F_m s_m^+ + F_k s_k^+) ,\end{aligned}\quad (22)$$

$$\hat{H}_3 = \frac{1}{4} \sum_{k\rho} \left\{ -\frac{1}{2} - \frac{\sqrt{3}\lambda}{2}(F_m - F_k) - \frac{3\lambda}{2}(G_{km} + F_k F_m) \right\} . \quad (23)$$

Here the summation over k runs over all triangular lattice sites, while the summation over ρ is over the three directed nearest-neighbour vectors that point from A to B, B to C, and C to A as required by the explicit bond directionality in the Hamiltonian given by Eq. (19), and the index $m \equiv k + \rho$. The operators F_k and G_{km} are defined as follows,

$$F_k \equiv \sum_{l=1}^{\infty} l \sum_{i_1 \dots i_{l-1}} \mathcal{S}_{ki_1 \dots i_{l-1}} s_{i_1}^+ \dots s_{i_{l-1}}^+ , \quad (24)$$

$$G_{km} \equiv \sum_{l=2}^{\infty} l(l-1) \sum_{i_1 \dots i_{l-2}} \mathcal{S}_{kmi_1 \dots i_{l-2}} s_{i_1}^+ \dots s_{i_{l-2}}^+ . \quad (25)$$

Equations (10) and (23) show that the ground-state energy is now given exactly in terms of $x_1 \equiv \mathcal{S}_{k,k+\rho}$, the nearest-neighbour two-body cluster correlation coefficient, as

$$\frac{E_g}{N} = -\frac{3}{8} (1 + 6\lambda x_1) . \quad (26)$$

We note that $x_1 \equiv \mathcal{S}_{k,k+\rho}$ is independent of k and ρ by the translational and point-group symmetries of the lattice. Clearly the term involving x_1 gives the correction to the classical value arising from quantum fluctuations. We further note that Eqs. (10) and (23) would also lead to a contribution from the one-spin correlation coefficient $\mathcal{S}_k$ if this were not identically zero. Although we have explicitly included this configuration in all our LSUB m derivations, as mentioned previously, the corresponding CCM equations always allow the solution $\mathcal{S}_k \equiv 0$, and general symmetry arguments prefer this solution. Furthermore, our method of solution of the equations, discussed below, always actually finds only this solution. Thus, the LSUB m equations are obtained by evaluating all non-zero contributions to Eq. (15). There is one such coupled nonlinear equation for every fundamental configuration which we retain, and hence N_F equations in N_F coefficients, in each level of approximation.

The actual derivation of the ket-state equations from Eqs. (15) and (21)-(23) is thus seen to reduce essentially to a pattern-matching exercise of each retained fundamental configuration and all of its allowed symmetry-equivalent counterparts to each of the 35 terms in the similarity-transformed Hamiltonian given in Eqs. (21)-(23). We have described elsewhere [18] how this procedure may be computationally implemented in a very efficient manner. The CCM ket-state equations are then solved by the Newton-Raphson method for nonlinear equations. Specifically, we start from

Table 1

Results obtained for the spin-half triangular-lattice HAF using CCM LSUB m approximations ($m = 2, 3, 4, 5, 6$). N_F denotes the number of fundamental configurations (which are further decomposed as a sum of connected and disconnected ones respectively). The ground-state energy per spin, E_g/N , and the sublattice magnetisation, M^+ , at the isotropic Heisenberg point ($\lambda = 1$) are shown for each LSUB m approximation, together with the extrapolated results in the limit $m \rightarrow \infty$. The terminating anisotropy parameters, λ_{c_1} and λ_{c_2} , which correspond respectively to a phase transition at $\lambda = -\frac{1}{2}$ and another believed [34] to be near $\lambda = 1$, are also given for each LSUB m approximation. Note that there is no terminating point in the LSUB2 approximation.

m	N_F	$E_g/N (\lambda = 1)$	$M^+ (\lambda = 1)$	λ_{c_1}	λ_{c_2}
2	2 (2+0)	-0.50290	0.8578	-	-
3	8 (6+2)	-0.51911	0.8045	-0.86	5.47
4	30 (16+24)	-0.53427	0.7273	-0.65	2.20
5	143 (53+90)	-0.53869	0.6958	-0.60	1.98
6	758 (200+558)	-0.54290	0.6561	-0.55	1.77
7	4427 (837+3590)	?	?	?	?
∞		-0.5505	0.51		

the point $\lambda = 0$ at which we know the exact solution is where all the cluster correlation coefficients $\{S_{i_1, \dots, i_n}; n = 1, 2, \dots\}$ are zero. We then use this known solution as an initial input in solving the CCM solutions for a slightly increased nonzero value of the anisotropy parameter, λ . This procedure is then iterated to obtain the numerical results reported below in Sec. 4. The (linear) bra-state equations may also be derived in an analogous fashion, and then solved using a standard decomposition technique for linear equations, such as the LU decomposition method, once the ket-state cluster correlation coefficients have been obtained and used as known input.

