

A coupled-cluster treatment of spin- 1/2 systems with nearest- and next-nearest-neighbour interactions

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1994 J. Phys.: Condens. Matter 6 5521

(<http://iopscience.iop.org/0953-8984/6/28/024>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.147

The article was downloaded on 12/05/2010 at 18:54

Please note that [terms and conditions apply](#).

A coupled-cluster treatment of spin- $\frac{1}{2}$ systems with nearest- and next-nearest-neighbour interactions

D J J Farnell and J B Parkinson

Department of Mathematics, UMIST, PO Box 88, Manchester M60 1QD, UK

Received 7 December 1993, in final form 15 April 1994

Abstract. The coupled-cluster method of quantum many-body theory is applied to 1D and 2D spin- $\frac{1}{2}$ systems with nearest-neighbour and next-nearest-neighbour isotropic exchange. Several simple approximation schemes based on a Néel model state are investigated and are found to give satisfactory results in the antiferromagnetic regime. Results are given for the ground-state energy, the order parameter and the sublattice magnetization. We obtain evidence of a phase transition.

1. Introduction

In a recent series of papers (Bishop *et al* 1991a, b, 1992a, b) the coupled-cluster method (CCM) has been established as an effective method of treating quantum spin systems, following the initial work of Roger and Hetherington (1990a, b). Two important features of the method are firstly, that it is an *ab initio* method and yet is capable of giving evidence of zero-temperature phase changes as the parameters of the Hamiltonian are varied, and secondly, that it gives numerical results for the ground-state energy per spin and other quantities, which are good at a low order of approximation and can be systematically improved.

In this paper we apply the method to two spin- $\frac{1}{2}$ quantum spin systems with isotropic nearest- and next-nearest-neighbour exchange. In 1D the model is the so-called Majumdar–Ghosh (MG) Hamiltonian (Majumdar and Ghosh 1969a, b; see also Haldane 1982), given by

$$\mathcal{H} = J_1 \sum_l \mathbf{s}_l \cdot \mathbf{s}_{l+1} + J_2 \sum_l \mathbf{s}_l \cdot \mathbf{s}_{l+2} \quad (1.1)$$

where the sum over l is over all N atoms with periodic boundary conditions.

In 2D we consider a square lattice and the Hamiltonian is

$$\mathcal{H} = \frac{1}{2} J_1 \sum_l \sum_{\rho} \mathbf{s}_l \cdot \mathbf{s}_{l+\rho} + \frac{1}{2} J_2 \sum_l \sum_{\delta} \mathbf{s}_l \cdot \mathbf{s}_{l+\delta} \quad (1.2)$$

where the sum over l is over all N atoms with periodic boundary conditions. The sum over ρ is over the four nearest neighbours along the edges of the squares, while that over δ is over the four next-nearest neighbours along the diagonals of the squares.

We shall also use the notation $J_1 = \cos \omega$ and $J_2 = \sin \omega$, and put $\alpha = J_2/J_1 = \tan \omega$. The models become isotropic Heisenberg models when $J_2 = 0$, and become two decoupled Heisenberg models when $J_1 = 0$.

For the 1D MG system exact results are available at both these points using the Bethe *ansatz* (Bethe 1931, Orbach 1958, Yang and Yang 1966a, b), for either sign of the exchange integrals. In addition the ground state is known exactly at the point $J_2 = \frac{1}{2}J_1$ with $J_1 > 0$ ($\omega = \theta_1 = \tan^{-1}(\frac{1}{2})$, the MG point), where it has a dimerized form.

The zero-temperature phase diagram of the MG model is shown in figure 1. The three regimes are ferromagnetic ($\theta_2 - \pi < \omega < -\pi/2$), antiferromagnetic (AF) ($-\pi/2 < \omega < \theta_1$) and frustrated ($\theta_1 < \omega < \theta_2$), where $\theta_2 = \tan^{-1}(-\frac{1}{4})$, the MG point being the boundary between the AF and frustrated regimes (see Tonegawa and Harada 1987). There is also a phase change *within* the AF regime from a gapless 'spin-fluid' regime to a 'dimer' regime with a non-zero gap. The position of this phase change is given by Okamoto and Nomura (1992) as $\alpha = 0.2411$. At the present level of approximation the CCM cannot identify this more subtle phase change with any reliability.

