Induced magnetization of an easy-plane spin-one ferromagnet

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Abstract

The characteristic angle (CA) method, which was introduced in a previous work, is applied to calculate the induced magnetization of an easy-plane spin-one ferromagnet. The harmonic approximation which is often applied in a spin-Bose expansion is found to be invalid and may even lead to wrong physical results when calculating the induced magnetization of the easy-plane spin-one ferromagnet. Then the complete Bose transformation (CBT) is used to transform the spin operator into a Bose operator, so that high-order terms in the Bose expansion can be taken into account based on an independent Bose representation. Comparison of the result calculated by the CBT and by the harmonic approximation shows that high-order terms in the CBT are helpful in determining a reasonable ground state and getting accurate physical results. Diagrams of the induced magnetization versus the external magnetic field for a simple-cubic lattice are presented for small and large anisotropy, respectively.

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1. Introduction

Single-ion anisotropy \((D(S_i^z)^2)\) is often occurs in magnetic systems with spin greater than one half [1], and many methods have been developed to consider the thermodynamic properties of such magnetic systems [1-3]. For instance, in order to study the long-wavelength spin-wave excitation in random anisotropic magnetism (RAM), i.e. for a Heisenberg ferromagnet with randomly directed single-ion anisotropy [2], a method of introducing local coordinate systems (LC method) was applied to determine the spin configuration in the ground state by the variation method, then the spin-wave excitation was studied based on such a ground state using a Holstein-Primakoff (HP) transformation. However, this method was found to work well only when the single-ion anisotropy is the “easy-axis” case (i.e. \(D < 0\)). When the anisotropy is the “easy-plane” case (i.e. \(D > 0\)), this method was much worse [4]. In fact, for an easy-plane ferromagnet, which is a special kind of RAM with fixed anisotropic direction, if the LC method is applied to study the ground state properties of such a system, an imaginary or negative spin-wave excitation energy for the “\(k = 0\)” mode will always be encountered, no matter how weak the anisotropy parameter \((D)\) is. It is also useless to apply a HP transformation [5] naively to an easy-plane ferromagnet for the same reason. To overcome this difficulty, the matching of metrics elements method
(MME method) [3] was introduced for the easy-plane magnetic systems. Several authors have used this method to discuss various kinds of magnetic properties of such systems [3,6-9]. Recently, some numerical results of magnetization for an easy-plane spin-one ferromagnet have been worked out [10,11].

In Ref. [1], a new method, the characteristic angle (CA) method, was developed successfully for an easy-plane spin-one ferromagnet. In that paper, we took a harmonic approximation of the HP transformation to calculate the quantum properties of such a system in the case of a zero external magnetic field. Comparison with the MME method and the numerical result showed that the magnon dispersion relation for the CA method was the same as that for the MME method, and the spontaneous magnetization for the CA method was quite close to the numerical result [4], although that for the MME method not, especially for a large anisotropy parameter.

On the other hand, among various kinds of spin-Bose transformations, such as the HP transformation [5], Dyson-Maleev (DM) transformation [12,13] etc., the complete Bose transformation (CBT) [14] is one which can present high-order terms more precisely, because the constraint that the number of excited bosons should not exceed 2S has been considered in such a spin-Bose expansion through the use of the step operator technique [14]. Usually, a harmonic approximation is believed to be enough in the spin-Bose expansion when calculating the spin wave excitation in magnetic systems, but sometimes high-order contributions in the Bose expansion may become important, especially when the off-diagonal interactions are large. For example, it was shown in Ref. [15] that the ground state energy of a two-dimensional antiferromagnet on a square lattice became closer to the numerical result after considering high-order contributions by the CBT [15]. So, it may be interesting to discuss whether the high-order terms in the spin-Bose expansion are necessary or not in the magnetic systems, and how we can obtain a more precise result by considering the high-order contribution.

The main purpose of the present work is to calculate the induced magnetization of the easy-plane spin-one ferromagnet with the help of the CA method and to discuss what the improvements are to such a magnetic system brought by the high-order contributions in the spin-Bose expansion.

