An extension of the characteristic angle method to the easy-plane spin-$\frac{3}{2}$ ferromagnet

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Abstract

The characteristic angle (CA) method [J. Phys. A 27 (1994) 5599], developed previously for the easy-plane spin-1 magnetic systems, has been successfully extended to the spin-$\frac{3}{2}$ case. A compact form of the CA spin-$\frac{3}{2}$ operator transformation is given. Then the ground state energy, the magnon dispersion relation and the spontaneous magnetization are discussed for an easy-plane spin-$\frac{3}{2}$ ferromagnet by using the CA method. A comparison with the old theoretical methods is made.

Keywords: Characteristic angle; Easy-plane; Single-ion; Spin-$\frac{3}{2}$

1. Introduction

"Easy-plane" single-ion anisotropy ($D(S^z)^2$, $D > 0$) is often occurs in magnetic systems with a spin greater than one half. Such systems have been attracting much attention for years [1–11]. On the theoretical side, the spin-wave excitations in such systems are very difficult to handle due to the off-diagonal terms introduced by the "easy-plane" single-ion anisotropy term. Actually, many straightforward methods which are good to deal with for "easy-axis" single-ion anisotropy ($D(S^z)^2$, $D < 0$) are usually found to be invalid for the "easy-plane" magnetic systems, no matter how weak the anisotropy parameter $D$ will be [4,11–13]. For example, applying the Holstein-Primakoff (HP) transformation [12] naively to study the magnon excitations in the easy-plane magnetic systems must lead to an imaginary value for the energy of the "$k = 0$" mode [4,11], and introducing a vector rotation of the spins in the $XZ$ plane to optimize the spontaneous magnetized direction also does not help [13] the excitation energy in a harmonic approximation under such an approach will either be negative or imaginary. In fact, due to the off-diagonal terms ($D((S_+^+)^2 + (S_-^+)^2)$) in the Hamiltonian introduced by the single-ion anisotropic terms, the proper eigenstate of the Hamiltonian must be a mixture of the single-site spin states $|n\rangle$ with $|n + 2\rangle$ and $|n - 2\rangle$ [3,4]. Such a spin-states mixing effect is very significant in the present
"easy-plane" case. As the result, an ordinary method which fails to consider such an effect must be invalid for such systems. The matching of matrix elements (MME) method is one possible way to take this effect into account perturbatively [3,4], and many applications of this method have been implemented in a first order approximation of the anisotropy term [3–7]. Some numerical methods have also been developed for the easy-plane spin-1 ferromagnetic systems where the authors considered the spin-states mixing effect [9,10]. Recently, a new method – the characteristic angle (CA) method – was developed successfully for the easy-plane spin-1 magnetic systems [1], in which the spin operators are transformed to a new set of quasi-spin operators, taking into account the spin-states mixing effect by a variation parameter – the characteristic angle (CA). The ground state properties of an easy-plane spin-1 ferromagnet, such as the ground state energy, the spontaneous magnetization and the magnon dispersion relation, are more reasonable in the CA approach than those in the MME method [1]. The induced magnetization of the easy-plane spin-1 ferromagnet has also been studied based on such an approach [11].

In this paper, we would like to extend the CA method to the easy-plane spin-$\frac{3}{2}$ magnetic systems. Although the main idea has been proposed in Ref. [1], an extension of this approach to the larger spin case is still nontrivial because the extension makes it possible to study the magnetic systems with single-ion anisotropy in the larger spin case. Actually, the extension is not very easy because the number of variation parameters will increase and the expression of the CA transformation will become more complicated than that in spin-1 case. This paper is organized as follows. After diagonalizing the single-site Hamiltonian part, we derive the CA spin operator transformation for the $S = \frac{3}{2}$ case successfully in Section 2. Then we present the main physical results for an easy-plane spin-$\frac{3}{2}$ ferromagnet using the CA method in Section 3. A comparison with the MME method and other methods is made thereafter. Finally, the conclusions are outlined in Section 4.

2. Characteristic angle transformation for $S = \frac{3}{2}$

The Hamiltonian of an easy-plane spin-$\frac{3}{2}$ ferromagnet can be given as

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

(1)

where $(i, j)$ means summation restricted on nearest-neighbor pairs. The spin vectors are forced into the YZ plane by the anisotropy term $(D > 0)$, so that the spontaneous magnetized direction must be in the YZ plane. Without losing any generality, the Z direction is chosen to be the spontaneous magnetized direction, and an external magnetic field $h$ will be applied along the Z direction, which will be set to zero in the end.

