High-order coupled-cluster method for general spin-lattice problems: An illustration via the anisotropic Heisenberg model

D. J. J. Farnell, K. A. Gernoth, and R. F. Bishop

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

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A high-order coupled cluster method (CCM) for the zero-temperature ground states of quantum lattice spin systems of general spin quantum number ($s \geq 1/2$) is described and illustrated via the spin-1 anisotropic Heisenberg antiferromagnet on the square lattice. Results for the ground-state energy and sublattice magnetization are seen to be in excellent agreement with the best of other approximate methods. Furthermore, we are able to follow the solution to the CCM equations at a given level of approximation with respect to the anisotropy parameter Δ from the trivial Ising limit ($\Delta \rightarrow \infty$) down to a critical value Δ_c , at which point the physical solution terminates. The results for the ground-state energy, sublattice magnetization, and phase transition point thus support our choice of this model as a good nontrivial test case of our CCM formalism.

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The field of quantum magnetic insulating systems at zero temperature has become increasingly well understood for one-dimensional (or quasi-one-dimensional) lattices via the existence of well-known exact solutions such as the Bethe ansatz^{1,2} (BA) and also via more recent density matrix renormalization group (DMRG) calculations.^{3–5} Similarly, zero-temperature quantum Monte Carlo (QMC) calculations^{6,7} have been shown to yield very accurate results for spin- $\frac{1}{2}$, two-dimensional systems. QMC techniques, however, are severely limited in their range of application by the presence of the infamous “sign problem,” although we note that for non-frustrated spin systems it is often possible to determine a “sign rule”^{8,9} which completely circumvents this minus-sign problem. By contrast, the technique of quantum many-body theory known as the coupled cluster method (CCM) is limited neither by the presence of frustration nor by the spatial dimensionality of the lattice.^{10–15} Indeed, a great strength of this method is that it is able to determine with great accuracy the positions of quantum phase transition points of quantum systems within an *ab initio*, and thus essentially unbiased, framework. These quantum phase transitions typically arise as some parameter within the Hamiltonian is varied, thus driving the system from one phase into another.

The behavior of the quantum Heisenberg antiferromagnet (HAF) on the linear chain is highly dependent on whether the quantum spin number s has an integer or a half-odd-integer value. Indeed, Haldane¹⁶ predicted that the spin-1 isotropic HAF would contain an excitation energy gap, and this prediction has subsequently and conclusively been shown numerically to be correct by exact diagonalizations of short chains¹⁷ and by more recent and extremely accurate DMRG calculations.⁵ This behavior is in stark contrast to the exact BA solution^{1,2} of the spin- $\frac{1}{2}$ isotropic HAF for the linear chain, which contains no such gap. However, such exact diagonalizations and DMRG calculations are considerably more difficult for systems of higher spatial dimensionality. In this article we wish to describe a high-order coupled cluster method ground-state formalism at zero temperature for quantum lattice spin systems of general spin quantum number ($s \geq 1/2$). We choose the spin-1 anisotropic Heisenberg anti-

ferromagnet on the square lattice as a good nontrivial test case of this formalism.

The spin-1 anisotropic HAF is given by,

$$H = \sum_{\langle i,j \rangle} \{s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z\}, \quad (1)$$

where the symbol $\langle i,j \rangle$ indicates nearest-neighbor bonds on the square lattice and where each bond is counted once and once only. For $\Delta \geq 1$, the ground state of this model contains nonzero Néel-like order. The precise value of the phase transition point at which this ordering breaks down is not exactly known, although it is believed to be at (or near to) the Heisenberg point at $\Delta = 1$. Very accurate results for the values of various ground-state properties of this model have been obtained via spin-wave theory¹⁸ (SWT) and cumulant series expansions.¹⁹ Both sets of results indicate that approximately 80% of the classical ordering remains for the spin-1, square-lattice HAF model at $\Delta = 1$. We note, however, that cumulant series expansions make an explicit assumption that the position of the phase transition point is exactly at $\Delta = 1$ in order to perform Padé resummations of the otherwise divergent perturbation series. Also, conventional SWT essentially appears to “build in” a phase transition point at $\Delta = 1$ for any lattice, at which point the excitation spectrum becomes soft. This is, of course, now known to be incorrect^{5,16,17} for the spin-1 linear-chain HAF model, as noted above.

