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Unified spin-wave theory for quantum spin systems with single-ion anisotropies

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Abstract. By introducing a new spin-Bose transformation which incorporates the single-site spin-states mixing effect self-consistently, we establish a unified spin-wave approach, applicable to an arbitrary spin-number case and general spin configurations, for quantum spin systems with single-ion anisotropies. The conventional Holstein–Primakoff (HP) method *completely fails* for such systems with easy-plane anisotropy and *sometimes fails* for those with easy-axis anisotropy, while these difficulties have been overcome successfully by the new method. In some limiting cases, the present method recovers the results of old theories which are valid in such cases. Applications to magnetic multilayers show that the new method is useful to remove the unphysical instability predicted by the conventional HP method.

1. Introduction

The single-ion term $D(S_i^z)^2$ is the most widely adopted form in quantum spin models to describe the anisotropies in magnetic systems [1–7]. When $D < 0$, the z axis is a magnetic easy axis, otherwise the xy plane turns to become an easy plane. The conventional treatment for such a system is straightforward†—one first introduces a local coordinate (LC) system, then one determines the spin configuration via the variation method, and finally one obtains spin-wave spectra with the help of the Holstein–Primakoff (HP) transformation [8]. Such an approach, denoted by the conventional HP method, has been applied to various magnetic systems with single-ion anisotropies, for example, randomly anisotropic magnets [3], magnetic multilayers [4–7], etc. However, the conventional HP method is not always successful. First, it *completely* fails for a magnetic system with any 'easy-plane' anisotropy. When using this approach to study even the simplest easy-plane model, one may find that: whenever the magnetized direction is different from the anisotropic axis, the excitation energies of some modes turn out to be imaginary. Second, even for the easy-axis model, the conventional HP method is *not always* valid. In some cases, for example when an external field forces the spin to rotate from its easy axis to its hard axis, the same problem arises.

Generally, these problems are induced by neglecting a very important quantum effect—the single-site spin-states mixing (SSM) effect. After the LC transformation, off-diagonal interactions $((S^+)^2 + (S^-)^2)$ may appear in the Hamiltonian. Such terms have a tendency to mix the single-site spin states $|n\rangle$ with $|n \pm 2\rangle$ etc to form the proper eigenstates. However, such an effect was completely neglected by the conventional HP method [2]. Several methods have already been developed to solve these problems, such as the matching of the matrix elements (MME) method [9–11], the characteristic angle (CA) method [12–14], and a numerical

† A review of the conventional method is decribed in [2].

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method [15]. Unfortunately, all of them have limitations. The MME method is a perturbative one, so that it can only be applied to small anisotropy cases; furthermore, it cannot combine with the LC transformation to deal with general spin configurations [9–11]. Although the CA method has been combined successfully with the LC transformation, it can only be applied to spin-1 systems [12–14]. The numerical method is limited in spin-1 systems [15]. Thus, to our knowledge, a satisfactory theory for quantum spin systems with single-ion anisotropy remains a great challenge to theoretical researchers.

In the present paper, we propose a unified spin-wave approach, which is applicable to arbitrary spin-number systems and general spin configurations, for quantum spin systems with single-ion anisotropies. The key point of this method is a new set of spin-Bose transformations which is different from the HP one and incorporates the SSM effect automatically. This paper is organized as follows: first we outline the theoretical formalism based on a homogeneous easy-plane model in the next section; we then compare the present method with existing theories in section 3. Section 4 is devoted to the applications to magnetic multilayers. Finally, the conclusions are summarized in the last section.

2. Theoretical formalism

2.1. The Hamiltonian

Let us illuminate the basic ideas of the new method based on the simplest case—a bulk easy-plane ferromagnet in an external field. The Hamiltonian is given by

$$H = -J\sum_{(ij)} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + D\sum_i (S_i^z)^2 - h\sum_i S_i^z \tag{1}$$

where the exchange interactions are within nearest neighbours, D is the anisotropy constant, and h is the external field. Considering the competition between the anisotropy and the external field, it is helpful to introduce the LC transformation [2]:

$$S_i^z = \cos\theta S_i^{z'} - \sin\theta S_i^{x'} \qquad S_i^y = S_i^{y'} \qquad S_i^x = \cos\theta S_i^{x'} + \sin\theta S_i^{z'} \tag{2}$$

to optimize the magnetization direction. After the transformation, the Hamiltonian becomes

$$\begin{aligned} H = {} & -J\sum_{(ij)} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + D\cos^2\theta \sum_i (S_i^{z'})^2 + D\sin^2\theta \sum_i (S_i^{x'})^2 - h\cos\theta \sum_i S_i^{z'} \\ & - D\sin\theta\cos\theta \sum_i (S_i^{z'} S_i^{x'} + S_i^{x'} S_i^{z'}) + h\sin\theta \sum_i S_i^{x'}. \end{aligned} \tag{3}$$

It is clear that except $\theta = 0$, there is a single-site off-diagonal term $(S_i^{x'})^2$ in the Hamiltonian (3) which contributes the SSM effect.

In the standard spin-wave theory, one usually applies a spin-Bose transformation to the Hamiltonian and then tries to solve the Boson system. If the resulting Boson Hamiltonian can be *exactly* solved, it does not matter what kind of spin-Bose transformation has been applied. However, an exact solution is unfortunately hard to obtain, so that usually some approximations (for example, the harmonic approximation) are necessary. Such approximations assume that high-order Boson terms are relatively unimportant to determine the ground state and the low-lying spin waves, so that only low-order terms are retained. However, this assumption is correct *only if* the (local) Boson representation has been chosen in such a way that the off-diagonal effects in the low-order terms are as small as possible. Otherwise, renormalizations of high-order interactions will generate *non-negligible* effects to the final results. Thus, it is of much importance to select an appropriate (local) Boson representation where the off-diagonal interactions are as small as possible and a further spin-wave analysis can be performed. Usually,

the (local) Boson representation should be chosen to approach the exact eigenstates as close as possible. In the conventional HP method, the (local) Boson representation has been chosen as the single-site eigenstates of $S_i^{z'}$. However, such a choice, although appropriate for isotropic spin systems, is not for the present anisotropic systems because a proper single-site eigenstate would be a mixture of $|n\rangle$ with $|n\pm 2\rangle \ldots$ rather than a naive $|n\rangle$. In order to take account of such an effect, let us first select an appropriate single-site Hamiltonian to include as many as possible messages from the total Hamiltonian (3), and then determine a (local) Boson representation based on diagonalizing such a Hamiltonian.

First consider the exchange term:

$$\begin{aligned}\boldsymbol{S}_i \cdot \boldsymbol{S}_j = &-\langle S_i^{z'}\rangle\langle S_j^{z'}\rangle + \langle S_i^{z'}\rangle S_j^{z'} + S_i^{z'}\langle S_j^{z'}\rangle \\ &+(S_i^{z'} - \langle S_i^{z'}\rangle)(S_j^{z'} - \langle S_j^{z'}\rangle) + \tfrac{1}{2}(S_i^{+'}S_j^{-'} + S_i^{-'}S_j^{+'}).\end{aligned} \tag{4}$$

Since the second line of the above expression must contribute high-order correlation terms rather than single-site ones, the contributions to the single-site Hamiltonian can be written as $2\overline{S}S_i^{z'}$ where $\overline{S} = \langle S_i^{z'}\rangle$ should be determined later self-consistently. Thus, all the single-site terms from equation (3) can be collected as follows:

$$H_s = -2JZ\overline{S}S_i^{z'} + D\cos^2\theta(S_i^{z'})^2 + D\sin^2\theta(S_i^{x'})^2 - h\cos\theta S_i^{z'} \tag{5}$$

where Z is the number of nearest neighbours of a given site in a lattice. In principle, the single-site Hamiltonian should depend on the site. In the present homogeneous system, however, it is not necessary to consider the site dependence because every site is equivalent. In inhomogeneous systems such as the magnetic multilayers which will be studied in section 4, we have to consider the layer dependence since spins in different layers are no longer equivalent.

Terms in the second line of equation (3) are not included in H_s. Later we will show that an appropriate value of θ can be chosen to eliminate their influences to the total Hamiltonian. It should be noted that the single-site Hamiltonian (5) *only* serves to determine the (local) Boson representation and a set of spin-Bose transformations to help us perform further analysis. After we have found the spin-Bose transformation, we will come back to the total Hamiltonian (3) to consider all the terms.

