Coherent Approaches to Fluctuations

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THE COUPLED CLUSTER METHOD AS A COHERENT AB INITIO APPROACH TO QUANTUM FLUCTUATIONS: APPLICATIONS TO PHASE TRANSITIONS IN ANISOTROPIC ANTIFERROMAGNETS

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ABSTRACT

The coupled cluster method (CCM) has long been recognized as providing one of the most powerful ab initio formulations of quantum many-body theory available for studying the properties of a wide variety of physical systems. By specific application to anisotropic spin-half antiferromagnets on square and triangular lattices, we show how the method is now also capable of providing a coherent approach to quantum phase transitions and the study of the criticality properties associated with the quantum order. The CCM is seen to be equally capable of dealing with (non-frustrated) bipartite and frustrated systems.

1. Introduction

There are now many physical systems characterized by novel ground states which display quantum order in some regions of the relevant parameter space, delimited by critical values marking the corresponding quantum phase transitions. The critical phenomena of the quantum systems often differ profoundly from any classical counterparts, where such exist, and the subtle correlated states usually cannot sensibly be viewed within the traditional language of, for example, Landau's theory of Fermi liquids or other comparable phenomenological approaches. Examples of areas of physics which are covered by such general remarks on quantum order are heavy fermions, the fractional quantum Hall effect, high-temperature superconductors, new quantum states in the condensed phases of helium, and various phases of antiferromagnetic materials.

The standard many-body techniques (e.g., perturbation theory, variational calculations) which have been developed for conventional systems typically fail completely for systems characterized by novel quantum order. One of the key challenges for modern quantum many-body theory will now be to develop and exploit microscopic techniques capable of handling both these novel and the more traditional systems. One of the prime aims of our own recent work has been to show that at least one such modern technique, namely the coupled cluster method (CCM), is already capable of bridging this divide. The CCM is nowadays recognized as providing one of the most powerful, most widely applicable, and most accurate at attainable levels of implementation of all ab initio microscopic techniques of quantum many-body/field theory. In recent years it has successfully been applied to various lattice Hamiltonian
systems,\textsuperscript{4–7} producing results which are the best or among the best available, in terms of accuracy and power. What we now further demonstrate, by explicit applications to various spin-lattice models on both bipartite (unfrustrated) and frustrated lattices, is how the CCM also enables us to study the quantum phase transitions of these systems in a very systematic and unbiased manner.\textsuperscript{5,8,9}

2. Overview of the CCM Formalism

Since detailed descriptions of the basic CCM formalism\textsuperscript{1} and its applications to spin-lattice problems\textsuperscript{6} are available in the literature, we only highlight the essential ingredients here. In the so-called single-reference version of the CCM considered here we first require the choice of a single model state $|\Phi\rangle$, in terms of which a quantitative and systematic description of the multi-spin correlations (or fluctuations) can be given. This model state $|\Phi\rangle$ must have the property that it is a cyclic vector with respect to which two Abelian subalgebras of multi-configurational creation operators $\{C^+_I\}$ and their Hermitian-adjoint destruction operators $\{C^-_I\}$ can be defined. The exponential parametrization of the exact ground-state ket wave function $|\psi\rangle$, which lies at the heart of the CCM, is now written as

$$|\psi\rangle = e^S|\Phi\rangle ; \quad S = \sum_{I \neq 0} s_I C^+_I ,$$

where the cluster correlation operator $S$ is decomposed wholly in terms of mutually commuting creation operators $\{C^+_I; I \neq 0\}$ (where $C^+_0 \equiv 1$), for distinct multi-spin excitations with respect to the state $|\Phi\rangle$. Here $\{s_I\}$ denote the corresponding correlation coefficients which we wish to determine. The exponentiated form of the ground-state parametrization ensures both the proper counting of the independent fluctuations of excited multi-spin groups with respect to $|\Phi\rangle$ present in the exact ground state $|\psi\rangle$, and the exact incorporation of the Goldstone linked-cluster theorem. The latter, in turn, guarantees the size-extensivity of all relevant physical quantities.

