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Many-body correlations in quantum antiferromagnets: A microscopic coupled-cluster approach

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The coupled-cluster method of many-body theory is applied to anisotropic quantum antiferromagnets in one and two dimensions. It is found to give good results for ground-state and excited-state energies and the staggered magnetization. It also gives a qualitatively correct description of the entire one-dimensional Heisenberg-Ising phase and the phase change in one dimension as the anisotropy decreases.

The coupled-cluster method[1-5] (CCM) of quantum many-body theory has been outstandingly successful in recent years in many areas. Its main advantages are its wide applicability, its automatic avoidance of unphysical divergences in the thermodynamic limit, and its systematic hierarchies of approximation schemes. The CCM can be used to calculate ground-state and excited-state energies, and also such other physical quantities as correlation functions and density matrices.

A recent paper by Roger and Hetherington[6] has pioneered its application to quantum spin lattices. In particular they obtained good results for the ground-state energies of spin-$\frac{1}{2}$ Heisenberg lattices in one dimension (1D) and 2D. They then used the method to investigate the ground state of solid ^{3}He. In this paper we wish to show how the CCM can be applied to quantum spin systems with a range of parameters. Our main result is that the CCM may be good enough, even at low levels of truncation, to predict the existence of phase transitions in these models at $T=0$ as the parameters are varied. Furthermore, the qualitative behavior of the staggered magnetization and of the elementary excitations is correctly described over an entire phase and also at the transition point.

We shall present results for spin-$\frac{1}{2}$ lattices with a nearest-neighbor antiferromagnetic XXZ interaction in both 1D and 2D (square). For 1D, exact results for the ground and excited states are available[7] from the Bethe *ansatz* although this does not readily give information about the correlation functions. Nevertheless, recent developments[8] using the quantum inverse scattering method have enabled information about correlation functions to be obtained from the general algebraic structure of the Bethe *ansatz* solutions.

The Hamiltonian is

$$\mathcal{H}=\tfrac{1}{2}\sum_i\sum_\rho(\Delta s_i^z s_{i+\rho}^z+s_i^x s_{i+\rho}^x+s_i^y s_{i+\rho}^y)\,,$$

where the sum over i is over all N sites of the lattice and the sum over ρ is over all ν nearest neighbors. The total z component of spin $s_T^z=\sum_i s_i^z$ is a good quantum number. We shall assume periodic boundary conditions, and work with Pauli spin operators σ_i^α, defined in the usual way: $\sigma_i^\alpha=2s_i^\alpha$, $\alpha=x,y,z$.

The starting point of the CCM is the choice of an uncorrelated model state $|\phi\rangle$ which we shall take as the usual two-sublattice Néel state. It is convenient to perform a notional rotation of 180° on one sublattice[6] so that the model state has all spins pointing down. Defining raising and lowering operators $\sigma_i^\pm=\frac{1}{2}(\sigma_i^x\pm i\sigma_i^y)$ for i on the "down" sublattice and $\sigma_i^\pm=\frac{1}{2}(-\sigma_i^x\pm i\sigma_i^y)$ for i on the "up" sublattice, then $\sigma_i^-|\phi\rangle=0$ for all i, while $\sigma_i^+|\phi\rangle$ is a state with the ith spin reversed with respect to the model state. The Hamiltonian becomes

$$\mathcal{H}=-\sum_i\sum_\rho[(\Delta/8)\sigma_i^z\sigma_{i+\rho}^z+\tfrac{1}{4}(\sigma_i^+\sigma_{i+\rho}^++\sigma_i^-\sigma_{i+\rho}^-)]\,.$$