We now briefly describe the general CCM formalism, and the interested reader is referred to Refs. 10–15 for further details. The exact ket and bra ground-state energy eigenvectors $|\Psi\rangle$ and $\langle\tilde{\Psi}|$ of a many-body system described by a Hamiltonian H are parametrized within the single-reference CCM as follows:

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

$$\langle \tilde{\Psi} | = \langle \Phi | \tilde{S} e^{-S}, \quad \tilde{S} = 1 + \sum_{I \neq 0} \tilde{S}_I C_I^- . \quad (2)$$

The single model or reference state $|\Phi\rangle$ is required to have the property of being a cyclic vector with respect to two well-defined Abelian subalgebras of *multiconfigurational* creation operators $\{C_I^+\}$ and their Hermitian-adjoint destruction counterparts $\{C_I^- \equiv (C_I^+)^\dagger\}$. Thus, $|\Phi\rangle$ plays the role of a vacuum state with respect to a suitable set of (mutually commuting) many-body creation operators $\{C_I^+\}$. Note that $C_I^- |\Phi\rangle = 0$, $\forall I \neq 0$, and that $C_0^- \equiv 1$, the identity operator.

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

The CCM equations are defined by the following coupled set of equations:

$$\langle \Phi | C_I^- e^{-S} H e^S | \Phi \rangle = 0, \quad \forall I \neq 0, \quad (3)$$

$$\langle \Phi | \tilde{S} e^{-S} [H, C_I^+] e^S | \Phi \rangle = 0, \quad \forall I \neq 0. \quad (4)$$

We furthermore note that the ground-state energy at the stationary point has the simple form

$$E_g = E_g(\{S_I\}) = \langle \Phi | e^{-S} H e^S | \Phi \rangle. \quad (5)$$

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

The CCM formalism is exact in the limit of inclusion of all possible multispin cluster correlations for S and $\tilde{S}$, although in any real application this is usually impossible to achieve. It is therefore necessary to utilize various approximation schemes within S and $\tilde{S}$. The three most commonly employed schemes previously utilized 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 localized LSUB m scheme, in which all multispin correlations over distinct locales on the lattice defined by m or fewer contiguous sites are retained. We note that in order to carry out such LSUB m or SUB n - m calculations to high order in the truncation indexes n and m we must rely on computer-algebra techniques in order to generate the corresponding sets of coupled equations. These computational techniques are based on the fact that the similarity transformed Hamiltonian in Eqs. (3)–(5) may be written *purely* in terms of creation operators acting on the model state, so that evaluation of Eq. (3) becomes purely a matter

of pattern matching. The interested reader is referred to Refs. 12 and 15 for a full explanation of how this is achieved for spin- $\frac{1}{2}$ models. We note that the generalization of this procedure to the case of arbitrary quantum spin number s is relatively straightforward, although detailed, and will be described fully elsewhere.²⁰

We now apply the CCM formalism outlined above to the specific case of the anisotropic HAF, and we choose the Néel state, in which the spins lie along the z axis, to be the model state. Furthermore, we perform a rotation of the local axes of the up-pointing spins by 180° about the y axis, so that spins on both sublattices may be treated equivalently. The (canonical) transformation is described by

$$s^x \rightarrow -s^x, \quad s^y \rightarrow s^y, \quad s^z \rightarrow -s^z. \quad (6)$$

The model state now appears *mathematically* to consist of purely down-pointing spins in these rotated local axes. In terms of the spin raising and lowering operators $s_k^\pm \equiv s_k^x \pm is_k^y$ the Hamiltonian may be written in these local axes as

$$H = -\frac{1}{4} \sum_{\langle i,j \rangle} \{s_i^+ s_j^+ + s_i^- s_j^- + 2\Delta s_i^z s_j^z\}, \quad (7)$$

where i and j runs over all nearest neighbors, although each nearest-neighbor bond is counted once and once only. Furthermore, the sublattice magnetization M (after rotation of the local spin axes) is given by

$$M = -\frac{1}{N} \sum_{i=1}^N s_i^z. \quad (8)$$

In the limit $\Delta \rightarrow \infty$ we note that the model state is the exact ground eigenstate of the Hamiltonian of Eq. (7). Hence, all of the CCM correlation coefficients are zero at this point. We may track this solution for decreasing values of Δ until we reach a *critical point* Δ_c , at which point the real solution to our CCM equations for the LSUB m and SUB m - m approximation schemes terminates. This is associated with a phase transition in the real system.^{12–15} Similar behavior was also seen for the CCM SUB2 approximation for this model (see Ref. 11), and once more this was associated with a phase transition of the real system.