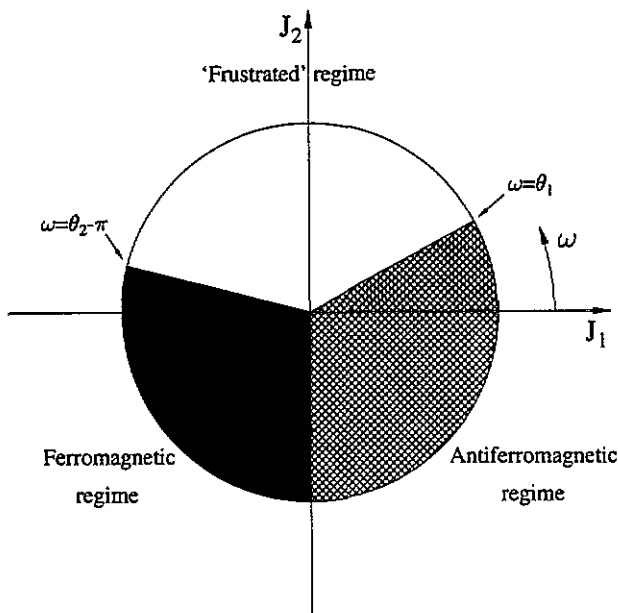


Figure 1. The zero-temperature phase diagram for the 1D model.

The *classical* ground state in the frustrated regime (which has a slightly different boundary with the AF regime, namely $\omega = \tan^{-1}(\frac{1}{4})$) is a spiral whose real-space periodicity increases monotonically from two at the AF boundary to infinity at the ferromagnetic boundary. There is evidence of similar behaviour in the quantum system from study of the correlation functions (Tonegawa and Harada 1987). In this paper we shall present results for the AF regime.

The 2D Hamiltonian has attracted a great deal of interest recently because it is believed to describe the antiferromagnetic undoped cuprate systems that are precursors of one of the principal classes of high- T_c superconductors (see Manousakis 1991 and Birgeneau 1990 for reviews of these materials). Numerical studies have been carried out by Dagotto and Moreo (1989a), reviewed by Dagotto (1991), and we shall compare our results with these in sections 3 and 4.

The zero-temperature phase diagram is believed to be similar to the 1D case, although there are very few exactly known features in 2D. The boundaries of the ferromagnetic regime are at $\omega = -\pi/2$ and $\omega = \tan^{-1}(-\frac{1}{2})$. The boundary between the AF and frustrated regimes is not known exactly but probably lies fairly close to the classical value, $\omega = \tan^{-1}(\frac{1}{2})$ (Chandra and Doucot 1988). The classical ground state in the frustrated regime consists of two interpenetrating Néel-like sublattices with arbitrary angle between the sublattice magnetizations. Quantum mechanically the arbitrary angle would obviously be correct at $J_1 = 0$ but for non-zero values a parallel or antiparallel (collinear) structure seems likely (Dagotto and Moreo 1989a, b). Other recent studies of this regime include those of Xu and Ting (1990) and Chubukov and Jolicoeur (1991). Again, however, our results apply primarily to the AF rather than the frustrated regime.

In this paper we shall frequently refer to the article by Bishop *et al* (1991b), in which a detailed description of the method is given, and this will be denoted as I.

2. Approximation schemes

We begin by selecting our model or reference state, $|\Phi\rangle$, which we shall take as the usual two-sublattice Néel state. A notional rotation of 180° on one sublattice is performed so that the model state may be referred to as having all spins pointing down. This model state is clearly particularly suitable for the AF regime. Although in principle the CCM is valid for any model state, a choice physically unrelated to the true ground state leads to results that converge too slowly to be useful. Consequently we do not expect the CCM based on this model state to work well in the frustrated regime.

We shall work with Pauli spin operators σ_i^α , related to the spin angular momentum operators in the usual way: $\sigma_i^\alpha = 2s_i^\alpha$, $\alpha = x, y, z$. Defining raising or lowering operators $\sigma_i^\pm = \frac{1}{2}(\sigma_i^x \pm i\sigma_i^y)$ for index i on the 'down' sublattice and $\sigma_j^\pm = \frac{1}{2}(-\sigma_j^x \pm i\sigma_j^y)$ for index j on the 'up' sublattice, then $\sigma_l^-|\Phi\rangle = 0$ for index l on either sublattice, while $\sigma_l^+|\Phi\rangle$ is a state with the l th spin reversed with respect to the model state (and see I for further details).

