AB INITIO CALCULATIONS OF THE
SPIN-HALF XY MODEL

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Abstract

In this article, the correlated basis-function (CBF) method is applied for the first time to the quantum spin-half XY model on the linear chain, the square lattice, and the simple cubic lattice. In this treatment of the quantum spin-half XY model a Jastrow ansatz is utilised to approximate the ground-state wave function. Results for the ground-state energy and the sublattice magnetisation are presented, and evidence that the CBF detects the quantum phase transition point in this model is also presented. The CBF results are compared to previous coupled cluster method (CCM) results for the spin-half XY model, and the two formalisms are then compared and contrasted.

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

\begin{equation}
H = \frac{1}{8} \sum_{i,j} \left[(1 + \gamma)\sigma_i^x \sigma_j^x + (1 - \gamma)\sigma_i^y \sigma_j^y \right],
\end{equation}

in the regime $0 < \gamma \leq 1$. Note that the index $i$ runs over all $N$ lattice sites and that the index $j$ runs over the $z$ nearest-neighbour to $i$ on the linear chain ($z = 2$), the square lattice ($z = 4$), and the cubic lattice ($z = 6$).

In the regime $0 < \gamma \leq 1$ the ground state is believed to exhibit Néel ordering in the $x$-direction, and for $-1 < \gamma \leq 0$ the ground state is again believed to possess Néel ordering in the $y$-direction. We note that a phase transition point occurs for the linear chain model at exactly $\gamma = 0$, and that Néel ordering is found to disappear at this point. For spatial dimensionality greater than one, the phase transition point of the anisotropic model is also believed to be at (or
very near to) $\gamma = 0$ from approximate calculations. The ground state of the spin-half XY model on the square and cubic lattices at $\gamma = 0$ is also believed to be Néel-ordered in the $xy$-plane.

The spin-half XY model was solved exactly by Lieb, Schultz and Mattis for the linear chain using the Jordan-Wigner transformation. Since then the ground- and excited-state properties have been extensively studied by many authors (see, for examples, Refs. [2,3]). However, no exact results exist for higher spatial dimensionality, although approximate results such as those from spin-wave theory, Monte-Carlo (QMC) methods, series expansions and the coupled cluster method (CCM) has proven to be highly successful. Extrapolated finite size calculations have also been performed for $\gamma = 0$.

The correlated basis function (CBF) method is a widely applied and accurate method of modern-day quantum many-body theory. Recently, this method has been applied with great success to the Ising model in a transverse magnetic field at zero temperature. In this article we wish to apply the CBF method to the spin-half XY model. We begin this process by firstly performing a number of unitary transformations on the local spin axes on two sublattices $\{A, B\}$ in order to simplify the problem. The first such transformation on the $A$-sublattice is given by,

$$
\sigma_x \rightarrow \sigma_z ; \quad \sigma_y \rightarrow \sigma_x ; \quad \sigma_z \rightarrow \sigma_y ,
$$

and the second transformation on the $B$-sublattice is given by,

$$
\sigma_x \rightarrow -\sigma_z ; \quad \sigma_y \rightarrow -\sigma_x ; \quad \sigma_z \rightarrow \sigma_y .
$$

Note that both of these transformations are simply rotations of the local spin-axes of the spins, and that the eigenvalue spectrum of the problem is left unchanged because these transformations are unitary. The Hamiltonian may now be rewritten in terms of these new spin-axes as

$$
H = -\frac{1}{8} \sum_{i,j} \left[ (1 - \gamma)\sigma_i^x \sigma_j^x + (1 + \gamma)\sigma_i^z \sigma_j^z \right] .
$$

We may now define a ground-state trial wave function, given by

$$
|\psi\rangle = \exp(U) \mid 0 \rangle ; \quad U = \frac{1}{2} \sum_{i<j} u(\mathbf{r}_{ij}) \sigma_i^x \sigma_j^x ,
$$

where $u(\mathbf{r}_{ij})$ is the pseudopotential. The reference state $\mid 0 \rangle$ is given by a tensor product of spin states which have eigenvalues of $+1$ with respect to $\sigma^z$, and this state is an exact ground eigenstate of the Hamiltonian Eq. when $\gamma = 1$. Translational invariance also implies that the pseudopotential, $u(\mathbf{r}_{ij})$, depends only on the relative distance, $\mathbf{n} = \mathbf{r}_i - \mathbf{r}_j \equiv \mathbf{r}_{ij}$. 