2.2. The spin-Bose transformation

We will formulate a new set of spin-Bose transformations, which is *formally exact* in this subsection. Since the transformation is independent on the site, we omit the site index for simplicity. Single-site Hamiltonian H_s can be easily diagonalized by the following orthogonal transformation:

$$|\tilde{n}\rangle = \sum_m P_{mn}(\overline{S},\theta)|m\rangle \tag{6}$$

yielding

$$H_s|\tilde{n}\rangle = E_n|\tilde{n}\rangle \tag{7}$$

where $\{|m\rangle, m = 0, 1, \ldots, 2S\}$ represent the eigenstates of $S^{z'}$ defined by $S^{z'}|m\rangle = (S - m)|m\rangle$, $m = 0, 1, \ldots, 2S\}$, and $\{|\tilde{n}\rangle, n = 0, 1, \ldots, 2S\}$ are the eigenstates of H_s. The sequence of the eigenstates $\{|\tilde{n}\rangle\}$ has been arranged by $E_{n+1} > E_n$ so that $|\tilde{0}\rangle$ is the 'ground state' in a single site. The transformation matrix $P_{mn}(\overline{S},\theta)$, obtained by diagonalizing the Hamiltonian matrix $\langle n|H_s|m\rangle$, is certainly dependent on $\overline{S}$ and θ. The matrix forms of the spin operators in the new representation can be evaluated by

$$\langle\tilde{n}|T|\tilde{n_1}\rangle(\overline{S},\theta) = \sum_{mm_1} P_{mn}(\overline{S},\theta)P_{m_1n_1}(\overline{S},\theta)\cdot\langle m_1|T|m\rangle \tag{8}$$

where T stands for the operators $S^{+'}$, $S^{z'}$, etc, and the matrix elements $\langle m_1|S^{+'}|m\rangle$, $\langle m_1|S^{z'}|m\rangle$ are very easy to calculate. To study the low-lying spin-wave excitations, we transform the spin operators into Bose expansions in $a^\dagger$, a which are defined in the *diagonalized* single-site representation (rather than the original representation) as

$$a^\dagger|\tilde{n}\rangle_B = \sqrt{n+1}\widetilde{|n+1\rangle}_B \qquad a|\tilde{n}\rangle_B = \sqrt{n}\widetilde{|n-1\rangle}_B \tag{9}$$

where $|\tilde{n}\rangle_B$ are the Bose states related to the spin states as: $|\tilde{n}\rangle_B = |\tilde{n}\rangle$ (for $n \leqslant 2S$). Since the Boson space is semi-infinite but the spin space is finite, only these states $\{|\tilde{n}\rangle, n \leqslant 2S\}$ have physical definitions, which will construct the physical Boson space. The remainder states $\{|\tilde{n}\rangle, n > 2S\}$ then construct the unphysical Boson space.

It is the core of the present approach to select the (local) Boson representation as the *diagonalized* representation of the approximate single-site Hamiltonian H_s as shown by equation (9). The HP transformation [8], on the other hand, defines the Boson representation as the naive eigenstates of $S_i^{z'}$. The Bose operators in the HP transformation are defined by

$$a^\dagger|n\rangle_B = \sqrt{n+1}|n+1\rangle_B \qquad a|n\rangle_B = \sqrt{n}|n-1\rangle_B. \tag{10}$$

Compared with the HP method, the merit of our choice is very clear—for example, although the zero-Boson state $|\tilde{0}\rangle$ in the present definition is still not the exact ground state, it should be closer to the exact ground state than the zero-Boson state $|0\rangle$ defined in the HP method. The same arguments also hold for low-lying exciting states. In fact, later we will show that the improvement over the conventional spin-wave theory essentially comes from the choice of the local basis equation (9) rather than (10), since the off-diagonal terms in the total Hamiltonian based on such a (local) Boson representation are *indeed* much smaller than those based on equation (10). However, the price to pay is that our spin-Bose transformation will be much more complicated than the HP transformation.

Now let us determine the spin-Bose transformation. Due to the fact that an eigenstate $|\tilde{n}\rangle$ of Hamiltonian H_s of form (5) must be a linear combination of $|n\rangle$, $|n\pm2\rangle$, $|n\pm4\rangle$, ..., the non-zero matrix elements are then: $\langle\tilde{n}|S^{+'}|\widetilde{n+2p+1}\rangle$, $\langle\tilde{n}|S^{z'}|\widetilde{n+2p}\rangle$. Generally, the spin-Bose transformation can be written as

$$\begin{aligned} S^{+'} &= \Theta\cdot\left\{\sum_{p=0}^{2p+1\leqslant 2S}\sum_{l=0}^{2S-2p-1}[A_l^{(p)}a^{\dagger l}a^{l+2p+1} + B_l^{(p)}a^{\dagger l+2p+1}a^l]\right\}\cdot\Theta \\ S^{z'} &= \Theta\cdot\left\{\sum_{l=0}^{2S}C_l^{(0)}a^{\dagger l}a^l + \sum_{p=1}^{2p\leqslant 2S}\sum_{l=0}^{2S-2p}C_l^{(p)}(a^{\dagger l}a^{l+2p} + a^{\dagger l+2p}a^l)\right\}\cdot\Theta \end{aligned} \tag{11}$$

where Θ is the step operator to project out the unphysical states, and is defined by [16]

$$\Theta = \sum_l G_l a^{\dagger l}a^l \tag{12}$$

in which the coefficients are

$$G_l = \begin{cases} \dfrac{(-1)^{l-1}(l-1)(l-2)\ldots(l-2S)}{(2S)!l!} & l \geqslant 0 \\ 0 & l < 0. \end{cases} \tag{13}$$

According to [16], the step operator Θ has the following properties:

$$\begin{aligned} &\Theta|\tilde{n}\rangle = |\tilde{n}\rangle \qquad n \leqslant 2S \\ &\Theta|\tilde{n}\rangle = 0 \qquad n > 2S. \end{aligned} \tag{14}$$

Thus, for an arbitrary operator $\hat{T}$, we have

$$\begin{aligned} &\langle\tilde{n}|\Theta\hat{T}\Theta|\tilde{m}\rangle = \langle\tilde{n}|\hat{T}|\tilde{m}\rangle \qquad n, m \leqslant 2S \\ &\langle\tilde{n}|\Theta\hat{T}\Theta|\tilde{m}\rangle = 0 \qquad \text{otherwise} \end{aligned} \tag{15}$$

which means that the step operator can automatically eliminate the contributions of a given operator in the unphysical Boson space. Thus, we only need to consider the matrix contributions in the physical Boson space.

All the coefficients $\{A_l^{(p)}, B_l^{(p)}, C_l^{(p)}\}$ defined in equation (11) can be determined uniquely by the matrix elements of $S^{+'}$ and $S^{z'}$ obtained by equation (8). Taking $A_l^{(0)}$ as an example, by equating the matrix elements between $\langle\tilde{n}|$ and $|\widetilde{n+1}\rangle$ (both states are in physical Boson space) calculated by the two sides of equation (11), we find that:

$$\begin{aligned}\langle\tilde{n}|S^{+'}|\widetilde{n+1}\rangle &= \langle\tilde{n}|\Theta\cdot\left\{\sum_{p=0}^{2p+1\leqslant 2S}\sum_{l=0}^{2S-2p-1}[A_l^{(p)}a^{\dagger l}a^{l+2p+1}+B_l^{(p)}a^{\dagger l+2p+1}a^l]\right\}\cdot\Theta|\widetilde{n+1}\rangle\\ &= \langle\tilde{n}|\sum_{p=0}^{2p+1\leqslant 2S}\sum_{l=0}^{2S-2p-1}[A_l^{(p)}a^{\dagger l}a^{l+2p+1}+B_l^{(p)}a^{\dagger l+2p+1}a^l]|\widetilde{n+1}\rangle\\ &= \langle\tilde{n}|\sum_{l=0}^{2S-1}A_l^{(0)}a^{\dagger l}a^{l+1}|\widetilde{n+1}\rangle\\ &= \sum_{l=0}^{n}\frac{\sqrt{(n+1)!n!}}{(n-l)!}A_l^{(0)}\end{aligned} \tag{16}$$

in which equations (9), (14) have been used.

Following this method, all the coefficients $\{A_l^{(p)}, B_l^{(p)}, C_l^{(p)}\}$ can be *uniquely* determined by the following coupled equations:

$$\begin{aligned}&\sum_{l=0}^{n}\frac{\sqrt{(n+2p+1)!n!}}{(n-l)!}A_l^{(p)} = \langle\widetilde{n}|S^{+'}|\widetilde{n+2p+1}\rangle \qquad n+2p+1 \quad 2p+1\leqslant 2S\\ &\sum_{l=0}^{n}\frac{\sqrt{(n+2p+1)!n!}}{(n-l)!}B_l^{(p)} = \langle\widetilde{n+2p+1}|S^{+'}|\widetilde{n}\rangle \qquad n+2p+1 \quad 2p+1\leqslant 2S\\ &\sum_{l=0}^{n}\frac{\sqrt{(n+2p)!n!}}{(n-l)!}C_l^{(p)} = \langle\widetilde{n}|S^{z'}|\widetilde{n+2p}\rangle \qquad n+2p \quad 2p\leqslant 2S.\end{aligned} \tag{17}$$

Equation (17) can be solved step by step. For example, in the case of $p=0, n=0$, we have $A_0^{(0)} = \langle\widetilde{0}|S^{+'}|\widetilde{1}\rangle$, $B_0^{(0)} = \langle\widetilde{1}|S^{+'}|\widetilde{0}\rangle$, and $C_0^{(0)} = \langle\widetilde{0}|S^{z'}|\widetilde{0}\rangle$. Some lowest-order coefficients are listed in table 1. The larger S is, the larger the number of coefficients. In a definite-spin case, the number of coefficients is always finite. For example, only $A_0^{(0)}, A_1^{(0)}, B_0^{(0)}, B_1^{(0)}, C_0^{(0)}, C_1^{(0)}, C_2^{(0)}, C_0^{(1)}$ are needed in the case of $S=1$.