The 1D Hamiltonian (1.1) becomes

$$\mathcal{H} = -J_1 \sum_i [(\frac{1}{4})\sigma_i^z\sigma_{i+1}^z + \frac{1}{2}(\sigma_i^+\sigma_{i+1}^+ + \sigma_i^-\sigma_{i+1}^-)] + J_2 \sum_i [(\frac{1}{4})\sigma_i^z\sigma_{i+2}^z + \frac{1}{2}(\sigma_i^+\sigma_{i+2}^- + \sigma_i^-\sigma_{i+2}^+)] \quad (2.1)$$

while in 2D we obtain from (1.2)

$$\mathcal{H} = -\frac{1}{2}J_1 \sum_i \sum_\rho [(\frac{1}{4})\sigma_i^z\sigma_{i+\rho}^z + \frac{1}{2}(\sigma_i^+\sigma_{i+\rho}^+ + \sigma_i^-\sigma_{i+\rho}^-)] + \frac{1}{2}J_2 \sum_i \sum_\delta [(\frac{1}{4})\sigma_i^z\sigma_{i+\delta}^z + \frac{1}{2}(\sigma_i^+\sigma_{i+\delta}^- + \sigma_i^-\sigma_{i+\delta}^+)]. \quad (2.2)$$

In the CCM the true ground state is written

$$|\Psi\rangle = e^S|\Phi\rangle.$$

The CCM correlation operator S is constructed entirely out of creation operators with respect to the model state, i.e. out of a sum of terms containing all possible C_i^+ , where C_i^+ is a product of creation operators from $\{\sigma_i^+\}$ consistent with the conserved quantities. For the ground state we require that $s_i^z \equiv \sum_l s_l^z = 0$. Any particular approximation consists of selecting a subset of these terms.

We shall use the following approximation schemes, all of which were described in I.

(i) *Full SUB2*. In this scheme S includes all possible products of two spin-flip operators. In 1D this has the form

$$S = \frac{1}{2} \sum_i \sum_r b_r \sigma_i^+ \sigma_{i+r}^+ \quad (2.3)$$

where i runs over all N sites and r is a positive or negative odd integer with $|r| \leq N/2$. This ensures that there is one flip on each sublattice. By symmetry $b_{-r} = b_r$. In 2D i and r become two component vectors and b_r satisfies the square lattice symmetry.

(ii) *SUB2-2*. This is a subset of full SUB2 in which all b_r are set to zero except the term involving nearest neighbours, whose coefficient is denoted b_1 in both 1D and 2D.

(iii) *LSUB4*. This contains all the configurations obtained by flipping spins within a 'locale' of four adjacent spins and is defined differently in 1D and 2D.

In 1D the 'locale' is a line of four adjacent spins so LSUB4 consists of the $b_{\pm 1}$ and $b_{\pm 3}$ terms from full SUB2 together with a term involving four flips on adjacent sites, leading to

$$S = b_1 \sum_i \sigma_i^+ \sigma_{i+1}^+ + b_3 \sum_i \sigma_i^+ \sigma_{i+3}^+ + g_4 \sum_i \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ \sigma_{i+3}^+. \quad (2.4)$$

In 2D the 'locale' is a square block of four adjacent spins so LSUB4 consists of the b_1 terms of SUB2-2 together with a term in which all four adjacent spins in a single square are flipped, leading to

$$S = b_1 \sum_i (\sigma_i^+ \sigma_{i+\rho_1}^+ + \sigma_i^+ \sigma_{i+\rho_2}^+) + g_4 \sum_i \sigma_i^+ \sigma_{i+\rho_1}^+ \sigma_{i+\rho_2}^+ \sigma_{i+\rho_1+\rho_2}^+ \quad (2.5)$$

where ρ_1 , and ρ_2 are vectors connecting adjacent sites in the positive x and y directions respectively.

We denote the similarity transform with respect to S of any operator by $\tilde{}$, and for each scheme we calculate the transform of the spin operators, for example

$$\tilde{\sigma}_i^+ = e^{-S} \sigma_i^+ e^S.$$

An important feature of the CCM is that the expansion of this expression in terms of nested commutators will always terminate after a finite (small) number of terms. Using these the transformed Hamiltonian $\tilde{\mathcal{H}}$ can be obtained. The ground-state Schrödinger equation $\mathcal{H}|\Psi\rangle = E_g|\Psi\rangle$ can then be written

$$\tilde{\mathcal{H}}|\Phi\rangle = E_g|\Phi\rangle. \quad (2.6)$$

Operating on this equation with $\langle\Phi|$ yields the following equation for the ground-state energy in terms of the coefficients in S :

$$E_g/N = (-J_1\kappa + J_2)z/8 \quad (2.7)$$

where $\kappa = 1 + 2b_1$ and z is the number of nearest neighbours. This equation is valid in both 1D and 2D for all the approximation schemes. Its simple form is a consequence of the localized form of the interactions in (1.1) and (1.2).

