A complete Hartree-Fock mean field method for spin systems at finite temperatures

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Abstract

We develop a complete Hartree-Fock mean-field method to study ferromagnetic systems at finite temperatures. With the help of the complete Bose transformation, we renormalize all the high-order interactions including both the dynamic and the kinetic ones based on an independent Bose representation, and obtain a set of compact self-consistent equations. Using our method, the spontaneous magnetization of an Ising model on a square lattice is investigated. The result is quite close to the exact one. Finally, we discuss the temperature dependences of the coercivities for magnetic systems and show the hysteresis loops at different temperatures. © 1997 Elsevier Science B.V.

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1. Introduction

Spin systems have long been an interesting and challenging subject. Experimentally, many interesting effects are strongly related to the magnetic order, such as the high-$T_c$ superconductivity, the giant magnetoresistance effect, the giant magneto-impedance effect, the magnetic-optical recording, etc. Many theoretical methods have been developed for magnetic systems. The traditional approaches are the Holstein-Primakoff (HP) [1] transformation and the Dyson-Maleev (DM) [2,3] one, by which one can project the spin operators into Bose ones so as to study the low-lying Bose-like excitations. Such methods are found to be successful at very low temperatures and for ferromagnetic systems. At finite temperatures or for antiferromagnetic systems, high-order interactions should be considered to renormalize the effective excitation spectrum. Some authors have recently employed a Green's function method (for Bose operators) to renormalize the remaining interaction terms left in the DM transformation [4]. However, their method neglects the kinetic interactions. Since the Hilbert space of the spin operator is not the same as that of a Bose one, there must be a constraint in the transformation to confine the Hilbert space to a finite range ($|n|, n < 2S + 1$). As a result, the remaining interactions are not only the dynamic ones, which have been included in the traditional transformations, but also the additional kinetic ones which are introduced by...
the constraints. Some authors have even applied a so-called well-ordered HP transformation to get the $H_4$ terms which includes the kinetic interactions [5], and then considered the renormalization of the thermally excited spin waves using a conventional Hartree–Fock approximation [6–9]. However, since the interaction terms are actually infinite, when the temperature is not very low, interacting terms higher than $H_4$ probably become significant. Therefore, these methods cannot be applied to a not very low temperature region.

To systematically treat the kinetic interactions, a new approach, the complete Bose transformation (CBT), was established with the help of the step operator's technique [10]. In the zero-temperature case, a schematic approximation method has been developed to consider both the dynamic and the kinetic interactions perturbatively [10], and the method has been applied to study the ground state energy of a spin-$\frac{1}{2}$ antiferromagnet on a square lattice [11] and the induced magnetization of an easy-plane spin-1 ferromagnet [12]. The ground state energy of the system is quite close to the numerical result [11].

In this paper, we would like to extend that method to the finite temperature case, and use it to discuss the temperature dependence of the coercivity which is interesting for recording materials. Based on the CBT, we renormalize the thermally excited spin waves using a Hartree–Fock approximation considering all the remaining interactions included by the local constraints. The self-consistent equations for a general anisotropic ferromagnet are presented in compact forms. With the help of this method, we examine the temperature dependence of the spontaneous magnetization for an Ising model on a square lattice, and show that it agrees well with the exact result. Other systems, including the isotropic Heisenberg models, have also been investigated, the results show that the temperature region of application of the current method is larger for the magnetic system with a higher anisotropy. Finally, we present the temperature dependence of the coercivity for a magnetic system, and compare the hysteresis loops at different temperatures.

This paper is organized as follows. In Section 2, the model Hamiltonian and the complete Bose transformation will be introduced. Then, the complete Hartree–Fock (CHF) approximation is described in Section 3. Section 4 is devoted to the discussions of the results, while the conclusions are summarized in the last section.

2. The model and the transformation

The model we study in this paper is a ferromagnetic model with anisotropic interactions. In general, the Hamiltonian can be presented as

$$H = \sum_{\langle i,j \rangle} H_{\langle i,j \rangle}(S)$$

$$= -\sum_{\langle i,j \rangle} \left[ J_z S_i^z S_j^z + \frac{1}{2} J_{xy} (S_i^+ S_j^- + S_i^- S_j^+) \right]$$

$$- D \sum_i (S_i^z)^2 - h \sum_i S_i^z.$$  \hspace{1cm} (1)