The validity of our spin-Bose transformation equation (11) is ensured by the fact that the Bose expansion has *exactly* the same matrix elements as the original spin operator in the *physical* Boson space, and has *zero* matrix elements in the *unphysical* Boson space. The Bose expansions of the spin operators certainly satisfy all the commutation rules of the angular momentum

$$\begin{aligned}&[S_i^{+'}, S_j^{-'}] = 2S_i^{z'}\delta_{ij}\\ &[S_i^{z'}, S_j^{\pm'}] = \pm\delta_{ij}S_i^{\pm'}\end{aligned} \tag{18}$$

because the transformation P_{nm} is orthogonal.

Inserting (12) into (11), we can further expand the transformations to infinite Bose series

Table 1. Coefficients of the new Bose expansion up to the fourth-order terms. $\{J_l^{(p)}\}$ and $\{K_l^{(p)}\}$ can be obtained through replacing $S^{+'}$ by $S^{z'}S^{x'}$ in the expressions of $\{A_l^{(p)}\}$ and $\{B_l^{(p)}\}$. $\{E_l^{(p)}\}$ and $\{F_l^{(p)}\}$ can be obtained through replacing $S^{z'}$ by $(S^{z'})^2$ and $(S^{x'})^2$ in the expressions of $\{C_l^{(p)}\}$, respectively. The site index i has been omitted.

p	l	$A_l^{(p)}$	$B_l^{(p)}$	$C_l^{(p)}$
0	0	$\langle\tilde{0}\|S^{+'}\|\tilde{1}\rangle$	$\langle\tilde{1}\|S^{+'}\|\tilde{0}\rangle$	$\langle\tilde{0}\|S^{z'}\|\tilde{0}\rangle$
0	1	$\frac{\langle\tilde{1}\|S^{+'}\|\tilde{2}\rangle}{\sqrt{2}} - \langle\tilde{0}\|S^{+'}\|\tilde{1}\rangle$	$\frac{\langle\tilde{2}\|S^{+'}\|\tilde{1}\rangle}{\sqrt{2}} - \langle\tilde{1}\|S^{+'}\|\tilde{0}\rangle$	$\langle\tilde{1}\|S^{z'}\|\tilde{1}\rangle - \langle\tilde{0}\|S^{z'}\|\tilde{0}\rangle$
0	2	$\frac{\langle\tilde{2}\|S^{+'}\|\tilde{3}\rangle}{\sqrt{12}} - \frac{\langle\tilde{1}\|S^{+'}\|\tilde{2}\rangle}{\sqrt{2}} + \frac{1}{2}\langle\tilde{0}\|S^{+'}\|\tilde{1}\rangle$	$\frac{\langle\tilde{3}\|S^{+'}\|\tilde{2}\rangle}{\sqrt{12}} - \frac{\langle\tilde{2}\|S^{+'}\|\tilde{1}\rangle}{\sqrt{2}} + \frac{1}{2}\langle\tilde{1}\|S^{+'}\|\tilde{0}\rangle$	$\frac{1}{2}\langle\tilde{2}\|S^{z'}\|\tilde{2}\rangle - \langle\tilde{1}\|S^{z'}\|\tilde{1}\rangle + \frac{1}{2}\langle\tilde{0}\|S^{z'}\|\tilde{0}\rangle$
1	0	$\frac{\langle\tilde{0}\|S^{+'}\|\tilde{3}\rangle}{\sqrt{6}}$	$\frac{\langle\tilde{3}\|S^{+'}\|\tilde{0}\rangle}{\sqrt{6}}$	$\frac{\langle\tilde{0}\|S^{z'}\|\tilde{2}\rangle}{\sqrt{2}}$
1	1	$\frac{\langle\tilde{1}\|S^{+'}\|\tilde{4}\rangle}{\sqrt{24}} - \frac{\langle\tilde{0}\|S^{+'}\|\tilde{3}\rangle}{\sqrt{6}}$	$\frac{\langle\tilde{4}\|S^{+'}\|\tilde{1}\rangle}{\sqrt{24}} - \frac{\langle\tilde{3}\|S^{+'}\|\tilde{0}\rangle}{\sqrt{6}}$	$\frac{\langle\tilde{1}\|S^{z'}\|\tilde{3}\rangle}{\sqrt{6}} - \frac{\langle\tilde{0}\|S^{+'}\|\tilde{2}\rangle}{\sqrt{2}}$

in normal order:

$$\begin{aligned} S^{+'} &= \sum_{p=0}^{2p+1\leqslant 2S}\sum_{l=0}^{\infty}[A_l^{(p)}a^{\dagger l}a^{l+2p+1} + B_l^{(p)}a^{\dagger l+2p+1}a^l] \\ S^{z'} &= \sum_{l=0}^{\infty}C_l^{(0)}a^{\dagger l}a^l + \sum_{p=1}^{2p\leqslant 2S}\sum_{l=0}^{\infty}C_l^{(p)}(a^{\dagger l}a^{l+2p} + a^{\dagger l+2p}a^l). \end{aligned} \tag{19}$$

It has been proved in [16] that the projection operator has no influence on the coefficients of those Boson terms in physical space which have been determined in equation (17). To avoid the unnecessary introduction of too many symbols, we have used the same ones ($\{A_l^{(p)}, B_l^{(p)}, C_l^{(p)}\}$ etc) in the above expansions to denote the *whole* set of coefficients for the infinite series including those for unphysical Boson terms which are not determined by equation (17).

Let us now take the $S = 1$ case as an example. Equations (11) can be rewritten as

$$\begin{aligned} S^{+'} &= \Theta\cdot[A_0^{(0)}a + A_1^{(0)}a^\dagger a^2 + B_0^{(0)}a^\dagger + B_1^{(0)}a^{\dagger 2}a]\cdot\Theta \\ &= [A_0^{(0)}a + A_1^{(0)}a^\dagger a^2]\cdot\Theta + \Theta\cdot[B_0^{(0)}a^\dagger + B_1^{(0)}a^{\dagger 2}a] \\ S^{z'} &= \Theta\cdot[C_0^{(0)} + C_1^{(0)}a^\dagger a + C_2^{(0)}a^{\dagger 2}a^2 + C_0^{(1)}a^{\dagger 2} + C_0^{(1)}a^2]\cdot\Theta \\ &= [C_0^{(0)} + C_1^{(0)}a^\dagger a + C_2^{(0)}a^{\dagger 2}a^2]\cdot\Theta + \Theta_i\cdot C_0^{(1)}a^{\dagger 2} + C_0^{(1)}a^2\cdot\Theta. \end{aligned} \tag{20}$$

Every term in equation (20) can be expanded to infinite Bose series arranged in normal order. For instance,

$$\begin{aligned} A_0^{(0)}a\cdot\Theta &= \sum_l G_l A_0^{(0)}aa^{\dagger l}a^l = \sum_l G_l A_0^{(0)}[a^{\dagger l}a^{l+1} + la^{\dagger l-1}a^l] \\ &= \sum_l [G_l + (l+1)G_{l+1}]A_0^{(0)}a^{\dagger l}a^{l+1}. \end{aligned} \tag{21}$$

After a careful calculation, the final form of the coefficients are found to be

$$\begin{aligned} A_l^{(0)} &= [G_l + (l+1)G_{l+1}]A_0^{(0)} + [G_{l-1} + 2lG_l + (l+1)lG_{l+1}]A_1^{(0)} \\ B_l^{(0)} &= [G_l + (l+1)G_{l+1}]B_0^{(0)} + [G_{l-1} + 2lG_l + (l+1)lG_{l+1}]B_1^{(0)} \\ C_l^{(0)} &= G_lC_0^{(0)} + [lG_l + G_{l-1}]C_1^{(0)} + [G_{l-2} + 2(l-1)G_{l-1} + l(l-1)G_l]C_2^{(0)} \\ C_l^{(1)} &= [G_l + 2(l+1)G_{l+1} + (l+1)(l+2)G_{l+2}]C_0^{(1)}. \end{aligned} \tag{22}$$

As we have stated, the step operator does not change the coefficients of those physical Boson terms—one may check this point by examining the cases of $l = 0, 1$. It can be seen from equation (22) that the high-order terms are derived *uniquely* from the low-order terms which

are determined by equation (17). Actually, the high-order terms have no matrix contributions in the physical Boson space. They only serve to cancel the matrix contribution of the low-order terms in the unphysical Boson space.

