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Coupled-cluster treatment of the XY-model

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Abstract. We study quantum spin systems in the 1D, 2D square and 3D cubic lattices with nearest-neighbour XY-exchange. We use the coupled-cluster method (CCM) to calculate the ground-state energy, the $T = 0$ sublattice magnetization and the excited-state energies, all as functions of the anisotropy parameter γ. We consider the case with $S = 1/2$ in detail and give some results for higher S. In 1D these results are compared with the exact $S = 1/2$ results and in 2D with Monte Carlo and series expansions. We obtain critical points close to the expected value $\gamma = 0$ and our extrapolated LSUBn results for the ground-state energy are well converged for all γ except very close to the critical point.

1. Introduction and the coupled-cluster-method formalism

In this paper we consider the $T = 0$ properties of the quantum spin system known as the XY-model, described by the Hamiltonian

$$H = \frac{1}{2}\sum_{l,p}[(1+\gamma)s_l^x s_{l+p}^x + (1-\gamma)s_l^y s_{l+p}^y] \qquad \text{in the region } 0 \leqslant \gamma \leqslant 1 \tag{1}$$

where index l runs over all N lattice sites with periodic boundary conditions, and p over the z nearest-neighbour sites.

For $s = 1/2$ and 1D, this model was solved exactly by Lieb *et al* (1961) and its properties have been studied by many authors (see Niemeyer (1967) and Barouch and McCoy (1971), for example). For higher spin in 1D or in 2D (square) and 3D (simple cubic), useful results have been obtained using spin-wave theory (Zheng *et al* 1991), Monte Carlo methods (Ding 1992, Zhang and Runge 1992), series expansions (Hamer *et al* 1991) and, for $\gamma = 0$, finite-size extrapolations (Betts *et al* 1996).

In a recent paper (Bishop *et al* (1996), referred to as I), the coupled-cluster method (CCM) was applied to the XXZ-model in the $|\Delta| < 1$ regime. It was found that good results could be obtained by using a *planar* model state in which the spins are aligned in the xy-plane, as in the classical ground state, rather than along the z-axis. Here we shall use a similar model state for (1), again motivated by the classical ground state.

For a description of the CCM applied to spin systems, see Bishop *et al* (1991) and also the references given in I. To calculate the ground-state wave function $|\Psi\rangle$ of a spin system, we start with a *model state* $|\Phi\rangle$ and a *correlation operator* S such that

$$|\Psi\rangle = \mathrm{e}^S|\Phi\rangle.$$

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For the Hamiltonian (1), we expect that in the ground state the spins are aligned in the xy-plane. We choose $|\Phi\rangle$ to be a Néel state with spins aligned parallel and antiparallel to the x-axis. In 1D this has the form

$$|\Phi\rangle = |\cdots \quad \longleftarrow \quad \longrightarrow \quad \longleftarrow \quad \longrightarrow \quad \longleftarrow \quad \longrightarrow \quad \longleftarrow \quad \longrightarrow \quad \longleftarrow \quad \longrightarrow \quad \cdots\rangle.$$

It is useful to introduce *local axes* such that each spin in $|\Phi\rangle$ is pointing in the negative z-direction, by means of the following transformation:

$$s^x \to -s^z,\ s^y \to s^y,\ s^z \to s^x \qquad \text{left-pointing spins}$$
$$s^x \to s^z,\ s^y \to s^y,\ s^z \to -s^x \qquad \text{right-pointing spins.}$$

Thus (1) becomes (with $s^{\pm} = s^x \pm \mathrm{i}s^y$)

$$H = \frac{1}{2}\sum_{l,p}[As_l^z s_{l+p}^z + B(s_l^+ s_{l+p}^+ + s_l^- s_{l+p}^-) + C(s_l^+ s_{l+p}^- + s_l^- s_{l+p}^+)] \tag{2}$$

with

$$A \equiv -(1+\gamma) \qquad B \equiv -\frac{1}{4}(1-\gamma) \qquad C = -B.$$

For the correlation operator S we choose a linear combination of creation operators relative to $|\Phi\rangle$, a creation operator being any combination of spin-raising operators (s^+ in the local axes). Because of the form of (2), the total number of spin flips in each creation operator must be even.

