High-Order Coupled Cluster Method (CCM) Calculations Via Parallel Processing: An Application To The Kagomé Antiferromagnet

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Abstract

A simple “brute-force” parallelisation procedure for the computational implementation of high-order coupled cluster method (CCM) calculations is presented here. This approach is investigated and illustrated by an application of high-order CCM to the Heisenberg antiferromagnet on the Kagomé lattice with nearest- and next-nearest-neighbour bonds. Ferromagnetic next-nearest-neighbour bonds are used to stabilise a model state which contains three sublattices in which the spins make angles of 120° to each other. Ground-state results for up to approximately 10000 fundamental clusters are presented, and our best estimate for the ground-state energy per spin of the spin-half Kagomé lattice antiferromagnet with only nearest-neighbour bonds is $E_g/N = -0.43104$. We believe that further increases (of at least another order of magnitude) in the number of fundamental clusters might be possible in future by using parallel processing techniques. The extension of high-order CCM calculations in order to consider non-Néel (e.g., dimer solid) model states, simulation of excitation spectra, lattice boson and fermion models, and finite-sized systems is very briefly considered.
I. INTRODUCTION

The coupled cluster method (CCM) is a highly successful and widely applied technique of modern-day quantum many-body theory. In particular, the CCM has been applied to quantum magnetic systems at zero temperature over the last ten years or so. Indeed, the use of computational approaches of the CCM for quantum systems has been found to be particularly efficacious. We note that the subsequent application of these highly accurate computational CCM techniques to other types of quantum system is ripe.

In this article, we present a simple parallelisation procedure for high-order coupled cluster method (CCM) calculations. This approach is investigated and illustrated by the application to the Heisenberg antiferromagnet on the Kagomé lattice with nearest- and next-nearest-neighbour bonds. In particular, we note that we may consider up to approximately 10000 fundamental clusters, although we believe that further increases (of at least another order of magnitude) in the number of fundamental clusters might be possible in future by using such techniques.

II. FORMALISM

The exact ket and bra ground-state energy eigenvectors, $|\Psi\rangle$ and $\langle \tilde{\Psi}|$, of a general many-body system described by a Hamiltonian $H$, 

$$H |\Psi\rangle = E_g |\Psi\rangle ; \quad \langle \tilde{\Psi}| H = E_g \langle \tilde{\Psi}| ,$$

are parametrised within the single-reference CCM as follows:

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

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

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 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 $\{C_I^+\}$. Note that $C_I^- |\Phi\rangle = 0, \forall I \neq 0$, and that $C_0^- \equiv 1,$
the identity operator. These operators are furthermore complete in the many-body Hilbert (or Fock) space. Also, the correlation operator $S$ is decomposed entirely in terms of these creation operators $\{C^+_I\}$, which, when acting on the model state $\{C^+_I|\Phi\rangle\}$, create excitations from it. We note that although the manifest Hermiticity, $\langle \tilde{\Psi}|T|\Psi\rangle = \langle \Psi|T|\Psi\rangle = \langle \Phi|\Phi\rangle \equiv 1$ are explicitly imposed. The correlation coefficients $\{S_I, \tilde{S}_I\}$ are regarded as being independent variables, and the full set $\{S_I, \tilde{S}_I\}$ thus provides a complete description of the ground state. For instance, an arbitrary operator $A$ will have a ground-state expectation value given as,

$$\bar{A} \equiv \langle \tilde{\Psi}|A|\Psi\rangle = \langle \Phi|\tilde{S}e^{-S}He^SE\Phi\rangle = \bar{A}\left(\{S_I, \tilde{S}_I\}\right). \quad (3)$$

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 $|\Phi\rangle$ 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 determination of the correlation coefficients $\{S_I, \tilde{S}_I\}$ is achieved by taking appropriate projections onto the ground-state Schrödinger equations of Eq. (1). Equivalently, they may be determined variationally by requiring the ground-state energy expectation functional $\bar{H}(\{S_I, \tilde{S}_I\})$, defined as in Eq. (3), to be stationary with respect to variations in each of the (independent) variables of the full set. We thereby easily derive the following coupled set of equations,

$$\delta \bar{H}/\delta \tilde{S}_I = 0 \Rightarrow \langle \Phi|C^+_Ie^{-S}He^S|\Phi\rangle = 0, \quad I \neq 0 ; \quad (4)$$

$$\delta \bar{H}/\delta S_I = 0 \Rightarrow \langle \Phi|\tilde{S}e^{-S}[H, C^+_I]e^S|\Phi\rangle = 0, \quad I \neq 0. \quad (5)$$