Similarly, $S^{z'}S^{x'}$, $(S^{z'})^2$ and $(S^{x'})^2$ can be expanded into Bose series:

$$\begin{aligned} S^{z'}S^{x'} &= \sum_{p=0}^{2p+1\leqslant 2S}\sum_{l=0}^{\infty}[J_l^{(p)}a^{\dagger l}a^{l+2p+1} + K_l^{(p)}a^{\dagger l+2p+1}a^l] \\ (S^{z'})^2 &= \sum_{l=0}^{\infty}E_l^{(0)}a^{\dagger l}a^l + \sum_{p=1}^{2p\leqslant 2S}\sum_{l=0}^{\infty}E_l^{(p)}(a^{\dagger l}a^{l+2p} + a^{\dagger l+2p}a^l) \\ (S^{x'})^2 &= \sum_{l=0}^{\infty}F_l^{(0)}a^{\dagger l}a^l + \sum_{p=1}^{2p\leqslant 2S}\sum_{l=0}^{\infty}F_l^{(p)}(a^{\dagger l}a^{l+2p} + a^{\dagger l+2p}a^l). \end{aligned} \tag{23}$$

Basically, the coefficients $\{J_l^{(p)}, K_l^{(p)}, E_l^{(p)}, F_l^{(p)}\}$ can be determined by the coefficients $\{A_l^{(p)}, B_l^{(p)}, C_l^{(p)}\}$ uniquely. However, it is more efficient to derive them directly from the corresponding matrix elements calculated from equation (8), following the method described above. Actually, in equation (17) and table 1, one may just substitute $S^{+'}$ by $S^{z'}S^{x'}$ to determine $J_l^{(p)}$ and $K_l^{(p)}$ and substitute $S^{z'}$ by $(S^{z'})^2$ and $(S^{x'})^2$ to determine $E_l^{(p)}$ and $F_l^{(p)}$, respectively.

Thus, we have formulated a new spin-Bose transformation which is *formally exact* and have considered the SSM effect explicitly, rather than the conventional HP spin-Bose transformation [8] and others. Although the expressions seem rather complicated, in practical cases, one rarely applies the infinite series but rather takes only the lowest several order terms (say, up to harmonic terms) to catch the main physics†. In the remainding parts of this paper, we will present some applications of our method under the harmonic approximation, and show that the method is applicable to some problems where the conventional methods fail under the harmonic approximation.

2.3. The spin-wave excitations under the harmonic approximation

Since we have obtained a set of spin-Bose transformation based on the Boson representation defined by the single-site Hamiltonian, now we go back to the total Hamiltonian (3) to consider all the other terms. Applying our new Bose transformation (19)–(23) to Hamiltonian (3) and then applying a Fourier transformation, under the harmonic approximation, we find that

$$H = H_0(\overline{S},\theta) + H_1(\overline{S},\theta) + \sum_{\boldsymbol{k}}P(\boldsymbol{k})a_{\boldsymbol{k}}^{\dagger}a_{\boldsymbol{k}} + \sum_{\boldsymbol{k}}Q(\boldsymbol{k})(a_{\boldsymbol{k}}^{\dagger}a_{-\boldsymbol{k}} + a_{\boldsymbol{k}}a_{-\boldsymbol{k}}) + \cdots \tag{24}$$

where

$$H_0 = N(-JZC_0^{(0)2} + D\cos^2\theta E_0^{(0)} + D\sin^2\theta F_0^{(0)} - h\cos\theta C_0^{(0)}) \tag{25}$$

$$H_1 = \sum_{\boldsymbol{k}}[-D\sin\theta\cos\theta(K_0^{(0)} + J_0^{(0)}) + \tfrac{1}{2}h\sin\theta(A_0^{(0)} + B_0^{(0)})](a_{\boldsymbol{k}}^{\dagger} + a_{-\boldsymbol{k}}) \tag{26}$$

$$\begin{aligned} P(\boldsymbol{k}) = {} & -2JZC_0^{(0)}C_1^{(0)} - JZ[(A_0^{(0)})^2 + (B_0^{(0)})^2]\gamma_{\boldsymbol{k}} + D\cos^2\theta E_1^{(0)} + D\sin^2\theta F_1^{(0)} \\ & -h\cos\theta C_1^{(0)} \end{aligned} \tag{27}$$

$$Q(\boldsymbol{k}) = -JZA_0^{(0)}B_0^{(0)}\gamma_{\boldsymbol{k}} + [-2JZC_0^{(0)}C_0^{(1)} + D\cos^2\theta E_0^{(1)} + D\sin^2\theta F_0^{(1)} - h\cos\theta C_0^{(1)}]. \tag{28}$$

Here, $\gamma_{\boldsymbol{k}}$ is defined as

$$\gamma_{\boldsymbol{k}} = (1/Z)\sum_{\boldsymbol{\delta}}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}} \tag{29}$$

† Effects of higher-order terms in the infinite series have been considered by some authors, see [14, 16].

in which the summation runs over Z nearest neighbours.

According to the arguments leading to (5), we understand the parameter $\overline{S}$ is used to take account of appropriate contributions from the exchange term to the single-site representation. In the zero-temperature case which is considered here, according to equation (11), it is thus appropriate to use the equation

$$\overline{S} = \langle S_i^{z'} \rangle = C_0^{(0)}(\overline{S}, \theta) \tag{30}$$

to determine the parameter $\overline{S}$ self-consistently, where $\langle S_i^{z'} \rangle$ is the local Boson ground state expectation of $S_i^{z'}$. On the other hand, θ is chosen to cancel the non-harmonic part of interaction: $H_1(\theta, \overline{S})$, that is

$$-D \sin\theta \cos\theta [J_0^{(0)}(\overline{S}, \theta) + K_0^{(0)}(\overline{S}, \theta)] + \tfrac{1}{2} h \sin\theta [A_0^{(0)}(\overline{S}, \theta) + B_0^{(0)}(\overline{S}, \theta)] = 0. \tag{31}$$

In fact, the above terms just come from the second line of the total Hamiltonian (3). Although such terms are not included in the approximate single-site Hamiltonian (5) to determine the (local) Boson representation, their influences upon the total Hamiltonian are indeed eliminated by choosing an appropriate value of the canting angle θ, at least under the harmonic approximation adopted here.

It should be emphasized that since all of the coefficients (i.e. $A_l^{(p)}$, $B_l^{(p)}$, $C_l^{(p)}$, etc) are related to the matrix elements (see equation (17) and table 1) which are the functions of the two parameters $\overline{S}$ and θ according to equation (8), all of the coefficients presented in equations (24)–(28) (i.e. $A_0^{(0)}$, $B_0^{(0)}$ etc) are then the implicit functions of the two parameters $\overline{S}$ and θ. Thus, equations (30), (31) are two nonlinearly coupled equations serving to determine these two parameters. Once equations (30), (31) are solved, every parameter appearing in Hamiltonian (24) has a fixed value. We can diagonalize the Hamiltonian with the help of the Bogolyubov transformation and obtain

$$H = H_0' + \sum_{\boldsymbol{k}} E(\boldsymbol{k}) \alpha_{\boldsymbol{k}}^{\dagger} \alpha_{\boldsymbol{k}} + \cdots \tag{32}$$

where the ground state energy H_0' and the spin-wave dispersion relation $E(\boldsymbol{k})$ are defined as

$$H_0' = H_0 + \tfrac{1}{2} \sum_{\boldsymbol{k}} \left[-P(\boldsymbol{k}) + \sqrt{P(\boldsymbol{k})^2 - 4Q(\boldsymbol{k})^2} \right] \tag{33}$$

$$E(\boldsymbol{k}) = \sqrt{P(\boldsymbol{k})^2 - 4Q(\boldsymbol{k})^2}. \tag{34}$$

Then all the physical properties can be calculated readily.