The exact ground state has the CCM form $|\psi\rangle=\exp(S)|\phi\rangle$, where the operator S is constructed from products of creation operators only with respect to $|\phi\rangle$; in this case from $\{\sigma_i^+\}$ only. We thus put $S=\sum_{n=1}^N S_n$, where S_n creates a linear combination of configurations with n spins flipped with respect to the Néel state. As usual it is necessary to consider various approximation schemes for S. Perhaps the most straightforward of these is the well-known SUBn scheme, in which only the configurations are retained with at most n spins flipped with respect to the Néel state. The most interesting results have been obtained using the SUB2 approximation scheme in which $S\rightarrow S_2=\frac{1}{2}\sum_i\sum_r b_r\sigma_i^+\sigma_{i+r}^+$. Since the true ground state has $s_T^z=0$ the two spin flips must take place on opposite sublattices, so we require r to be a vector connecting sites on opposite sublattices. We assume the $\{b_r\}$ have the corresponding lattice symmetry (e.g., $b_{-r}=b_r$ in 1D) and define $b_1=b_\rho$ for all ρ. Note that a SUB1 scheme is not possible here as a single spin flip takes the system out of the $s_T^z=0$ subspace. From the Schrödinger equation $\mathcal{H}|\psi\rangle=E_g|\psi\rangle$ we obtain the equation $E_g=-(N\nu/8)(\Delta+2b_1)$, while a set of coupled equations for the $\{b_r\}$ is obtained from the condition $\langle r|e^{-S}\mathcal{H}e^S|\phi\rangle=0$, where $\langle r|=\sum_i\langle\phi|\sigma_i^-\sigma_{i+r}^-$. These equations have the form

$$\nu K b_r-K_1\sum_\rho\delta_{r\rho}-\tfrac{1}{2}\sum_s b_s\sum_\rho b_{r+\rho+s}=0\,,\qquad(1)$$

where $K=\Delta+2b_1$ and $K_1=\frac{1}{2}+\Delta b_1+b_1^2$.

Subapproximations within SUB2 involve truncation of this system of coupled nonlinear equations, so that the SUB2-n scheme has $b_r\equiv0$ for relative lattice vectors r of length not less than those between nth nearest neighbors. The simplest of these, SUB2-2, is of some interest, giving in 1D the equation $3b_1^2+2\Delta b_1-1=0$ and hence $E_g/N=-[\Delta+2(\Delta^2+3)^{1/2}]/12$. At $\Delta=1$ this gives E_g/N

$=-5/12=-0.41667$, compared to the exact result -0.44315. It is interesting to note that our SUB2-2 wave function has the same form as that employed in a variational calculation of Sachdev[9] at $\Delta=1$. He minimizes the expectation value of $\mathcal{H}$ with respect to b_1 and obtains $E_g/N\simeq -0.428$.

The full SUB2 equations (1) can be solved by Fourier transform. Henceforth we shall consider only the 1D case with $N\rightarrow\infty$, except where indicated. The result is, for any integer m,

$$b_{2m-1}=\frac{K}{2\pi}\int_{-\pi}^{\pi}dx[1-f(x;k^2)]\frac{\cos[(m-\frac{1}{2})x]}{\cos(\frac{1}{2}x)}, \quad (2)$$

where $k^2=2K_1/K^2$ and

$$f(x;k^2)=[1-k^2\cos^2(\tfrac{1}{2}x)]^{1/2}.$$

Putting $m=1$ in Eq. (2) leads to a self-consistent equation for b_1, which is easily solved numerically. In this way we obtain the value $E_g/N=-0.41862$ at $\Delta=1$. Both the full SUB2 and the SUB2-2 results have the correct asymptotic form for large Δ which is $E_g/N\rightarrow -\frac{1}{4}(\Delta+\Delta^{-1})$.

The most interesting feature of the full SUB2 results, however, is that a real solution for b_1 only exists provided $k\leq 1$ which requires $\Delta\geq\Delta_c$, where $\Delta_c\simeq 0.37275$. In Fig. 1 we show the values of E_g/N for the SUB2-2 and full SUB2 approximations as well as the exact result as a function of Δ. The absence of a solution for $\Delta<\Delta_c$ signals a possible phase transition in the physical system, even though the value of Δ_c is not very close to the exact critical value 1. Clearly it is desirable to have additional evidence that it is not merely a mathematical breakdown in the SUB2 approximation.