The simplest possible choice for S is to flip two spins, known as the SUB2 approximation scheme:

$$S = \sum_{l=1}^{N}\left(\frac{1}{2}\sum_r b_r s_l^+ s_{l+r}^+\right) \tag{3}$$

where r runs over all distinct lattice vectors ($r \neq 0$ for $s = 1/2$).

The full SUB4 scheme involves four-flip configurations as well as two-flip ones, and is too complicated to handle in general. However, the most important extra term is the one with four flips on adjacent sites. Including this term gives the SUB2 + LSUB4 scheme, which we have applied only in 1D:

$$S = \sum_{l=1}^{N}\left(\frac{1}{2}\sum_r b_r s_l^+ s_{l+r}^+ + g_4 s_l^+ s_{l+1}^+ s_{l+2}^+ s_{l+3}^+\right). \tag{4}$$

A third approximation scheme is to include in S all possible combinations of spin flips within a region of size n, known as the LSUBn scheme. This is particularly useful for numerical extrapolation as a function of n, and will be discussed in detail in section 5.

From the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$, we obtain the equation for the ground-state energy:

$$E = \langle\Phi|\mathrm{e}^{-S}H\mathrm{e}^{S}|\Phi\rangle = \frac{1}{2}zN\left(\frac{1}{4}A + b_1 B\right). \tag{5}$$

This equation is exact whatever approximations are made for S.

To determine the coefficients b_r and g_4 in the SUB2 + LSUB4 scheme, we operate on the Schrödinger equation with $\exp(-S)$, then with one of the destruction operators and then with $\langle\Phi|$:

$$\langle\Phi|s_l^- s_{l+r}^-\mathrm{e}^{-S}H\mathrm{e}^{S}|\Phi\rangle = \sum_p\Bigg[B\sum_{r'} b_{r'}b_{r-r'+p} - (A + 4Bb_1)b_r$$

$$+ 2Cb_{r-p} + (B(2b_1^2 + 2g_4 + 1) + Ab_1)\delta_{p,r} + Bg_4\delta_{3p,r}\Big] = 0 \tag{6}$$

$$\langle\Phi|s_l^- s_{l+1}^- s_{l+2}^- s_{l+3}^- \mathrm{e}^{-S} H \mathrm{e}^{S}|\Phi\rangle = A(b_1^2 + 3b_2^2 + 2b_1b_3) - 4B(b_1b_2b_4 + b_1b_3^2 + b_2^2b_3)$$
$$- 4C(2b_1b_2 + b_2b_3) + g_4[B(2b_5 - 2b_3 - 8b_1) - A] = 0. \tag{7}$$

The corresponding equations for the SUB2 scheme are obtained by setting $g_4 = 0$ everywhere in the first of these and ignoring the second.

These coupled *non-linear* equations are solved by first Fourier transforming equation (6) and then solving the resulting equations and equation (10) self-consistently. For dimension d we obtain

$$\Gamma(q) \equiv \sum_r \mathrm{e}^{\mathrm{i}rq} b_r \qquad b_r = \int_{-\pi}^{\pi} \mathrm{d}^d q\ (2\pi)^{-d} \mathrm{e}^{-\mathrm{i}rq}\Gamma(q) \qquad \gamma(q) = \frac{1}{z}\sum_p \mathrm{e}^{\mathrm{i}pq}$$

$$b_1 = \int_{-\pi}^{\pi} \mathrm{d}^d q\ (2\pi)^{-d}\gamma(q)\Gamma(q) \qquad X_1 \equiv \sum_r b_r b_{r+p} = \int_{-\pi}^{\pi} \mathrm{d}^d q\ (2\pi)^{-d}\gamma(q)\Gamma^2(q)$$

leading to

$$a\Gamma^2(q) + b\Gamma(q) + c = 0$$

where

$$a \equiv B\gamma(q) \qquad b \equiv -A - 4Bb_1 + 2C\gamma(q)$$
$$c \equiv [B(2b_1^2 + 2g_4 + 1) + Ab_1)]\gamma(q) + Bg_4\gamma(3q) - BX_1 - 2Cb_1$$

with the usual solution

$$\Gamma(q) = \frac{-b + \sqrt{b^2 - 4ac}}{2a}.$$

The equations can now be solved numerically in a self-consistent way.