Following Ref. [1], let us start by diagonalizing the single-site part of the Hamiltonian. The matrix form of the single-site Hamiltonian $D(S^z)^2 - hS^z$ in the $S^z$ representation is found to be

$$\mathcal{A} = \begin{pmatrix}
\frac{3}{2}D - \frac{3}{2}h & 0 & 0 & 0 \\
0 & \frac{3}{2}D - \frac{3}{2}h & 0 & \frac{1}{2}\sqrt{3}D \\
0 & \frac{1}{2}\sqrt{3}D & \frac{3}{2}D + \frac{1}{2}h & 0 \\
0 & 0 & \frac{1}{2}\sqrt{3}D & \frac{3}{2}D + \frac{3}{2}h
\end{pmatrix},$$

(2)

where the matrix elements are defined by $\mathcal{A}_{mn} = \langle m | D(S^z)^2 - hS^z | n \rangle$ in which the bases $| m \rangle$ are the complete set of eigenstates of the operator $S^z$ with eigenvalues ($\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$).
A new representation can be defined as follows, in which the complete set of bases $|\tilde{m}\rangle$ are related to the old ones by the following orthogonal transformation,

$$|\tilde{m}\rangle = \sum_n |n\rangle \mathcal{P}_{nm},$$  \hspace{1cm} (3)

$$\mathcal{P} = \begin{pmatrix}
\cos \theta_1 & 0 & \sin \theta_1 & 0 \\
0 & \cos \theta_2 & 0 & -\sin \theta_2 \\
-\sin \theta_1 & 0 & \cos \theta_1 & 0 \\
0 & \sin \theta_2 & 0 & \cos \theta_2
\end{pmatrix}. $$  \hspace{1cm} (4)

Then, after the transformation, the matrix form of the operator $D(S^z)^2 - hS^z$ in the new representation $|\tilde{m}\rangle$ will be

$$\tilde{A} = \mathcal{P}^T \mathcal{A} \mathcal{P}. $$  \hspace{1cm} (5)

It is easy to check that only when

$$\tan 2\theta_1 = \frac{\sqrt{3}D}{D + 2h}, $$  \hspace{1cm} (6)

$$\tan 2\theta_2 = \frac{\sqrt{3}D}{D - 2h}, $$  \hspace{1cm} (7)

the matrix $\tilde{A}$ can be exactly diagonalized with the following eigenvalues

$$\lambda_1 = -\frac{3}{2}D - \frac{1}{2}h - \sqrt{D^2 + h^2 + Dh}, \quad \lambda_2 = -\frac{3}{2}D + \frac{1}{2}h + \sqrt{D^2 + h^2 + Dh}, $$

$$\lambda_3 = -\frac{3}{2}D - \frac{1}{2}h + \sqrt{D^2 + h^2 + Dh}, \quad \lambda_4 = -\frac{3}{2}D + \frac{1}{2}h - \sqrt{D^2 + h^2 + Dh}. $$  \hspace{1cm} (8)

Since the orthogonal transformation $\mathcal{P}$ can exactly diagonalize the single-site part of the Hamiltonian, then, if we apply this transformation to the total Hamiltonian (1), we can expect to obtain a reasonable representation of the easy-plane spin-$\frac{3}{2}$ ferromagnet after selecting appropriate values of the parameters $\theta_1, \theta_2$ by the variation method.

However, for the sake of simplification in this paper, we will only study the easy-plane spin-$\frac{3}{2}$ ferromagnet in a zero external magnetic field here (in other words, $h = 0$). Then the two variation parameters $\theta_1$ and $\theta_2$ should be the same. In fact, since the $Z$ direction is not specified in Hamiltonian (1), the state that all spins are at $|\frac{3}{2}\rangle$ and the state that all spins are at $|\frac{1}{2}\rangle$ will give the same physical results. So, from the definition of the transformation $\mathcal{P}$ (Eq. (4)), we may easily obtain $\theta_1 = \theta_2 = \theta$. Of course, if an external magnetic field $h$ is applied, the two parameters may not be the same and things are somewhat complicated then.

