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 magnetisation and the excited state energies, all as functions of the anisotropy parameter $\gamma$. We consider $S = 1/2$ 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 $\gamma$ except very close to the critical point.

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Short Title CCM for the XY model.
1. Introduction and CCM formalism

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

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

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, Schultz and Mattis (1961) and its properties have been studied by many authors (see Niemeyer, 1967, and Barouch et al., 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, Farnell and Parkinson, 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

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

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

$$|\Phi\rangle = |\ldots \leftarrow \rightarrow \leftarrow \rightarrow \leftarrow \rightarrow \leftarrow \rightarrow \leftarrow \rightarrow \ldots\rangle.$$

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:

$$s^x \rightarrow -s^z, s^y \rightarrow s^y, s^z \rightarrow s^x \quad \text{left-pointing spins}$$

$$s^x \rightarrow s^z, s^y \rightarrow s^y, s^z \rightarrow -s^x \quad \text{right-pointing spins}.$$
\[ H = \frac{1}{2} \sum_{l,p} [As^+_l s^z_{l+p} + B(s^+_l s^z_{l+p} + s^-_l s^-_{l+p}) + C(s^+_l s^-_{l+p} + s^-_l s^+_l)] \]  

with

\[ A \equiv -(1 + \gamma), \quad B \equiv -\frac{1}{4} (1 - \gamma), \quad C = -B. \]

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:

\[ S = \sum_{l=1}^{N} \left( \frac{1}{2} \sum_r b_r s^+_l s^+_l \right) \]  

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

The full SUB4 scheme involves 4-flip configurations as well 2 flips and is too complicated to handle in general. However the most important extra term is the one with 4 flips on adjacent sites. Including this term gives the SUB2+LSUB4 scheme which we have applied only in 1D:

\[ S = \sum_{l=1}^{N} \left( \frac{1}{2} \sum_r b_r s^+_l s^+_l + g_4 s^+_l s^+_l s^+_l s^+_l \right) \]  

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:

\[ E = \langle \Phi | e^{-S} H e^S |\Phi\rangle = \frac{1}{2} zN \left( \frac{1}{4} A + b_1 B \right) \]  

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 one of the destruction operators and then by \( \langle \Phi | \):
\[ \langle \Phi | s_t e^{-S} H e^{S} | \Phi \rangle = \sum_p [B \sum_{r,r'} b_r b_{r'-p} - (A + 4Bb_1)b_r \\
+ 2C b_{r-p} + (B(2b_1^2 + 2g_4 + 1) + Ab_1)\delta_{p,r} + Bg_4\delta_{3p,r}] = 0 \] (6)

\[ \langle \Phi | s_t s_{t+1}^{-1} s_{t+2}^{-1} s_{t+3} e^{-S} H e^{S} | \Phi \rangle = A(b_1^2 + 3b_2^2 + 2b_1b_3) - 4B(b_1b_2b_4 + b_1b_2^2 + b_2b_3) \\
- 4C(2b_1b_2 + b_2b_3) + g_4[B(2b_5 - 2b_3 - 8b_1) - A] = 0 \] (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 Eq.(6) and then solving the resulting equations and Eq.(10) self-consistently. For dimension \( d \) we obtain:

\[ \Gamma(q) \equiv \sum_r e^{irq}b_r, \quad b_r = \int_{-\pi}^{\pi} d^d q (2\pi)^{-d} e^{-irq}\Gamma(q), \quad \gamma(q) = \frac{1}{z} \sum_p e^{ipq} \]

\[ b_1 = \int_{-\pi}^{\pi} d^d q (2\pi)^{-d} \gamma(q)\Gamma(q), \quad X_1 \equiv \sum_r b_r b_{r+p} = \int_{-\pi}^{\pi} d^d q (2\pi)^{-d} \gamma(q)\Gamma^2(q) \]

leading to

\[ a\Gamma^2(q) + b\Gamma(q) + c = 0, \]

where

\[ a \equiv B\gamma(q), \quad b \equiv -A - 4Bb_1 + 2C\gamma(q), \]

\[ c \equiv [B(2b_1^2 + 2g_4 + 1) + Ab_1]\gamma(q) + Bg_4\gamma(3q) - BX_1 - 2Cb_1 \]

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.