Table 1. The ground-state energy and sublattice magnetization for the one-dimensional XY-model at $\gamma = 0$ compared to exact results of McCoy (1968). N_f indicates the number of fundamental configurations for a given LSUBn approximation level.

LSUBn	N_f	E_g/N	M
LSUB2	1	−0.303 813	0.837 286
SUB2	—	−0.310 377	0.779 517
LSUB4	4	−0.314 083	0.722 916
LSUB6	13	−0.316 301	0.660 064
LSUB8	43	−0.317 137	0.617 624
LSUB10	151	−0.317 542	0.586 067
LSUB∞	—	−0.318 29	—
Exact	—	−0.318 310	0.0

Results for the ground-state energy obtained using the SUB2 and SUB2 + LSUB4 approximation schemes are shown in figures 1 and 2, and tables 1 and 2 for 1D and 2D. The LSUBn results are discussed in section 5.

A notable feature of the CCM is the existence of terminating points as a function of γ. These are believed to correspond to the actual $T = 0$ phase changes, known to be at $\gamma = 0$ in 1D and believed also to be at $\gamma = 0$ on symmetry grounds for 2D and 3D. In 1D, terminating points only occur if correlations of infinite range are explicitly included in S and occur at $\gamma = -0.107\,89$ in SUB2 and at $\gamma = -0.096\,05$ in SUB2 + LSUB4. In 2D,

Table 2. The ground-state energy and sublattice magnetization for the square-lattice XY-model at $\gamma = 0$ compared to series expansion calculations of Hamer *et al* (1991). N_f indicates the number of fundamental configurations for a given LSUBn approximation level, and also shown are the critical values of γ for the anisotropic model—where the value in parentheses is the estimated error in the final decimal place shown.

LSUBn	N_f	E_g/N	M	$\gamma_c(n)$
LSUB2	1	−0.540 312	0.949 634	—
SUB2	—	−0.546 325	0.918 953	−0.030(1)
LSUB4	10	−0.547 267	0.915 768	−0.175(1)
LSUB6	131	−0.548 329	0.901 357	−0.073(1)
LSUB8	2793	−0.548 616	0.893 665	−0.04(1)
LSUB∞	—	−0.548 92	0.869	0.00(1)
Series expansion	—	−0.5488	0.872	0.0

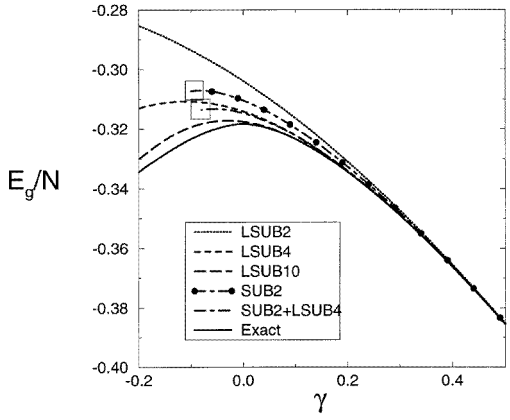

Figure 1. Results for the CCM ground-state energy of the one-dimensional XY-model. The terminating points of the SUB2 and SUB2 + LSUB4 schemes are indicated.

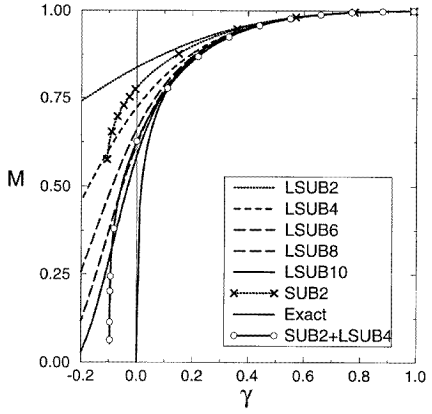

Figure 2. Results for the CCM ground-state sublattice magnetization of the one-dimensional XY-model.

there is a terminating point at $\gamma = -0.030\,33$ in SUB2. These values are reasonably close to $\gamma = 0$ considering the simple nature of these approximations.