We note that the “raw” results for the ground-state energy, sublattice magnetization, and critical points Δ_c have been obtained using both the LSUB m and SUB m - m approximation schemes. For both approximation schemes we may extrapolate these results as a function of m in the limit $m \rightarrow \infty$ in order to obtain even better results. We note that SUB2- m calculations and the full SUB2 calculation have also previously been performed¹¹ for the anisotropic square-lattice HAF with general quantum spin number. It was therefore possible to determine accurately the manner in which SUB2- m results scale as a function of m , namely, that as $m \rightarrow \infty$ the ground-state energy and the critical points $E_g(m)/N$ and $\Delta_c(m)$, respectively, scale linearly with $1/m^2$, and the sublattice magnetization $M(m)$ scales linearly with $1/m$. By analogy, we utilize a similar procedure here in order to extrapolate raw LSUB m and SUB m - m results. However, as we may utilize LSUB m and SUB m - m results for $m = \{2, 4, 6\}$

TABLE I. CCM results for the ground state of the spin-1 Heisenberg antiferromagnet at $\Delta=1$ on the square lattice using the LSUB m approximation with $m=\{2,4,6\}$. Values for the CCM critical points Δ_c of the anisotropic model as a function of the anisotropy Δ are also presented. Note that N_F indicates the number of fundamental clusters at each level of approximation.

	N_F	E_g/N	M	Δ_c
LSUB2	2	-2.295322	0.909747	0.3240
SUB2 ^a	—	-2.302148	0.8961	0.9109
LSUB4	30	-2.320278	0.869875	0.7867
LSUB6	1001	-2.325196	0.851007	0.8899
LSUB ∞	—	-2.3292	0.8049	0.98
SWT ^b	—	-2.3282	0.8043	—
Series expansions ^c	—	-2.3279(2)	0.8039(4)	—

^aSee Ref. 11.

^bSee Ref. 18.

^cSee Ref. 19.

only, a quadratic function is fitted to these data in order to obtain the best possible results. A full and comprehensive explanation of the extrapolation process of CCM LSUB m expectation values is given in Ref. 15 for the spin- $\frac{1}{2}$ XXZ model for a variety of lattices, and the interested reader is referred to this article for further information.

CCM results for the position of the critical point using the LSUB m and SUB m - m approximation schemes are presented in Tables I and II. The extrapolated result of $\Delta_c=0.98$ for both the LSUB m and SUB m - m approximation schemes indicates that the phase transition point is at (or perhaps slightly below) the isotropic Heisenberg point ($\Delta=1$). One of the strengths of the CCM is that it can provide such an accurate value for the position of the quantum phase transition point as a function of the anisotropy within an *ab initio*, and thus fully unbiased, framework.

TABLE II. CCM results for the ground state of the spin-1 Heisenberg antiferromagnet at $\Delta=1$ on the square lattice using the SUB m - m approximation with $m=\{2,4,6\}$. Values for the CCM critical points Δ_c of the anisotropic model as a function of the anisotropy Δ are also presented. Note that N_F indicates the number of fundamental clusters at each level of approximation.

	N_F	E_g/N	M	Δ_c
SUB2-2	1	-2.295041	0.910013	0.3499
SUB2 ^a	—	-2.302148	0.8961	0.9109
SUB4-4	15	-2.319755	0.871195	0.7843
SUB6-6	375	-2.324863	0.852559	0.8879
SUB ∞	—	-2.3291	0.8067	0.98
SWT ^b	—	-2.3282	0.8043	—
Series expansions ^c	—	-2.3279(2)	0.8039(4)	—

^aSee Ref. 11.

^bSee Ref. 18.

^cSee Ref. 19.

FIG. 1. CCM results for the ground-state energy per spin of the spin-1 anisotropic Heisenberg antiferromagnet on the square lattice using the LSUB m and SUB m - m approximations with $m=\{2,4,6\}$. The boxes indicate the CCM critical points.

Figure 1 and Tables I and II indicate that the results for the ground-state energy of the spin-1 HAF converge extremely quickly with m for both the LSUB m and SUB m - m schemes. Indeed, even the “raw” unextrapolated results provide excellent estimates of the ground-state energy, although the extrapolated results of $E_g/N=-2.3292$ for the LSUB m approximation scheme and $E_g/N=-2.3291$ for the SUB m - m approximate scheme are certainly even more accurate. By way of comparison, we note that third-order SWT (Ref. 18) gives a result of $E_g/N=-2.3282$ and cumulant series expansions¹⁹ a result of $E_g/N=-2.3279(2)$.