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The treatment of the spin-half \(XY\) model by the CBF method is continued by defining the lattice magnetisation (i.e., again the magnetisation in the \(z\)-direction in terms of the rotated local spin-axes), given by

\[
M = \frac{\langle \psi | \sigma^z_i | \psi \rangle}{\langle \psi | \psi \rangle},
\]
for a ground-state trial wave function, \(|\psi\rangle\). Furthermore, the ‘transverse’ magnetisation (in terms of the rotated local spin-axes) is given by,

\[
A = \frac{\langle \psi | \sigma^x_i | \psi \rangle}{\langle \psi | \psi \rangle}.
\]

We may now define a spatial distribution function (which plays a crucial part in any CBF calculation) in the following manner,

\[
G(n) = \frac{\langle \psi | \sigma^x_i \sigma^x_j | \psi \rangle}{\langle \psi | \psi \rangle}.
\]

Furthermore, we may also determine an expression for the expectation value of the ground-state energy of the spin-half \(XY\) Hamiltonian of Eq. (4), where

\[
E_N = \frac{\langle \psi | H | \psi \rangle}{N \langle \psi | \psi \rangle}.
\]

In the region \(\gamma \geq 0\) we now make the explicit assumption that \(A = 0\), which is in agreement with our Ansatz for the trial wave function of Eq. (2). This assumption furthermore implies that \(A/N = \langle P^+ - P^- \rangle = \rho^+ - \rho^- = 0\), where \(P^+\) and \(P^-\) are spin projection operators in the positive and negative \(x\)-directions respectively. However, we note that \(\rho^+ + \rho^- = 1\) must also be correct, which therefore implies that \(\rho^+ = \rho^- = 1/2\). Hence, we may treat this problem completely analogously to a binary-mixture of two types of bosons each with a density equal to one-half.

The expression in Eq. (9) may be determined via a hyper-netted chain (HNC) cluster expansion, and it is readily found using this procedure that the ground-state energy is given in terms of a functional with respect to the pseudopotential, \(u(n)\), where

\[
\frac{E}{N} = \frac{1}{8} \sum_n \Delta(n) \left[ (1 - \gamma) G(n) + (1 + \gamma) M^2 \cosh[u(n)] \right].
\]

Note that \(\Delta(n)\) is unity if \(n\) is a nearest-neighbour vector and is zero otherwise.

Self-consistent HNC equations may also be determined. These equations may be then iteratively solved, and thus \(G(n)\) (and so the ground-state energy) may be also obtained. The first method of finding the pseudopotential has a “variational” flavour, and we parametrise \(u(n)\) in the following way,

\[
u(n) = \alpha \Delta(n).
\]
$\Delta(n)$ is unity if $n$ is a nearest-neighbour vector and is zero otherwise. We now minimise the ground-state energy with respect to $\alpha$ at a given value of $\gamma$. Indeed, at $\gamma = 1$ we already know that all correlations have zero strength as our reference state $|0\rangle$ is an exact ground eigenstate of Eq. (4), and this implies that $\alpha = 0$. We thus track this solution at $\gamma = 1$ in the regime $\gamma < 1$, and the ground-state energy as a function of $\alpha$ for various values of $\gamma$ is plotted in Fig. 1 for the square lattice. We may see that at $\gamma = -0.36$ the minima that we have tracked from $\gamma = 0$ become a point of inflection.