4. RESULTS

4.1 Ground-State Energy

In Fig. 2 we show the ground-state energy per spin, E_g/N , as a function of the anisotropy parameter λ for various LSUB m approximations. The corresponding values at the isotropic Heisenberg point are also tabulated in Table 1. The highest-order calculation, LSUB6, which consists of 758 independent fundamental correlation

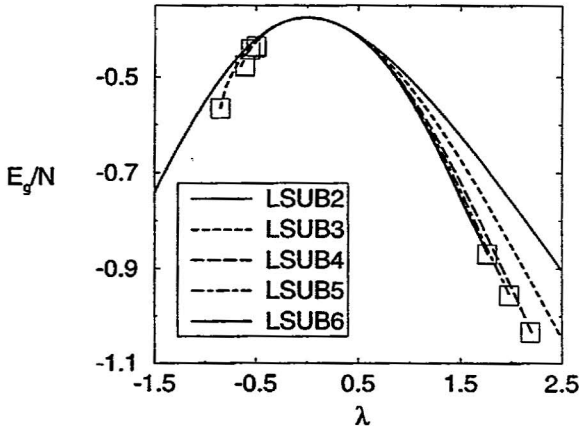


Figure 2. Results for the CCM ground-state energy for the spin-half triangular HAF. LSUB m critical points, λ_{c1} and λ_{c2} , are indicated by the boxes.

coefficients, yields $E_g/N \simeq -0.54290$. This value may be compared, for example, with the value -0.5445 extrapolated from finite-cluster diagonalisations of up to 36-spin clusters [24], and with the upper-bound value -0.5431 ± 0.0001 from a recent fixed-node GFMC simulation [31].

In order to compare our results with those cited above and in Sec. 3.1 from other methods, we also attempt a simple heuristic extrapolation of our LSUB m results to the limit $m \rightarrow \infty$ at the isotropic Heisenberg point ($\lambda = 1$). As has already been found elsewhere [13], our results seem to extrapolate well to their asymptotic value with a leading correction that scales as m^{-2} . In this way we obtain an extrapolated value for the ground-state energy per spin of $E_g/N \simeq -0.5505$ which is in good agreement, for example, with the series expansion calculations of Singh and Huse [34] who obtained a value for the ground-state energy of -0.551 . Compared with the corresponding classical value of -0.375 , it is safe to say that the LSUB6 CCM calculation captures at least 99% of the quantum corrections.

To make further contact with the highest-order series expansion known to date [34], we have computed the perturbative CCM solutions of E_g/N in terms of the anisotropy parameter λ . In Table 2 we tabulate the expansion coefficients from the LSUB6 approximation, together with the corresponding results from exact series expansions [34]. We note that the LSUB6 approximation reproduces the exact series expansion up to the sixth order. This result lends further strong support to the conjecture that the LSUB m approximation reproduces the *exact* series expansion to the same m th order [12(e)]. Moreover, the fact that the corresponding values of several of the higher-order expansion coefficients from both the CCM LSUB6 perturbative solution and the exact series expansion remain close to each other shows that the exponential parametrisation of the CCM with the inclusion of multi-spin correlations up to a certain order also captures the dominant contributions to correlations of a few higher orders in the series expansions.

Table 2

Expansion coefficients in powers of λ up to the 15th order for the ground-state energy per spin, E_g/N , and the sublattice magnetisation, M^+ , for the anisotropic spin-half triangular-lattice HAF obtained from the CCM equations in the LSUB6 approximation. The highest-order known exact series expansions up to the 11th order obtained by Singh and Huse [34] are also included for comparison.