In order to investigate how the transformation acts on the exchange interactions, we should first study how the transformation acts on the spin operators. The matrix form of the spin operator $S^+$ in the old $S^z$ representation is

$$(S^+) = \begin{pmatrix}
0 & \sqrt{3} & 0 & 0 \\
0 & 0 & 2 & 0 \\
0 & 0 & 0 & \sqrt{3} \\
0 & 0 & 0 & 0
\end{pmatrix}. $$  \hspace{1cm} (9)
After the orthogonal transformation, the matrix form of the operator $S^+$ in the new representation is found to be

$$
(S^+) = \mathcal{P}^T (S^+) \mathcal{P} = 
\begin{pmatrix}
0 & \sqrt{3} \cos 2\theta & 0 & -\sqrt{3} \sin 2\theta \\
-\sin 2\theta & 0 & \sin 2\theta & 0 \\
0 & \sqrt{3} \sin 2\theta & 0 & \sqrt{3} \cos 2\theta \\
2 \sin^2 \theta & 0 & -\sin 2\theta & 0
\end{pmatrix}.
$$

(10)

Now we may understand this transformation in another way: suppose the complete bases $|m\rangle$ stay unchanged, and instead the spin operators are transformed to new ones by a unitary transformation. Noticing some matrix identities for spin-$\frac{2}{2}$ operators such as

$$
(s(S^+))^2 = \begin{pmatrix}
-1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix},
$$

(11)

and

$$
((S^+)^2) = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix},
$$

(12)

we can easily obtain the following spin-operator transformation,

$$
P^S S^+ P = \tilde{S}^+ = \frac{1}{2} \cos 2\theta \left[ 1 + \sin(\pi S^+) \right] S^+ + \frac{1}{2} \sin 2\theta \left[ 1 - \sin(\pi S^+) \right] S^+ - \frac{1}{2} \sqrt{3} \sin 2\theta S^- \left[ 1 + \sin(\pi S^+) \right]
\left. + \frac{1}{2} \sqrt{3} \sin 2\theta S^- \left[ 1 - \sin(\pi S^+) \right] - \frac{1}{2} \sqrt{3} \sin 2\theta \left[ S^+ \left( S^+ \right)^{\dagger} \right] + \frac{1}{2} \sin^2 \theta \left[ S^- \left( S^- \right)^{\dagger} \right].
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3. Results and comparison

In order to study the ground state properties and the low-lying excitations for such a system, the HP transformation is introduced for the spin-$3\over 2$ operators

\[ S_i^+ = \frac{3}{2} - a_i^* a_i, \]
\[ S_i^- = \sqrt{3} - a_i^* a_i, \]
\[ S_i^z = a_i^* \sqrt{3} - a_i^* a_i. \]

Applying the above HP transformation, we can obtain the Bose expansions for CA spin-$3\over 2$ operators.

However, there exists another straightforward method to determine the first several order terms of the Bose expansions for the CA spin operators. We will consider $\tilde{S}^+$ as an example. After transforming the Hilbert space of the spin operator to that of the Bose operator, the vacuum state of the Bose operator $|0\rangle_B$ is defined to be the spin state $|0\rangle_S$, and the excited Bose states $|1\rangle_B, |2\rangle_B, |3\rangle_B$ are the corresponding spin states $|{3\over 2}\rangle_S, |-{1\over 2}\rangle_S, |-{3\over 2}\rangle_S$, respectively (the subscripts B and S denote the Bose state and the spin state, respectively). Other Bose states such as $|n\rangle_B, n > 3$ are unphysical states. In physical space, the matrix forms of some lower order Bose expansion can be written out readily,

\[ (a) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \]
\[ (a^2) = \begin{pmatrix} 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{6} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \]

etc. Then from the matrix form of the operator $\tilde{S}^+$ (Eq. (10)), it is very easy to write out the first order terms of CA spin operator $\tilde{S}^+$,

\[ \tilde{S}^+ = \sqrt{3} \cos 2\theta a - \sin 2\theta a^* + \ldots. \]  
\[ \text{(21)} \]

The Bose expansion of $\tilde{S}^z$ can be similarly derived as

\[ \tilde{S}^z = \frac{3}{2} - 2 \sin^2 \theta - a^* a + \frac{1}{2} \sqrt{2} \sin 2\theta (a^{*2} + a^2) + \ldots. \]  
\[ \text{(22)} \]

Other terms can be obtained easily.

Applying the CA transformation to Hamiltonian (1), we get

\[ \tilde{H} = -J \sum_{(i,j)} \tilde{S}_i \cdot \tilde{S}_j + D \sum_i (\tilde{S}_i^z)^2. \]  
\[ \text{(23)} \]

The transformed Hamiltonian $\tilde{H}$ must have the same eigenvalues as the original one since the transformation is an orthogonal one.