Equation (4) also shows that the ground-state energy at the stationary point has the simple form

$$E_g = E_g(\{S_I\}) = \langle \Phi|e^{-S}He^S|\Phi\rangle. \quad (6)$$

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, one can prove that the important Hellmann-Feynman theorem is preserved in all such approximations.
In the case of spin-lattice problems of the type considered here, the operators \( C_I^+ \) become products of spin-raising operators \( s_k^+ \) over a set of sites \( \{k\} \), with respect to a model state \( |\Phi\rangle \) in which all spins points “downward” in some suitably chosen local spin axes. The CCM formalism is exact in the limit of inclusion of all possible such 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 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, in which all multi-spin correlations over all distinct locales on the lattice defined by \( m \) or fewer contiguous sites are retained.

### III. A “BRUTE-FORCE” PARALLELISATION PROCEDURE

A simple “brute-force” approach in order to solve the CCM equations in parallel is firstly to rearrange Eqs. (4) and (5) for the ket and bra states, respectively, where

\[
S_I = f_I(S_1, \ldots, S_{I-1}, S_{I+1}, \ldots, S_N) ;
\]
\[
\tilde{S}_I = \tilde{f}_I(S_1, \ldots, S_N; \tilde{S}_1, \ldots, \tilde{S}_{I-1}, \tilde{S}_{I+1}, \ldots, \tilde{S}_N) ;
\]

and where \( N_f \) is the number of fundamental configurations. Note that there are therefore \( N_f \) equations for both \( f_I \) and \( \tilde{f}_I \), which refer to the ket and bra states, respectively. We note that each equation contains a finite-number of terms and that, indeed, this is always the case for the CCM for Hamiltonians that contain a finite number of creation and destruction operators.

The “brute-force” approach is to iterate the set of equations in Eq. (7) to convergence first in order to obtain the ket-state correlation coefficients. We then iterate the set of equations Eq. (8) to convergence. This approach appears to function adequately as long as one is in the region where the model state is a good starting point. Clearly, this approach will become more difficult as we approach any critical points in the CCM equations. A simple parallelisation technique is now to split the problem of determining and solving the \( N_f \) equations for both the bra and ket states of Eqs. (7) and (8) between each processor in
the parallel cluster. Thus, each equation for $I = \{1, \cdots, N_f\}$ is ever dealt with by one node in the cluster only and the results of each node are collected together at each iteration in the “brute-force” algorithm. (Again, we remember that we iterate the ket-state equations first and then the bra-state equations.) Thus, the set of equations for the ket and bra states are solved independently and in parallel.

This approach has a number of advantages. Firstly, we do not need to define a Jacobian (e.g., as for the Newton-Raphson technique) and so we save on RAM by using this procedure. Secondly, the task of evaluating and saving the CCM equations is reduced by a factor of the number of machines used. Indeed, in our implementation we saved all of the data for a particular set of equations to disk locally on each machine, although we note that one could even re-derive the CCM equations as and when necessary in order to further reduce disk usage. Finally, this a simple approach and so is easy to amend existing code and so be parallelised.

This very simple approach was found to be surprisingly successful, although we note that the number of iterations for such a direct iteration method is at least an order of magnitude greater than that for the Newton-Raphson technique, for example. Indeed, we were able to reproduce those results determined on a single machine up to the LSUB7 level of approximation by using our parallelised implementation. This was found to be an excellent test of the validity of our results. However, we were able to solve the LSUB8 approximation for the ground-state energy only by using parallel processing. We note that this approximation contained 10707 fundamental configurations and that this is twice as big as the previous “largest” CCM calculation for spin systems. We believe that further increases in the number of fundamental configurations by at least another order of magnitude might be possible even by using moderate levels of parallelisation (e.g., 10 or 20 nodes) and for our “brute-force” approach.