Let us now discuss the physical significance of our choice equation (30). Applying the spin-Bose transformation to the single-site Hamiltonian (5), we find that

$$\begin{aligned} H_s = {} & -2JZ\overline{S}C_0^{(0)} + D\cos^2\theta E_0^{(0)} + D\sin^2\theta F_0^{(0)} - h\cos\theta C_0^{(0)} \\ & + [-2JZ\overline{S}C_1^{(0)} + D\cos^2\theta E_1^{(0)} + D\sin^2\theta F_1^{(0)} - h\cos\theta C_1^{(0)}] a^{\dagger} a \\ & + [-2JZ\overline{S}C_0^{(1)} + D\cos^2\theta E_0^{(1)} + D\sin^2\theta F_0^{(1)} - h\cos\theta C_0^{(1)}](a^{\dagger 2} + a^2) + \cdots . \end{aligned} \tag{35}$$

Since $a, a^{\dagger}$ are defined in the diagonalized representation of H_s (see equation (9)), the off-diagonal interactions in the above equation should be zero, which means that

$$-2JZ\overline{S}C_0^{(1)} + D\cos^2\theta E_0^{(1)} + D\sin^2\theta F_0^{(1)} - h\cos\theta C_0^{(1)} \equiv 0. \tag{36}$$

Substituting equation (30) into the above equation yields

$$-2JZC_0^{(0)}C_0^{(1)} + D\cos^2\theta E_0^{(1)} + D\sin^2\theta F_0^{(1)} - h\cos\theta C_0^{(1)} = 0. \tag{37}$$

When comparing equation (37) with the off-diagonal term $Q(\boldsymbol{k})$ defined in equation (28), the physical meaning of our choice equation (30) is very clear—up to second order, all the single-site off-diagonal interactions in the Hamiltonian (collected in the bracket in equation (28), of the type $(a^2 + a^{\dagger 2})$) have been cancelled. This is the direct consequence of the local Boson representation defined by (9). Instead, there appears another off-diagonal term $-JZA_0^{(0)}B_0^{(0)}\gamma_{\boldsymbol{k}}$ in the expression of $Q(\boldsymbol{k})$. But the off-diagonal effect of this term is much less serious than that of the single-site terms. Those single-site off-diagonal terms are actually responsible for the failure of the conventional HP method.

In fact, the parameter $\overline{S}$ is used to indicate the strength of the SSM effect. The larger the deviation of $\overline{S}$ from S (i.e. $\Delta S = S - \overline{S}$) is, the stronger the SSM effect will be. In the isotropic case, i.e. $D = 0$, according to equations (5), (30), it is easy to find that $\overline{S} = S$ because the local Boson ground state expectation value of $S_i^{z'}$ is just the absolute value of S. In such a case, the SSM effect disappears. This is why the conventional HP method works well for the isotropic spin systems. However, in the presence of an anisotropy, ΔS will be non-zero caused by the off-diagonal interactions in H_s. In such cases, the SSM effect is never trivial. The conventional HP method, which fails to consider such an effect, will encounter problems in some cases.

The parameter θ still possesses its classical meaning—the canting angle of the spin vector. According to equation (32), the approximate ground state is defined by $\alpha_{\boldsymbol{k}}|G\rangle = 0$. It is easy to check that

$$\langle G|S_i^{x'}|G\rangle = 0 \qquad \langle G|S_i^{y'}|G\rangle = 0. \tag{38}$$

Thus, we have chosen θ in such a way that the spin will point along the local z axis, without expectation values along other directions.

The state described by the parameters $\overline{S}$ and θ can then be understood as follows. The spins still point along the local z axis defined by θ, however, the ground state $|\tilde{0}\rangle$ is no longer that for the isotropic Heisenberg ferromagnet (i.e. the state with the largest $S_i^{z'}$ expectation value), but rather a mixture of the isotropic ground state $|0\rangle$ and exciting states $|2\rangle$, $|4\rangle \ldots$. The mixing effect is dependent on the anisotropy and the canting angle θ, and is described by the deviation ΔS.

So far, we have outlined the basic formalism of the new approach based on a homogeneous easy-plane model in which only one set of parameters $(\overline{S}, \theta)$ are necessary. The method is certainly not limited in such a special case. Actually, for any micromagnetic models with single-ion anisotropy, one just applies the LC transformation, then selects an appropriate single-site Hamiltonian to determine the local Boson representation, and finally performs the spin-wave analysis based on such a local Boson representation. It is a rather routine job to apply the same ideas to study the easy-axis model

$$H = -J\sum_{(ij)} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - D\sum_i (S_i^x)^2 - h\sum_i S_i^z \tag{39}$$

and other more complicated systems. After making detailed comparisons with existing theories in the next section, we will study an inhomogeneous system—the magnetic multilayers in section 4.

3. Comparison with existing theories

3.1. The HP method

First, let us compare our method with the conventional HP method which is the most widely adopted in the literature to deal with such problems [2–7]. Instead of our spin-Bose

transformation (11), the conventional method applies the naive HP transformation [8]

$$\begin{aligned} S_i^{+'} &= \sqrt{2S - a_i^\dagger a_i}\, a_i = \sqrt{2S} a_i + \cdots \\ S_i^{z'} &= S - a_i^\dagger a_i \end{aligned} \tag{40}$$

to Hamiltonian (3) to study the spin waves.

Subsequently, we will show that the conventional HP method has chosen a (local) Boson representation based on such a single-site Hamiltonian in which the off-diagonal interactions are neglected. Actually, if we discard the off-diagonal terms in the single-site Hamiltonian (5), the transformation matrix P_{mn} becomes diagonal:

$$P_{mn} = \delta_{mn}. \tag{41}$$

According to equation (8) and table 1, one may obtain

$$\begin{aligned} &A_0^{(0)} = \sqrt{2S}, \ldots \qquad A_l^{(p)} = 0 \qquad p \neq 0 \\ &B_l^{(p)} = 0 \\ &C_0^{(0)} = S \qquad C_1^{(0)} = -1, \ldots \qquad C_l^{(p)} = 0 \qquad p \neq 0 \\ &J_0^{(0)} = S\sqrt{2S}/2, \ldots \qquad J_l^{(p)} = 0 \qquad p \neq 0 \\ &K_0^{(0)} = (S-1)\sqrt{2S}/2, \ldots \qquad K_l^{(p)} = 0 \qquad p \neq 0 \\ &E_0^{(0)} = S^2 \qquad E_1^{(0)} = 1 - 2S, \ldots \qquad E_l^{(p)} = 0 \qquad p \neq 0 \\ &F_0^{(0)} = S/2 \qquad F_1^{(0)} = S - 1/2 \\ &F_0^{(1)} = \sqrt{2S(2S-1)}/4, \ldots \qquad F_l^{(p)} = 0 \qquad p \neq 0, 1. \end{aligned} \tag{42}$$

By putting the coefficients defined in equation (42) into equations (11), we find the resulting transformation

$$\begin{aligned} S_i^{+'} &= \sqrt{2S} a_i + \cdots \\ S_i^{z'} &= S - a_i^\dagger a_i + \cdots \end{aligned} \tag{43}$$

is in fact the same as the conventional HP transformation (40) under the harmonic approximation†.

According to equation (42), the solution of equation (30) is just $\overline{S} = S$ and equation (31) now becomes

$$\cos\theta = \frac{h}{D(2S-1)}. \tag{44}$$

Substituting equations (44), (42) into (27), (28), we find that

$$P^{HP}(\boldsymbol{k}) = 2JSZ(1 - \gamma_{\boldsymbol{k}}) + \tfrac{1}{2}D(2S-1)\sin^2\theta \tag{45}$$

$$Q^{HP}(\boldsymbol{k}) = \tfrac{1}{4}D\sin^2\theta\sqrt{2S(2S-1)}. \tag{46}$$

It is very easy to check that the magnon excitation energies of the easy-plane model, calculated by

$$E^{HP}(\boldsymbol{k}) = \sqrt{(P^{HP}(\boldsymbol{k}))^2 - 4(Q^{HP}(\boldsymbol{k}))^2} \tag{47}$$

are always imaginary when $\boldsymbol{k} \longrightarrow 0$. One may understand that this problem is caused by neglecting completely the off-diagonal interactions when choosing the (local) Boson representation, so that the off-diagonal interactions [$Q^{HP}(\boldsymbol{k})$ in (46)] are so strong that a harmonic approximation fails.

† It should be noted that the conventional HP method (40) fails to cancel the contributions of the Bose expansions in the unphysical Boson space. As the result, high-order terms in HP transformation may be different from our transformation.

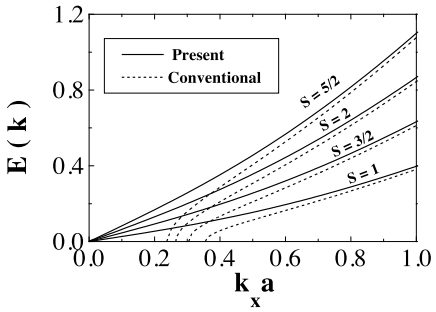

Figure 1. Magnon dispersion relations $E(\boldsymbol{k}) \sim k_x a$ ($k_y = k_z = 0$) calculated by the present method (solid curves) and the conventional HP method (dashed curves) for easy-plane model with anisotropy parameter $D/JZ = 0.2$ under zero external field (in this case, $\theta = \pi/2$) in spin-1,-3/2,-2,-5/2 cases, respectively.