The zero-temperature properties of such systems can be obtained very straightforwardly. An HP transformation is popularly used to investigate the ground state and the low-lying spin wave excitations. At very low temperatures, one uses Bose statistics to incorporate the thermal effect [13]. However, if the temperature is not so low, this method cannot be applied and the renormalization by the thermally excited bosons must be taken into account. In the present paper, we will apply the CBT instead of the HP transformation to take account of the dynamic interactions as well as the kinetic interactions. Following Ref. [10], the CBT of the spin operator is given as

$$S_i^z \rightarrow S_i^+ = (S - a_i^\dagger a_i) \theta_i = \sum_{l=0}^{\infty} D_l a_i^{(l+1)} a_i^\dagger,$$  \hspace{1cm} (2)

$$S_i^+ \rightarrow S_i^+ = \sqrt{2S - a_i^\dagger a_i} \theta_i = \sum_{l=0}^{\infty} C_{l+1} a_i^{(l+1)} a_i^\dagger,$$  \hspace{1cm} (3)

$$S_i^- \rightarrow S_i^+ = \theta_i a_i^\dagger \sqrt{2S - a_i^\dagger a_i} = \sum_{l=0}^{\infty} C_{l+1} a_i^{(l+1)} a_i^\dagger.$$  \hspace{1cm} (4)

where $\theta_i$ is a step operator to confine the Hilbert space into the physically permitted part ($|n\rangle, n < 2S + 1$). $C_l$, and $D_l$ can be found in Ref. [10] or be calculated following Ref. [10]. Other terms such as $(S_i^z)^2$ can be calculated similarly.

An exactly equivalent Hamiltonian can be found after the complete Bose transformation and a global constraint, namely.
$$H' = \sum_{(i,j)} \Theta_{i,j} \Theta_{j,i} H_{i,j}(S) \Theta_{i,j} \Theta_{j,i}$$

$$\equiv \sum_{(i,j)} \Theta_{i,j} H_{i,j}(\tilde{S}) \Theta_{j,i}, \quad (5)$$

where

$$\Theta_{(i,j)} = \prod_{k \neq i,j} \Theta_k, \quad (6)$$

$$H_{i,j}(\tilde{S}) = \theta_i \theta_j H_{i,j}(\tilde{S}) \theta_i \theta_j. \quad (7)$$

However, Hamiltonian $H'$ is very difficult to handle. Fortunately, it was proved in Ref. [10] that the following Hamiltonian has the same eigenvalues as the original Hamiltonian (1),

$$\hat{H} = \sum_{(i,j)} H_{i,j}(\tilde{S}), \quad (8)$$

so, in this paper, we will use this Hamiltonian to incorporate some kinetic interactions. After this transformation, we obtain

$$\hat{H} = \hat{H}_0 + \hat{H}_2 + \hat{H}_4 + \ldots \quad (9)$$

The harmonic part of Hamiltonian has the following form,

$$\hat{H}_2 = \sum_{(i,j)} \left[ J_z (a_i^\dagger a_i + a_j^\dagger a_j) + J_{xy} (a_i^\dagger a_j + a_j^\dagger a_i) \right]$$

$$+ \left[ (2S-1)D + h \right] \sum_i a_i^\dagger a_i, \quad (10)$$

which is the same for all the spin-Bose transformations. The interacting terms, even the $H_4$ term, are different due to the constraints. For example, in the usual HP transformation, $H_4$ can be obtained by a usual large-$S$ expansion as follows [14],

$$H_4 = -J_z \sum_{(i,j)} (\frac{3}{8} a_i^\dagger a_i^2 + a_j^\dagger a_j^2) + a_i^\dagger a_j^\dagger a_i a_j$$

$$+ \frac{1}{2} J_{xy} \sum_{(i,j)} [a_i^\dagger a_i^2 a_j^\dagger a_j + a_j^\dagger a_j^2 a_i a_i + h.c.]$$

$$- h \sum_i \frac{3}{8} a_i^\dagger a_i^2 \quad (11)$$

and for the $S = 1$ system, it is

$$H_4 = -J_z \sum_{(i,j)} (\frac{3}{8} a_i^\dagger a_i^2 + a_j^\dagger a_j^2) + a_i^\dagger a_j^\dagger a_i a_j$$

$$+ \frac{1}{2} J_{xy} \sum_{(i,j)} [a_i^\dagger a_i^2 a_j^\dagger a_j + a_j^\dagger a_j^2 a_i a_i + h.c.] - D \sum_i a_i^\dagger a_i^2. \quad (12)$$

Comparing Eq. (11) with Eqs. (12), (13), one may find that the additional contribution is non-trivial even for the $H_4$ term. Later we will show that the additional interacting terms included by the CBT become significant when the temperature increases and considering them will highly improve the final result.