Finally, we would wish to implement a more sophisticated solution of this problem using parallel processing in the future. A possible way of doing this would be to use PLAPACK, for example, in order to implement the Newton-Raphson technique “in parallel.” Other strategies might include numerical approximations to the Jacobian for the Newton-Raphson technique or other less memory-intensive ways of determining and solving the CCM equations of Eqs. 4 and 5.
IV. THE $J_1-J_2$ KAGOMÉ MODEL

The spin-half $J_1-J_2$ Kagomé Model model is given by

$$H = J_1 \sum_{\langle i,j \rangle} s_i \cdot s_j - J_2 \sum_{\{i,k\}} s_i \cdot s_k,$$

where $\langle i,j \rangle$ runs over all nearest-neighbour (n.n.) bonds and $\{i,k\}$ runs over all next-nearest-neighbour (n.n.n.) bonds on the Kagomé lattice. Note that each bond is counted once and once only, and that we now set $J_1 = 1.0$.

We choose a model state $|\Phi\rangle$ in which the lattice is divided into three sublattices, denoted \{A,B,C\}. The spins on sublattice A are oriented along the negative $z$-axis, and spins on sublattices B and C are oriented at $+120^\circ$ and $-120^\circ$, respectively, with respect to the spins on sublattice A. Our local axes are chosen by rotating about the $y$-axis the spin axes on sublattices B and C by $-120^\circ$ and $+120^\circ$ respectively, and by leaving the spin axes on sublattice A unchanged. The n.n.n. bonds for $J_2 > 0$ stabilise this type of Néel ordering in the quantum ground state.

Careful CCM and finite-sized calculations [28, 32, 33, 34] have been performed for the spin-half Kagomé antiferromagnet (KAF) ($J_2 = 0$), and these results indicate that the classical Néel-like ordering observed, for example, in the triangular-lattice antiferromagnet (TAF) is not seen for the quantum KAF model. The best estimate for the ground-state energy of the KAF via finite-sized calculations [34] stands at $E_g/N = -0.43$. Furthermore, CCM and series expansion results [28, 33] indicate that the ground-state of the KAF is disordered. Indeed, a variational calculation [35] which utilised a dimerised basis also found that the ground state of the KAF is some sort of spin liquid. Thus, it is highly likely that a quantum phase transition will occur at or near to $J_2 = 0$.

Our results for the ground-state energy per spin are given in Fig. 1 using the LSUB$m$ approximation with $m = \{2, 3, 4, 5, 6, 7\}$. We see that our results converge rapidly with $m$ across a wide range of $J_2$ up to an including the point $J_2 = 0$. Results for the special case $J_2 = 0$ are given in Table 1. (Note that these results are slightly different than previous CCM calculations in Ref. [28] due to a different underlying “interpolating” lattice in this case.) We are able to consider 10707 fundamental configurations using our parallel approach and a simple extrapolation in the limit $m \to \infty$ gives $E_g/N = -0.43104$, which should be considered to previous results of the best of other calculations [28, 34], namely, $E_g/N \approx$
FIG. 1: CCM results for the ground-state energy per spin of the $J_1$–$J_2$ model (with $J_1 = 1$) using the LSUB$m$ approximation with $m = \{2, 3, 4, 5, 6, 7\}$. We see that our results converge rapidly with $m$ across a wide range of $J_2$ up to an including the point $J_2 = 0$.

$-0.43$.

The sublattice magnetisation is defined by,

$$M = -\frac{2}{N} \sum_{k=1}^{N} s_k^z .$$

where $k$ runs over all lattice sites on the Kagomé lattice. Results for the sublattice magnetisation are given in Fig. 2 using the LSUB$m$ approximation with $m = \{2, 3, 4, 5, 6, 7\}$. Results for the special case $J_2 = 0$ are given in Table I. Note that CCM equations break down in the region $J < 0$ at their critical points. In the limit $m \to \infty$ we expect that this would occur at $J_2 = 0$. The “upturn” in $M$ for LSUB6 that occurs in the region $J_2 < 0$ is an artifact and such effects occur when the model state becomes an increasingly bad starting point. The CCM equations for LSUB7 break down at a critical point near to $J_2 = 0$, and we note that our results are consistent with the assertion that this model does not demonstrate Néel ordering at $J_2 = 0$. 