To investigate the Δ_c point further we have calculated the staggered magnetization $M=|\langle\sigma_i^z\rangle|$ and the correlation function $G_n=\langle\sigma_i^z\sigma_{i+n}^z\rangle$ as functions of Δ. In order to calculate any expectation value in the CCM it is necessary to construct a bra state corresponding to the ket ground state $|\psi\rangle$. This has the standard form[4] $\langle\tilde{\psi}|=\langle\phi|\tilde{S}\times\exp(-S)$ where the operator $\tilde{S}$ is composed entirely of destruction operators, i.e., of $\{\sigma_i^-\}$. Just as in constructing S various approximations are possible, but the obvious choice corresponding to the full SUB2 approximation is

$$\tilde{S}\rightarrow\tilde{S}_2=1+\tfrac{1}{2}\sum_i\sum_r\tilde{b}_r\sigma_i^-\sigma_{i+r}^-$$

where the sums over i and r are the same as for S_2. A linear set of equations for $\{\tilde{b}_r\}$ is obtained from the Schrödinger equation $\langle\tilde{\psi}|\mathcal{H}=\langle\tilde{\psi}|E_g$ of the form

$$\nu K\tilde{b}_r-K_2\sum_\rho\delta_{r\rho}-\sum_s b_s\sum_\rho\tilde{b}_{r+\rho+s}=0, \quad (3)$$

where $K_2=\frac{1}{2}+K\tilde{b}_1-2\sum_r\tilde{b}_r b_r$. Equation (3) is valid for arbitrary dimensions but again we consider only 1D in detail.

The subapproximation SUB2-2 in which only b_1 and $\tilde{b}_1$ are retained gives $\tilde{b}_1=\frac{1}{2}(\Delta^2+3)^{-1/2}$. The full set of coupled equations is again solved by Fourier transform to give

$$\tilde{b}_{2m-1}=\frac{D}{4K}\frac{1}{2\pi}\int_{-\pi}^{\pi}dx\frac{\cos(\frac{1}{2}x)\cos[(m-\frac{1}{2})x]}{f(x;k^2)}, \quad (4)$$

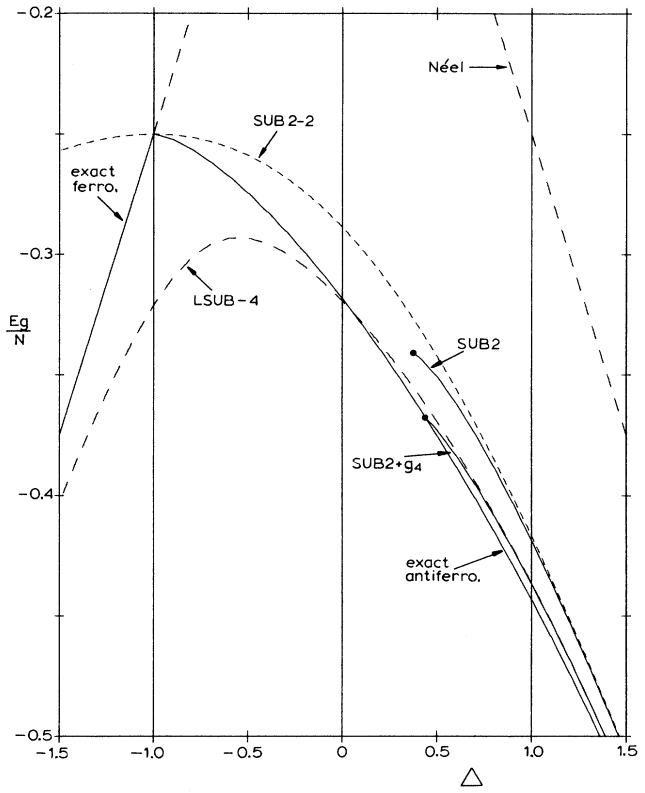

FIG. 1. Ground-state energy per spin for the 1D XXZ model with $s=\frac{1}{2}$ as a function of Δ, showing the exact result of Ref. 7, and results for the full SUB2, SUB2+g_4, SUB2-2, and LSUB-4 approximation schemes. The terminating points of the SUB2 and SUB2+g_4 schemes are clearly indicated. The exact result becomes critical at $\Delta=1$, although this is not obvious from the energy plot.

where

$$D^{-1}=\frac{1}{2\pi}\int_{-\pi}^{\pi}dx\,f^{-1}(x;k^2)f^2(x;\tfrac{1}{2})-\tfrac{1}{2}.$$

The leading asymptotic behavior of b_r and $\tilde{b}_r$, obtained from Eqs. (2) and (4), is

$$b_{2m-1}\underset{m\rightarrow\infty}{\longrightarrow}\begin{cases}O(\xi^{-2m})\\ \gamma m^{-2}\end{cases};\quad \tilde{b}_{2m-1}\underset{m\rightarrow\infty}{\longrightarrow}\begin{cases}O(\lambda^{-2m}), & \Delta>\Delta_c\\ \Gamma, & \Delta=\Delta_c\end{cases}$$

where ξ and λ are functions of Δ only, while γ and Γ are constants.