By taking the inner product of the Schrödinger equation in the form $e^{-S}He^S|\Phi\rangle = E_g|\Phi\rangle$, where $H$ is the Hamiltonian, with both (i) the reference state itself, and (ii) the complete set of multi-spin excitation states, $\{C^+_I|\Phi\rangle; I \neq 0\}$, we obtain respectively (i) the ground-state energy,

$$E_g = E_g[s_I] = \langle \Phi | e^{-S}He^S | \Phi \rangle ,$$

where we have used the intermediate normalization implied by Eq. (1), $\langle \Phi | \psi \rangle = \langle \Phi | \Phi \rangle \equiv 1$; and (ii) the coupled set of nonlinear equations,

$$\langle \Phi | C^-_I e^{-S}He^S | \Phi \rangle = 0 ; \quad I \neq 0 ,$$

from which the correlation coefficients $\{s_I\}$ may be determined. It is important to note that the otherwise infinite nested-commutator expansion

$$e^{-S}He^S = H + [H, S] + \frac{1}{2!}[[H, S], S] + \cdots ,$$

(4)
will always terminate at a finite order when $H$ is a finite-order multinomial of the elementary single-spin operators, due to the fact that the correlation operator $S$ is constructed from the mutually commuting set $\{C_I^{-}\}$.

Calculation of quantities other than $E_g$ also requires the ground bra state. It is crucial to the CCM that corresponding bra and ket states are parametrized independently, and that they are thus not explicitly constructed to be Hermitian-adjoint to each other. Indeed, the Hermiticity property may be lost when approximations are implemented. In the so-called normal version of the CCM employed here, the bra ground-state wave function $\langle \tilde{\Psi} I \rangle$ analogous to $|\Psi\rangle$ and thus obeying the Schrödinger equation, $\langle \tilde{\Psi} | H = \langle \tilde{\Psi} | E_g$, is parametrized as

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

Equations (1) and (5) imply the normalization $\langle \tilde{\Psi} | \tilde{\Psi} I \rangle = 1$. One may readily show from the bra- and ket-state Schrödinger equations that the coefficients $\{s_I\}$ are determined from the coupled set of linear equations,

$$\langle \tilde{\Phi} | \hat{S} e^{-S}[H, C_I^+] e^S | \tilde{\Phi} I \rangle = 0 ; \quad I \neq 0 . \quad (6)$$

Arbitrary ground-state expectation values may be calculated as

$$\hat{A} \equiv \langle \tilde{\Psi} | A | \Psi \rangle = \langle \tilde{\Phi} | \hat{S} e^{-S} A e^S | \tilde{\Phi} I \rangle = \hat{A}[s_I, \hat{s}_I] . \quad (7)$$

3. Application of the CCM to Spin-Lattice Models

We turn now to the application of the CCM outlined above to the specific spin-$1/2$ models considered here on the two-dimensional square and triangular lattices.

For the square lattice we consider the anisotropic Heisenberg (or XXZ) model, whose Hamiltonian is

$$H_1 = -\frac{1}{4} \sum_{\langle ij \rangle} \left\{ \frac{1}{2} \left( \sigma_i^+ \sigma_j^+ + \sigma_i^- \sigma_j^- \right) + \Delta \sigma_i^z \sigma_j^z \right\} , \quad (8)$$

where the summation runs over all nearest-neighbour bonds, and $\Delta$ is the anisotropy parameter. We note that Eq. (8) is expressed in local Néel coordinates, in which we have performed a spin rotation on one of the two equivalent sublattices of this bipartite lattice, namely the up-down transformation in which the Pauli matrices on the rotated sublattice undergo the (canonical) transformation: $\sigma^x \rightarrow -\sigma^x$, $\sigma^y \rightarrow \sigma^y$, $\sigma^z \rightarrow -\sigma^z$. Here $\sigma^\pm(\equiv \sigma^x \pm i \sigma^y)$ are the corresponding single-site creation and destruction operators in the rotated spin coordinates. The Hamiltonian of Eq. (8) becomes that of the usual Ising antiferromagnet at $\Delta \rightarrow \infty$, with a Néel-ordered ground state which is simply the fully aligned ferromagnetic configuration in the
local (rotated) spin coordinates. At $\Delta = 1$ we regain the Heisenberg antiferromagnet. We thus choose the Néel state as the reference state,

$$|\Phi\rangle = \bigotimes_{i=1}^{N} |\downarrow\rangle_i$$ \quad \text{in local quantization axes}, \quad \text{(9)}$$