2. Calculation procedure

The Hamiltonian of an easy-plane spin-one ferromagnet is given as

\[ H = -J \sum_{(i,j)} S_i \cdot S_j + D \sum_i (S_i^z)^2 - h \sum_i S_i^z, \]  

where \((i,j)\) means summation restricted to nearest-neighbor pairs. The spins are forced into the YZ plane by the anisotropy term \((D > 0)\), which means that the spontaneous magnetized direction must be in the YZ plane. To discuss the induced magnetization of such a system, an external magnetic field has been applied along the Z axis \((-h \sum S_i^z)\).

The LC method [2] cannot provide a reasonable representation for such systems. Following Ref. [2], a local coordinates (LC) system \((\hat{x}_i, \hat{y}_i, \hat{z}_i)\) can be introduced in which the spin components in the original coordinate system are related to those in the LC system as follows,

\[ S_i^x = \cos(\theta) S_i^x + \sin(\theta) S_i^y, \]
\[ S_i^y = S_i^y, \]
\[ S_i^z = \sin(\theta) S_i^x - \cos(\theta) S_i^y. \]

We apply the transformation (3)–(5) to Hamiltonian (1), and then a HP transformation. Hamiltonian (1) will then be

\[ H = U_0 + H^{(1)} + H^{(2)} + \ldots, \]

\[ \theta \] can be obtained by minimizing the ground state energy, which is now substituted by \(U_0\) in the first-order approximation,

\[ \frac{d}{d\theta} U_0 = 0. \]

This yields

\[ D \sin(\theta) \cos(\theta) + h \sin(\theta) = 0. \]

Substitute the nontrivial solution of the above equation back into Eq. (6) and diagonalize the harmonic part of the corresponding Hamiltonian. We then find

\[ H = U_0 + \sum_k \bar{\epsilon}_k \alpha_k^\dagger \alpha_k + \ldots. \]

It is easy to check that the excitation energy \(\bar{\epsilon}_k\) will either be negative or imaginary for the \("k = 0"\) mode,
which means that the ground state must be unstable. So, the LC method fails to give a reasonable representation for an easy-plane spin-one ferromagnet.

However, the characteristic angle (CA) method was found to be a good approach for such a system [4], so we will use the CA method to discuss the induced magnetization of the easy-plane spin-one ferromagnet in this paper. Following Ref. [4], the CA transformation of the spin-one operator can be presented as

\[ S_i^x = \cos(\theta) \tilde{S}_i^x + \sin(\theta) \tilde{S}_i^y \exp(i\pi \tilde{S}_i^z), \]  

\[ S_i^y = \cos(\theta) \tilde{S}_i^y + \sin(\theta) \exp(-i\pi \tilde{S}_i^z) \tilde{S}_i^x, \]  

\[ S_i^z = \frac{1}{2} [\tilde{S}_i^+, \tilde{S}_i^-] - , \]

where \((\tilde{S}_i^-, \tilde{S}_i^+, \tilde{S}_i^z)\) is a set of CA spin operators which has been proved to obey the usual spin-one operator commutation rules [4]. \(\theta\) is the characteristic angle (CA) which is actually a variational parameter and which will be determined later by minimizing the ground state energy [4].

According to Ref. [14], the complete Bose transformation of the spin-one operators is given as

\[ \tilde{S}_i^+ = \sum_{l=0}^{\infty} \frac{(-1)^{2l+1} (l-\sqrt{2})}{l!} (a_i^+)^l (a_i^0)^{l+1}, \]

\[ \tilde{S}_i^- = \sum_{l=0}^{\infty} \frac{(-1)^{2l+1} (l+\sqrt{2})}{l!} (a_i^+)^l (a_i^0)^{l+1}, \]

\[ \tilde{S}_i^z = \sum_{l=0}^{\infty} \frac{(-1)^{2l+1} (l+1) (l-2)}{2l!} (a_i^+)^l (a_i^0)^{l+1}, \]

where the constraint that the excited Bosons for a given state should not exceed \(2S\) has been considered automatically [14].