To find b_1 we obtain a set of coupled non-linear equations for the coefficients retained in each of the approximation schemes by operating on (2.6) with $\langle\Phi|C_I$, where C_I is the Hermitian conjugate of one of the strings of creation operators (combinations of σ_i^+) present in S .

3. The coupled non-linear equations

After carrying out the procedure described above for S given by (2.3), we operate on (2.6) with $\sum_i \sigma_i^- \sigma_{i+t}^-$ or $\sum_i \sigma_i^- \sigma_{i+t}^-$ in 1D or 2D respectively. This yields the following full SUB2 equations in 1D:

$$A \sum_{\rho} \delta_{t\rho} - Bb_t - 2\alpha \sum_{\delta} b_{t+\delta} + \sum_r \sum_{\rho} b_{t+\rho+r} b_r = 0 \quad (3.1)$$

with $\rho = \pm 1$, $\delta = \pm 2$ and t (like r) any positive or negative odd integer. The solution of (3.1) is given in section 4.

In 2D the full SUB2 scheme gives

$$A \sum_{\rho} \delta(r - \rho) - Bb_r - 2\alpha \sum_{\delta} b_{r+\delta} + \sum_s \sum_{\rho} b_{r+\rho+s} b_s = 0. \quad (3.2)$$

Here ρ is a nearest-neighbour vector and δ a next-nearest-neighbour vector, while s , like r , is any vector connecting sites on different sublattices. The solution of (3.2) is also given in the next section.

For both equations

$$\alpha = J_2/J_1 = \tan \omega \quad A = 1 + 2b_1 + 2b_1^2 \quad B = 2z(\kappa - \alpha).$$

For SUB2-2 the single equation in 1D is

$$-1 + 2b_1 + 3b_1^2 - 2\alpha b_1 = 0 \quad (3.3)$$

leading directly to

$$E_g/N = -J_1/12[1 - \alpha + 2\sqrt{4 - 2\alpha + \alpha^2}] \quad (3.4)$$

while in 2D the single SUB2-2 equation is

$$-1 + 6b_1 + 5b_1^2 - 4\alpha b_1 = 0 \quad (3.5)$$

leading directly to

$$E_g/N = J_1/10[1 + \alpha - 2\sqrt{4\alpha^2 - 12\alpha + 14}]. \quad (3.6)$$

In both (3.4) and (3.6) the positive sign of the square root has been taken to give agreement with the results of I where it was shown to be necessary to obtain the correct result in the Ising limit. The results are shown in figures 2 and 3.

For the LSUB4 approximation scheme in 1D, a similar procedure results in the three coupled equations

$$-1 + 2b_1 + 3b_1^2 - 2b_1b_3 - 2b_3^2 - 2g_4 - 2\alpha(b_1 - b_3) = 0 \quad (3.7a)$$

$$4b_3 - b_1^2 + 4b_1b_3 - g_4 + 2\alpha(b_1 - 2b_3) = 0 \quad (3.7b)$$

$$(1 + 4b_1 + b_3)g_4 - b_1^2 - 2b_1b_3 + 2b_1b_3^2 - 2\alpha g_4 = 0. \quad (3.7c)$$

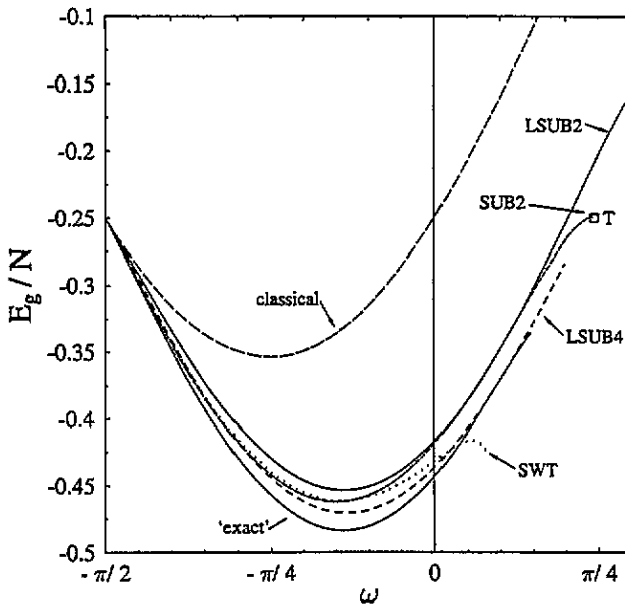


Figure 2. The ground-state energy per spin as a function of ω in 1D. We show the results of the full SUB2, the SUB2-2 and the LSUB4 approximation schemes. Also shown are the 'exact' results based on short-chain calculations extrapolated to $N = \infty$. Spin-wave theory (SWT) results are shown for comparison.