where $N$ is the number of lattice sites, and we always work directly in the limit $N \to \infty$. For the triangular lattice we choose the anisotropic Hamiltonian,

$$H_2 = \sum_{\langle i\rightarrow j \rangle} \left\{ \frac{-1}{2} \sigma^z_i \sigma^z_j + \frac{\sqrt{3} \lambda}{4} \left( \sigma^x_i \sigma^x_j + \sigma^y_i \sigma^y_j - \sigma^z_i \sigma^z_j - \sigma^z_i \sigma^z_j \right) \right. \right.$$

$$\left. + \frac{\lambda}{8} \left( \sigma^z_i \sigma^z_j + \sigma^z_i \sigma^z_j \right) - \frac{3 \lambda}{8} \left( \sigma^z_i \sigma^z_j + \sigma^z_i \sigma^z_j \right) \right\}, \quad \text{(10)}$$

where the Pauli matrices are again defined with respect to local quantization axes corresponding to the classical Ising ground state at $\lambda = 0$. This configuration, expressed in terms of global axes, has three sublattices, with spins on sublattice $A$ pointing along the negative $z$ direction, and with spins on sublattices $B$ and $C$ being rotated respectively through $-120^\circ$ and $+120^\circ$ away from the negative $z$-axis in the $xz$-plane. It is easy to show that at $\Delta = 1$ $H_2$ describes the conventional Heisenberg antiferromagnet. The model state $|\Phi\rangle$ is again chosen to be the fully aligned ferromagnetic configuration of Eq. (9) in the local spin coordinates already described. We note that the summation in Eq. (10) again runs over all nearest-neighbour bonds as in Eq. (8), but now also with directionality indicated by $i \rightarrow j$, which goes from $A$ to $B$, $B$ to $C$, and $C$ to $A$.

For both $H_1$ and $H_2$, with the choice of $|\Phi\rangle$ described by Eq. (9), the CCM operators $\{C^+_i\}$ now simply become products of single-spin raising operators $\{\sigma^+_i\}$. In principle these products should run over all such distinct multi-spin configurations allowed by the symmetries of the lattice and the Hamiltonian. In the latter case, for example, the Hamiltonian $H_1$ on the square lattice commutes with the total $z$-component of spin in global coordinates, and hence the configurations $\{I\}$ run only over those in which an equal number of sites are chosen on the two sublattices.

In practice we clearly need an approximation scheme to truncate the expansions of $\hat{S}$ and $\hat{S}$ in Eqs. (1) and (5) to some finite or infinite subset of the full set of multi-spin configurations $\{I\}$. The implementation of the CCM thus amounts to the two distinct problems of enumerating the set of independent configurations $\{I\}$ retained, and evaluating the corresponding sets of (finite) equations (3) and (6). For high-order approximations the use of computer algebra is particularly apposite, and a separate article in this volume gives further practical details of the implementation. Once the resulting equations are then solved for the retained coefficients $\{s_r, \tilde{s}_r\}$, Eq. (7) may be used to calculate arbitrary ground-state quantities in the corresponding approximation.
The three most commonly used truncation methods are: (i) the SUBn scheme, in which all correlations involving only n or fewer spins are retained, however far separated on the lattice; (ii) the simpler SUBn-m subapproximation, where only SUBn correlations spanning a range of no more than m adjacent lattice sites are retained; and (iii) the systematic local LSUBm scheme, which includes all multi-spin correlations over all possible distinct locales on the lattice defined by m or fewer contiguous lattice sites.

4. Results for the Square Lattice

At the Heisenberg point ($\Delta = 1$) on the square lattice, the SUB2 scheme gives a ground-state energy per spin, $E_g/N \approx -0.6508$, compared with the corresponding classical result of $-0.5$ and the results of $-0.6580$ from Anderson's lowest-order spin wave theory (SWT),$^{11}$ and approximately $-0.6693$ from quantum Monte Carlo (QMC) simulations.$^{12}$ The corresponding SUB2 result for the Heisenberg ($\Delta = 1$) sublattice magnetization $M_z$ is about 0.83, corresponding to a classical value of 1, and compared with an SWT value of 0.606, and with the best of the QMC results which vary between 0.68 ± 0.02 and 0.62 ± 0.04.

