High-Order Coupled Cluster Method (CCM) Formalism 3: Finite-Size CCM

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Abstract

Recent developments of high-order CCM have been to extend existing formalism and codes to \( s \geq \frac{1}{2} \) for both the ground and excited states, and independently to “generalised” expectation values for a wide range of one- and two-body spin operators. An advantage of the CCM is that the Goldstone linked-cluster theorem is obeyed at all levels of approximation and so it provides results in the infinite lattice limit \( N \to \infty \) from the outset. However, recent results have also shown that the CCM can provide exact (symmetry-breaking) results for the spin-half linear-chain \( J_1-J_2 \) at the Majumdar-Ghosh point \( J_2/J_1 = 0.5 \) by identifying special solutions of the CCM equations for the usual Néel model state. Interestingly, the CCM provides exact (non-symmetry-breaking) results for systems in which small magnetic clusters become de-coupled from each other when the bonds connecting them tend to zero. These exact results involve the identification of “special solutions” of the CCM equations for the Néel state. An example of this is given by a spin-half system with nearest-neighbour bonds for an underlying lattice corresponding to the magnetic material CaV\(_4\)O\(_9\) (CAVO) in which one of the two different types of bonds on the lattice tend to zero. Larger finite-sized systems may be considered by appropriate choice of the unit cell and the bonds on it. We show here that exact diagonalisation results for ground-state energy and excitation energy gap for the spin-half and spin-one linear Heisenberg model on chains of length up to \( N = 12 \) sites for \( s = 1/2 \) and \( N = 6 \) sites for \( s = 1 \) with periodic boundary conditions are reproduced exactly using high-order CCM via this “brute-force” approach; i.e., one in which none of the translational or point-group symmetries of the finite lattice are used.
I. INTRODUCTION

The coupled cluster method (CCM) is a well-known method of quantum many-body theory (QMBT). The CCM has been applied with much success in order to study quantum magnetic systems at zero temperature (see Refs. [10–52]). In particular, the use of computer-algebraic implementations of the CCM has been found to be very effective with respect to these spin-lattice problems. Recent developments of high-order CCM formalism and codes have been to treat systems with spin quantum number of \( s \geq \frac{1}{2} \) for both the ground and excited states [52]. Furthermore, the ground-state formalism and codes may also be used directly to find “generalised” expectation values [53]. These expectation values are defined for a wide range of one- or two-body spin operator that prior to the CCM calculation.

Here we show how the consideration of previous results for exact results for the (symmetry-breaking) 1D \( J_1-\tilde{J}_2 \) model at \( \tilde{J}_2/J_1 = 0.5 \) [50, 54] and a (non-symmetry-breaking) nearest-neighbour CAVO model [50] in the limits that various nearest-neighbour bond either go to zero or infinity leads on naturally to the treatment of finite lattices via the CCCM code [55]. This is achieved by the simple expedient of choosing the finite-lattice to be the fundamental unit cell and so this is a “brute-force” solution of the finite-lattice problem via high-order CCM.

II. METHOD

The details of the practical application of high-order coupled cluster method (CCM) formalism to lattice quantum spin systems are given in Refs. [22, 26, 32, 52] and also in the appendices to this article. However, we point out now that the ket and bra ground-state energy eigenvectors, \( |\Psi\rangle \) and \( \langle \tilde{\Psi}| \), of a general many-body system described by a Hamiltonian \( H \), are given by

\[
H|\Psi\rangle = E_g|\Psi\rangle \quad \text{and} \quad \langle \tilde{\Psi}|H = E_g\langle \tilde{\Psi}|. \tag{1}
\]

Furthermore, the ket and bra states are parametrised within the single-reference CCM as follows:

\[
|\Psi\rangle = e^S|\Phi\rangle \quad \text{and} \quad S = \sum_{I \neq 0} S_I C_I^+. \]

\[ \langle \tilde{\Psi} | = \langle \Phi | \tilde{S} e^{-S} ; \quad \tilde{S} = 1 + \sum_{I \neq 0} \tilde{S}_I C_I^- . \]  

(2)

One of the most important features of the CCM is that one uses a single model or reference state \( |\Phi\rangle \) that is normalised. We note that the parametrisation of the ground state has the normalisation condition for the ground-state bra and ket wave functions \( (\langle \tilde{\Psi} | \Psi \rangle \equiv \langle \Phi | \Phi \rangle = 1) \). The model state is required to have the property of being a cyclic vector with respect to two well-defined Abelian subalgebras of multi-configurational creation operators \( \{C_I^+\} \) and their Hermitian-adjoint destruction counterparts \( \{C_I^- \equiv (C_I^+)^\dagger\} \). The interested reader is referred to the Appendices and to Ref. [52] for more information regarding how the CCM problem is solved for.

