Phase Transition Of The Spin-One Square-Lattice Anisotropic Heisenberg Model

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The coupled cluster method (CCM) is applied to the spin-one anisotropic Heisenberg antiferromagnet (HAF) on the square lattice at zero temperature using a new high-order CCM ground-state formalism for general quantum spin number \( s \geq 1/2 \). The results presented constitute the first such application of this new formalism, and they are shown to be among the most accurate results for the ground-state energy and sublattice magnetisation of this model as yet determined. We “track” the solution to the CCM equations at a given level of approximation with respect to the anisotropy parameter, \( \Delta \), from the trivial Ising limit (\( \Delta \to \infty \)) down to a critical value \( \Delta_c \), at which point this solution terminates. This behaviour is associated with a phase transition in the system, and hence a primary result of these high-order CCM calculations is that they provide an accurate and unbiased (i.e., \textit{ab initio}) estimation of the position of the quantum phase transition point as a function of the anisotropy parameter. Our result is, namely, that this point occurs at (or slightly below) the isotropic Heisenberg point at \( \Delta = 1 \), for this model.

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The area 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 (BA) \([1, 2]\) and also via more recent density matrix renormalisation group (DMRG) calculations \([3, 4]\). Similarly, zero-temperature quantum Monte Carlo (QMC) calculations \([6, 7]\) have been shown to yield very accurate results for spin-half, 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 neither limited by the presence of frustration nor by the spatial dimensionality of the lattice \([10, 11, 12, 13, 14, 15]\). 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 \textit{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 behaviour 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, Haldane \([16]\) first predicted that the spin-one isotropic HAF would contain an excitation energy gap, and this prediction has subsequently and conclusively been shown numerically to be correct by exact diagonalisations of short chains \([17, 18]\) and by more recent and extremely accurate DMRG calculations \([19]\). We note that this is in stark contrast to the exact BA solution \([1, 2]\) of the spin-half isotropic HAF for the linear chain, which contains no such gap. However, such exact diagonalisations and DMRG calculations are considerably more difficult for systems of higher spatial dimensionality. In this article, we focus on the specific case of the spin-one anisotropic HAF on the square lattice at zero temperature using the CCM, especially in relation to its quantum phase transition, by applying a high-order CCM formalism for general quantum spin number for the first time.

The spin-one anisotropic HAF is given by,

\[
H = \sum_{\langle i,j \rangle} \left\{ s_i^z s_j^z + s_i^y s_j^y + \Delta s_i^x s_j^x \right\},
\]

where the symbol \( \langle i, j \rangle \) indicates nearest-neighbour bonds on the square lattice, and where each bond is counted once and once only. For \( \Delta \gtrsim 1 \), the ground state of this model contains non-zero 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 theory (SWT) \([18]\) and cumulant series expansions \([19]\). Both sets of results indicate that approximately 80% of the classical ordering remains for the spin-one, 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 \([10, 16, 17]\) for the spin-one linear-chain HAF model, as noted above.

We now briefly describe the general CCM formalism, and the interested reader is referred to Refs. \([10, 11, 12, 13, 14, 15]\) for further details. The exact ket and
The exact ground state is itself guaranteed the size-extensivity of all relevant incorporation of the Goldstone linked-cluster theorem, \( \{ C_I^+ \} \) and their Hermitian-adjoint destruction counterparts \( \{ C_I^- \} \). 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 parametrisation of Eq. (2) ensures the correct counting of the independent and excited correlated many-body clusters with respect to \( | \Psi \rangle \) 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,

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

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

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 multi-spin cluster correlations for \( S \) and \( \tilde{S} \), although in any real application this is usually impossible to achieve. It is therefore necessary to utilise various approximation schemes within \( S \) and \( \tilde{S} \). The three most commonly employed schemes previously utilised have been: (1) the \( \text{SUB}n \) 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 \( \text{SUB}n-m \) sub-approximation, in which all \( \text{SUB}n \) correlations spanning a range of no more than \( m \) adjacent lattice sites are retained; and (3) the localised \( \text{LSUB}m \) scheme, in which all multi-spin 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 \( \text{LSUB}m \) or \( \text{SUB}n-m \) 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 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.
TABLE I: CCM results for the ground state of the spin-one 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, $\Delta_c$, of the anisotropic model as a function of the anisotropy, $\Delta$, are also presented. Note that $N_F$ indicates the number of fundamental clusters at each level of approximation.