More interestingly, the SUB2 scheme yields a terminating point, $\Delta_c \approx 0.798$, below which no physical solution can be found. Although the CCM based on the Néel reference state 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 Néel ordering, we have clearly demonstrated$^8$ that this terminating point corresponds to (an approximation to) a true critical point of a phase transition. The nature of this critical point can be elucidated by studying the singular behaviour of various quantities. We find, for example, in SUB2 approximation,

$$M^z \xrightarrow{\Delta \to \Delta_c^+} M_c^z + k(\Delta - \Delta_c)^{\frac{1}{2}}$$  \hspace{1cm} (11)

$$\frac{\partial^2 (E_g/N)}{\partial \Delta^2} \xrightarrow{\Delta \to \Delta_c^+} D(\Delta - \Delta_c)^{-\frac{1}{2}}$$  \hspace{1cm} (12)

where $M_c^z$, $k$, and $D$ are constants. These critical exponents agree with those from SWT. This is, perhaps, not surprising since both the CCM SUB2 scheme and SWT include only two-body correlations.

In order to go beyond the essentially mean-field-like SUB2 approximation, we have also performed LSUBm calculations for $m = 2, 4, 6$. For the Hamiltonian $H_1$ on the square lattice, the number of independent configurations $\{I\}$ retained are respectively 1, 7, and 72. At the isotropic point ($\Delta = 1$), for example, we obtain in LSUB6 approximation $E_g/N \approx -0.6670$ and $M^z \approx 0.728$. We find heuristically that, for both the 1D chain and the 2D square lattice, our LSUBm results for $E_g/N$ and $M^z$ approach the asymptotic ($m \to \infty$) limits as $m^{-2}$ and $m^{-1}$, respectively. Our best extrapolated values for the square lattice at the Heisenberg point ($\Delta = 1$), based on
LSUBm results with \( m = 2, 4, 6 \) give \( E_g/N \approx -0.6691 \pm 0.0003 \) and \( M^z \approx 0.68 \pm 0.01 \), both in excellent agreement with the best available QMC results.

Interestingly, the LSUBm calculations with \( m > 2 \) also show corresponding critical points \( \Delta^m_c \); \( \Delta^4_c \approx 0.577, \Delta^6_c \approx 0.766 \). The corresponding SUB2-\( m \) results appear to approach the full SUB2 value for \( \Delta_c \) as \( m^{-2} \), and the same rule fitted to the LSUBm results yields a corresponding prediction for the extrapolated critical point at \( \Delta_c \approx \Delta^\infty_c \approx 0.92 \pm 0.01 \). This is clearly smaller than the value of 1 from SWT, and it will be of great interest to perform higher-order LSUBm calculations with \( m > 6 \) in order to confirm this difference.

The critical index for the singular term in \( E_g/N \) as \( \Delta \to \Delta^\tau_c \) can also be obtained from the LSUBm results. A particularly interesting possibility in this context is to employ a variant of the coherent anomaly method (CAM) of Suzuki. Thus, by direct evaluation of the anisotropy susceptibility, \( \chi_\alpha \equiv -\partial^2(E_g/N)/\partial \Delta^2 \), we find in LSUBm approximation, for \( m \geq 2 \),

\[
\chi^m_\alpha(\Delta) \to \chi^m_\alpha(\Delta - \Delta^m_c)^{-\alpha_0} ; \quad \Delta \to \Delta^m_c ,
\]

where \( \alpha_0 \approx 1.50 \). This behaviour appears to be identical to that of the SUB2-\( n \) subapproximations with finite \( n \), for which \( \alpha_0 = 3/2 \), whereas we know that in the full SUB2 approximation \( \alpha_0 = 1/2 \). However, just as for the SUB2-\( m \) series, the LSUBm data fit well with a pre-factor \( \chi^m_\alpha \) of the so-called coherent anomaly form,

\[
\chi^m_\alpha \to K (\Delta^\infty_c - \Delta^m_c)^\nu ; \quad \Delta \to \Delta^\infty_c ,
\]

where \( K \) is a constant. Thus, as explained by Suzuki, one may prove

\[
\chi_\alpha(\Delta) \sim (\Delta - \Delta^\infty_c)^{-\alpha_0 + \nu} ; \quad \Delta \to \Delta^\infty_c .
\]

A CAM analysis along these lines of the LSUBm results for \( m = 4, 6 \) gives \( \nu \approx 1.25 \pm 0.2 \), and hence a singular term in \( E_g/N \) near \( \Delta_c \) with a critical exponent \( 2 - \alpha_0 + \nu \approx 1.75 \pm 0.2 \), compared to the corresponding value of 3/2 from the mean-field-like CCM SUB2 and SWT approximations. Clearly, it will be of great interest to obtain LSUBm results for \( m > 6 \) in order to sharpen our results.