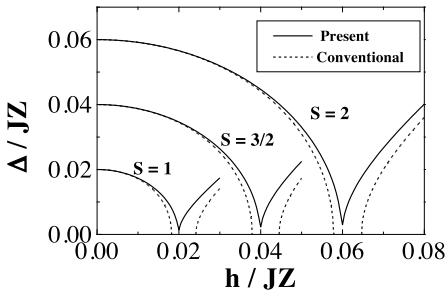

Figure 2. Magnon excitation gaps $\Delta(h)$ as functions of the external field calculated by the present method (solid curves) and the conventional HP method (dashed curves) for easy-axis models with anisotropy parameter $D/JZ = 0.02$ in spin-1,-3/2,-2 cases, respectively.

Some examples are helpful for comparison. Figure 1 presents the dispersion relations calculated by the present method (solid curve) and the conventional HP method (dashed curve) for the easy-plane model with a simple cubic lattice at zero external field. The imaginary excitation energies of those modes near the Γ point clearly show the failure of the conventional HP method, while such a problem has been overcome by the present method.

The magnon excitation gaps $\Delta(h)$ of an easy-axis model described by Hamiltonian (39) with a simple cubic lattice calculated by the two methods have been plotted together in figure 2 with respect to the external field. It is found that the conventional HP method is good for the easy-axis model in many cases. However, in some cases, i.e., in the vicinity $h \sim (2S-1)D$ when the spin is forced just parallel to the external field, the conventional HP method fails. We see that our method always gives a positive gap to the magnon dispersion relation.

Figure 3 presents the two parameters θ and $\overline{S}$ as the functions of the external field h for both the easy-plane and the easy-axis model. It is understood that the value of $S - \overline{S}$ describes the SSM effect—the larger this value, the more drastic the SSM effect. From figure 3, we find that, for the easy-plane model, the SSM effect is very significant when $\theta \neq 0$, and disappears when $\theta = 0$; while for the easy-axis model, the SSM effect is most significant when θ just approaches zero. Comparing figure 3 with figures 1 and 2, it is not difficult to understand that the failure of the conventional HP method is indeed caused by neglecting the SSM effect.

3.2. The MME method

Let us compare our new method with the MME method in this section [9–11]. In the MME method, when $h = 0$, the spin-Bose transformation has been derived which is correct to the lowest order in $d = D/2JZ$ for the easy-plane model [10, 11]. We will show that under the same conditions, our present method will give the same results as the MME method.

When $h = 0$, there is no competition between the anisotropy and the external field, so that the solution of equation (31) must be $\theta = \pi/2$—in another words, the spins have to lie in the easy plane (the xy plane). Then, the single-site Hamiltonian (5) is written as

$$H_s = 2JZ[-\overline{S}S_i^{z'} + d(S_i^{x'})^2]. \tag{48}$$

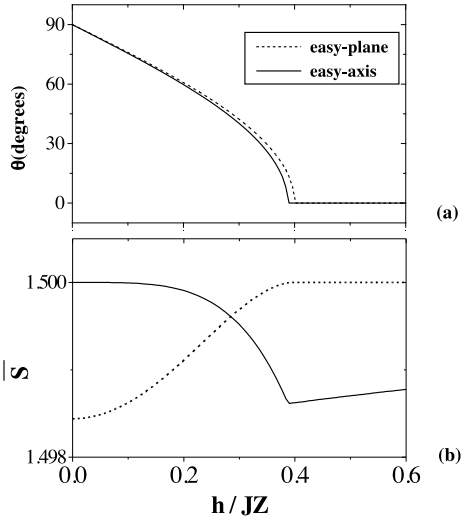

Figure 3. θ and $\overline{S}$ as the functions of the external field h for an easy-plane spin-3/2 model (solid curves) and an easy-axis spin-3/2 model (dashed curves) where the anisotropy parameters are $D/JZ = 0.2$ in the two models.

Treating $d(S_i^{x'})^2$ as a perturbation, we find the proper eigenstates of Hamiltonian (48) should be

$$\begin{aligned}
|\tilde{0}\rangle &= |0\rangle - \frac{\sqrt{4S(2S-1)}}{8\overline{S}}d|2\rangle + \mathrm{o}(d^2) \\
|\tilde{1}\rangle &= |1\rangle - \frac{\sqrt{6(2S-1)(2S-2)}}{8\overline{S}}d|3\rangle + \mathrm{o}(d^2) \\
|\tilde{2}\rangle &= \frac{\sqrt{4S(2S-1)}}{8\overline{S}}d|0\rangle + |2\rangle - \frac{\sqrt{12(2S-2)(2S-3)}}{8\overline{S}}d|4\rangle + \mathrm{o}(d^2).
\end{aligned} \tag{49}$$

According to table 1 and the above equation, we find that

$$\begin{aligned}
A_0^{(0)} &= \sqrt{2S} + \mathrm{o}(d^2) \\
B_0^{(0)} &= -\frac{\sqrt{2S}(S-\frac{1}{2})}{2\overline{S}}d + \mathrm{o}(d^2) \\
C_0^{(0)} &= S + \mathrm{o}(d^2) \\
C_1^{(0)} &= -1 + \mathrm{o}(d^2) \\
C_0^{(1)} &= \frac{\sqrt{2S(2S-1)}}{4\overline{S}}d + \mathrm{o}(d^2).
\end{aligned} \tag{50}$$

Correct to the first order in d, the solution of equation (30) is simply $\overline{S} = S$. Putting $\overline{S} = S$ into the above equation, we find that the resulting transformation is *exactly* the same as that in the MME method [10].

However, we have to emphasis here that the MME spin-Bose expansion [10] is only valid for the small d case, and more importantly, in the case of $h = 0$. If $h \neq 0$, we find from equations (30) and (31) that the two parameters θ and $\overline{S}$ cannot be determined independently. These two parameters must influence each other so that the final solution should be determined self-consistently rather than perturbatively. Clearly, the MME method cannot be applied naively to study the quantum spin systems in general spin configurations, but the present approach has included all the high-order contributions in d and can be applied to general spin configurations.

3.3. The CA method

Finally, we compare out method with the CA method which is developed for spin-1 systems [12–14]. We will show that, in the case of $S = 1$, our present method is *equivalent* to the CA method.

When $S = 1$, the eigenstates of Hamiltonian (5) must be

$$\begin{aligned} |\tilde{0}\rangle &= \cos\phi|0\rangle - \sin\phi|2\rangle \\ |\tilde{1}\rangle &= |1\rangle \\ |\tilde{2}\rangle &= \sin\phi|0\rangle + \cos\phi|2\rangle \end{aligned} \tag{51}$$

where ϕ needs to be determined. According to the above equation and table 1, we find that

$$\begin{aligned} &A_0^{(0)} = \sqrt{2}\cos\phi \\ &B_0^{(0)} = -\sqrt{2}\sin\phi \\ &C_0^{(0)} = \cos 2\phi \qquad C_1^{(0)} = -\cos 2\phi \qquad C_0^{(1)} = \sqrt{2}\sin\phi\cos\phi \\ &E_0^{(0)} = 1 \qquad E_1^{(0)} = -1 \qquad E_0^{(1)} = 0 \\ &F_0^{(0)} = \frac{1}{2}(1 - \sin 2\phi) \qquad F_1^{(0)} = \frac{1}{2}(1 + \sin 2\phi) \qquad F_0^{(1)} = \frac{1}{2\sqrt{2}}\cos 2\phi \\ &J_0^{(0)} = \frac{1}{\sqrt{2}}(\cos\phi + \sin\phi) \\ &K_0^{(0)} = 0. \end{aligned} \tag{52}$$

ϕ is selected to cancel the off-diagonal elements of the single-site Hamiltonian (5) in the representation $|\tilde{0}\rangle, |\tilde{1}\rangle, |\tilde{2}\rangle$. The only diagonal term is $\langle\tilde{0}|H_s|\tilde{2}\rangle$, so that we have the equation

$$\begin{aligned} \langle\tilde{0}|H_s|\tilde{2}\rangle = \langle\tilde{2}|H_s|\tilde{0}\rangle = -2JZ\overline{S}\sqrt{2}\sin\phi\cos\phi + D\sin^2\theta\frac{1}{2\sqrt{2}}\cos 2\phi \\ -h\cos\theta\sqrt{2}\sin\phi\cos\phi = 0 \end{aligned} \tag{53}$$

to fix ϕ. According to (52), equations (30), (31) now become

$$\overline{S} = \cos 2\phi \tag{54}$$

$$-D\sin\theta(\cos\phi + \sin\phi) + h\sin\theta(\cos\phi - \sin\phi) = 0. \tag{55}$$

Thus, we have three equations (53)–(55) to fix three parameters $\overline{S}$, θ and ϕ. Putting (54) into (53), we then have

$$-JZ\cos 2\phi\sin 2\phi + \frac{D}{4}\sin^2\theta\cos 2\phi - \frac{h}{2}\cos\theta\sin 2\phi = 0. \tag{56}$$

When comparing equations (56), (55) with the criterion in the CA method for the same model (equations (19), (20) in [13]), one may find that they are in fact *equivalent*. The parameter ϕ is just another variation parameter—the characteristic angle, in the CA method [12–14]. Substituting equation (52) into (24)–(28), it is rather easy to check that the resulting expressions are *exactly* the same as those presented in the CA method [13]. Thus, we have shown that in the case of $S = 1$, the present method is equivalent to the CA method. This result is not surprising, because the basic ideas of both methods are the same—to try to find out the best local Boson representations. However, the CA method is only applicable to spin-1 systems whereas the present method can be applied to arbitrary spin-number cases.