Results for the ground state energy using the SUB2 and SUB2+LSUB4 approximation schemes are shown in Figures 1 and 3, 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 \( \gamma \). 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 \( \gamma = -0.10789 \) in SUB2 and at \( \gamma = -0.09605 \) in SUB2+LSUB4. In 2D there is a terminating point at \( \gamma = -0.03033 \) in SUB2. These 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 Magnetisation

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

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

(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

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

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:

$$\frac{\partial \bar{H}}{\partial \tilde{b}_r} = N \sum_p \left[ 2B \sum_{r'} \tilde{b}_{r',r,-r+p} - (A + 4Bb_1) \tilde{b}_r + 2C \tilde{b}_{r-p} 
+ (B + (A + 4Bb_1) \tilde{b}_1 - 4B \sum_{r'} \tilde{b}_{r',r,p} \delta_{p,r} 
+ \tilde{g}_4 / 2 \left[ 4A(b_1 + b_3) - 8B(b_2 b_4 + b_2^3) - 16Bg_4 - 16Cb_2 \right] \delta_{p,r} 
+ [12Ab_2 - 8B(b_1 b_4 + 2b_2 b_3) - 8C(2b_1 + b_3)] \delta_{2p,r} 
+ [4Ab_1 - 8B(2b_1 b_3 + b_2^2) - 4Bg_4 - 8Cb_2] \delta_{3p,r} 
- 8Bb_1 b_2 \delta_{4p,r} + 4Bg_4 \delta_{5p,r} \right] = 0$$

(9)

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

(10)

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

Finally the results are used to calculate the magnetisation using the formula for SUB2:
\[ M = -2\langle \bar{\psi} | s_i^z | \psi \rangle = 1 - 2 \sum_r \bar{b}_r b_r \]

and for SUB2+LSUB4:

\[ M = -2\langle \bar{\psi} | s_i^z | \psi \rangle = 1 - 2 \sum_r \bar{b}_r b_r - 8g_4\bar{g}_4 \]

3. Excitations

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

\[ X_1 = \sum_i X_i s_i^+ , \quad i \text{ belongs to one sublattice only} \]

leading to

\[ \langle \Phi | s_i^- e^{-S[H,X_1]} - e^S | \Phi \rangle = -\frac{1}{2} z(A + 4Bb_1)X_i + B \sum_{r,p} b_r X_{i+r+p} = \varepsilon_i X_i \quad (11) \]

and hence, via Fourier transform

\[ \Rightarrow \varepsilon(q) = -\frac{1}{2} z(A + 4Bb_1) + Bz\gamma(q)\Gamma(q) \quad (12) \]

4. General spin \( s \), (SUB2 only)

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

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

\[ \langle \Phi | s_i^- s_{i+r}^- e^{-S[H,e^S]} | \Phi \rangle = 4s^2 \sum_p \left[ 4s^2 B \sum_{r'} b_r b_{r-r'+p} - 2s(A + 4Bb_1)b_r + 4sCb_{r-p} \right. \\
+ \left. (B(2b_1^2 + 1) + Ab_1)\delta_{p,r} \right] = 0 \quad (13) \]

and the energy is

\[ \langle \Phi | e^{-S[H,e^S]} | \Phi \rangle = 2s^2 zN \left( \frac{1}{4} A + b_1 B \right) \quad (14) \]
Using these equations we find for the ground-state energy per spin of the \( s = 1 \) system at the \( \gamma = 0 \) point the value \(-1.09179\). This compares with a numerical result from extrapolating rings with \( N \leq 14 \) of \(-1.1157 \pm 0.0003\). 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

\[
\frac{\partial \tilde{H}}{\partial \tilde{b}_r} = 4s^2N \sum_p \left[ 8s^2B \sum_{r'} \tilde{b}_{r'}\tilde{b}_{r'-p} - 2s(A + 4Bb_1)\tilde{b}_r + 4sC\tilde{b}_{r-p} 
+ (B + (A + 4Bb_1)\tilde{b}_1 - 8sB \sum_{r'} \tilde{b}_{r'}\tilde{b}_{r'})\delta_{p,r} \right] = 0
\]  

(15)

Finally the magnetisation is given by:

\[
M = -\frac{1}{s} \langle \tilde{\Psi}|s_z^x|\Psi \rangle = 1 - 4s \sum_r \tilde{b}_r b_r
\]  

(16)

5. The LSUB\( n \) Approximation

The LSUB\( n \) 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 less 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 LSUB\( n \) 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 Eq. (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 LSUB\( n \) approximation to include 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 lattice and the Hamiltonian have identical symmetries for the XY model.