The SUB2 values of the staggered magnetization and the correlation function are given by

$$M=1-2\alpha;\quad G_n=1+4\tilde{b}_n b_n-4\alpha(1-\delta_{n0}), \quad (5)$$

where $\alpha=\sum_r\tilde{b}_r b_r$. Using Eqs. (2) and (4), we find that $M\rightarrow 0$ as $\Delta\rightarrow\Delta_c$, as shown in Fig. 2. The exact result of Baxter[10] is also shown. Clearly the essential singularity at $M=0$ is not correctly given by the SUB2 approximation. Nevertheless, the critical region is very narrow and over most of the range our results have the correct general form. In particular, the exact asymptotic behavior, $M\rightarrow 1-\Delta^{-2}$ as $\Delta\rightarrow\infty$, is reproduced.

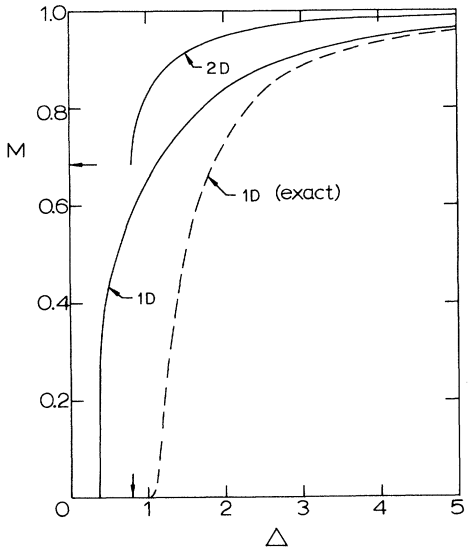

FIG. 2. Staggered magnetization M for the 1D and 2D XXZ models with $s=\frac{1}{2}$, as a function of Δ. The solid curves are our results in the SUB2 approximation, and the dashed curve is from Ref. 10. The values M_c and Δ_c in the 2D case are indicated by arrows.

For n even and nonzero, G_n is independent of n, which is an unphysical consequence of the approximation. For n odd, we observe the characteristic changeover in the long-range decay from exponential (for $\Delta>\Delta_c$) to algebraic (at $\Delta=\Delta_c$), although the exact critical exponent[8] is not obtained. It should also be noted that CCM approximations are intrinsically non-Hermitian. This manifests itself here in the fact that the asymptotic value for G_n as $n\rightarrow\infty$ is *not* identically equal to M^2, as can be seen from Eq. (5).

The behavior of both M and G_n near Δ_c is strongly suggestive of a phase transition at this point. In order to obtain a phase transition it is essential that the long-range correlations are not neglected. A necessary condition for this is that there should be terms in S of arbitrarily long range. However, from the point of view of obtaining more accurate numerical values for the ground-state energy at any particular value of Δ, it is important to include other short-range terms in S as these can be large.

Roger and Hetherington showed that at $\Delta=1$ a more accurate value for E_g can be obtained by including one term from SUB4, namely, in 1D

$$S_4\rightarrow S_4^{(1)}=\sum_i g_4\sigma_i^+\sigma_{i+1}^+\sigma_{i+2}^+\sigma_{i+3}^+ .$$

Clearly this involves a cluster of 4 adjacent spins. We call an approximation which includes all contributions within a range of n spins the LSUB-n approximation, the L indicating a "locale." The LSUB-4 approximation thus contains the b_1 and b_3 terms of S_2 together with $S_4^{(1)}$. The LSUB-4 results for E_g/N are also shown in Fig. 1. They lie closer to the exact results than SUB2 over the whole range of Δ. In particular $E_g/N\simeq -0.4363$ at $\Delta=1$. Remarkably, they even appear to give reasonable results in the ferromagnetic regime. It might be expected that an approximation scheme which has long-range contributions but with extra short-range contributions as well could continue to show a phase transition and also give better numerical accuracy. We have calculated results for a scheme which we call SUB2+g_4 in which *all* the SUB2 terms are kept as well as the $S_4^{(1)}$ given earlier. In this case analytic expressions can no longer be obtained as a function of Δ. However as can be seen from Fig. 1 the numerical results are encouraging. The phase transition now occurs at $\Delta_c\simeq 0.4355$, while the energy values are appreciably closer to the exact values than for SUB2.