5. Results for the triangular lattice

At the isotropic Heisenberg point (\( \lambda = 1 \)) we find in SUB2 approximation, \( E_g/N \approx -2.015 \), compared with the classical value of -1.5 and a value of -2.21 \( \pm 0.01 \) obtained from a series expansion. Clearly, the full SUB2 approximation for the triangular lattice captures fewer quantum corrections to the classical energy than for the square lattice, since three-spin correlations play an important role for the former, whereas they are not present for the latter. As for the square lattice, we also find a SUB2 terminating point for \( H_2 \), namely at \( \lambda_c \approx 1.33525 \). We also find that in SUB2 approximation the power-law singularities for the triangular lattice model are exactly
as in Eqs. (11) and (12). This provides strong evidence that both transitions belong to the same universality class, and also strongly supports the existence of nonzero three-sublattice ordering in the frustrated triangular antiferromagnet. This is consistent with the result for the sublattice magnetization computed within the SUB2 approximation, which we find to be about 85% of its classical value at the isotropic ($\lambda = 1$) Heisenberg point. Further results, including LSUB$m$ calculations, will be reported elsewhere.\textsuperscript{9,10}

Finally, we comment on the structure of the ground-state ket wave functions obtained in the SUB2 approximation. For the Hamiltonian $H_1$ on the bipartite square lattice the Marshall sign theorem\textsuperscript{15} guarantees the positivity of all multi-spin correlation coefficients $\{s_J\}$, when the spin-raising operators $\{\sigma_i^+\}$ are expressed in terms of the local spin quantization axes used here. The SUB2 approximation for the square lattice is observed to preserve this exact theorem. We note also that it is the existence of the Marshall sign theorem which enables QMC simulations for the spin-$\frac{1}{2}$ square lattice models to be performed. By contrast, no such theorem exists for the frustrated triangular lattice, and the associated "minus sign problem" has so far prevented QMC simulations for the Hamiltonian $H_2$. However, by contrast to the square lattice case, the two-spin CCM correlation coefficients in the SUB2 approximation are found to exhibit an intriguing oscillatory behaviour in their signs as a function of separation distance on the triangular lattice. It is our hope that this SUB2 information might represent a sufficiently accurate description of the nodal structure of the exact wave function as to permit a successful implementation of a fixed-node Monte Carlo approach for this system for the first time.

6. Conclusions

We have shown how the CCM can be successfully applied to spin-$\frac{1}{2}$ spin-lattice problems on both bipartite and frustrated lattices, in order to obtain results for the ground-state properties which are competitive with the best available alternative calculations and to study quantitatively the critical properties of the associated phase transitions. The SUB2 calculations presented here share much in common with those of SWT. Thus, both methods use a Gaussian parametrization of the ground-state ket wave function with an infinite number of parameters. By contrast with SWT, however, the CCM SUB2 approximation provides an unbiased estimate of the location of the critical point, whereas in SWT its existence can only be ascertained qualitatively.

Furthermore, the LSUB$m$ results, which consider localized independent multi-spin correlations over any $m$ adjacent lattice sites, also provide a coherent approach to the accurate incorporation of quantum fluctuations. In particular, a variant of Suzuki's CAM approach permits a quantitative evaluation of the critical exponents.

Two particular advantages of the CCM are: (i) that we always deal from the outset with infinite lattices, and hence never have to concern ourselves with finite-size corrections; and (ii) the fact that we have closed sets of analytic equations for the
cluster correlation coefficients \( \{s_I, \tilde{s}_I\} \) enables us to calculate directly all finite-order derivatives of any ground-state quantity with respect to the parameter driving the transition (i.e., the anisotropy parameters \( \Delta \) and \( \lambda \) here). On the joint basis of the results presented here and the very general nature of the CCM, we believe that the method will find wide applicability to other systems which exhibit quantum order and quantum phase transitions.

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8. References

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