Order	LSUB6: E_g/N	Exact: E_g/N	LSUB6: M^+	Exact: M^+
0	-0.3750000	-0.3750000	1	1
1	0	0	0	0
2	-0.1687500	-0.1687500	-0.27	-0.27
3	0.0337500	0.0337500	0.108	0.108
4	-0.0443371	-0.0443371	-0.2726916	-0.2726916
5	0.0204259	0.0204259	0.1717951	0.1717951
6	-0.0283291	-0.0283291	-0.3315263	-0.3315263
7	0.0311703	0.0315349	0.4060277	0.4110737
8	-0.0357291	-0.0476598	-0.5331858	-0.7382203
9	0.0541263	0.0685087	0.8894023	1.1781303
10	-0.0771681	-0.1025446	-1.3927395	-2.0109889
11	0.1294578	0.1565522	2.4179612	3.4012839
12	-0.1848858	?	-4.0426184	?
13	0.2857225	?	6.8086538	?
14	-0.4463496	?	-11.488761	?
15	0.7021061	?	19.388053	?

As already displayed in Fig. 2, the LSUB m ground-state energy curves for $m \geq 3$ terminate at lower and upper critical values of the anisotropy, λ_{c_1} and λ_{c_2} respectively, beyond which no physical solution of the CCM ket-state equations exists. We have also tabulated λ_{c_1} and λ_{c_2} for various LSUB m approximations in Table 1. Although the CCM based on the model state given in Eq. (12) with the three-sublattice magnetic ordering is bound to break down in the region of the anisotropy parameter space where the true ground-state wave function possesses a different symmetry from that of the model state, it has been strongly argued [12,13] that the terminating points may correspond to the critical points of a phase transition. Within

our analytic approach the derivatives of the ground-state energy with respect to the anisotropy parameter may be directly determined, and these derivatives of second and higher orders are found to diverge at the corresponding terminating anisotropy parameters λ_{c_1} and λ_{c_2} .

We observe that the lower terminating point λ_{c_1} clearly converges to a value of about -0.5 , as argued by Singh and Huse [34]. However, the upper terminating point λ_{c_2} , as tabulated in Table 1, remains considerably larger than the value of unity which was obtained via Padé analysis of the series expansion by Singh and Huse [34]. Higher orders of approximation are needed to clarify this disagreement, although it is possible that the upper terminating point is highly singular and so convergence may be very slow. The detailed behaviour of the sublattice magnetisation near λ_{c_2} is particularly suggestive with regard to this point, as discussed below in Sec. 4.2. Also, further work is necessary in order to determine the singularity exponents of the ground-state energy at the two critical points.

Finally, we note that previous CCM calculations for the spin-half triangular HAF using the full SUB2 approximation [15], in which *all* two-spin correlations are retained (however far apart on the lattice) but all m -spin correlations with $m > 2$ are neglected, gave a value for $E_g/N \simeq -0.504$. The CCM pair correlations on top of the three-sublattice Néel state thus seem to account for scarcely more than 70% of the quantum corrections to the classical value for the ground-state energy. Nevertheless, this full SUB2 calculation gave an upper critical point $\lambda_{c_2} \simeq 1.335$, which is much closer to the expected critical value of unity than the corresponding LSUB m results with $m \leq 6$. This is probably an indication of the particular importance of long-range correlations in the vicinity of the presumed phase transition near the Heisenberg point for this triangular lattice case.

4.2 Sublattice Magnetisation

Once both the ket- and bra-state cluster correlation coefficients are known we may calculate the simplest order parameter for any Néel antiferromagnet, namely the sublattice magnetisation, $M^+ \equiv -2\langle s^z \rangle$, which is defined as the average over the entire lattice of s^z in the *local* (rotated) spin coordinates, or, equivalently over a single sublattice of the corresponding unrotated component of the spin in the original *global* coordinates. Thus, $M^+ = 1$ for the Néel model state, with perfect ferromagnetic order on each of the three sublattices separately. Quantum fluctuations (i.e., multi-spin correlations) present in the exact interacting ground state are expected to reduce M^+ below unity. We would expect, *a priori*, that a phase transition would be marked by M^+ becoming zero (or, in an approximate calculation, singular) at some critical value of the coupling parameter, namely λ for the present anisotropic model.

By inserting the CCM parametrisations of Eq. (5) we find,

$$M^+ = -\frac{2}{N} \sum_{k=1}^N \langle \tilde{\Psi} | s_k^z | \Psi \rangle = -\frac{2}{N} \sum_{k=1}^N \langle \Phi | \tilde{S} e^{-S} s_k^z e^S | \Phi \rangle, \quad (27)$$

where s_k^z is in the local coordinates of each sublattice. In the notation of Eq. (24) we

find

$$\begin{aligned}
M^+ &= 1 - \frac{2}{N} \sum_{k=1}^N \langle \Phi | \tilde{S} F_k s_k^+ | \Phi \rangle \\
&= 1 - \frac{2}{N} \sum_{n=1}^{\infty} n(n!) \sum_{i_1 \dots i_n} \tilde{S}_{i_1 \dots i_n} S_{i_1 \dots i_n} .
\end{aligned} \tag{28}$$