Applying the CA spin operator transformation (2)–(4) and the CBT (5)–(7) into Hamiltonian (1), and then applying a usual Fourier transformation, we may obtain the transformed Hamiltonian as follows,

\[ H = H_0 + \sum_k A_k a_k^+ a_k + \sum_k B_k (a_k^+ a_{-k} + a_k a_{-k}) \]

\[ + H_4 + \ldots, \]

where

\[ H_0 = [-JZ \cos^2(2\theta) - \frac{1}{2} D \sin(2\theta) \]

\[ + \frac{1}{2} D - h \cos(2\theta)]N, \]

\[ A_k = 2JZ \left[ \cos^2(2\theta) - \gamma_k \right] + \frac{1}{2} D \sin(2\theta) \]

\[ + \frac{1}{2} D + h \cos(2\theta), \]

\[ B_k = \frac{1}{2} \sqrt{2} [-JZ \sin(4\theta) + \frac{1}{2} D \cos(2\theta) - h \sin(2\theta) \]

\[ + JZ \sin(2\theta) \gamma_k. \]

It is not surprising that \(H_0\) and \(A_k, B_k\) are the same as in Ref. [4], because the CBT will yield the same results in a harmonic approximation with a HP transformation, which was applied in Ref. [4]. But, they are different in the fourth-order terms.

Applying a Bogolyubov transformation

\[ a_k^+ = U_k a_k^0 + V_k a_{-k}, \]

\[ a_k = U_k a_k^0 - V_k a_{-k}, \]

where

\[ U_k = \left\{ \frac{1}{2} + \frac{1}{2} \sqrt{\frac{A_k^2}{(A_k^2 - 4B_k^2)}} \right\}^{1/2}, \]

\[ V_k = \left\{ -\frac{1}{2} + \frac{1}{2} \sqrt{\frac{A_k^2}{(A_k^2 - 4B_k^2)}} \right\}^{1/2}, \]

to Hamiltonian (15), we get

\[ H = E_0 + \sum_k \epsilon_k a_k^0 a_k + \ldots, \]

\[ E_0 = H_0 + \sum_k \left[ -\frac{1}{2} A_k(\theta) + \frac{1}{2} \sqrt{A_k^2 - 4B_k^2} \right], \]

\[ \epsilon_k = \sqrt{A_k^2 - 4B_k^2}. \]

In the independent boson representation, the ground state \(\left| 0 \right\rangle\) can be defined by

\[ \alpha_k\left| 0 \right\rangle = 0, \]

then the ground state energy \(E(\theta)\) in this representation will be

\[ E(\theta) \simeq \langle 0 | H | 0 \rangle = H_0 + \langle 0 | H_2 | 0 \rangle + \langle 0 | H_4 | 0 \rangle + \ldots. \]

After the Bogolyubov transformation (10), (11), all the high-order terms will have expectation values in the ground state, and they all take small factors \(V, U, P_{ij}\) and \(W_{ij}\).

\[ V = \langle 0 | a_k^0 a_i | 0 \rangle = \frac{1}{N} \sum_k V_k^2. \]
\[ U = \langle 0 | a_i^+ a_i^0 | 0 \rangle = \frac{1}{N} \sum_k U_k V_k, \quad (29) \]

\[ P_{ij} = \langle 0 | a_i^+ a_j^0 | 0 \rangle = \langle 0 | a_i a_j^+ | 0 \rangle = \frac{1}{N} \sum_k \exp\{ik \cdot (r_j - r_i)\} V_k^2, \quad (30) \]

\[ W_{ij} = \langle 0 | a_i^+ a_j^0 | 0 \rangle = \langle 0 | a_i a_j^+ | 0 \rangle = \frac{1}{N} \sum_k \exp\{ik \cdot (r_j - r_i)\} U_k V_k. \quad (31) \]