In 2D and 3D, terminating points can also occur within the LSUBn scheme as described in section 5.

2. In-plane sublattice magnetization

In the CCM the bra ground state is not in general the Hermitian conjugate of the ket state. Instead we introduce a new operator $\tilde{S}$ such that

$$\langle\tilde{\Psi}| = \langle\Phi|\tilde{S}\exp(-S).$$

The SUB2 + LSUB4 approximation for $\tilde{S}$ is

$$\tilde{S} = 1 + \sum_{l=1}^{N}\left(\frac{1}{2}\sum_{r}\tilde{b}_r s_l^- s_{l+r}^- + \tilde{g}_4 s_l^- s_{l+1}^- s_{l+2}^- s_{l+3}^-\right) \tag{8}$$

where r runs over all distinct lattice vectors (with $r \neq 0$ for $s = 1/2$).

The bra-state equations are found variationally by taking the partial derivatives of

$$\bar{H} = \langle\tilde{\Psi}|H|\Psi\rangle$$

with respect to the ket-state coefficients. By CCM theory (Bishop *et al* 1991) these derivatives must be equal to 0. Hence we obtain two bra-state equations:

$$\begin{aligned}\frac{\partial\bar{H}}{\partial b_r} = N\sum_p\Big[&2B\sum_{r'}\tilde{b}_{r'}b_{r'-r+p} - (A+4Bb_1)\tilde{b}_r + 2C\tilde{b}_{r-p}\\
&+ (B + (A+4Bb_1)\tilde{b}_1 - 4B\sum_{r'}\tilde{b}_{r'}b_{r'})\delta_{p,r}\\
&+ (\tilde{g}_4/2)\{[4A(b_1+b_3) - 8B(b_2b_4+b_3^2) - 16Bg_4 - 16Cb_2]\delta_{p,r}\\
&+ [12Ab_2 - 8B(b_1b_4+2b_2b_3) - 8C(2b_1+b_3)]\delta_{2p,r}\\
&+ [4Ab_1 - 8B(2b_1b_3+b_2^2) - 4Bg_4 - 8Cb_2]\delta_{3p,r}\\
&- 8Bb_1b_2\delta_{4p,r} + 4Bg_4\delta_{5p,r}\}\Big] = 0\end{aligned} \tag{9}$$

$$\frac{\partial\bar{H}}{\partial g_4} = N[B(2\tilde{b}_1+\tilde{b}_3) + \tilde{g}_4(2B(b_5-b_3-4b_1) - A)] = 0. \tag{10}$$

Again we perform a Fourier transform on equation (9), and the resulting equations and equation (10) may be solved self-consistently in order to obtain the bra-state correlation coefficients.

Finally the results are used to calculate the magnetization using the formula for SUB2:

$$M = -2\langle\tilde{\Psi}|s_l^z|\Psi\rangle = 1 - 2\sum_r\tilde{b}_r b_r$$

and for SUB2 + LSUB4:

$$M = -2\langle\tilde{\Psi}|s_l^z|\Psi\rangle = 1 - 2\sum_r\tilde{b}_r b_r - 8g_4\tilde{g}_4.$$

3. Excitations

A similar method can be used for the excited-state energies, introducing the operator

$$X_1 = \sum_i \mathcal{X}_i s_i^+ \qquad i \text{ belongs to one sublattice only}$$

leading to

$$\langle\Phi|s_l^-\mathrm{e}^{-S}[H, X_1]\mathrm{e}^{S}|\Phi\rangle = -\frac{1}{2}z(A+4Bb_1)\mathcal{X}_l + B\sum_{r,p}b_r\mathcal{X}_{l+r+p} = \varepsilon_l\mathcal{X}_l \tag{11}$$

and hence, via Fourier transformation,

$$\Rightarrow \varepsilon(q) = -\frac{1}{2}z(A + 4Bb_1) + Bz\gamma(q)\Gamma(q). \tag{12}$$

4. General spin s (SUB2 only)

We have also considered the general case of $s \geqslant 1/2$ within the SUB2 approximation scheme. The main features are as follows.