Tables 1, 2, and 3 show the numbers of fundamental configurations for given LSUB\( n \) 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 LSUB\( n \) equations computationally also. A full explanation of the computational method used here is given in Zeng et al. (1997). It is now possible to obtain values for the ground-state energy and sublattice magnetisation for the LSUB\( n \) approximation scheme. Results for these quantities are given in Figs.
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 magnetisation has also been carried out by plotting the ground-state energy against $1/n^2$ and the sublattice magnetisation against $1/n$, and then performing polynomial fits on this data. The extrapolated LSUB$\infty$ results obtained from this simple, ‘naive’ approach are shown in Tables 1, 2, and 3. The results are clearly at least as good as 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 ground state of the system (Zeng et al., 1997), and the results for given LSUB$n$ approximation level 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 be (in all dimensions), with increasing approximation level. Again, a simple extrapolation of the LSUB$n$ critical points is attempted by plotting $\gamma_c(n)$ against $1/n^2$, as in Bishop et al. (1994), and the extrapolated results are also shown in Tables 2 and 3.

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Figure captions

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

Fig.2
Results for the CCM ground-state sublattice magnetisation of the one dimensional $XY$ model.

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

Fig.4
Results for the CCM ground-state sublattice magnetisation of the square lattice $XY$ model.
Table 1: Ground-state energy and sublattice magnetisation 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 $\text{LSUB} n$ approximation level.

| $\text{LSUB} n$ | $N_f$ | $E_g/N$   | $M$     |
|-----------------|-------|-----------|---------|
| $\text{LSUB}2$ | 1     | -0.303813 | 0.837286|
| $\text{SUB}2$  |       | -0.310377 | 0.779517|
| $\text{LSUB}4$ | 4     | -0.314083 | 0.722916|
| $\text{LSUB}6$ | 13    | -0.316301 | 0.660064|
| $\text{LSUB}8$ | 43    | -0.317137 | 0.617624|
| $\text{LSUB}10$| 151   | -0.317542 | 0.586067|
| $\text{LSUB}\infty$ |       | -0.31829  |          |
| Exact           |       | -0.318310 | 0.0      |

Table 2: Ground-state energy and sublattice magnetisation for the square lattice XY model at $\gamma = 0$ compared to series expansion calculations of Hamer, Oitmaa and Zheng [2]. $N_f$ indicates the number of fundamental configurations for a given $\text{LSUB} n$ approximation level, and also shown are the critical values of $\gamma$ for the anisotropic model – where the value in parentheses is the estimated error in the final decimal place shown.

| $\text{LSUB} n$ | $N_f$ | $E_g/N$   | $M$     | $\gamma_c(n)$ |
|-----------------|-------|-----------|---------|----------------|
| $\text{LSUB}2$ | 1     | -0.540312 | 0.949634|                |
| $\text{SUB}2$  |       | -0.546325 | 0.918953| -0.030(1)      |
| $\text{LSUB}4$ | 10    | -0.547267 | 0.915768| -0.175(1)      |
| $\text{LSUB}6$ | 131   | -0.548329 | 0.901357| -0.073(1)      |
| $\text{LSUB}8$ | 2793  | -0.548616 | 0.893665| -0.04(1)       |
| $\text{LSUB}\infty$ |       | -0.54892  | 0.869   | 0.00(1)        |
| Series Expansion |       | -0.5488   | 0.872   | 0.0            |

Table 3: Ground-state energy and sublattice magnetisation for the cubic lattice XY model at $\gamma = 0$. $N_f$ indicates the number of fundamental configurations for a given $\text{LSUB} n$ approximation level, and also shown are the critical values of $\gamma$ for the anisotropic model – where the value in parentheses is the estimated error in the final decimal place shown.

| $\text{LSUB} n$ | $N_f$ | $E_g/N$   | $M$     | $\gamma_c(n)$ |
|-----------------|-------|-----------|---------|----------------|
| $\text{LSUB}2$ | 1     | -0.786866 | 0.971488|                |
| $\text{SUB}2$  |       | -0.790901 | 0.958282| -0.01666(1)    |
| $\text{LSUB}4$ | 13    | -0.791224 | 0.958648| -0.172(1)      |
| $\text{LSUB}6$ | 327   | -0.791702 | 0.954759| -0.071(1)      |
| $\text{LSUB}\infty$ |       | -0.79201  | 0.948   | 0.01(1)        |
\[ \frac{E_g}{N} \]

\[ \gamma \]

Graph showing the relationship between \( \frac{E_g}{N} \) and \( \gamma \). The graph includes curves labeled as LSUB2, LSUB4, LSUB10, SUB2, SUB2+LSUB4, and Exact. The exact values of the points are not provided in the image.