Thus the ground state energy \( E(\theta) \) can be expanded to series in \( U, V, P_{ij} \) and \( W_{ij} \) by means of the Wick theorem. We will give one term as an example. Consider a simple-cubic lattice, then \( P_{ij} = P \) and \( W_{ij} = W \). One term in the expression of \( E \) (Eq. (15)) is found to be

\[ \langle 0 | \tilde{S}_0^0 | 0 \rangle = \sum_{l=0}^{\infty} \frac{(-1)^{l+1}(l+1)(l-2)}{2l!} \langle 0 | (a_i^+)^l a_i^0 | 0 \rangle. \quad (32) \]

As we know from Wick’s theorem,

\[ \langle 0 | (a_i^+)^{2m} | 0 \rangle = \langle 0 | (a_i^+)^{2m} | 0 \rangle = \frac{(2m)!}{2^m m!} U^m, \quad (33) \]

thus,

\[ \langle 0 | (a_i^+)^{2l} a_i^0 | 0 \rangle = \sum_{k=0}^{l} \frac{(C_{2l}^{2l})^2}{(2l-2k)!} (2l-2k)!, \quad (34) \]

\[ \langle 0 | (a_i^+)^{2l+1} a_i^0 | 0 \rangle = \sum_{k=0}^{l} \frac{(C_{2l+1}^{2l+1})^2}{(2l+1)!} (2l+1)!, \quad (35) \]

So, considering Eqs. (20)–(23), \( \langle 0 | \tilde{S}_0^0 | 0 \rangle \) can be expanded as

\[ \langle 0 | \tilde{S}_0^0 | 0 \rangle = \sum_{l=0}^{\infty} \sum_{k=0}^{l} \frac{(2l-1)(2l+2)!}{2(2k+1)(l-k)!(l-k)!} \times \left( \frac{2l-2}{2l-2k} V_{2k+1} \right) + \frac{(2l-2)(2l+1)!}{2l!(l-k)!(l-k)!} \times \left( \frac{2l-2}{2l-2k} V_{2k} \right). \quad (36) \]

Other terms in Eq. (15) can be expanded similarly. Determine the value of \( \theta \) by minimizing the ground state energy \( E \) and substitute it into the following expression,

\[ M = \langle 0 | \tilde{S}_e^e | 0 \rangle = \cos(2\theta) \langle 0 | \tilde{S}_e^e | 0 \rangle - \sin(\theta) \cos(\theta) \langle 0 | (\tilde{S}_e^e)^2 \exp(-i\pi \tilde{S}_e^e) | 0 \rangle + \langle 0 | \exp(i\pi \tilde{S}_e^e) (\tilde{S}_e^e)^2 | 0 \rangle. \quad (37) \]

We then can obtain the induced magnetization of this system. However, it is very difficult to derive an analytical expression for the infinite summations. Fortunately, \( U, V, \) and \( W \) are all small factors, and higher-order terms in the expressions will give smaller contributions to the final results. So we may do the calculation with the help of a computer. Terms up to the order \( l = 80 \) are kept in calculating the ground state energy and the induced magnetization.

3. Discussion and comparison

Now we will discuss the effects of the high-order terms for such a system.

In Table 1, the values of the ground state energy are listed when different number of high-order terms are kept in the calculation, where the parameters are fixed.

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<th>Number of terms retained</th>
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<tr>
<td>80</td>
<td>-1.008366621348486</td>
</tr>
</tbody>
</table>

Other terms in Eq. (15) can be expanded similarly. Determine the value of \( \theta \) by minimizing the ground state energy \( E \) and substitute it into the following expression,

\[ M = \langle 0 | \tilde{S}_e^e | 0 \rangle = \cos(2\theta) \langle 0 | \tilde{S}_e^e | 0 \rangle - \sin(\theta) \cos(\theta) \langle 0 | (\tilde{S}_e^e)^2 \exp(-i\pi \tilde{S}_e^e) | 0 \rangle + \langle 0 | \exp(i\pi \tilde{S}_e^e) (\tilde{S}_e^e)^2 | 0 \rangle. \quad (37) \]

We then can obtain the induced magnetization of this system. However, it is very difficult to derive an analytical expression for the infinite summations. Fortunately, \( U, V, P \) and \( W \) are all small factors, and higher-order terms in the expressions will give smaller contributions to the final results. So we may do the calculation with the help of a computer. Terms up to the order \( l = 80 \) are kept in calculating the ground state energy and the induced magnetization.
Fig. 1. Energy $E$ of an easy-plane spin-one ferromagnetic simple-cubic lattice as the function of $\sin(2\theta)$, where $D/4JZ = 0.1$ and $h/JZ = 0.4$ based on the CBT (solid line) and the harmonic approximation (dotted line). $M$ is the minimum point of the solid line and $R_1$, $R_2$ are two minimum points of the dotted line.