A very similar analysis is possible for the 2D square lattice, where very few exact results are known. For example, Ising-like behavior has only been rigorously proved[11] for $\Delta>1.78$. In this case the possible approximation schemes are more complicated. We have considered a number of these but the most striking results still occur for the SUB2 scheme, where we again find a terminating point. (In fact, it is straightforward to show that such a point occurs for other lattices and also in 3D.) The critical value of Δ for the 2D square lattice is $\Delta_c\simeq 0.7985$, closer to the classical value of 1 than for 1D.

However, unlike in the 1D case, the staggered magnetization, shown in Fig. 2, now approaches a *nonzero* value, $M_c\simeq 0.682$ as $\Delta\rightarrow\Delta_c$, at which point $E_g/N\simeq -0.5836$. For comparison, spin-wave (SW) theory[12] breaks down when $\Delta<1$ in *all* dimensions. At $\Delta=1$ the staggered magnetization in SW theory diverges in 1D and is given by $M_c\simeq 0.606$ in 2D. Our own SUB2 2D results at $\Delta=1$ are $E_g/N\simeq -0.6508$, and $M\simeq 0.827$. Finally, Monte Carlo calculations are also available in 2D for $\Delta=1$,[13] giving the results $E_g/N\simeq -0.6692(2)$ and $M\simeq 0.62(4)$. Our CCM results suggest a phase transition in 2D also (albeit with some different features to the 1D case), although more work is clearly needed.

As a final piece of evidence that Δ_c does correspond to a phase transition we have examined the elementary excitations as functions of Δ. Within the CCM this is done by constructing the excited-state wave functions $|\psi_e\rangle$ from the ground state by means of a linear operator X, so that $|\psi_e\rangle=X|\psi\rangle$. The excitation operator X is chosen like S to be formed solely from creation operators, so we write $X\rightarrow X_1=\sum_r x_r\sigma_r^+$ as the simplest approximation. The excitation energies are the eigenvalues of $(e^{-S}\mathcal{H}e^S-E_g)$ within the subspace spanned by states of the form $\sigma_r^+|\phi\rangle$, and the $\{x_r\}$ are the components of the corresponding eigenvectors. These excitations have $s_T^z=1$. Our result in 1D, using the SUB2 approximation for $|\psi\rangle$, is that the excitation energy for a state with wave vector q is given by $\varepsilon(q)=Kf(2q;k^2)$. This has a gap for $\Delta>\Delta_c$ but at Δ_c has the form $\varepsilon_c(q)=K_c\sin(q)$, where $K_c\simeq 1.3642$. This behavior closely parallels that of the exact excitation energies above and at the exact transition point $\Delta=1$, where $\varepsilon_c(q)=\frac{1}{2}\pi\sin(q)$.

In conclusion we believe that the CCM is potentially a very powerful tool in the study of quantum spin systems. It should be emphasized that it is an *ab initio* method which does not presuppose any knowledge of phase transitions, or any other phenomena. It cannot be expected to give very detailed descriptions of critical behavior. However, it is very encouraging that even low-level approxima-

tions are capable of qualitative predictions in these respects, as well as giving accurate numerical values for quantities such as the ground-state energy. The other important feature of the CCM is that it is capable of systematic improvement.

The CCM will be especially useful in studying systems which are not integrable such as 2D lattices and 1D systems with $s > \frac{1}{2}$. We are hopeful that relatively simple approximations for the operators S, $\tilde{S}$, and X will lead to accurate results, which will complement the existing methods such as direct diagonalization for small N, Monte Carlo for somewhat larger N,[13,14] and perturbation theory.[15] Clearly there are possibilities for using computer algebraic methods for generating and solving the coupled nonlinear equations which lie at the core of the CCM. For other spin systems different model states will be more appropriate. The method should also be useful for lattice field theories.

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