Here, we use the Néel state as the model state for the antiferromagnetic Heisenberg model given by

\[ H = J \sum_{\langle i,j \rangle} s_i \cdot s_j . \]  

(3)

For the bipartite lattices, we perform a rotation of the local axes of the up-pointing spins by 180° about the y-axis. The transformation is described by,

\[ s^x \rightarrow -s^x, \quad s^y \rightarrow s^y, \quad s^z \rightarrow -s^z . \]  

(4)

The model state now appears mathematically to consist of purely down-pointing spins. In terms of the spin raising and lowering operators \( s^\pm_k \equiv s^x_k \pm i s^y_k \) the Hamiltonian may be written in these local axes as,

\[ H = -J \sum_{\langle i,j \rangle} \left[ s^+_i s^+_j + s^-_i s^-_j + 2 s^+_i s^-_j \right] , \]  

(5)

where the sum on \( \langle i,j \rangle \) again counts all nearest-neighbour pairs once on the lattice.

The CCM formalism is exact in the limit of inclusion of all possible multi-spin cluster correlations within \( S \) and \( \tilde{S} \), although this is usually impossible to achieve practically. Hence, we generally make approximations in both \( S \) and \( \tilde{S} \). The three most commonly employed approximation schemes previously utilised have been: (1) the SUBn scheme, in which all correlations involving only \( n \) or fewer spins are retained, but no further restriction is made concerning their spatial separation on the lattice; (2) the SUBn-m sub-approximation, in which all SUBn correlations spanning a range of no more than \( m \) adjacent lattice sites are retained; and (3) the localised LSUBm scheme, in which all multi-spin correlations over all...
distinct locales on the lattice defined by $m$ or fewer contiguous sites are retained. Another important feature of the method is that the bra and ket states are not always explicitly constrained to be Hermitian conjugates when we make such approximations, although the important Helmann-Feynman theorem is always preserved. We remark that the CCM provides results in the infinite-lattice limit $N \to \infty$ from the outset.

Key to understanding the application of the CCM to spin problems is the concept of the unit cell and the Bravais lattice. The unit cell contains a number of sites at specific positions (given by the “primitive” lattice vectors) that are replicated at all possible multiples of the Bravais lattice vectors. Thus, for example, we have a single site in the unit cell for the linear chain, say, at position $(0,0)$ and a single Bravais lattice vector $\hat{a} = (1,0)^T$. The lattice is formed by translating the single site in the unit cell by all integer multiples of $\hat{a}$. Two-dimensional lattices have two Bravais lattice vectors. For example the square lattice has a single site in the unit cell and the lattice vectors are $\hat{a} = (1,0)^T$ and $\hat{b} = (0,1)^T$. The triangular lattice is given by vectors $\hat{a} = (1,0)^T$ and $\hat{b} = (1/2, \sqrt{3}/2)^T$ and so on for other lattices. We see also that the basic building blocks of unit cell, Bravais lattice, and bonds/interactions in the Hamiltonian placed on the lattice gives us a broad canvas to work with. For example, we may form models that interpolate between different lattices (and even different spatial dimensions) by varying the strengths of various bonds that have been carefully placed with respect to the underlying lattice. Hence, the number of possible such quantum spin systems is enormous. Furthermore, the development in the number and complexity of these theoretical models is often driven by the magnetic materials studied in experiment.