4. Applications in magnetic multilayers

In principle, the method described in section 2 can be applied to any quantum spin system with single-ion anisotropy. Here, we apply the method to study one kind of inhomogeneous

system—the magnetic multilayer system. Our results may reveal that the remarkable merit of the new method is that it can clarify some unphysical instabilities which are predicted by the conventional HP method.

Generally, a magnetic multilayer can be well described by the following micromagnetic model:

$$H = \sum_{m,m'} \sum_{\boldsymbol{r},\boldsymbol{r}'} I_{m,m'} \boldsymbol{S}_m(\boldsymbol{r}) \cdot \boldsymbol{S}_{m'}(\boldsymbol{r}') + \sum_{m,\boldsymbol{r}} D_m [S_m^{z_m^0}(\boldsymbol{r})]^2 - h \sum_{m,\boldsymbol{r}} S_m^z(\boldsymbol{r}) \tag{57}$$

where m, m' label the layer and $\boldsymbol{r}, \boldsymbol{r}'$ are the lattice sites within the plane. The anisotropic axes $\{\hat{z}_m^0\}$ can be different from layer to layer, and the anisotropy $\{D_m\}$ can be of easy-plane or easy-axis type. For simplicity, we assume that $\{\hat{z}_m^0\}$ are in the xz plane and $\hat{z}_m^0 \cdot \hat{z} = \cos\eta_m$.

As we have already mentioned, in magnetic multilayers, the spins in different layers are no longer equivalent. We have to adopt different parameters $\{\theta_m, \overline{S}_m\}$ to describe spins in different layers. After a LC transformation similar to (2) but with angles θ_m different from layer to layer, we find the following single-site Hamiltonian for each layer:

$$\begin{aligned} H_m^s = -\Bigg[& 2I_{mm} Z \overline{S}_m + \sum_{m'} 2I_{mm'} \cos(\theta_m - \theta_{m'}) \overline{S}_{m'} + h \cos\theta_m \Bigg] S_m^{z_m}(\boldsymbol{r}) \\ & + D_m \cos^2(\theta_m - \eta_m) [S_m^{z_m}(\boldsymbol{r})]^2 + D_m \sin^2(\theta_m - \eta_m) [S_m^{x_m}(\boldsymbol{r})]^2 \\ & m = 1, 2, \ldots . \end{aligned} \tag{58}$$

The spin-Bose transformation for the mth layer is determined based on its own Hamiltonian H_m^s. Thus, we have

$$\begin{aligned} S_m^+(\boldsymbol{r}) &= \sum_{p=0}^{2p+1 \leqslant 2S_m} \sum_{l=0}^{\infty} [A_{l,m}^{(p)} a_m^{\dagger l}(\boldsymbol{r}) a_m^{l+2p+1}(\boldsymbol{r}) + B_{l,m}^{(p)} a_m^{\dagger l+2p+1}(\boldsymbol{r}) a_m^l(\boldsymbol{r})] \\ S_m^{z_m}(\boldsymbol{r}) &= \sum_{l=0}^{\infty} C_{l,m}^{(0)} a_m^{\dagger l}(\boldsymbol{r}) a_m^l(\boldsymbol{r}) + \sum_{p=1}^{2p \leqslant 2S_m} \sum_{l=0}^{\infty} C_{l,m}^{(p)} [a_m^{\dagger l}(\boldsymbol{r}) a_m^{l+2p}(\boldsymbol{r}) + a_m^{\dagger l+2p}(\boldsymbol{r}) a_m^l(\boldsymbol{r})] \end{aligned} \tag{59}$$

where the parameters $\{A_{l,m}^{(p)}, B_{l,m}^{(p)}, C_{l,m}^{(p)}\}$ are determined following the same procedures described in section 2, with single-site Hamiltonian (5) in section 2 replaced by H_m^s.

By using the transformation (59), we expand the Hamiltonian into the following Bose series under the harmonic approximation:

$$\begin{aligned} H = {} & H_0(\{\overline{S}_m\}, \{\theta_m\}) + H_1(\{\overline{S}_m\}, \{\theta_m\}) \\ & + \sum_{m,m'\boldsymbol{k}} \{P_{mm'}(\boldsymbol{k}) a_m^\dagger(\boldsymbol{k}) a_{m'}(\boldsymbol{k}) + Q_{mm'}(\boldsymbol{k}) [a_m^\dagger(\boldsymbol{k}) a_{m'}^\dagger(-\boldsymbol{k}) \\ & + a_m(\boldsymbol{k}) a_{m'}(-\boldsymbol{k})]\} + \cdots \end{aligned} \tag{60}$$

where

$$\begin{aligned} H_0 = \sum_m \{ & -I_{mm} Z [C_{0,m}^{(0)}]^2 + D_m \cos^2(\theta_m - \eta_m) E_{0,m}^{(0)} + D_m \sin^2(\theta_m - \eta_m) F_{0,m}^{(0)} - h \cos\theta_m C_{0,m}^{(0)} \\ & - \sum_{m'} I_{mm'} \cos(\theta_m - \theta_{m'}) C_{0,m}^{(0)} C_{0,m'}^{(0)} \} \times N \end{aligned} \tag{61}$$

$$\begin{aligned} H_1 = \sum_m [& \sum_{m'} I_{mm'} \sin(\theta_m - \theta_{m'}) C_{0,m'}^{(0)} (A_{0,m}^{(0)} + B_{0,m}^{(0)}) - D_m \sin(\theta_m - \eta_m) \cos(\theta_m - \eta_m) \\ & \times (J_{0,m}^{(0)} + K_{0,m}^{(0)}) + \tfrac{1}{2} h \sin\theta_m (A_{0,m}^{(0)} + B_{0,m}^{(0)})] [a_m^\dagger(\boldsymbol{k}) + a_m(-\boldsymbol{k})] \end{aligned} \tag{62}$$

and

$$P_{mm}(\boldsymbol{k}) = -2I_{mm} Z C_{0,m}^{(0)} C_{1,m}^{(0)} - I_{mm} Z [(A_{0,m}^{(0)})^2 + (B_{0,m}^{(0)})^2] \gamma_{\boldsymbol{k}} + D_m \cos^2(\theta_m - \eta_m) E_{1,m}^{(0)}$$

$$+D_m \sin^2(\theta_m - \eta_m) F^{(0)}_{1,m} - h \cos\theta_m C^{(0)}_{1,m}$$
$$-2\sum_{m'} I_{mm'} \cos(\theta_m - \theta_{m'}) C^{(0)}_{0,m'} C^{(0)}_{1,m} \tag{63}$$

$$Q_{mm}(\boldsymbol{k}) = -I_{mm} A^{(0)}_{0,m} B^{(0)}_{0,m} Z\gamma_{\boldsymbol{k}} + \{-2I_{mm} Z C^{(0)}_{0,m} C^{(1)}_{0,m} - h\cos\theta_m C^{(1)}_{0,m}$$
$$+D_m \cos^2(\theta_m - \eta_m) E^{(1)}_{0,m} + D_m \sin^2(\theta_m - \eta_m) F^{(1)}_{0,m}$$
$$-\sum_{m'} 2I_{mm'} \cos(\theta_m - \theta_{m'}) C^{(0)}_{0,m'} C^{(1)}_{0,m}\} \tag{64}$$

$$P_{mm'}(\boldsymbol{k}) = -\tfrac{1}{2} I_{mm'}[1 + \cos(\theta_m - \theta_{m'})] \cdot (A^{(0)}_{0,m} A^{(0)}_{0,m'} + B^{(0)}_{0,m} B^{(0)}_{0,m'})$$
$$+\tfrac{1}{2} I_{mm'}[1 - \cos(\theta_m - \theta_{m'})] \cdot (A^{(0)}_{0,m} B^{(0)}_{0,m'} + A^{(0)}_{0,m'} B^{(0)}_{0,m}) \tag{65}$$

$$Q_{mm'}(\boldsymbol{k}) = -\tfrac{1}{4} I_{mm'}[1 + \cos(\theta_m - \theta_{m'})] \cdot (A^{(0)}_{0,m} B^{(0)}_{0,m'} + A^{(0)}_{0,m'} B^{(0)}_{0,m})$$
$$+\tfrac{1}{4} I_{mm'}[1 - \cos(\theta_m - \theta_{m'})] \cdot (A^{(0)}_{0,m} A^{(0)}_{0,m'} + B^{(0)}_{0,m'} B^{(0)}_{0,m}). \tag{66}$$