The correlation operators S and $\tilde{S}$ are the same as before (without g_4). The ket-state equations become

$$\langle\Phi|s_l^- s_{l+r}^- \mathrm{e}^{-S} H \mathrm{e}^{S}|\Phi\rangle = 4s^2 \sum_p \Bigg[4s^2 B \sum_{r'} b_{r'} b_{r-r'+p} - 2s(A + 4Bb_1)b_r + 4sCb_{r-p} + (B(2b_1^2 + 1) + Ab_1)\delta_{p,r} \Bigg] = 0 \tag{13}$$

and the energy is

$$\langle\Phi|\mathrm{e}^{-S} H \mathrm{e}^{S}|\Phi\rangle = 2s^2 zN\left(\frac{1}{4}A + b_1 B\right). \tag{14}$$

Using these equations we find for the ground-state energy per spin of the $s = 1$ system at the $\gamma = 0$ point the value $-1.091\,79$. This compares with a numerical result from extrapolating rings with $N \leqslant 14$ of -1.1157 ± 0.0003. This is a very similar accuracy to that obtained using SUB2 for $s = \frac{1}{2}$ at the same point.

There are similar modifications to the bra-state equations, which become

$$\frac{\partial \bar{H}}{\partial b_r} = 4s^2 N \sum_p \Bigg[8s^2 B \sum_{r'} \tilde{b}_{r'} b_{r'-r+p} - 2s(A + 4Bb_1)\tilde{b}_r + 4sC\tilde{b}_{r-p} + (B + (A + 4Bb_1)\tilde{b}_1 - 8sB \sum_{r'} \tilde{b}_{r'} b_{r'})\delta_{p,r} \Bigg] = 0. \tag{15}$$

Finally the magnetization is given by

$$M = -\frac{1}{s}\langle\tilde{\Psi}|s_l^z|\Psi\rangle = 1 - 4s \sum_r \tilde{b}_r b_r. \tag{16}$$

5. The LSUBn approximation

The LSUBn scheme contains all possible (connected and disconnected) terms in S which are contained within a 'locale' of size n. We use all possible connected configurations of n spins to define this locale; in 1D we may see that this locale is simply a chain of length n. Disconnected and connected configurations of fewer than n spins are then generated by successively removing sites from the original connected configurations of n spins, thus covering all possibilities. The lowest-order LSUBn approximation scheme is the LSUB2 (i.e. SUB2-2) approximation in which only a single nearest-neighbour, two-body term is retained in S. We note that the Hamiltonian of equation (2) includes products of the spin operators which contain even numbers of these spin operators only. This means that the ground state contains only even numbers of spin flips with relation to the model state. We restrict the LSUBn approximation to including only those configurations which contain an even number of spin-raising operators. A further restriction is that each *fundamental*

configuration must be independent of all others under the symmetries of both the lattice and the Hamiltonian; we note that both the lattice and the Hamiltonian have identical symmetries for the XY-model.

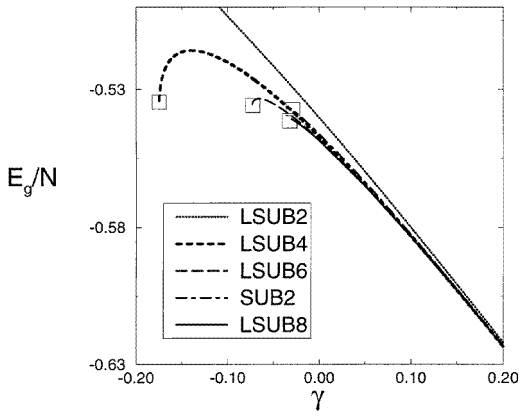

Figure 3. Results for the CCM ground-state energy of the square-lattice XY-model. All of the approximation schemes have terminating points except LSUB2.

Table 3. The ground-state energy and sublattice magnetization for the cubic-lattice XY-model at $\gamma = 0$. N_f indicates the number of fundamental configurations for a given LSUBn approximation level, and also shown are the critical values of γ for the anisotropic model—where the value in parentheses is the estimated error in the final decimal place shown.