III. RESULTS

A. The Spin-Half $J_1-J_2$ Model on the Linear Chain

The Hamiltonian for this spin-half model has nearest-neighbour bonds of strength $J_1$ and next-nearest-neighbour bonds of strength $J_2$. We use a Néel model state in which nearest-neighbour spins on the linear chain are anti-parallel. We rotate the spin coordinates of the ‘up’ spins so that notationally they become ‘down’ spins in these locally defined axes. The
relevant Hamiltonian in rotated coordinates is then given by

$$H = -J_1 \sum_{\langle i,j \rangle} (s_i^+ s_j^z + s_i^z s_j^- + 1/2 \{ s_i^- s_{j+1}^- + s_i^+ s_{j+1}^+ \}) + J_2 \sum_{\langle\langle i,k \rangle\rangle} (s_i^+ s_k^z + 1/2 \{ s_i^- s_k^- + s_i^+ s_k^+ \})$$

(6)

where $\langle i, j \rangle$ runs over all nearest-neighbour sites on the lattice counting each pair once and once only and $\langle\langle i, k \rangle\rangle$ runs over all next-nearest-neighbor sites on the lattice, again counting each pair once and once only. Henceforth we put $J_1 = 1$ and consider $J_2 > 0$.

The ground-state properties of this system have been studied using methods such as exact diagonalisations [57, 62], DMRG [17, 58–60], CCM [14, 16, 42], and field-theoretical approaches [60] (see Refs. [60, 61] for a general review). We shall not go into detail about this model here except to note that there are two degenerate simple exact dimer-singlet product ground states at the Majumdar-Ghosh point $J_2/J_1 = 0.5$.

We now consider how this model can be treated at the Majumdar-Ghosh point $J_2/J_1 = 0.5$ by the CCM via the identification of a special dimerised solution of the CCM equations for a Néel model state. We use a doubled unit cell including two neighbouring sites for a spin-half system on the linear chain at points (0,0,0) and (1,0,0) and a single Bravais vector $(2,0,0)^T$ to take into account the symmetry breaking. There are thus two distinct types of two-spin nearest-neighbour ket-state correlation coefficients and again these are denoted as $S_a^2$ and $S_b^2$ for $S_2 = S_a^2 \sum_{i_a} s_{i_a}^+ s_{i_a+1}^+ + S_b^2 \sum_{i_b} s_{i_b}^+ s_{i_b+1}^+$ with respect to the CCM ket state of Eq. (2), and where $i_a$ runs over all sites with odd-numbered indices and $i_b$ runs over all sites with even-numbered indices. The exact ground state at $J_2/J_1 = 0.5$ is obtained by setting $S_a^2 = 1$ and all other coefficients equal to zero. This result is found to hold for all levels of LSUB$m$ approximation. The exact ground-state energy of $E_g/N = -0.375J_1$ is thus obtained at the point $J_2/J_1 = 0.5$, as expected. Furthermore, the sublattice magnetisation is found to be zero at this point at all levels of approximation. We find values [54] for the excitation energy gap of $0.35250, 0.34170, 0.30548, 0.28732, 0.27559$, and $0.26760$ at the LSUB$m$ levels of approximation with $m = \{4, 6, 8, 10, 12, 14\}$. A simple extrapolation of these results in the limit $m \to \infty$ using a quadratic function gives a value for the gap of $0.2310$. This result is in agreement with results of exact diagonalisations that predict a gap of $0.234$ [63].
FIG. 1: The CAVO lattice. The nearest-neighbour bonds that connect two sites on a four-site plaquette are shown by the solid lines and have a bond strength given by $J$ ($=1$). The nearest-neighbour bonds that connect two sites on different plaquettes (dimer bonds) are shown by the dotted lines and have a bond strength given by $J'$. The unit cell of the lattice is shown by the square with the grey dashed lines.

B. The $J$–$J'$ Heisenberg antiferromagnet on the CAVO lattice

In the previous section, we saw that the exact dimerised state at the Majumdar-Ghosh point may be obtained for the Néel model state by appropriate choice of ket-state correlation coefficients. However, this is a case in which the translational symmetry of the lattice (the linear chain) is spontaneously broken. We now wish to a case in which dimerised and plaquette exact solutions follow the symmetry of the Hamiltonian and so do not form symmetry-broken states. We consider an antiferromagnetic Heisenberg model in which the basic geometric unit cell contains four neighbouring lattice sites on the underlying crystallographic lattice of the magnetic material CaV$_4$O$_9$ (CAVO), shown in Fig. 1. There are two non-equivalent antiferromagnetic nearest-neighbour bonds $J$ and $J'$ belonging to dimers ($J'$) and to four-spin plaquettes ($J$) respectively. The ground state of the quantum model depends on the ratio $J'/J$ of the competing bonds. Using a unit cell as defined in Fig. 1, the plaquette bonds $J$ are inside the four-site unit cell and the dimer bonds $J'$ connect sites in different unit cells. We note that this model is not frustrated but the two non-equivalent
nearest-neighbour bonds lead to a competition in the quantum system. Henceforth, we choose an energy scale such that $J = 1$.