The second such method of determining the pseudopotential is to determine the optimal value for the function $u(n)$ with respect to the ground-state energy, $E/N$. This is stated as,

$$\frac{\delta E}{\delta u(n)} = 0,$$

which may be determined analytically from Eq. (10). In the context of this article, this approach shall be referred to as the Paired-Phonon Approximation (PPA), in analogy with a binary mixture of two types of bosons, for example. Note that we do not explicitly state here the resulting PPA equations for this model, although the treatment is fully analogous to that performed for the transverse Ising model and the interested reader is referred to Ref. [22] for a full account of this calculation.

For details of the specific application of the CCM to the spin-half $XY$ model the interested reader is referred to Ref. [8]. We note however that two types
Figure 2: CBF results for the ground-state energy of the spin-half XY model on the square lattice compared to results of high-order CCM results of Ref. [8].

of approximations are made, namely, the SUB2 approximation which retains all two-body correlations in the approximate CCM ground-state wave function, and the LSUB\textit{m} which retains all correlations in a locale defined by \textit{m}.

Results for the CBF ground-state energy of the spin-half XY model on the square lattice compared to results of high-order CCM results are given in Fig. \ref{fig:energy} and, for the isotropic point (\(\gamma = 0\)) only, in Table \ref{tab:results}. We may see from Fig. \ref{fig:energy} that both sets of results are in excellent qualitative agreement over a wide range of \(\gamma\). It is furthermore seen from Tables \ref{tab:results} that CBF results are in excellent quantitative agreement with LSUB2 CCM results at \(\gamma = 0\). This is a perfectly reasonable result because both the CBF and CCM LSUB2 results only utilise two-body correlations. It is, however, expected that the inclusion of higher-order correlations in the CBF trial wave function would produce more accurate results for the energy, as is seen for the CCM. Thus, from Tables \ref{tab:results} we see that the CBF results at \(\gamma = 0\) capture about 59\% of the correlation energy for the linear chain, 76\% of the correlation energy for the square lattice and 85\% of the correlation energy for the cubic lattice (in comparison with exact and extrapolated CCM results). Indeed, the extrapolated CCM results present some of the most accurate results yet seen for the isotropic XY model on the square and cubic lattices. (Results for the linear chain and cubic lattice are qualitatively similar to the results presented for the square lattice in Fig. \ref{fig:energy} and so are not plotted here.)

Results for the sublattice magnetisation of the spin-half XY model on the square lattice are presented in Fig. \ref{fig:magnetisation} and in Table \ref{tab:results} for the isotropic point,
\[ \gamma = 0 \]. Again, it is seen from Fig. 3 that the CBF results are in good qualitative agreement with the known results of this model. However, the CBF result for the sublattice magnetisation at the isotropic point \((\gamma = 0)\) is slightly too high, although it is again expected that higher accuracy would be achieved with the inclusion of higher-order correlations in the approximate CBF ground-state wave function. Again, results for the linear chain and cubic lattice are fully analogous to the square lattice case and so are presented only for the isotropic model in Tables 1 and 3.

Results for the phase transitions points predicted by the CCM method are also given in Tables 1-3, although no such results are explicitly given for the CBF method in these tables. It is however noted here that the loss of “minima” within the parametrized HNC CBF approach (at \(\gamma = -0.36\) for the square lattice) may be associated with a phase transition within this system. This constitutes a powerful result for such a simple variational-style calculation. Note that similar behaviour is also seen for both the linear chain and cubic lattices. An analogous change in the energy surface with respect to \(u(n)\) for the CBF PPA approach seems to occur for varying values of \(\gamma\). However, in this case, the situation is much less clear-cut because, near to this point, convergence of the PPA equations becomes very difficult.