| $N_F$ | $E_g/N$ | $M$ | $\Delta_c$ |
|-------|---------|-----|-----------|
| 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$\infty$ | $-2.3292$ | 0.8049 | 0.98 |
| SWT$^b$ | $-2.3282$ | 0.8043 | $-2.3279(2)$ |
| Series Expansions$^c$ | $-2.3279(2)$ | 0.8039(4) |

$^a$ See Ref. [11]  
$^b$ See Ref. [12]  
$^c$ See Ref. [13]

be written purely in terms of creation operators acting on the model state, so that evaluation of Eq. (4) becomes purely a matter of pattern matching. The interested reader is referred to Refs. [12] and [13] for a full explanation of how this is achieved for spin-half models. We note that the generalisation 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,

$$s^x \rightarrow -s^x, \ s^y \rightarrow s^y, \ s^z \rightarrow -s^z.$$  

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 $s^\pm_k \equiv s^x_k \pm is^y_k$, the Hamiltonian may be written in these local axes as,

$$H = -\frac{1}{4} \sum_{i,j} \left( s^+_i s^+_j + s^-_i s^-_j + 2\Delta s^z_i s^z_j \right),$$  

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

$$M = -\frac{1}{N} \sum_{i=1}^{N} s^z_i.$$  

In the limit $\Delta \rightarrow \infty$ we note that the model state is the exact ground eigenstate of the Hamiltonian of Eq. (6). Hence, all of the CCM correlation coefficients are zero at this point. We may track this solution for decreasing values of $\Delta$ until we reach a critical point, $\Delta_c$, 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, 13, 14, 15]. Similar behaviour was also seen for this model 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 magnetisation, and critical points, $\Delta_c$, 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 performed [11] 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 magnetisation, $M(m)$, scales linearly with $1/m$. By analogy, we utilise a similar procedure here in order to extrapolate raw LSUB$m$ and SUB$m-m$ results. However, as we may utilise LSUB$m$ and SUB$m-m$ results for $m = \{2, 4, 6\}$ 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-half XXZ model for a variety of lattices, and the interested reader is referred to this article.

TABLE II: CCM results for the ground state of the spin-one 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, $\Delta_c$, of the anisotropic model as a function of the anisotropy, $\Delta$, are also presented. Note that $N_F$ indicates the number of fundamental clusters at each level of approximation.

| $N_F$ | $E_g/N$ | $M$ | $\Delta_c$ |
|-------|---------|-----|-----------|
| 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$\infty$ | $-2.3291$ | 0.8067 | 0.98 |
| SWT$^b$ | $-2.3282$ | 0.8043 | $-2.3279(2)$ |
| Series Expansions$^c$ | $-2.3279(2)$ | 0.8039(4) |

$^a$ See Ref. [11]  
$^b$ See Ref. [13]  
$^c$ See Ref. [15]
for further information.

CCM results for the position of the critical point using the LSUBm and SUBb_m approximation schemes are presented in Tables I and II. The extrapolated result of \( \Delta_c = 0.98 \) for both the LSUBm and for the SUBb_m approximation scheme indicates that the phase transition point is at (or perhaps slightly below) the isotropic Heisenberg point \( (\Delta = 1) \). The strength 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 \textit{ab initio}, and thus fully unbiased, framework.

Figure 1 and Tables I and II indicate that the results for the ground-state energy of the spin-one HAF converge extremely quickly with \( m \) for both the LSUBm and SUBb_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 LSUBm approximation scheme and \( E_g/N = -2.3291 \) for SUBb_m approximation scheme are certainly even more accurate. By way of comparison, we note that third-order SWT \cite{18} gives a result of \( E_g/N = -2.3282 \) and cumulant series expansions \cite{19} a result of \( E_g/N = -2.3279(2) \).

CCM results for the sublattice magnetisation are found to be similarly well converged as a function of the truncation index \( m \) for both the LSUBm and SUBb_m schemes, as indicated in Fig. 2. The extrapolated results of \( M = 0.8049 \) and \( M = 0.8067 \) for the LSUBm and SUBb_m schemes, respectively, are again in excellent agreement with the results of third-order SWT \cite{18} and cumulant series expansions \cite{19}, which give values of \( M = 0.8043 \) and \( M = 0.8039(4) \) respectively.