3. The complete Hartree–Fock mean field method

In this section, we will introduce the Hartree–Fock approximation.

In the zero-temperature case, it is reasonable to diagonalize $\hat{H}_2$ to get the one-boson spin wave excitations, high-order interactions (both dynamic and kinetic) make no contribution to these eigenstates. In the finite temperature case, however, things are different. Even the one-boson excitations would be substantially modified by the interactions since they depend on other excitations present. It is surely impossible to take all kinds of renormalization into account since the interacting terms are infinite. so we will only consider the Hartree–Fock like renormalization from all the remaining interactions, and sum them in the end. The self-consistent equations are obtained in compact forms.

Introduce the ansatz that the renormalized independent boson representation (RIBR) has the following form,
\[ H \simeq U_0'(T) + \sum_{(i,j)} [J^R_x(T) \langle a_i^+ a_i + a_i^+ a_j \rangle \\
- J^R_{xy}(T) \langle a_i^+ a_j + a_i^+ a_j \rangle \\
+ [D^R(T) + h^R(T)] \sum_i a_i^+ a_i, \quad (14) \]

where \( J^R_x(T), J^R_{xy}(T), D^R(T), h^R(T) \) are the renormalized values of the interaction parameters, which will be self-consistently determined later.

The RIBR can be diagonalized by a Fourier transformation

\[ H = U_0'(T) + \sum_k \epsilon_k^R(T) a_k^+ a_k, \quad (15) \]

where

\[ \epsilon_k^R(T) = 2SZ [ J^R_x(T) - J^R_{xy}(T) \gamma_k ] \\
+ D^R(T) + h^R(T) \]

in which \( \gamma_k = (1/Z) \sum_\delta \exp(ik \cdot r_\delta) \) and \( Z \) is the number of nearest neighbors.

In this representation, only the following two terms contribute,

\[ n(T) = \langle a_i^+ a_i \rangle = \frac{1}{N} \sum_k \langle a_k^+ a_k \rangle \\
= \frac{1}{N} \sum_k \exp(\beta \epsilon_k^R) - 1, \quad (17) \]

\[ g(T) = \langle a_i^+ a_j^+ a_i a_j \rangle = \frac{1}{N} \sum_k \langle \cos(k \cdot [r_i - r_j]) \rangle \langle a_k^+ a_k \rangle \\
= \frac{1}{N} \sum_k \cos(k \cdot [r_i - r_j]) \frac{1}{\exp(\beta \epsilon_k^R) - 1}, \quad (18) \]

other terms such as \( \langle a_i^+ a_j^+ \rangle, \langle a_i^+ a_j^+ \rangle, \langle a_i a_i \rangle \) and \( \langle a_i a_i \rangle \) are zero.

Based on the Hartree–Fock approximation, all the high-order terms can be decoupled into harmonic ones. According to Eqs. (17), (18), we get generally

\[ \langle a_i^+ a_j^+ a_i^+ a_j^+ \rangle \sim \langle a_i^+ a_i \rangle (l + 1) (k + 1) \times \langle a_i^+ a_j^+ a_j^+ \rangle \\
+ \langle a_i^+ a_j^+ \rangle \times \langle a_i^+ a_j^+ a_i^+ a_j^+ \rangle \\
+ \langle a_i^+ a_i \rangle (l + 1) \times \langle a_i^+ a_j^+ a_j^+ \rangle \\
+ \langle a_i^+ a_j \rangle (k + 1) \times \langle a_i^+ a_j^+ a_i^+ a_j^+ \rangle, \quad (19) \]

Every expectation value can be calculated exactly in the RIBR with the help of Wick’s theorem. For example,

\[ \langle a_i^+ a_j^+ a_i^+ a_j^+ \rangle = [l!/n_1] [k!/n_2] \\
+ g^2 [l!/n_1^{-1}] [k!/n_2^{-1}] + \ldots \\
+ \left( \frac{g^2}{m!} \right)^2 [l \ldots (l - m + 1) l!n_1^{-m}] \\
\times [k \ldots (k - m + 1) k!n_2^{-m}] + \ldots, \quad (20) \]