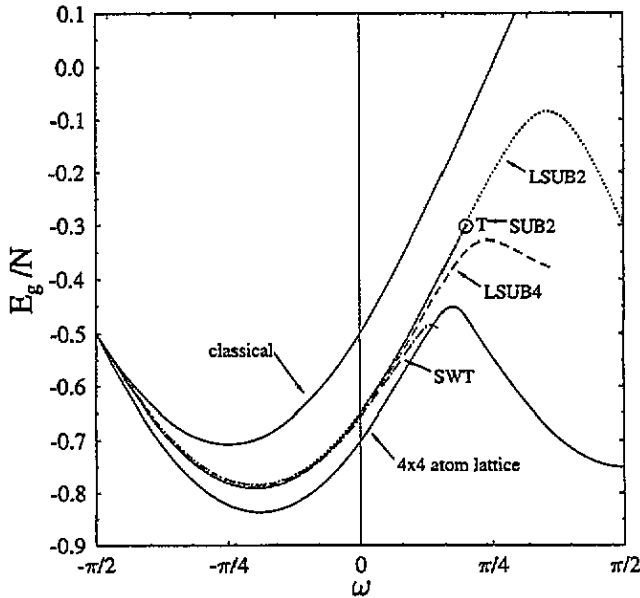


Figure 3. The ground-state energy per spin as a function of ω in 2D. Also shown are the numerical results for a 4×4 lattice.

In 2D the two equations are

$$-1 + 6b_1 + 5b_1^2 - 2g_4 - 4\alpha b_1 = 0 \quad (3.8a)$$

$$2\kappa g_4 - 2b_1^2 - 3\alpha g_4 = 0. \quad (3.8b)$$

In both cases a numerical solution of these equations can be obtained by a simple iterative technique and the resulting value of b_1 used in (2.7). These results are also plotted in figures 2 and 3, and discussed in the next section.

For comparison purposes, accurate values for the true ground-state energy in the AF regime in 1D were obtained by first directly diagonalizing short chains with $N \leq 14$. Then plots of E_g/N against $1/N^2$ were extrapolated to $N \rightarrow \infty$ to produce the results labelled 'exact' in figure 2. They are indistinguishable visually on this figure from the exact results where these are known. We see that even the very simple SUB2-2 approximation scheme gives much better results than the classical approximation while the LSUB4 scheme represents a further significant improvement.

For 2D we compare our results with Lanczos calculations on a 4×4 lattice. Where comparable, these agree exactly with the values given by Dagotto and Moreo (1989a).

4. Solution of the full SUB2 equations

The full SUB2 equations, (3.1) and (3.2), can be solved using Fourier transforms as described in appendix A of I. The result in 1D is

$$b_r = \frac{1}{\pi} \int_0^\pi dq \frac{\cos(rq)}{\cos(q)} [G(q) - \sqrt{D(q)}] \quad (4.1)$$

with

$$G(q) = \kappa - 2\alpha \sin^2(q) \quad D(q) = G^2(q) - A \cos^2(q). \quad (4.2)$$

A and α are defined in section 3 and κ in section 2.

In 2D

$$b_r = \frac{1}{(2\pi)^2} \int_{-\pi}^\pi dq_x \int_{-\pi}^\pi dq_y \frac{\exp(-\mathbf{q} \cdot \mathbf{r})}{\gamma_1(\mathbf{q})} [G(\mathbf{q}) - \sqrt{D(\mathbf{q})}] \quad (4.3)$$

with

$$\gamma_1(\mathbf{q}) = \frac{1}{2}(\cos q_x + \cos q_y) \quad (4.4)$$

$$\gamma_2(\mathbf{q}) = \cos q_x \cos q_y \quad (4.5)$$

$$G(\mathbf{q}) = \kappa + \alpha(\gamma_2(\mathbf{q}) - 1) \quad (4.6)$$

$$D(\mathbf{q}) = G^2(\mathbf{q}) - A\gamma_1^2(\mathbf{q}). \quad (4.7)$$

As in section 3, we choose the sign of the square roots for consistency with I, which in turn was chosen to be correct in the Ising limit. The choice $r = 1$ in 1D or $r = \rho$ in 2D in these equations gives an integral equation for b_1 that can be solved numerically. The resulting ground-state energy given by (2.7) is also shown in figures 2 and 3.