Following section 2, $\{\overline{S}_m\}$ should be determined self-consistently by the following equations:

$$\overline{S}_m = \langle 0|S^{z_m}_m|0\rangle = C^{(0)}_{0,m} \qquad m = 1, 2, \ldots \tag{67}$$

and the canting angles $\{\theta_m\}$ are obtained by letting $H_1 = 0$, i.e.,

$$\sum_{m'} I_{mm'} \sin(\theta_m - \theta_{m'}) C^{(0)}_{0,m'} (A^{(0)}_{0,m} + B^{(0)}_{0,m}) - D_m \sin(\theta_m - \eta_m)\cos(\theta_m - \eta_m)(J^{(0)}_{0,m} + K^{(0)}_{0,m})$$
$$+\tfrac{1}{2} h \sin\theta_m (A^{(0)}_{0,m} + B^{(0)}_{0,m}) = 0. \tag{68}$$

Since all the coefficients shown in equations (67), (68) (i.e. $C^{(0)}_{0,m}$, $A^{(0)}_{0,m}$, $B^{(0)}_{0,m}$, etc) are the implicit functions of $\{\theta_m\}$ and $\{\overline{S}_m\}$, $\{\theta_m\}$ and $\{\overline{S}_m\}$ can be determined by solving equations (67) and (68) self-consistently. Putting the solutions into Hamiltonian (60), we have

$$H = H'_0 + \sum_{m,\boldsymbol{k}} E_m(\boldsymbol{k}) \alpha^{\dagger}_m(\boldsymbol{k}) \alpha_m(\boldsymbol{k}) + \cdots \tag{69}$$

where the spin-wave excitations $E_m(\boldsymbol{k})$ are calculated following [5]. All the physically interesting properties can be examined.

The first example we study is a six-layer sandwich-type magnetic multilayer, where the first two layers and the last two layers have easy-plane anisotropies while the middle two layers have perpendicular easy-axis anisotropies. The lattice structure is assumed to be simple cubic-like, and the structural parameters have been specified in the caption of figure 4†. For such a system, following the method outlined in [6], two non-trivial spin configurations (denoted by configurations (*a*) and (*b*)) are found to exist at zero external field—see the caption of figure 4. If we are using the conventional HP method, we find that both spin configurations are *unstable*!—see the spin-wave spectra (dashed curves) depicted in figures 4(*a*) and (*b*). In fact, such problems exist generally in magnetic multilayers with easy-plane anisotropies—we have examined many other systems with easy-plane anisotropy and have found that soft modes exist for *any* canted spin configurations.

However, is it true that the canted spin configurations are *all* unstable in such kinds of systems?

Using the present method to recalculate the same system, we find that spin configuration (*b*) is really unstable; however, spin configuration (*a*) is stable. The instability of spin configuration (*a*) is caused by missing the SSM effect, not a physical one.

† It should be noted that in this paper, in order to show just the main physical picture, the anisotropy parameters are selected to be somewhat larger than practical values. Actually, for small anisotropy, such an effect still exists.

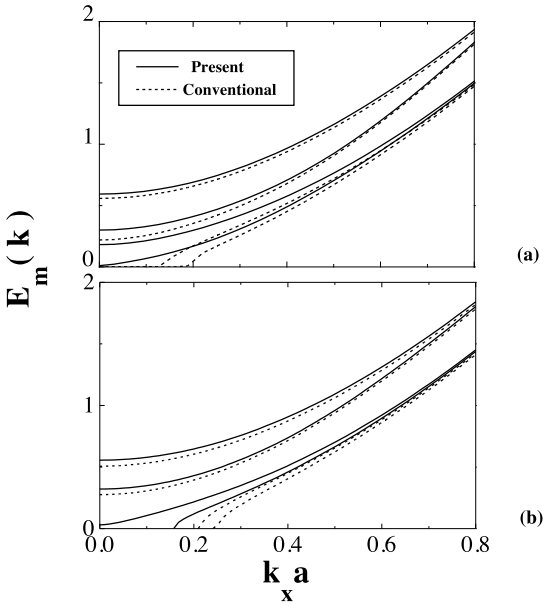

Figure 4. Magnon dispersion relations $E_m(\boldsymbol{k}) \sim k_x a$ $(k_y = 0)$ (lowest four modes) calculated by the present method (solid curves) and the conventional HP method (dashed curves) for a six-layer magnetic multilayer with model parameters: $I_{m,m} = 1$, $I_{m,m+1} = I_{m,m-1} = 0.1$; $m = 1, 2, 5, 6$: $D_m = 0.5$, $S_m = 1$, $\eta_m = 0$; $m = 3, 4$: $D_m = -0.1$, $S_m = 3/2\eta_m = 0$; $h = 0$ at spin configuration (*a*): $\theta_1 = 1.50, \theta_2 = 1.33, \theta_3 = 0.81, \theta_4 = 0.81, \theta_5 = 1.33, \theta_6 = 1.50$; and spin configuration (*b*): $\theta_1 = -1.45, \theta_2 = -1.16, \theta_3 = -0.21, \theta_4 = 0.21, \theta_5 = 1.16, \theta_6 = 1.45$.

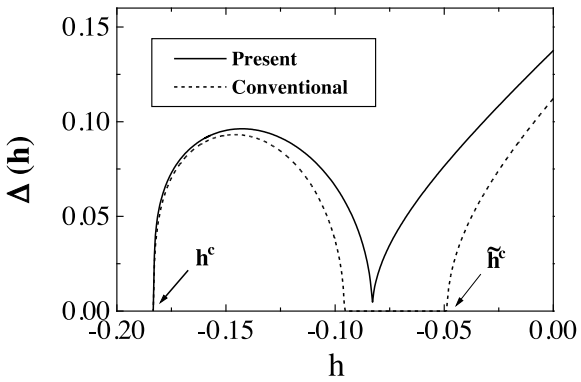

Figure 5. Magnon excitation gap $\Delta(h)$ calculated by the present method (solid curve) and the conventional HP method (dashed curve) as the function of the external field for a six-layer magnetic multilayer with model parameters: $I_{m,m} = 1$, $I_{m,m+1} = I_{m,m-1} = 0.5$; $m = 1, 2$: $D_m = -0.2$, $S_m = 1$, $\eta_m = \pi/2$; $m = 3, 4, 5, 6$: $D_m = -0.2$, $S_m = 3/2$, $\eta_m = 0$.

We will investigate another example to show the usefulness of our new method. Let us consider a six-layer system in which the first two layers have magnetic easy axes along the x direction in the plane and the remaining four layers have perpendicular easy axes. By using both the conventional HP method and the present new one, we have calculated the magnon excitation gaps $\Delta(h)$ as functions of the external field applied along the $-z$ direction, and compared the results in figure 5. According to the quantum theory for coercive fields

established in [5], we know that the field at which the magnon excitation gap approaches zero is simply the coercive field h^c, since at this point the present spin state is no longer stable so that a spin reversal transition should take place. From figure 5, it is very interesting to find that the coercive field $\tilde{h}^c \simeq 0.5$ calculated by the conventional HP method is considerably smaller than that calculated by the new method $h^c \simeq 1.7$. Once more, $\tilde{h}^c$ corresponds to an unphysical instability caused by missing the SSM effect, which has been removed by the new method.

In principle, the method established here is applicable to any micromagnetic models with single-ion anisotropy—one just substitutes the conventional HP transformation by our spin-Bose transformation (11). Although some physical properties (such as the ground state energy, the magnetization) may not be modified very much, the low-lying spin-wave excitations, however, can be improved considerably by our new method. The latter may be important in determining the stability of an arbitrary spin configuration in a complicated magnetic system.

5. Conclusions

To summarize, we have established a unified spin-wave approach for quantum spin systems with single-ion anisotropies, which can be applied to remedy the problems encountered by the conventional HP method, and is applicable to the arbitrary spin-number case and general spin configurations. The key element of our method is a new spin-Bose transformation which is quite different with the conventional HP transformation and other spin-Bose transformations. In the new spin-Bose transformation, the single-site spin-states mixing effect has been considered self-consistently, so that the largest part of off-diagonal terms in the Hamiltonian have been cancelled by this transformation, while it is actually those terms which are responsible for the failure of the conventional HP method.

The present method has been compared with other existing theories. Treating the anisotropy in a first-order approximation and in the case of zero external field, the present method gives the same results as the MME method which is valid in such a case. For spin-1 systems, the present method recovers the results of the CA method which is developed only for spin-1 systems.

The method has also been applied to study some magnetic multilayer systems; the results show that it is helpful to clarify the unphysical instability predicted by the conventional HP method.

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