Then we can apply the HP transformation to the Hamiltonian (23) keeping a harmonic approximation. We obtain

\[ \tilde{H} = U_0 + H_3 + \ldots. \]  
\[ \text{(24)} \]

\[ U_0 = \left[-J Z \left(\frac{3}{2} - 2 \sin^2 \theta\right) + \left(\frac{3}{2} D - D \cos^2 \theta - \frac{1}{2} \sqrt{3} D \sin 2\theta\right)\right] N, \]  
\[ \text{(25)} \]
Taking a Fourier transformation to the momentum $k$ space, we obtain the following Hamiltonian,

\[ H' = U_0 + \sum_k A_k a_k^+ a_k + \sum_k B_k (a_k^+ a_{-k} + a_k a_{-k}) + \ldots, \]

where

\[ \gamma_k = \frac{1}{Z} \sum_\delta \exp(ik \cdot r), \]

in which the $\delta$ summation runs over the $Z$ nearest-neighbor sites of a given site.

The approximate Hamiltonian (27) can be diagonalized by a Bogolyubov transformation,

\[ \tilde{H} - E_0 = \sum_k \epsilon_k \alpha_k^+ \alpha_k + \ldots, \]

\[ E_0 - U_0 = \frac{1}{2} \sum_k A_k + \frac{1}{2} \sum_k \sqrt{A_k^2 - 4B_k^2}, \]

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

The spontaneous magnetization for the easy-plane spin-$\frac{3}{2}$ ferromagnet in the harmonic approximation can be derived as

\[ M_0 = \langle 0 | \tilde{S}^z | 0 \rangle = 2 - 2 \sin^2 \theta - \frac{1}{N} \sum_k \frac{1}{2} A_k + \frac{\sqrt{2}}{\sqrt{A_k^2 - 4B_k^2}}. \]

As we know, the value of variation parameter $\theta$ should be determined by minimizing the ground state energy $E_0$. An analytical expression of $\theta$ with respect to the anisotropy parameter seems very difficult to obtain. However, an expansion in $d = D/J_2$ can be determined order by order. As a first step, suppose $d$ is very small so that $\theta$ is also small, then by minimizing the ground state energy, keeping only the first order terms in $d$, we obtain the following equation,

\[ \frac{d}{d \theta} E = \frac{d}{d \theta} U_0 = -2JZ \sin 4\theta - (2JZ + D) \sin 2\theta + \sqrt{3} D \cos 2\theta \]

\[ = -2JZ \times 4\theta - 2JZ \times 2\theta + \sqrt{3} D = 0. \]

Then

\[ \theta \approx \frac{1}{4\theta} \sqrt{3} d. \]

Applying this solution into Eqs. (21), (22), it is easy to obtain

\[ \tilde{S}^z = \sqrt{3} a - \frac{1}{6} \sqrt{3} d a^+ + \ldots, \]
\( \tilde{S} = \sqrt{3} a^+ - \frac{1}{\sqrt{3}} d a \ldots, \) \hspace{1cm} (38)
\( \tilde{S}^z = \frac{3}{2} - a^+ a + \frac{1}{\sqrt{6}} d (a^+ a^2 + a^2) \ldots . \) \hspace{1cm} (39)

Then from Eqs. (32), (33), we obtain the ground state energy and the magnon dispersion relation as follows,

\[ E_0 = -JZ \left( \frac{3}{4} - \frac{1}{4} d \right) - \frac{1}{2} JZ \sum_k \sqrt{3(1 - \gamma_k) + d^2} - (d \gamma_k)^2, \] \hspace{1cm} (40)
\[ \epsilon_k = JZ \sqrt{3(1 - \gamma_k) + d^2} - (d \gamma_k)^2. \] \hspace{1cm} (41)

It is easy to check that \( \epsilon_k \to 0 \) when \( k \to 0. \)

Comparing the transformation (37)–(39) and the results (40), (41) to those of the MME method which are obtained in a first order approximation of \( d \) \([4,6]\), we find that they are exactly the same.