The four-site plaquettes in the unit cell become de-coupled only in the limit $J'/J \to 0$. The ground state is a product of such four-site plaquette singlets in this limit. In the limit that $J'/J \to \infty$ dimers are formed on the $J'$ bonds. To model such states using the CCM we start again from the Néel model state; namely, a state in which the spins on nearest-neighbour sites are anti-parallel. To create an exact plaquette-singlet product VBC ground state at $J'/J = 0$ using the CCM we have to adjust the nearest-neighbour correlation coefficients $S^a_2$ and $S^b_2$ and a single four-body plaquette correlation coefficient $S^p_4$ containing all four sites properly. (Note that $S^a_2$ represents those ket-state coefficients for the nearest-neighbour two-body cluster connecting sites on a plaquette indicated by the solid lines in Fig. 1 whereas $S^b_2$ represents those ket-state coefficients for the nearest-neighbour two-body cluster connecting sites on a dimer indicated by the dotted lines in the same figure. The coefficient $S^p_4$ represents those ket-state coefficients for the four-body cluster corresponding to a plaquette indicated by the solid lines in Fig. 1.) Indeed, it is easy to show that setting the ket-state correlation coefficients $S^a_2$ and $S^p_4$ to a value of 0.5 and all other ket-state correlation coefficients (including $S^b_2$) to zero the plaquette-singlet product valence-bond crystal state is obtained exactly. Furthermore, we are also able to reproduce exactly the dimer-singlet product ground state in the limit $J'/J \to \infty$. In this limit, the nearest-neighbour ket-state correlation coefficient $S^b_2$ on the dimer bonds (dotted lines in Fig. 1) has a value of one and all other coefficients (e.g., $S^a_2$ and $S^p_4$) are zero.

An important point is that in the limits $J'/J \to 0$ and $|J'/J| \to \infty$ the system is comprised of independent clusters. However, the system is two-dimensional for all other values of $J'/J$. This system therefore “interpolates” between a zero-dimensional and two-dimensional lattice with the bond strengths $J'/J$. This model (and similar models) may therefore be used to study the differences between zero-dimensional and two-dimensional systems. They may also be used to investigate the effects of “linking” magnetic clusters in order to form an extended two-dimensional material. Such models are of interest in the subject of quantum computational. We remark that the CCM solution at intermediate values of $J'/J$ may be found by “tracking” the exact CCM solution by making small incremental changes in $J'/J$ from either of the exact limits $J'/J \to 0$ and $|J'/J| \to \infty$ (see Ref. 50 for details).
FIG. 2: CCM results for the ground-state energy of the $J-J'$ Heisenberg antiferromagnet on the CAVO lattice (with $J = 1$).

We remark that the correct ground-state energies (with $J = 1$) are reproduced in the limits $J'/J \to 0$ and $J'/J \to \infty$, namely, $E_g/N = -0.5$ and $E_g/N = -0.375J'$, respectively. These results for the ground-state energy are shown in Fig. 2 and we see that LSUB8 and LSUB10 results agree extremely well over the region considered. Hence, we conclude that the CCM also provides excellent results for intermediate values of $J'/J$ that interpolates between the two (exact) limits, $J'/J \to 0$ and $J'/J \to \infty$.

C. The Spin-Half and Spin-One Heisenberg Model on Finite-Sized Chains

We have seen in the previous sections that an appropriate choice of the unit cell and values for the CCM correlation coefficients can reproduce exact results for Néel model states. This was observed, namely, for the symmetry-breaking solution to the $J_1-J_2$ model at $J_2/J_1 = 0.5$ or for the CAVO model with two types of bonds in the limits $J'/J \to 0$ and $|J'/J| \to \infty$. We now consider if exact solutions for larger unit cells may be found by “brute force”, i.e., without using any of the translational or point-group symmetries of the finite lattice.