In this article it has been shown that the coupled cluster method (CCM) provides quantitatively accurate results for the ground-state properties of the spin-one square-lattice isotropic HAF by comparison with results of third-order spin-wave theory (SWT) and cumulant series expansions. Furthermore, we note that the results presented in this article constitute the first application of the CCM using a new high-order CCM ground-state formalism for general \( (s \geq 1/2) \) quantum spin number. (A fuller account of this new high-order formalism will be published elsewhere \cite{20}.) The best estimates of the ground-state energy of this model were found to be \( E_g/N = -2.3292 \) using the LSUBm approximation scheme and \( E_g/N = -2.3291 \) using the SUBb_m approximation scheme via heuristic extrapolation to the (exact) limit \( m \to \infty \). The best estimates of the sublattice magnetisation are \( M = 0.8049 \) using the LSUBm approximation scheme and \( M = 0.8067 \) using the SUBb_m approximation scheme, again via extrapolation to the limit \( m \to \infty \). The most important result of the CCM calculations presented here for this model is the prediction that the phase transition point of the spin-one square-lattice anisotropic HAF is at (or slightly below) the isotropic Heisenberg point. A strength of the method is that this prediction may be made using an unbiased (i.e., \textit{ab initio}) treatment.

\begin{thebibliography}{99}

\bibitem{1} H. A. Bethe, \textit{Z. Phys.} \textbf{71}, 205 (1931).
\bibitem{2} L. Hulthén, \textit{Ark. Mat. Astron. Fys.} \textbf{A 26}, No. 11 (1938).
\bibitem{3} S.R. White and R. Noack, \textit{Phys. Rev. Lett.} \textbf{68}, 3487 (1992).
\bibitem{4} S.R. White, \textit{Phys. Rev. Lett.} \textbf{69}, 2863 (1992).
\bibitem{5} S.R. White, \textit{Phys. Rev. B} \textbf{48}, 10345 (1993).
\bibitem{6} K. J. Runge, \textit{Phys. Rev. B} \textbf{45}, 12292 (1992); \textit{ibid.} \textbf{45}, 7229 (1992).
\bibitem{7} A.W. Sandvik, \textit{Phys. Rev. B} \textbf{56}, 11678 (1997).
\bibitem{8} R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, \textit{Phys. Rev. B} \textbf{61}, 6775 (2000).
\bibitem{9} R.F. Bishop and D.J.J. Farnell, in \textit{Advances in Quantum Many-Body Theory}, Vol. \textit{3}, edited by R.F. Bishop, K.A. Gernoth, N.R. Walet, and Y. Xian (UMIST, Manchester, UK) – in press.
\bibitem{10} R.F. Bishop, J.B. Parkinson, and Y. Xian, \textit{Phys. Rev. B} \textbf{44}, 9425 (1991).
\bibitem{11} R.F. Bishop, J.B. Parkinson, and Yang Xian, \textit{Phys. Rev. B} \textbf{46}, 880 (1992).
\bibitem{12} D.J.J. Farnell, S.A. Krüger, and J.B. Parkinson, \textit{J. Phys.: Condens. Matter} \textbf{9}, 7601 (1997).
\bibitem{13} C. Zeng, D.J.J. Farnell, and R.F. Bishop, \textit{J. Stat. Phys.} \textbf{90}, 327 (1998).
\bibitem{14} R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, \textit{Phys. Rev. B} \textbf{58}, 6394 (1998).
\bibitem{15} R.F. Bishop, D. J. J. Farnell, S.E. Krüger, J. B. Parkinson, J. Richter, and C. Zeng, \textit{J. Phys.: Condens. Matter} \textbf{12}, 6887 (2000).
\bibitem{16} F.D.M. Haldane, \textit{Phys. Lett.} \textbf{93A}, 464 (1983).
\bibitem{17} J.B. Parkinson and J.C. Bonner, \textit{Phys. Rev. B} \textbf{32}, 4703 (1985).
\bibitem{18} C.J. Hamer, W.H. Zheng, and P. Arndt, \textit{Phys. Rev. B} \textbf{46}, 6276 (1992).
\bibitem{19} W.H. Zheng, J. Oitmaa, and C.J. Hamer, \textit{Phys. Rev. B} \textbf{43}, 8321 (1991).
\bibitem{20} D. J. J. Farnell, K. A. Gernoth, and R. F. Bishop, \textit{to be published}.
\end{thebibliography}