The sum in Eq. (28) may be rewritten in terms of the independent correlation coefficients $\tilde{\mathcal{X}}_r$ and $\mathcal{X}_r$ associated with the N_F fundamental configurations of a given LSUB m approximation, which were introduced in Sec. 2, to give the LSUB m estimate for M^+ ,

$$\begin{aligned}
M^+ &= 1 - 2 \sum_{r=1}^{N_F} n_r (n_r!)^2 \nu_r \tilde{\mathcal{X}}_r \mathcal{X}_r \\
&= 1 - 2 \sum_{r=1}^{N_F} n_r (n_r!) \tilde{x}_r x_r ,
\end{aligned} \tag{29}$$

where n_r is the number of spin flips with respect to $|\Phi\rangle$ for the r th fundamental configuration, and where we have introduced the notation $x_r \equiv \mathcal{X}_r$ and $\tilde{x}_r \equiv (n_r!) \nu_r \tilde{\mathcal{X}}_r$, in terms of the cluster coefficients $\mathcal{X}_r$ and $\tilde{\mathcal{X}}_r$ defined in Sec. 2. For the triangular lattice under consideration, and from the symmetry of the Hamiltonian under only the 6-point group, we see that the replication factor $\nu_r = 3$ or 6 for all allowed fundamental configurations.

Our results at the isotropic ($\lambda = 1$) Heisenberg point for the sublattice magnetisation are shown in Table 1 for various LSUB m approximations. The highest-order LSUB6 approximation gives rise to a value of 0.6561. We once again attempt a simple heuristic extrapolation of our LSUB m results for M^+ at the Heisenberg point to the limit $m \rightarrow \infty$, in order to compare with other calculations. As has been found elsewhere [13], our results for M^+ extrapolate reasonably well to the asymptotic value with a leading correction that scales as m^{-1} . Our extrapolated value for the sublattice magnetisation is thus 0.51, which now brings our results fully into line with those from the most careful analysis [24] to date of those from finite-size diagonalisation results and with the second-order spin-wave calculations, which were discussed above in Sec. 3.1. We suspect that the corresponding result of $M^+ \simeq 0.60$ from the fixed-node GFMC simulation [31] is likely to be too high, probably because the trial wave function on which it is based contains only two- and three-spin correlations.

The divergence in $\langle s^z \rangle$ seen in Fig. 3 near the critical points is a natural consequence of the approximate nature of the calculation. As we approach a critical point for a given LSUB m approximation, one of the CCM correlation coefficients x_r becomes very large. The contribution to $\langle s^z \rangle$ from this coefficient also becomes very large and so the sublattice magnetisation diverges. The puzzling “upturn” of M^+ observed for the LSUB5 and the LSUB6 approximations near their respective upper critical points λ_{c_2} remains elusive to us at the present, although this behaviour is undoubtedly correlated with the slow and erratic convergence of this antiferromagnetic critical point.

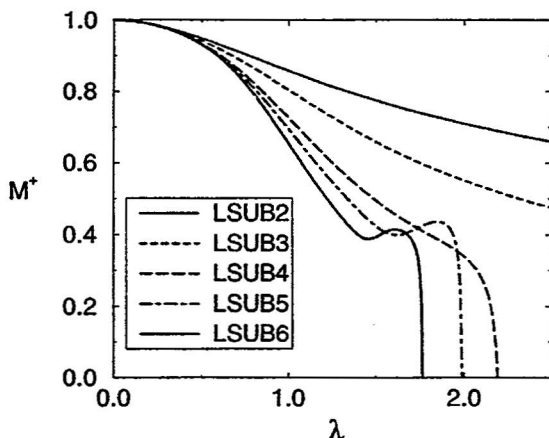


Figure 3. Results for the CCM ground-state sublattice magnetisation for the spin-half triangular HAF.