We start by defining the unit cell to be of size $N = \{2, 4, 6, 8, 10, 12\}$. We use the
Hamiltonian of Eq. (3) and we rotate the “up” spins as usual. The Hamiltonian in the new spin coordinates is then given by Eq. (5). Hence, we form bonds (of strength \( J = 1 \)) between all nearest-neighbour sites in the unit cell. However, we do not “link” the bonds by forming an intermediate bond between the unit cells, and so, in effect, the unit cells become isolated clusters. A technical point is that we set the single Bravais lattice vector to be of magnitude \( +N \) for this “brute force” approach; again, even though the clusters/unit cells are not linked by intermediate bonds. Furthermore, we may also provide an additional bond between the first and last sites (again of strength \( J = 1 \)). In effect, this bond acts as a “boundary condition” that creates a “ring” of sites for the finite lattice. These results should be compared to those of ED with periodic boundary conditions.

High-order CCM SUBn-m results for the antiferromagnetic Heisenberg model (with periodic conditions) for finite-sized chains of length \( N \) with SUBn-m with \( n = m = N \) for \( s = 1/2 \) and \( n/2 = m = N \) for \( s = 1 \) in Tables I and II respectively. We remark that CCM results for the ground-state energy and excitation energy gap agree to at least six decimal places with exact diagonalisations obtained using the SpinPack code of Joerg Schulenburg [64]. We may also study the manner in which LSUBm results behave with increasing \( m \) for a set value of chain length \( N \). Table III presents LSUBm results for the spin-half Heisenberg chain of length \( N = 12 \). The ground-state energies decrease monotonically with increasing LSUBm level of approximation, although no simple extrapolation “rule” may be seen. By contrast, the LSUBm data for the excitation energy gap is only monotonically decreasing up to LSUB10. Indeed, the gap for LSUB10 lies lower than that of the (exact) LSUB12 result. We note again that the LSUBm approximation for the spin-half system and the SUB2m-m approximation for the spin-one system reproduce exact results for the chains of length \( N \) when we set \( m = N \).

The CCM results in Tables I to III arise from “special solutions” of the CCM equations in exactly the same manner as for the nearest-neighbour CAVO problem in the limits \( J'/J \to 0 \) and \( |J'/J| \to \infty \). However, it is clearly more complicated in this case because we are dealing with unit cells (i.e., finite-sized 1D lattices here) of greater size than 4 sites. Interestingly though, the CCM ground-state equations were found to converge readily to this “special solution” and for a wide range of starting values at all levels of SUBn-m approximation attempted here. For example, setting the initial ket-state correlation coefficients to a small (positive) non-zero value was found to work quite well. Indeed, the ground-state solution
TABLE I: CCM $L_{SUBm}$ results for the ground-state energy and excitation energy gap of spin-half antiferromagnetic Heisenberg chains of $N$ length with periodic boundary conditions.

| $N$ | CCM $E_g/N$ | CCM Gap |
|-----|-------------|---------|
| 4   | $-0.5$      | 1       |
| 6   | $-0.46712928$ | 0.684740 |
| 8   | $-0.45638668$ | 0.522676 |
| 10  | $-0.45154464$ | 0.423239 |
| 12  | $-0.44894924$ | 0.355848 |

TABLE II: CCM $S_{UBn-m}$ results (with $n = 2N$ and $m = N$) for the ground-state energy and excitation energy gap of spin-one antiferromagnetic Heisenberg chains of $N$ length with periodic boundary conditions.

| $N$ | $E_g/N$ | Gap |
|-----|--------|-----|
| 2   | $-1.263853992$ | $1.4876903286$ |
| 4   | $-1.29781459$  | $1.038539433$  |
| 6   | $-1.436237197$ | $0.720627363$  |

was found to be very stable, as is generally also the case for extended systems ($N \to \infty$) in which the model state is known to be a “good starting point”.

These results prove the principle that the CCM may be used to study finite-sized lattices.

IV. CONCLUSIONS

Again, we remark that recent developments of high-order CCM have been to extend existing formalism and codes to $s \geq \frac{1}{2}$ for both the ground and excited states [52], and independently to “generalised” expectation values for a wide range of one- and two-body spin operators [53]. We note that the CCM is that the Goldstone linked-cluster theorem is obeyed at all levels of approximation and so it provides results in the infinite lattice limit $N \to \infty$ from the outset. In this article, we have shown the exact ground state for the
TABLE III: CCM \( \text{LSUB}m \) results for the ground-state energy and excitation energy gap of spin-half antiferromagnetic Heisenberg chains of length \( N = 12 \) with periodic boundary conditions.