Over much of the AF regime the results for the ground-state energy per spin in the full SUB2 scheme do not differ greatly from those obtained using the SUB2-2 scheme. However, one interesting aspect of the full SUB2 approximation scheme, as noted in I, is the possible existence of a terminating point. Clearly (4.1) or (4.3) has no real solution if D becomes negative for some value of q or q .

In 1D we find that this does occur, but the value of q at which D is a minimum is not at 0 or π , but at $q = q_0$ given by

$$\cos(2q_0) = 1 - \kappa/\alpha + A/(4\alpha^2). \quad (4.8)$$

Taking $D = 0$ at $q = q_0$ gives

$$A - 8\kappa\alpha + 16\alpha^2 = 0 \quad (4.9)$$

and furthermore \sqrt{D} can be evaluated exactly to give a term linear in $\cos(2q)$, which enables the integral to be evaluated analytically. This requires some care, and the range of integration needs to be divided into two at $q = q_0$ to ensure that \sqrt{D} always has the sign given in (4.1). We find the exact self-consistency expression for b_1 at this point is

$$b_1 = \kappa - \alpha - 2\alpha \sin(2q_0)/\pi + \alpha(4q_0 - \pi) \cos(2q_0)/\pi. \quad (4.10)$$

Solving the simultaneous equations (4.9) and (4.10) we obtain the critical value of ω beyond which there is no real solution of (4.1) as $\omega_c = 0.7660$. The corresponding value of the ground-state energy is $E_g/N = -0.2495$. This critical or terminating point is marked T in figure 2.

Turning now to 2D we find $D(q)$ becomes zero at $q = (0, \pm\pi)$ or $(\pm\pi, 0)$. In either case we find $b_1 = 0.2471$ and $\omega = 0.6416$, $E_g/N = -0.299$. This point is marked T in figure 3.

We believe (see the discussion in I) that each of these terminating points represents a phase change to a phase with a fundamentally different ground state from the model state. For the Hamiltonians described by (1.1) and (1.2) this would probably correspond to a change from an AF to a frustrated phase. In 1D the value ω_c at which this phase change takes place is clearly not accurate at this level of approximation, since the true value is believed to be $\omega = \tan^{-1}(\frac{1}{2}) = 0.4636$, and in 2D the accuracy is probably not significantly better. Nevertheless to obtain a phase change in an *ab initio* calculation of this type is encouraging.

If we compare the CCM results for the different approximation schemes with the SWT results, we see excellent agreement for $\omega \lesssim 0$ between all the methods. For $\omega \gtrsim 0$ the results of the different methods diverge. The CCM has the potential for systematic improvement as was shown by Bishop *et al* (1991b) and we would expect that successive approximations of the LSUB n type would be suitable for obtaining accurate values of the ground-state energy per spin over the whole of the AF regime.

5. Correlation functions and magnetization

To calculate an expectation value we need the bra ground state as well as the ket ground state. It is important to note that the CCM does not give a unitary transformation between the model ground state and the constructed approximate true ground state. For this reason the bra state is not the Hermitian conjugate of the ket state and has to be constructed separately.

However, a linear rather than exponential transformation is adequate, and is known as the normal CCM (NCCM). An exponential transformation is possible, known as the extended CCM (ECCM), as described by Arponen *et al* (1987), but will not be used here.