LSUBn	N_f	E_g/N	M	$\gamma_c(n)$
LSUB2	1	−0.786 866	0.971 488	—
SUB2	—	−0.790 901	0.958 282	−0.016 66(1)
LSUB4	13	−0.791 224	0.958 648	−0.172(1)
LSUB6	327	−0.791 702	0.954 759	−0.071(1)
LSUB∞	—	−0.792 01	0.948	0.01(1)

Tables 1, 2, and 3 show the numbers of fundamental configurations for given LSUBn approximation level, and we can see from these tables that the number of configurations grows very rapidly with n. Hence, for higher-order approximations we need to enumerate all possible configurations computationally, and we furthermore need to obtain and solve the CCM LSUBn equations computationally also. A full explanation of the computational method used here is given by Zeng *et al* (1997). It is now possible to obtain values for the ground-state energy and sublattice magnetization for the LSUBn approximation scheme. Results for these quantities are given in figures 1, 2, 3, and 4, and results at the isotropic point of $\gamma = 0$ are given in tables 1, 2, and 3. A simple extrapolation of the ground-state energy and sublattice magnetization has also been carried out by plotting the ground-state energy against $1/n^2$ and the sublattice magnetization against $1/n$, and then performing polynomial fits on these data. The extrapolated LSUB∞ results obtained from this simple, 'naive' approach are shown in tables 1, 2, and 3. The results are clearly at least as good as are obtained by series expansion. Results in 2D and 3D are especially valuable since no exact results are available.

Another consequence of this approximation scheme is that the second derivative of the ground-state energy is found to diverge for some *critical* value of the anisotropy parameter, denoted $\gamma_c(n)$, in 2D and 3D only. These points are related to phase transitions of the true

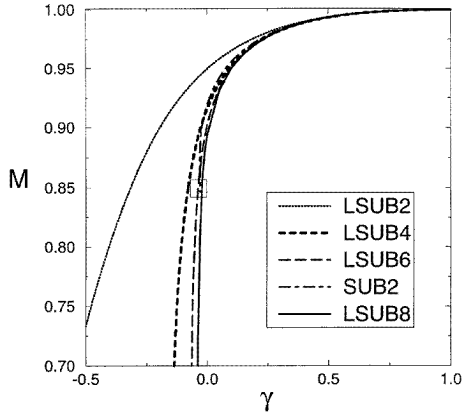

Figure 4. Results for the CCM ground-state sublattice magnetization of the square-lattice XY-model.

ground state of the system (Zeng *et al* 1997), and the results for given LSUBn approximation levels are shown in tables 2 and 3. We note that critical $\gamma_c(n)$ approaches $\gamma = 0$, the point at which the true phase transition point is believed to lie (in all dimensions), with increasing approximation level. Again, a simple extrapolation of the LSUBn critical points is attempted by plotting $\gamma_c(n)$ against $1/n^2$, as was done by Bishop *et al* (1994), and the extrapolated results are also shown in tables 2 and 3.

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References

Barouch E and McCoy B M 1971 *Phys. Rev.* A **3** 786–804
Betts D D, Matsui S, Vats N and Stewart G E 1996 *Can. J. Phys.* **74** 54–64
Bishop R F, Farnell D J J and Parkinson J B 1996 *J. Phys.: Condens. Matter* **8** 11 153–65
Bishop R F, Hale R G and Xian Y 1994 *Phys. Rev. Lett.* **73** 3157–60
Bishop R F, Parkinson J B and Xian Y 1991 *Phys. Rev.* B **44** 9425–43
Ding H-Q 1992 *Phys. Rev.* B **45** 230–42
Hamer C J, Oitmaa J and Zheng W 1991 *Phys. Rev.* B **43** 10 789–96
Lieb E, Schultz T and Mattis D 1961 *Ann. Phys., NY* **16** 407–66
McCoy B M 1968 *Phys. Rev.* **173** 531–41
Niemeyer T 1967 *Physica* **36** 377–419
Zeng C, Farnell D J J and Bishop R F 1997 to be published
Zhang S and Runge K J 1992 *Phys. Rev.* B **45** 1052–5
Zheng W, Oitmaa J and Hamer C J 1991 *Phys. Rev.* B **44** 11 869–81