| \( \text{LSUB}m \) | \( E_g/N \)          | Gap            |
|-----------------|---------------------|----------------|
| 4               | -0.421064786        | 0.589781571    |
| 6               | -0.42329432         | 0.440170513    |
| 8               | -0.42397557         | 0.375801129    |
| 10              | -0.424415368        | 0.348833726    |
| 12              | -0.448949243        | 0.355847514    |

\( J_1-J_2 \) model at \( J_2/J_1 = 0.5 \) may be reproduced using a Néel model state. Using a similar model state in 2D, exact results for a nearest-neighbour CAVO model were reproduced using high-order CCM in the limits \( J'/J \to 0 \) (4-site plaquette) and \( J'/J \to \infty \) (2-site dimers). These results lead on naturally to a “brute-force” approach for solving finite-sized lattices, i.e., without using any of the translational or point-group symmetries of the finite lattice. Indeed, we have shown here that high-order CCM \( \text{SUB}n-m \) results for the antiferromagnetic Heisenberg model (with periodic conditions) for finite-sized chains of length \( N \) with \( \text{SUB}n-m \) with \( n = m = N \) for \( s = 1/2 \) and \( n/2 = m = N \) for \( s = 1 \) were found to agree with exact-diagonalisation (ED) results for the ground-state energy and excitation energy gap agree to at least six decimal places.

We note that results for the case of finite clusters for \( s = 1 \) were obtained via new high-order formalism for the CCM excited state outlined in Refs. \[52, 54\]. Furthermore, new code \[55\] has been written to implement this new formalism for the excited state for \( s \geq 1 \). The agreement between ED results for the ground-state energy and excitation energy gap for chains of up to \( N = 6 \) for \( s = 1 \) is an excellent test of the validity of this new code. These solutions for the finite chains were found to be stable numerically. Hence, we have “proven the principle” that the high-order CCM code may be used directly to study (relatively small-sized) finite lattices by a somewhat “brute-force” approach. Indeed, this approach is still somewhat inefficient in comparison to exact diagonalisations (ED) because ED results use translational and point-group symmetries of the finite lattice in order to reduce the size of the matrix to be diagonalised, and so ED may to go to much larger lattice sizes.
For periodic boundary conditions, the manner in which this is achieved for ED is by identifying common states for a given $k$-value via a complex phase factor $e^{-i k \cdot r}$ for states that are related by a translational vector $r$ on the finite lattice (again: note periodic boundary conditions are assumed). The Hamiltonian then links only those states of common $k$. Point-group (PG) symmetries/permutations of indices may then be used to form states with real components only, thus simplifying the computational problem. In principle, we ought to be able to employ the finite lattice translational and point-group symmetries analogously in order to simplify the finite-size problem with periodic boundary conditions also for the CCM. However, it is unclear how one might do this in practice for the exponentiated $S$ in the ground ket and bra states. The use of translational and PG symmetries for finite-lattice CCM will be the subject of future research.

Despite the fact that translational and PG symmetries for the finite lattice were not used directly here, we were still able to treat finite-lattices of size $N = 12$ for the spin-half case using high-order CCM with only relatively meagre computational resources. (A MacBook with a “Core Duo” processor and 1 GIG RAM was used in this case was used to carry out this calculation.) Still larger lattices are possible using the CCCM code [55], which has been implemented to work in parallel on a cluster of processors. We note that the addition of intermediate bonds that link the isolated clusters in order to form extended lattices of infinite numbers of sites requires only relatively small increases in computational effort for high-order CCM compared to treating the case of isolated magnetic clusters alone. Excellent results were seen here for such a model that interpolated between finite clusters and an extended lattice, namely, for the n.n. CAVO model (e.g., see the results for the ground state energy in Fig. 2. High-order CCM might provide a good choice for the study of a whole range of such “interpolating” models between finite clusters and infinite lattices.

[1] F. Coester, Nucl. Phys. 7, 421 (1958); F. Coester and H. Kümmel, ibid. 17, 477 (1960).
[2] J. Čižek, J. Chem. Phys. 45, 4256 (1966); Adv. Chem. Phys. 14, 35 (1969).
[3] R.F. Bishop and K.H. Lührmann, Phys. Rev. B 17, 3757 (1978); ibid. 26, 5523 (1982).
[4] H. Kümmel, K.H. Lührmann, and J.G. Zabolitzky, Phys Rep. 36C, 1 (1978).
[5] J.S. Arponen, Ann. Phys. (N.Y.) 151, 311 (1983).
[6] R.F. Bishop and H. Kümmel, Phys. Today 40(3), 52 (1987).