In the case of a large anisotropy \( d \), the first order approximation is not enough, a numerical calculation must be made. We have studied a simple-cubic lattice in the present paper, the characteristic angle \( \theta \). The ground state energy \( E_0 \) and the spontaneous magnetization \( M \) are shown in Figs. 1–3 as a function of the anisotropy parameter \( D/JZ \). The most interesting thing is that the easy-plane spin-\( \frac{1}{2} \) ferromagnet does not exhibit a phase transition from the ferromagnetic phase to the non-ferromagnetic one as \( D/JZ \) is increased (Fig. 3). This is quite different from the spin-1 systems \([1,9]\). Actually, when \( D \gg JZ \), the single-ion term is dominant. In this case, one may find from Eqs. (6), (7) that \( \theta = \frac{1}{3} \pi \). According to Eq. (22), we obtain that when \( D \gg JZ \), \( M \to 1 \). However, in spin-1 systems, one may find that when \( D > D_0 (< 4JZ) \), \( M \to 0 \) \([1,9]\).

In the rest of this section, we will compare the CA method with the MME method and other old methods in details. The total Hamiltonian of an easy-plane spin-\( \frac{1}{2} \) ferromagnet can be divided into two parts,

\[ H = -J \sum_{(i,j)} (S_i^z S_j^z + S_i^z S_j^z) + D \sum_i (S_i^z)^2 = H_0 + H_{\text{int}} + \text{const}, \] \hspace{1cm} (42)
\[ H_0 = -2JZ \sum_i S_i^z + D \sum_i (S_i^z)^2, \] \hspace{1cm} (43)
\[ H_{\text{int}} = -J \sum_{(i,j)} \left[ S_i^z S_j^z + (S_i^z - S)(S_j^z - S) \right]. \] \hspace{1cm} (44)

The main question in such systems is to find a best "starting point" to perform the spin waves calculation. It is just because the "starting points" are chosen unreasonably that the methods mentioned in the introduction are invalid for the easy-plane magnetic systems \([4,11–13]\). For example, the "starting point" in the HP transforma-
tion method is the ordinary ferromagnetic state that all spins are aligned parallel to each other. However, this "starting point" does not consider the spin-states mixing effect at all so that it must be considered unreasonable.

According to the MME method [4], the "starting point" is the ferromagnetic state in the diagonalized representation of Hamiltonian $H_0$ (Eq. (43)). Treating the anisotropy term $D(S^i)^2$ as a perturbation, the Hamiltonian $H_0$ can be diagonalized in terms of $d = D/JZ$ order by order. Based on this, the spin-Bose transformation was applied to the total Hamiltonian to study the magnetic properties of the system. In such an approach, it should be noted that the $H_{\text{int}}$ part of the Hamiltonian has been neglected when determining the "starting point", so this approximation may be valid only when the anisotropy is very small.

However, we believe that the "starting point" in the CA approach will be more reasonable because the $H_{\text{int}}$ has also been taken into account when determining the "starting point". As we can see in this paper, the CA transformation is applied to the total Hamiltonian and $\theta$ is determined by minimizing the total ground state energy $E_0$ (Eq. (32)). Actually, $H_{\text{int}}$ has been considered through its contribution to $E_0$. Since $H_{\text{int}}$ will contribute the second order terms in $d$ to the ground state energy $E_0$, it is very easy to understand that the CA method gives the same physical results as the MME method in the first order approximation of $d$, which has been demonstrated in the present work. However, for the large $d$ case, when higher order terms in $d$ should be considered, the CA method may give more accurate results than the MME method because the CA method has considered more contributions than the MME method when choosing the "starting point".

Of course, the CA method can only deal with the spin-1 and the spin-$\frac{3}{2}$ cases at the present time. However, the MME method can deal with the arbitrary spin case perturbatively.

4. Conclusions

In this paper, we have successfully extended the characteristic angle method to the easy-plane spin-$\frac{3}{2}$ magnetic systems. Based on the diagonalization of the single-site part of the Hamiltonian, a compact form of the CA transformation for the spin-$\frac{3}{2}$ operators has been derived, in which the spin-states mixing effect is considered automatically by the variation parameters. After applying the CA transformation and the HP spin-Bose transformation, a model Hamiltonian which has the same eigenvalues as the original Hamiltonian is presented by the Bose operators. The Bogolyubov transformation is applied to diagonalize the Hamiltonian in the harmonic approximation, and the variation parameter $CA$ is determined by minimizing the ground state energy. Analytical results of the magnetic properties are obtained in a first order approximation of $d = D/JZ$, which are found to recover the MME method. Numerical calculations are carried out in the large $d$ case for the easy-plane spin-$\frac{3}{2}$ ferromagnet, and a detailed comparison with the MME method and other methods is made.
We find that the CA method has considered more contributions than the MME method and other methods for the spin-1 and spin-\(\frac{3}{2}\) easy-plane magnetic systems.

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