In this article, the CBF method has been applied with much success to the quantum spin-half \(XY\) model on the linear chain, the square lattice, and the cubic lattice in order to obtain accurate results for the ground-state energy and the sublattice magnetisation. These results were found to be in excellent qualita-
Table 1: Ground-state energy and sublattice magnetisation for the one-
dimensional $XY$ model at $\gamma = 0$ compared to exact results of Ref. [3] and
CCM results of Ref. [8]. The critical values of $\gamma$ for the anisotropic model are
also given.

| $\text{LSUB}\ n$ | $E_g/N$ | $M$ | $\gamma_c(n)$ |
|----------------|--------|-----|--------------|
| Parametrised CBF | $-0.29025$ | $0.8919$ | $-$ |
| PPA CBF | $-0.29030$ | $0.8904$ | $-$ |
| LSUB2 | $-0.30381$ | $0.8373$ | $-$ |
| SUB2 | $-0.31038$ | $0.7795$ | $-0.10789$ |
| LSUB$\infty$ | $-0.31829$ | $-$ | $-$ |
| Exact | $-0.318310$ | $0.0$ | $0$ |

We note that the CBF approach utilises a Jastrow wave function and its
bra states are always the explicit Hermitian adjoint of the corresponding ket
state. Hence, for the CBF approach, an upper bound to the true ground-state
energy is, in principle, obtainable, although the approximations made in calcu-
lating the energy may destroy it. By contrast, the CCM uses a bi-variational
approach in which the bra and ket states are not manifestly constrained to be
Hermitian adjoints and hence an upper bound to the true ground-state energy is
not necessarily obtained. Also, the CCM uses creation operators with respect to
Table 2: Ground-state energy and sublattice magnetisation for the square lattice $XY$ model at $\gamma = 0$ compared to CCM calculations of Ref. [8] and series expansion calculations of Ref. [7]. The critical values of $\gamma$ for the anisotropic model are also given, where the value in parentheses is the estimated error in the final decimal place shown.

| $L_{SUB}n$   | $E_g/N$   | $M$     | $\gamma_c(n)$ |
|--------------|-----------|---------|----------------|
| Parametrised CBF | $-0.53738$ | 0.9524  |                |
| PPA CBF      | $-0.53774$ | 0.9515  |                |
| LSUB2        | $-0.54031$ | 0.9496  |                |
| SUB2         | $-0.54633$ | 0.9190  | $-0.030(1)$    |
| LSUB$\infty$ | $-0.54892$ | 0.869   | 0.00(1)        |
| Series Expansion | $-0.5488$   | 0.872   |                |

some suitably normalised model state in order to span the complete set of (here) Ising states. The CBF method, in essence, uses projection operators to form the Jastrow correlations with respect to a reference state, $|0\rangle$. In some sense, the CCM is found to contain less correlations than the others at ‘equivalent’ levels of approximation (e.g., the CCM LSUB2 approximation versus Hartree and nearest-neighbour Jastrow correlations). A strength of the CCM is that it is well-suited to the inclusion of high-order correlations in the approximate ground-state wavefunction (for example, via computational techniques). Furthermore, the CCM requires no information other than the approximation in $S$ and $\tilde{S}$ in order to determine an approximate ground state of a given system. The CBF method, however, may require that only a certain subset of all possible diagrams are summed over (e.g., the HNC/0 approximation).

We finally note that the results of one method reinforce and sometimes elucidate the results of the other, and the application, in parallel, of two such methods to the same model can lead to a deeper understanding of the behaviour of it.

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Table 3: Ground-state energy and sublattice magnetisation for the cubic lattice XY model at $\gamma = 0$ compared to CCM results of Ref. [8]. The critical values of $\gamma$ for the anisotropic model are also given, where the value in parentheses is the estimated error in the final decimal place shown.

| $\text{LSUB}_n$ | $E_g/N$  | $M$   | $\gamma_c(n)$ |
|----------------|---------|-------|----------------|
| Parametrised CBF | $-0.78572$ | 0.9710 | --             |
| PPA CBF          | $-0.78625$ | 0.9695 | --             |
| $\text{LSUB2}$  | $-0.78687$ | 0.9715 | --             |
| $\text{SUB2}$   | $-0.79090$ | 0.9583 | $-0.01666(1)$  |
| $\text{LSUB}\infty$ | $-0.79201$ | 0.948 | $0.01(1)$      |

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