[7] J.S. Arponen, R.F. Bishop, and E. Pajanne, Phys. Rev. A 36, 2519 (1987); ibid. 36, 2539 (1987); in: Condensed Matter Theories, Vol. 2, P. Vashishta, R.K. Kalia, and R.F. Bishop, eds. (Plenum, New York, 1987), p. 357.

[8] R.J. Bartlett, J. Phys. Chem. 93, 1697 (1989).

[9] R.F. Bishop, Theor. Chim. Acta 80, 95 (1991).

[10] M. Roger and J.H. Hetherington, Phys. Rev. B 41, 200 (1990); Europhys. Lett. 11, 255 (1990).

[11] R.F. Bishop, J.B. Parkinson, and Y. Xian, Phys. Rev. B 44, 9425 (1991).

[12] R.F. Bishop, J.B. Parkinson, and Y. Xian, Phys. Rev. B 46, 880 (1992).

[13] R.F. Bishop, J.B. Parkinson, and Y. Xian, J. Phys.: Condens. Matter 5, 9169 (1993).

[14] D.J.J. Farnell and J.B. Parkinson, J. Phys.: Condens. Matter 6, 5521 (1994).

[15] R.F. Bishop, R.G. Hale, and Y. Xian, Phys. Rev. Lett. 73, 3157 (1994).

[16] Y. Xian, J. Phys.: Condens. Matter 6, 5965 (1994).

[17] R. Bursill, G.A. Gehring, D.J.J. Farnell, J.B. Parkinson, T. Xiang, and C. Zeng, J. Phys.: Condens. Matter 7, 8605 (1995).

[18] R.G. Hale. Ph.D. Thesis, UMIST, Manchester, United Kingdom (1995).

[19] R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, J. Phys.: Condens. Matter 8, 11153 (1996).

[20] D.J.J. Farnell, S.A. Krüger, and J.B. Parkinson, J. Phys.: Condens. Matter 9, 7601 (1997).

[21] R.F. Bishop, Y. Xian, and C. Zeng, in: Condensed Matter Theories, Vol. 11, E.V. Ludeña, P. Vashishta, and R.F. Bishop, eds. (Nova Science, Commack, New York, 1996), p. 91.

[22] C. Zeng, D.J.J. Farnell, and R.F. Bishop, J. Stat. Phys. 90, 327 (1998).

[23] R.F. Bishop, D.J.J. Farnell, and J.B. Parkinson, Phys. Rev. B 58, 6394 (1998).

[24] R.F. Bishop in Microscopic Many-Body Theories and Their Applications, Lecture Notes in Physics 510, J. Navarro and A. Polls, eds. Lecture Notes in Physics Vol. 510 (Springer-Verlag, Berlin, 1998), p. 1.

[25] J. Rosenfeld, N.E. Ligterink, and R.F. Bishop, Phys. Rev. B 60, 4030 (1999).

[26] R.F. Bishop, D.J.J. Farnell, S.E. Krüger, J.B. Parkinson, J. Richter, and C. Zeng, J. Phys.: Condens. Matter 12, 6887 (2000).

[27] R.F. Bishop, D.J.J. Farnell, and M.L. Ristig, Int. J. Mod. Phys. B 14, 1517 (2000).