In order to make comparison again with the highest-order series expansion results, we perform a series expansion of the sublattice magnetisation for a given LSUB m order of approximation, and results for LSUB6 are shown in Table 2. We may also perform an Euler transformation and then re-sum these series, in the same way as has been performed by Singh and Huse [34] using the exact series which is known to 11th order. We use precisely the same form of the Euler transform as these authors in order to compare their results with those of our CCM LSUB m calculations. The results are shown in Fig. 4, where the sublattice magnetisation is plotted against $r^{-0.5}$ (r is the series expansion order). We can see that the LSUB6 series expansion results are converged up to approximately $r^{-0.5} \approx 0.3$, (i.e., up to order $r \approx 11$), and also that each LSUB m plot tends to the results obtained via direct evaluation of the CCM equations in the limit $r^{-0.5} \rightarrow 0$. However, we also see that if only a limited order of series terms are used – say fewer than about fifteen terms – then it is very easy to extrapolate to an incorrect LSUB m value, for the higher values of m , due to the ‘oscillation’ which develops in the re-summed value of the sublattice magnetisation as m increases. This presents the possibility that the re-summed exact series expansion results of Singh and Huse (also shown in Fig. 4) were obtained at too low an order to observe this oscillation, which we believe might persist in the exact series limit, thus producing an incorrect extrapolation of the sublattice magnetisation. Hence, from these results, and that of our extrapolated LSUB m results, we believe that the ground state of the triangular lattice HAF does indeed possess Néel-like long-range order.

In summary, compared with earlier applications of the CCM on the triangular HAF which have already revealed interesting oscillatory behaviour in long-ranged two-spin correlations [15], the present high-order CCM calculations (with the systematic inclusion of multi-spin correlations on up to six contiguous lattice sites) have

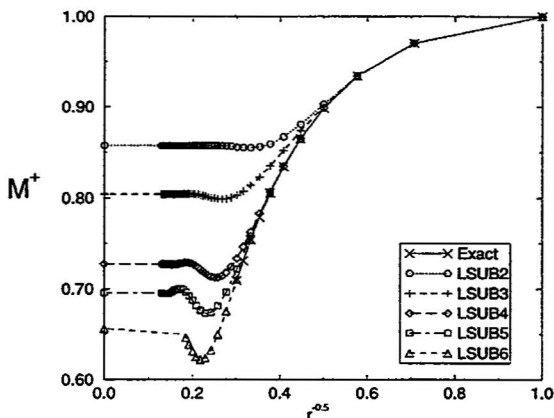


Figure 4. The re-summed series expansions of the sublattice magnetisation plotted against $r^{-0.5}$ where r is the series order. The Euler transform was used with a value of $a=1/3$, and the resulting series re-summed. The CCM LSUB m re-summed values for the sublattice magnetisation converge to the analytical results shown in Table 2 as $r^{-0.5} \rightarrow 0$, and the exact series of Singh and Huse [34] is also shown.

now obtained results for the ground-state energy and sublattice magnetisation which are fully competitive with those obtained from other methods, and which are clearly among the best available. Further detailed analysis of the large number of ket-state coefficients already obtained for the LSUB6 approximation, in order to achieve a better understanding of the nodal surface of the ground-state wave function, may provide a more microscopic justification of, and an extension to, the above-mentioned variational wave function. This may in turn lead to a better trial wave function for QMC simulations.

5. CONCLUSIONS AND FUTURE PROSPECTS

The usefulness of the coupled cluster method (CCM) in providing both a qualitative and quantitative description of the various phases of a wide variety of spin-lattice models has been amply demonstrated in the past [12-17]. One of our aims in the present paper has been to show that we now have at our disposal a rather powerful computational implementation of the CCM, which provides an efficient and effective general-purpose tool for studying the complex magnetic behaviour of spin-lattice models, including their quantum phase transitions between states of different quantum order. The CCM has thus clearly become fully competitive with other available microscopic techniques, including large scale QMC simulations, but does not suffer from the inherent minus-sign problem of the latter, as the detailed application here to the spin-half triangular HAF has demonstrated. One of our hopes for the future

is to use the information from the CCM calculations, concerning the structure of the nodal surface of the ground-state wave function for such frustrated systems, as input data for improved QMC simulations. Such a marriage of the best aspects of both the CCM and QMC methods offers an excellent prospect for further research.

One of the biggest challenges facing modern quantum many-body theory is the development and exploitation of explicit microscopic techniques which are capable of describing both "conventional" many-body systems and the many recent "unconventional" systems characterised by novel quantum order and non-Fermi-liquid behaviour. Apart from the various phases of (antiferro-)magnetic materials and low-dimensional quantum spin lattices discussed here, other examples of such unconventional many-body systems and related phenomena include heavy fermion materials, the fractional quantum Hall effect, high-temperature superconductors, and other strongly correlated electronic materials, new quantum states in the condensed phases of helium, and the confinement/deconfinement phase transition in lattice gauge field theories. It is our hope and expectation, from the successful study using the CCM of spin-lattice problems, that the CCM is now a prime candidate for use in addressing this key challenge.

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