The NCCM form of the bra state is

$$\langle \tilde{\Psi} | = \langle \Phi | \tilde{S} e^{-S} \quad (5.1)$$

where the new operator \tilde{S} is constructed from a linear combination of the C_l destruction operators, consistent with the conserved quantities. We shall use the full SUB2 version given in 1D by

$$\tilde{S} = 1 + \frac{1}{2} \sum_l \sum_r \tilde{b}_r \sigma_l^- \sigma_{l+r}^- \quad (5.2)$$

where $1 \leq l \leq N$ is an integer labelling the lattice sites and r is any positive or negative odd integer, corresponding to the difference between any two sites on opposite sublattices. The coupled linear equations for the coefficients of this operator are

$$K_1 \sum_\rho \delta_{r\rho} - 4\kappa \tilde{b}_r + 2 \sum_\rho \sum_s b_s \tilde{b}_{\rho+s+r} + 2\alpha(2\tilde{b}_r - \tilde{b}_{r+2} - \tilde{b}_{r-2}) = 0 \quad (5.3)$$

where $\rho = \pm 1$, s is also a positive or negative odd integer, and the b_s are the solutions of (4.1). The constant K_1 is defined by

$$K_1 = 1 + 2\kappa \tilde{b}_1 - 4\Xi \quad (5.4)$$

with

$$\Xi = \sum_r \tilde{b}_r b_r. \quad (5.5)$$

In 2D the equations are rather similar. We write

$$\tilde{S} = 1 + \frac{1}{2} \sum_l \sum_r \tilde{b}_r \sigma_l^- \sigma_{l+r}^- \quad (5.6)$$

where the l are the position vectors of the lattice sites and r connects any two sites on opposite sublattices. The coupled linear equations for the coefficients of this operator are

$$K_1 \sum_\rho \delta_{r\rho} - 8\kappa \tilde{b}_r + 2 \sum_\rho \sum_s b_s \tilde{b}_{\rho+s+r} + 2\alpha \sum_\delta (\tilde{b}_r - \tilde{b}_{r+\delta}) = 0 \quad (5.7)$$

where ρ is a nearest-neighbour vector and δ a next-nearest-neighbour vector, as before, and the b_δ are the solutions of (4.3). The constant K_1 is defined by (5.4) and

$$\Xi = \sum_r \tilde{b}_r b_r. \quad (5.8)$$

These equations can be solved by Fourier transformation. Details are given only for 1D, the 2D equations being analogous in the same way as in the last section. We find

$$\tilde{b}_r = \frac{K_1}{2\pi} \int_0^\pi dq \cos(rq) \frac{\cos(q)}{\sqrt{D}} \quad (5.9)$$

and the constant Ξ can also be expressed as an integral as shown in appendix B of I as

$$\Xi = K_1 \left[-\frac{1}{2} + \frac{1}{2\pi} \int_0^\pi dq \frac{G(q)}{\sqrt{D}} \right]. \quad (5.10)$$

Hence, using (5.4) and (5.9) with $r = 1$ we obtain

$$K_1^{-1} = -1 + \frac{1}{\pi} \int_0^\pi dq \frac{[2G(q) - \kappa \cos^2(q)]}{\sqrt{D}}. \quad (5.11)$$

These equations can be solved numerically.

Using the bra state we have calculated the following quantities:

(i) the order parameter μ , defined by

$$\mu = \lim_{r \rightarrow \infty} \langle \sigma_i^z \sigma_{i+r}^z \rangle \quad (5.12)$$

and

(ii) the sublattice magnetization M^z , defined by

$$M^z = -\frac{2}{N} \sum_i \langle \sigma_i^z \rangle. \quad (5.13)$$

As discussed in I we take r odd in (5.12) and obtain the results $\mu = 1 - 4\Xi$ and $M^z = 1 - 2\Xi$. The fact that $(M^z)^2$ is not equal to μ in any given level of approximation is another consequence of the non-unitary nature of the CCM.

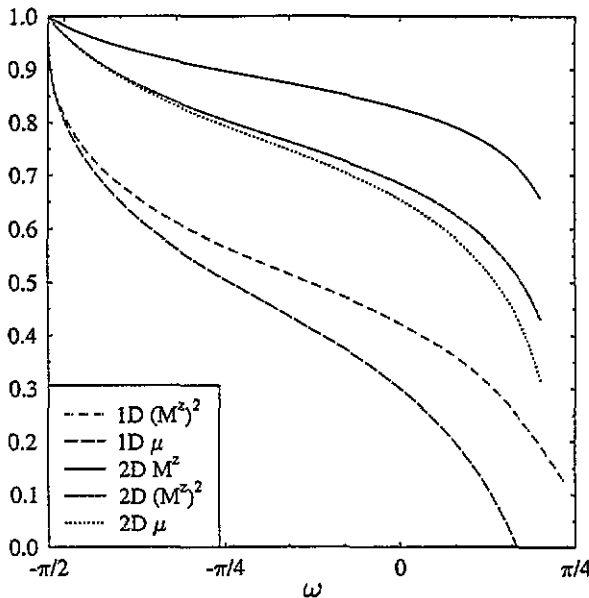


Figure 4. The order parameter μ , the sublattice magnetization M^z and the square of M^z as functions of ω , in both 1D and 2D.