Thus, all the terms in Eq. (9) can be decoupled into the harmonic ones following the method described above. Fortunately, those terms can be collected, and we finally get the analytical forms of the renormalized coefficients. Part of this technique has been presented in Refs. [10,11], we only give the final results as follows. For the \( S = \frac{1}{2} \) case, we have

\[ J^R_x(T) = J_x - \frac{1 + 2x}{(1 + n)^4 (1 - x)^4} \]

\[ J^R_{xy}(T) = 4g \frac{1 + x}{(1 + n)^4 (1 - x)^3}, \quad (23) \]

\[ J^R_y(T) = -J_y - \frac{1 + 3x}{(1 - x)^3 (1 + n)^4} \]

\[ J^R_z(T) = \frac{2 + x}{(1 - x)^4} \]

\[ D^R(T) = 0, \quad (24) \]

\[ h^R(T) = \frac{2}{(1 + n)^3}, \quad (25) \]

while in the case of \( S = 1 \), the functions are
\begin{align}
J_z^R(T) &= J_z \left( \frac{4(2 + 4x)}{(1 + n)^4(1 - x)^4} 
+ \frac{3(1 + 6x + 3x^2)}{(1 + n)^6(1 - x)^6} \right.
\nonumber
&\quad \left. - \frac{10 + 34x + 4x^2}{(1 + n)^6(1 - x)^5} \right) 
\nonumber
- J_{xy} g \left( \frac{(2 + \sqrt{2})(10 + 2x)}{(1 + n)^6(1 - x)^4} 
\nonumber
- \frac{2(2 + \sqrt{2})^2}{(1 + n)^5(1 - x)^3} \right. 
\nonumber
&\quad \left. - \frac{12(1 + x)}{(1 + n)^7(1 - x)^5} \right), 
\label{eq:27}
\end{align}

\begin{align}
J_x^R(T) &= \frac{1}{2} J_x \left( \frac{(2 + \sqrt{2})^2(1 + 3x)}{(1 + n)^4(1 - x)^3} 
\nonumber
- \frac{2(2 + \sqrt{2})(2 + 10x)}{(1 + n)^5(1 - x)^4} \right. 
\nonumber
&\quad \left. + \frac{4 + 34x + 10x^2}{(1 + n)^6(1 - x)^5} \right) 
\nonumber
+ J_z g \left( \frac{4(2 + 2x)}{(1 + n)^6(1 - x)^4} + \frac{9 + 18x + 3x^2}{(1 + n)^8(1 - x)^5} \right) 
\nonumber
\nonumber
- \frac{24 + 24x}{(1 + n)^5(1 - x)^5}, 
\label{eq:28}
\end{align}

\begin{align}
D^R(T) &= D \frac{1 + 2n^2}{(1 + n)^4}, 
\label{eq:29}
\end{align}

\begin{align}
h^R(T) &= h \frac{1 + 4n}{(1 + n)^4}, 
\label{eq:30}
\end{align}

where

\begin{align}
x(T) &= \frac{g}{(1 + n)^2}. 
\label{eq:31}
\end{align}

Eqs. (23)-(30) are self-consistent equations. All the physical properties such as the ground state energy \( E(T) \), the spontaneous or induced magnetization \( M(T) \) and the effective magnon excitation spectrum \( \epsilon_k \) including the excitation gap \( \Delta = \min \{ \epsilon_k \} \) can be calculated as functions of temperature, provided that those equations have been solved. In the case \( S = \frac{1}{2} \), we have the following expressions,

\begin{align}
E(T) &= -J_z Z N \left( \frac{4(1 + x)}{(1 + n)^4(1 - x)^3} 
\nonumber
+ \frac{1 + x^2 + 4x}{(1 + n)^6(1 - x)^5} \right. 
\nonumber
&\quad \left. - \frac{4 + 8x}{(1 + n)^5(1 - x)^4} \right) 
\nonumber
- J_{xy} Z N g \left( \frac{(2 + \sqrt{2})^2}{(1 + n)^4(1 - x)^2} 
\nonumber
+ \frac{4 + 2x}{(1 + n)^6(1 - x)^4} \right. 
\nonumber
&\quad \left. - \frac{4(2 + \sqrt{2})}{(1 + n)^5(1 - x)^3} \right) 
\nonumber
- D N \frac{1 + 2n + 2n^2}{(1 + n)^3} - h N \frac{1 + 2n}{(1 + n)^3}, 
\label{eq:32}
\end{align}

\begin{align}
M(T) &= \frac{1 + 2n}{(1 + n)^3}, 
\label{eq:33}
\end{align}

4. Results and discussions

In this section, we shall study some systems using the method described in the last section and compare our method with other ones.