In the $D/4JZ = 0.6$ case, respectively. The results are shown in Fig. 2.

In the remaining part of this section, we will make a clear comparison with the MME method. For the magnetic systems with “easy-plane” single-ion anisotropy, the MME method is one which can give a reasonable representation, and many authors have used it to discuss various kinds of properties for such systems. However, the following discussion will show that the CA method is better than the MME method for an “easy-plane” spin-one ferromagnet.

According to the MME method [6], the total Hamiltonian of an easy-plane spin-one ferromagnet Eq. (1) can be divided into two parts,

$$H = H_0 + H_{\text{int}} + \text{const},$$

$$H_0 = -(2JZS + h) \sum_i S_i^z + D \sum_i (S_i^z)^2,$$

$$H_{\text{int}} = -J \sum_{(i,j)} [S_i^+ S_j^- + (S_i^- - S)(S_j^- - S)].$$

The main point of the MME method is to find a reasonable “starting point” by diagonalizing the $H_0$ part of the Hamiltonian first, then take account of the $H_{\text{int}}$ part of the Hamiltonian based on this representation. However, for the current spin-one case, one may find that the MME method has been included by the CA approach. Actually, applying the CA spin-operator transformation (9)–(11) to the Hamiltonian $H_0$, we find
\[ H_0 = D (S_i^+)^2 - (h + 2JZ) S_i^- \]
\[ = \frac{1}{2} D \sin(2\theta) [\hat{S}_i^+ \exp(i\pi\hat{S}_i^-) + \text{h.c.}] + \frac{1}{2} D + (\frac{1}{2} h + JZ) \cos(2\theta) ] \hat{S}_i^+ \hat{S}_i^- \]
\[ + \{ \frac{1}{2} D \cos(2\theta) - (\frac{1}{2} h + JZ) \sin(2\theta) \} \hat{S}_i^+ \hat{S}_i^- \]
\[ + \text{h.c.}. \] (41)

When the variation parameter \( \theta \) is selected to satisfy
\[ D \cos(2\theta) - (2h + 4JZ) \sin(2\theta) = 0, \] (42)
the off-diagonal terms in braces of Eq. (41) will be canceled. So, all the results in the MME method can be recovered after setting the variation parameter \( \theta \) to be the solution of the above equation in the CA approach.

Unfortunately, such a selection of the variation parameter could not warrant the "ground state" in the MME method to be the most reasonable one because the \( H_{\text{int}} \) part of the Hamiltonian has been neglected. In other words, the MME method is equivalent to a special case in the CA approach, where only the function \( E(\theta) = \langle 0 \vert H_0 \vert 0 \rangle \) is minimized. However, in the current method, both \( H_0 \) and \( H_{\text{int}} \) have been considered to choose the most reasonable representation of an easy-plane spin-one ferromagnet in an external field. So, the CA method should give a more reasonable representation for the easy-plane spin-one ferromagnet than the MME method.

4. Conclusions

To summarize, in this paper the CA method has been applied to calculate the induced magnetization of an easy-plane spin-one ferromagnet with respect to the external magnetic field. Based on an independent boson representation, high-order terms have been taken into account as much as necessary by means of the CBT. Numerical calculations are carried out for a simple-cubic lattice, and the diagrams of the induced magnetization versus magnetic field \( h \) in the cases of small and large anisotropy are given. Comparison of the results based on the CBT and those based on the harmonic approximation shows that the harmonic approximation is poor in such a case since this approximation may even introduce wrong physical results, high-order contributions in the CBT are necessary. We also compared the CA method with the old methods for an easy-plane spin-one ferromagnet.

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