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FIG. 2: CCM results for the sublattice magnetisation of the $J_1$–$J_2$ model (with $J_1 = 1$) using the LSUB$m$ approximation with $m = \{2, 3, 4, 5, 6, 7\}$. Note that the CCM equations for the LSUB7 approximation “break down” at a critical point near to $J_2 = 0$, and that such behaviour is often associated with a phase transition in the “real” system.

TABLE I: CCM results for the ground-state energy per spin and sublattice magnetisation of the KAF model ($J_2 = 0$) using the LSUB$m$ approximation with $m = \{2, 3, 4, 5, 6, 7, 8\}$. $N_f$ is the number of fundamental configurations used. (The symbol “***” indicates that this result is yet to be determined.) Comparison is made in the last row with the results of other calculations.

| $m$ | $E_g/N$ | $M$ | $N_f$ |
|-----|--------|-----|-------|
| 2   | −0.377964 | 0.806536 | 2     |
| 3   | −0.394312 | 0.736248 | 9     |
| 4   | −0.408728 | 0.641403 | 29    |
| 5   | −0.414235 | 0.583833 | 117   |
| 6   | −0.418052 | 0.544218 | 521   |
| 7   | −0.420677 | 0.497977 | 2358  |
| 8   | −0.423554 | **   | 10707 |

c.f. Refs. [32, 33, 34, 35]
V. CONCLUSION

We have shown that it is possible to parallelise the high-order CCM problem implemented using computational techniques. A simple "brute-force" method was used, although more sophisticated approaches were briefly considered.

An application to the spin-half \( J_1- J_2 \) model on the Kagomé lattice was considered. Results for the ground-state energy and sublattice magnetisation (with respect to three-sublattice Néel ordering, as for the triangular lattice antiferromagnet) was considered. It was seen that our results were highly converged over a large range of \( J_2 \). Our results were consistent with the assertion that this model demonstrates no Néel ordering at \( J_2 = 0 \). All results were determined using the parallelised approach and with a single processor, except for a single result for the ground-state energy at \( J_2 = 0 \) which contained 10707 fundamental configurations and which was only able to be carried out "in parallel." Our best estimate for the ground-state energy per spin of the spin-half Kagomé lattice antiferromagnet with nearest-neighbour terms only \( (J_2 = 0) \) was \( E_g/N = -0.43104 \).

The increasing accuracy of the high-order CCM technique and its ability to be applied to even strongly frustrated systems (such as the model considered here) are strong advantages. However, there are many possible future extensions of high-order CCM which would make a parallel implementation even more useful. The CCM has been used previously [20] to determine the excitation energies of the XXZ model on one-, two-, and three-dimensional lattices with great accuracy using "localised" approximation schemes. We note that it is, in principle, straightforward to extend these treatments in order to determine the excitation spectra of even highly frustrated spin systems with equal accuracy and for lattices of complex crystallographic symmetries. Indeed, the use of existing codes would make this process simpler.

Such determination of the excitation spectra of quantum spin systems using high-order CCM techniques might be made even more useful by the utilisation of "non-Néel" model states. The model considered here uses just such a "Néel" model state and typically we perform some kind of notational rotation of the spin axis such that all of the spin "point downwards". This is then the starting point for our calculations. We note that non-Néel model states (such as the dimer solid state) have already been used at low orders of approximation to consider spin systems which demonstrate novel ordering. It would again
be a straightforward process to develop our high-order CCM approach for the “localised”
approximation schemes in order to consider such non-Néel model states.

Another extension of the current calculations is to bosonic or fermionic systems. Indeed,
the formalism has already been developed for lattice bosonic systems, which we note
have much in common (from a “CCM notational” point-of-view) which large quantum spin
number, \( s \), spin systems previously considered using high-order CCM techniques [30].

The above calculations were presented for the infinite-lattice case, \( N \to \infty \). We note that
it is also possible to consider the case where \( N \) is finite, and, again, high-order techniques
would be invaluable here.

The application of the CCM to quantum spin systems at non-zero temperature might also
be accomplished in future. Indeed, the application of the CCM at both zero- and non-zero
temperatures might help to explain the subtle interplay of quantum and thermal fluctuations
in driving phase transitions over a wide range of physical parameters.

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