The first example is a two-dimensional Ising model (IM) on a square lattice. In this case, the model parameters are \( S = \frac{1}{2}, J_{xy} = 0, J_z = J, D = 0, h = 0 \). With the help of the complete Hartree–Fock (CHF) method, the spontaneous magnetization \( M(T) \) as a function of temperature is shown in Fig. 1, where the exact result [15], the linear spin wave theory (LSWT) result, and the usual HP method result are also shown for comparison. We find that in a very wide temperature range the CHF result agrees well with the exact result and is better than the other two results. From the figure, one may find a critical temperature \( T_c \) above which the CHF method cannot be applied. The critical temperature is a little lower than the Curie temperature \( T_c \) of the Ising model. This is reasonable. When the temperature approaches the phase transition point, an independent boson representation can never be valid and the correlations are important in this case. On the contrary, in the usual HP method which neglects the kinetic interactions, the result drastically deviates from the exact one when it approaches the Curie temperature.

We then study a spin-\( \frac{1}{2} \) Heisenberg model (HM) on a simple-cubic lattice. The temperature dependences of the spontaneous magnetization in the CHF method, in the LSWT method and in the usual HP method (\( J_{xy} \)
method, a spontaneous magnetization can still be non-zero when the temperature is higher than \( T_c \) (Fig. 2), which is unreasonable. The CHF method gives a qualitatively correct tendency in the high-temperature region, the independent boson representation can be found only in a region \( T < \tilde{T}_c \) (\( < T_c \)).

Some other systems have been studied using the CHF method. The critical temperatures \( \tilde{T}_c \) are listed in Table 1 where the Curie temperatures \( T_c \) of the same system are also listed for comparison. It is very interesting to find that the temperature region of application of the CHF representation (denoted by \( \tilde{T}_c / T_c \)) is larger for an Ising system than for a Heisenberg system. The physical explanation is that there is a large gap in the excitation of the Ising model. Since we only incorporate the local constraints in the transformed Hamiltonian (8), the many-boson states still have some components in the improper spin space. This is a fundamental deficiency of any spin-Bose transformation method. Fortunately, since there is a large gap in the excitation spectrum of the Ising models, the contribution of many-boson states is highly suppressed by the factor \( e^{\theta \Delta} \) and thus the errors arising in those terms are also much deduced. As result, the stronger the anisotropy of the magnetic systems, the larger the temperature region where the CHF method can be applied.

Since we have shown that the CHF method is reasonable for anisotropic magnetic systems, it is interesting to discuss the temperature dependence of the coercivity using this method. According to the quantum theory for coercivity [19], the coercive field is defined as the negative field at which the magnon excitation gap becomes zero, \( \Delta(T, h_c) = 0 \). As an illustration, in Fig. 3, the coercive field of a three-dimensional recording system has been shown as a function of the temperature, where the parameters are fixed at \( S = 1, J_z = J_{xy} = J, JZ/D = 3.0 \). The coercivity of a magnetic system decreases faster and faster as the temperature becomes higher. The hysteresis loops of the same systems are shown in Fig. 4 at different temperatures.

5. Conclusions

In conclusion, we have developed a complete Hartree–Fock mean field method to study anisotropic ferromagnets at finite temperatures. The Hamiltonian is presented in the Bose representation with the help
Table 1
Temperature regions where the complete Hartree–Fock method is applicable for various magnetic models

<table>
<thead>
<tr>
<th>Models</th>
<th>$K_B T_c/J$</th>
<th>$K_B T_c/J$</th>
<th>$T_c/T_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2d IM on square lattice</td>
<td>1.135 (^a)</td>
<td>1.047</td>
<td>0.923</td>
</tr>
<tr>
<td>2d IM on triangular lattice</td>
<td>1.822 (^b)</td>
<td>1.570</td>
<td>0.862</td>
</tr>
<tr>
<td>3d spin-$\frac{1}{2}$ HM on sc lattice</td>
<td>1.978</td>
<td>1.366</td>
<td>0.691</td>
</tr>
<tr>
<td>3d spin-$\frac{1}{2}$ HM on sc lattice</td>
<td>5.276</td>
<td>4.337</td>
<td>0.822</td>
</tr>
<tr>
<td>3d spin-$\frac{1}{2}$ HM on bcc lattice</td>
<td>2.871</td>
<td>1.856</td>
<td>0.647</td>
</tr>
<tr>
<td>3d spin-$\frac{1}{2}$ HM on bcc lattice</td>
<td>7.656</td>
<td>5.680</td>
<td>0.742</td>
</tr>
</tbody>
</table>

\(^a\) Exact result [13].
\(^b\) Obtained using renormalization group theory [13]. Others obtained using the Green’s function method [17].

![Fig. 3. Temperature dependence of the coercivity for a 3d spin-1 anisotropic ferromagnet.](image)

![Fig. 4. Comparison of the hysteresis loops at different temperatures. Solid line: a high temperature; dashed line: low temperature.](image)

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References