[28] S.E. Krüger, J. Richter, J. Schulenberg, D.J.J. Farnell, and R.F. Bishop, Phys. Rev. B 61, 14607 (2000).
[29] D.J.J. Farnell, R.F. Bishop, and K.A. Gernoth, Phys. Rev. B 63, 220402R (2001).
[30] D.J.J. Farnell, K.A. Gernoth, and R.F. Bishop, Phys. Rev. B 64, 172409 (2001).
[31] S.E. Krüger and J. Richter, Phys. Rev. B 64, 024433 (2001).
[32] D.J.J. Farnell, R.F. Bishop, and K.A. Gernoth, J. Stat. Phys. 108, 401 (2002).
[33] N.B. Ivanov, J. Richter, and D.J.J. Farnell, Phys. Rev. B 66, 014421 (2002).
[34] D.J.J. Farnell and R.F. Bishop, arxiv.org/abs/cond-mat/0311126.
[35] S.E. Krüger, D.J.J. Farnell, and J. Richter, Int. J. Mod. Phys. B 17, 5347 (2003).
[36] R. Darradi, J. Richter, and D.J.J. Farnell, Phys. Rev. B. 72, 104425 (2005).
[37] R. Darradi, J. Richter, and D.J.J. Farnell, J. Phys.: Condens. Matter 17, 341 (2005).
[38] D.J.J. Farnell, J. Schulenberg, J. Richter, and K.A. Gernoth, Phys. Rev. B. 72, 172408 (2005).
[39] S.E. Krüger, R. Darradi, J. Richter, and D.J.J Farnell, Phys. Rev. B 73, 094404 (2006).
[40] D. Schmalfuß, R. Darradi, J. Richter, J. Schulenberg, and D. Ihle, Phys. Rev. Lett. 97, 157201 (2006).
[41] D.J.J. Farnell and R.F. Bishop, arxiv.org/abs/cond-mat/0606060.
[42] J. Richter, R. Darradi, R. Zinke, and R.F. Bishop, Int. J. Mod. Phys. B 21, 2273 (2007).
[43] R. Zinke, J. Schulenberg, and J. Richter, Eur. Phys. J. B 61, 147 (2008).
[44] R.F. Bishop, P.H.Y. Li, R. Darradi, and J. Richter, J. Phys.: Condens. Matt. 20 255251 (2008).
[45] R.F. Bishop, P.H.Y. Li, R. Darradi, J. Schulenberg, and J. Richter, Phys. Rev. B 78, 054412 (2008).
[46] R.F. Bishop, P.H.Y. Li, R. Darradi, and J. Richter, Europhys. Lett. 83, 47004 (2008).
[47] R.F. Bishop, P.H.Y. Li, R. Darradi, J. Richter, and C.E. Campbell, J. Phys.: Condens. Matt. 20, 415213 (2008).
[48] R. Darradi, O. Derzhko, R. Zinke, J. Schulenberg, S.E. Krüger, and J. Richter, Phys. Rev. B 78, 214415 (2008).
[49] D.J.J. Farnell and R.F. Bishop, Int. J. Mod. Phys. B. 22, 3369 (2008).
[50] D.J.J. Farnell, J. Richter, R. Zinke, and R.F. Bishop, J. Stat. Phys. 135, 175 (2009).
[51] P. Li, D.J.J. Farnell, and R.F. Bishop, Phys. Rev. B 79, 174405 (2009).
[52] D.J.J. Farnell, arXiv:0909.1226
[53] D.J.J. Farnell, arXiv:0911.5150
[54] D.J.J. Farnell, in Condensed Matter Theories – in print.
[55] A GPL licensed version of the ‘Crystallographic Coupled Cluster Method’ (CCCM) code of
D.J.J. Farnell and J. Schulenburg is available online at: [http://www.ovgu.de/jschulen/ccm/](http://www.ovgu.de/jschulen/ccm/)

[56] C.K Majumdar and D.K. Ghosh, J. Math. Phys. 10, 1388 (1969); J. Math. Phys. 10, 1399 (1969).

[57] T. Tonegawa and I. Harada, J. Phys. Soc. Japan 56, 2153 (1987).

[58] K. Nomura and K. Okamoto, Phys. Lett. 169A, 433 (1992); J. Phys. Soc. Japan 62, 1123 (1993); J. Phys. A.: Math. Gen. 27, 5773 (1994).

[59] R. Chitra, S. Pati, H.R. Krishnamurthy, D. Sen, and S. Ramasesha, Phys. Rev. B 52, 6581 (1995).

[60] S. R. White and I. Affleck, Phys. Rev. B 54, 9862 (1996).

[61] H.-J. Mikeska and A. K. Kolezhuk, in Quantum Magnetism, Lecture Notes in Physics 645, U. Schollwöck, J. Richter, D.J.J. Farnell, and R.F. Bishop, eds. (Springer-Verlag, Berlin, 2004), pp 1-83.

[62] A.A. Aligia, C.D. Batista, and F.H.L. Eßler, Phys. Rev. B 62, 3259 (2000).

[63] W.J. Caspers, in: Spins Systems (World Scienti c, 1989) p. 107. 29

[64] The exact diagonalisations SpinPack code of J. Schulenburg is available under GPL licence at: [http://www.ovgu.de/jschulen/spin/](http://www.ovgu.de/jschulen/spin/)