CCM results for the sublattice magnetization are found to be similarly well converged as a function of the truncation index m for both the LSUB m and SUB m - m schemes, as

FIG. 2. CCM results for the sublattice magnetization of the spin-1 anisotropic Heisenberg antiferromagnet on the square lattice using the LSUB m and SUB m - m approximations with $m=\{2,4,6\}$.

indicated in Fig. 2. The extrapolated results of $M=0.8049$ and $M=0.8067$ for the LSUB m and SUB m - m schemes, respectively, are again in excellent agreement with the results of third-order SWT (Ref. 18) and cumulant series expansions,¹⁹ which give values of $M=0.8043$ and $M=0.8039(4)$, respectively.

In conclusion, we have shown that the coupled cluster method provides quantitatively accurate results for the ground-state properties of the spin-1 square-lattice isotropic HAF, by comparison with results of third-order spin-wave theory and cumulant series expansions. Our best estimates of the ground-state energy of this model were found to be $E_g/N = -2.3292$ using the LSUB m approximation scheme and $E_g/N = -2.3291$ using the SUB m - m approximation scheme via heuristic extrapolation to the (exact) limit m

$\rightarrow \infty$. These results are within 0.05% of the best results of other methods. Our best extrapolated estimates of the sublattice magnetization are $M=0.8049$ using the LSUB m approximation scheme and $M=0.8067$ using the SUB m - m approximation scheme. These results are, respectively, within about 0.1% and 0.3% of the best results of other approximate methods. Furthermore, results for the position of the phase transition point of this model with respect to the anisotropy (via the fully *ab initio* CCM treatment) are in excellent agreement with the expected behavior of this model. We conclude that the new high-order CCM ground-state formalism for general ($s \geq 1/2$) spin quantum number has successfully passed its first test. A fuller account of this high-order formalism will be published elsewhere,²⁰ and we hope to apply it soon to more complicated systems.

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- ¹H.A. Bethe, Z. Phys. **71**, 205 (1931).
²L. Hulthén, Ark. Mat., Astron. Fys. **26**, No. 11 (1938).
³S.R. White and R. Noack, Phys. Rev. Lett. **68**, 3487 (1992).
⁴S.R. White, Phys. Rev. Lett. **69**, 2863 (1992).
⁵S.R. White, Phys. Rev. B **48**, 10 345 (1993).
⁶K.J. Runge, Phys. Rev. B **45**, 12 292 (1992); **45**, 7229 (1992).
⁷A.W. Sandvik, Phys. Rev. B **56**, 11 678 (1997).
⁸R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, Phys. Rev. B **61**, 6775 (2000).
⁹R.F. Bishop and D.J.J. Farnell, in *The Proceedings of the 10th International Conference on Recent Progress in Many-Body Theories*, edited by R. F. Bishop, K. A. Gernoth, N. R. Walet, and Y. Xian, Advances in Quantum Many-Body Theory, Vol. 3 (World Scientific, Singapore, 2000), p. 457.
¹⁰R.F. Bishop, J.B. Parkinson, and Y. Xian, Phys. Rev. B **44**, 9425 (1991).
¹¹R.F. Bishop, J.B. Parkinson, and Yang Xian, Phys. Rev. B **46**, 880 (1992).
¹²D.J.J. Farnell, S.A. Krüger, and J.B. Parkinson, J. Phys.: Condens. Matter **9**, 7601 (1997).
¹³C. Zeng, D.J.J. Farnell, and R.F. Bishop, J. Stat. Phys. **90**, 327 (1998).
¹⁴R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, Phys. Rev. B **58**, 6394 (1998).
¹⁵R.F. Bishop, D.J.J. Farnell, S.E. Krüger, J.B. Parkinson, J. Richter, and C. Zeng, J. Phys.: Condens. Matter **12**, 6887 (2000).
¹⁶F.D.M. Haldane, Phys. Lett. **93A**, 464 (1983).
¹⁷J.B. Parkinson and J.C. Bonner, Phys. Rev. B **32**, 4703 (1985).
¹⁸C.J. Hamer, W.H. Zheng, and P. Arndt, Phys. Rev. B **46**, 6276 (1992).
¹⁹W.H. Zheng, J. Oitmaa, and C.J. Hamer, Phys. Rev. B **43**, 8321 (1991).
²⁰D.J.J. Farnell, R.F. Bishop, and K.A. Gernoth, UMIST preprint (UMIST:Phys:TP:1–8) (unpublished).