Our 1D results for these quantities are shown in figure 4. The exact values for μ and M^z are believed to be zero in the AF regime, so our results are clearly not correct. Note, however, the infinite slope of the curves at $\omega = -\pi/2$, which would be consistent with a sudden change to zero at this point. Also the results are considerably better than those of AF SWT, which predicts divergences in both over the whole regime except at $\omega = -\pi/2$ where $M^z \rightarrow 1$.

The results for 2D are also shown in figure 4. The essential features are that the values of M^z lie higher than in 1D and that the gradient at the ferromagnetic boundary is not infinite. In 2D the magnetization is believed not to be zero over the whole of the AF regime. Although our results are not accurate enough to confirm this, these features do give it some support. It would be interesting to try better approximations for the bra state to shed further light on this question.

6. Conclusions

Of the three main $T = 0$ phases of the quantum spin systems given by (1.1) and (1.2), the ferromagnetic has the simplest ground state, the AF the next simplest and the frustrated the most complicated. We have shown how the CCM based on a Néel model state can produce useful results for the AF phase, including evidence of a phase transition at a critical value of ω , probably to the frustrated phase. At the present stage in the application of CCM to quantum spin systems, we can obtain reasonably accurate numerical results for the ground-state energy, and results for the order parameter and the sublattice magnetization better than those from SWT.

The behaviour of the 1D model in the vicinity of the transition between the AF and frustrated phases is known to be complex, with gapless and non-zero gap regimes as well as regimes with different spatial periodicity (Tonegawa and Harada 1987). Higher-order approximation schemes involving many extra terms in S would be necessary in order to obtain useful results on the subtle differences between these phases. Nevertheless this is possible in principle for the CCM and in practice would probably involve use of computer algebra packages to generate the coupled non-linear equations.

A much more difficult problem is the frustrated phase. The numerical results on short chains are in agreement with the classical picture of a spiral ground state in 1D whose periodicity in real space varies with ω . To apply the CCM requires both a suitable model state and a complete set of creation operators from that state, and these have not been considered in this paper.

Acknowledgments

We have benefited greatly from discussions with R F Bishop and Yang Xian. D J J Farnell acknowledges a postgraduate award from the Science and Engineering Research Council of Great Britain. We also thank one of the referees for drawing the numerical work of Dagotto to our attention.

References

- Arponen J S, Bishop R F and Pajanne E 1987 *Phys. Rev. A* **36** 2519–38
- Bethe H A 1931 *Z. Phys.* **71** 205–26

- Birgeneau R J 1990 *Am. J. Phys.* **58** 28-40
Bishop R F, Parkinson J B and Xian Yang 1991a *Phys. Rev. B* **43** 13 782-5
—— 1991b *Phys. Rev. B* **44** 9425-43
—— 1992a *Phys. Rev. B* **46** 880-8
—— 1992b *J. Phys.: Condens. Matter* **4** 5783-94
Chandra P and Doucot B 1988 *Phys. Rev. B* **38** 9335-8
Chubukov A V and Jolicoeur T 1991 *Phys. Rev. B* **44** 12050-3
Dagotto E 1991 *Int. J. Mod. Phys. B* **5** 907-35
Dagotto E and Moreo A 1989a *Phys. Rev. B* **39** 4744-7
—— 1989b *Phys. Rev. Lett.* **63** 2148-51
Haldane F D M 1982 *Phys. Rev. B* **25** 4925-8
Majumdar C K and Ghosh D K 1969a *J. Math. Phys.* **10** 1388-98
—— 1969b *J. Math. Phys.* **10** 1399-402
Manousakis E 1991 *Rev. Mod. Phys.* **63** 1-62
Okamoto K and Nomura K 1992 *Phys. Lett.* **169A** 433-7
Orbach R 1958 *Phys. Rev.* **112** 309-16
Roger M and Hetherington J H 1990a *Phys. Rev. B* **41** 200-19
—— 1990b *Europhys. Lett.* **11** 255-60
Tonogawa T and Harada I 1987 *J. Phys. Soc. Japan* **56** 2153-67
Xu J H and Ting C S 1990 *Phys. Rev. B* **42** 6861-4
Yang C N and Yang C P 1966a *Phys. Rev.* **150** 321-7
—— 1966b *Phys. Rev.* **150** 327-39