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Abstract. In this paper, we develop a new method of spin operator transformation for an easy-plane spin-one ferromagnet:

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

The ground-state energy E_0, the magnetization M and the magnon dispersion relation ϵ_k are calculated analytically, and the contrast with other methods and numerical results are given.

Crystal-field anisotropy plays an important role in the thermodynamic properties of magnetic systems with spin greater than one half [1]. In this paper we consider an easy-plane spin-one ferromagnet at $T = 0$. It represents a non-trivial system with single-ion anisotropy $(D \sum_i (S_i^x)^2)$. In these systems, even non-interacting spin wave theory is not trivial, owing to the diagonal effects of the anisotropy on single-ion energy levels. For instance, a naive use of the well ordered Holstein–Primakoff transformation (H-P transformation) lead to an imaginary value for the energy of the $k = 0$ mode [2]. To overcome these difficulties, the matching of metrics elements method (the MME method) was introduced in 1974 [3]. From then on, many applications [2, 4–6] of this method have been implemented, making it possible to examine the easy-plane ferromagnetic systems. In 1990, surface spin waves in these systems were discussed using Green's function method [7].

In reviewing these papers, one may find that the MME method can give a very good magnon dispersion relation in the case of small anisotropy, but its magnetization is quite different from the numerical result [8]. In this paper, we try to introduce a new transformation method, the so-called characteristic angle (CA) spin-operator transformation method, to deal with such systems. The main point in our method is that an angle, CA, is introduced to optimize the magnetized direction which will be used in the Holstein–Primakoff transformation. In fact, the angle is a variation parameter which is fixed by minimizing the ground-state energy. Using our method, we can not only get a good magnon dispersion relation, which is same as the one in MME method, but also more reasonable ground-state energy and magnetization.

The Hamiltonian is given as

$$H = -J \sum_{(i,j)} S_i \cdot S_j + D \sum_i (S_i^x)^2 - h \sum_i S_i^z \tag{1}$$

where (i, j) means summation restricted to the nearest-neighbour pairs, and h is the external magnetic field along the Z axis, used here to determine the magnetization of this system. The spins will be forced into the YZ plane by the anisotropy term $(D > 0)$. The Hamiltonian (1) can be rewritten as

$$H = -J \sum_{(i,j)} (S_i^z S_j^z + S_i^+ S_j^-) + (D/4) \sum_i (S_i^+ S_i^+ + S_i^- S_i^+ + \text{c.c.}) - h \sum_i S_i^z. \tag{2}$$

We introduce the following CA spin-operator transformation for $S = 1$:

$$S_j^+ = \cos\theta \tilde{S}_j^+ + \sin\theta \tilde{S}_j^- \exp(i\pi \tilde{S}_j^z) \tag{3}$$

$$S_j^- = \cos\theta \tilde{S}_j^- + \sin\theta \exp(-i\pi \tilde{S}_j^z) \tilde{S}_j^+ \tag{4}$$

$$S_j^z = \tfrac{1}{2}[S_j^+, S_j^-]_-. \tag{5}$$

Here $(\tilde{S}_j^-, \tilde{S}_j^+, \tilde{S}_j^z)$ is a set of CA spin operators which obey the usual angular momentum's commutation rules, and θ is the characteristic angle which will be determined later. In the appendix, we proove that the transformation (3)–(5) does not affect the commutation relations of operators (S_j^-, S_j^+, S_j^z). In fact, the transformation just means a kind of rotation in the spin space. After the transformation, the Hamiltonian can be presented by new spin operators $(\tilde{S}_j^-, \tilde{S}_j^+, \tilde{S}_j^z)$ as follows:

$$H = -J \sum_{(i,j)} H_{ij}^1 + \sum_i H_i^2 \tag{6}$$

$$\begin{aligned}
H_{ij}^1 =\ & [\cos\theta \tilde{S}_j^+ + \sin\theta \tilde{S}_j^- \exp(i\pi \tilde{S}_j^z)] \times [\cos\theta \tilde{S}_j^- + \sin\theta \exp(-i\pi \tilde{S}_j^z) \tilde{S}_j^+] \\
& + [\cos 2\theta \tilde{S}_i^z - \sin\theta \cos\theta ((\tilde{S}_i^+)^2 \exp(-i\pi \tilde{S}_i^z) + \exp(i\pi \tilde{S}_i^z)(\tilde{S}_i^-)^2)] \\
& \times [\cos 2\theta \tilde{S}_j^z - \sin\theta \cos\theta ((\tilde{S}_j^+)^2 \exp(-i\pi \tilde{S}_j^z) + \exp(i\pi \tilde{S}_j^z)(\tilde{S}_j^-)^2)]
\end{aligned} \tag{7}$$

$$\begin{aligned}
H_i^2 =\ & (D/4)[(\cos\theta \tilde{S}_i^+ + \sin\theta \tilde{S}_i^- \exp(i\pi \tilde{S}_i^z)) \times (\cos\theta \tilde{S}_i^- + \sin\theta \exp(-i\pi \tilde{S}_i^z) \tilde{S}_i^+) \\
& + (\cos\theta \tilde{S}_i^+ + \sin\theta \tilde{S}_i^- \exp(i\pi \tilde{S}_i^z))^2 + \text{c.c.}] \\
& - h[\cos 2\theta \tilde{S}_i^z - \sin\theta \cos\theta ((\tilde{S}_i^+)^2 \exp(-i\pi \tilde{S}_i^z) + \exp(i\pi \tilde{S}_i^z)(\tilde{S}_i^-)^2)].
\end{aligned} \tag{8}$$

Let us define a ground state $|0\rangle$ by

$$\tilde{S}_j^z |0\rangle = |0\rangle, \quad \tilde{S}_j^+ |0\rangle = 0. \tag{9}$$

The meaning of (9) is that the new spins will point along the direction described by choosing the angle θ for decreasing the ground-state energy as low as possible. The H-P transformation is introduced for $(\tilde{S}_i^-, \tilde{S}_i^+, \tilde{S}_i^z)$

$$\tilde{S}_i^z \rightarrow 1 - a_i^+ a_i \tag{10}$$

$$\tilde{S}_i^+ \rightarrow \sqrt{2}\sqrt{1 - (a_i^+ a_i/2)}\, a_i \tag{11}$$

$$\tilde{S}_i^- \rightarrow \sqrt{2} a_i^+ \sqrt{1 - (a_i^+ a_i/2)}. \tag{12}$$

It is very tedious to write down the expansions of all the terms in expressions (7) and (8) when applying the H-P transformation; we will only give one of them since the others are similar. For example, some terms in H_i^2 are found to be proportional to

$$\begin{aligned}
& \tilde{S}_i^z \exp(i\pi \tilde{S}_i^z) + \exp(-i\pi \tilde{S}_i^z) \tilde{S}_i^z \\
&= -\exp(-i\pi a_i^+ a_i) + a_i^+ a_i \exp(-i\pi a_i^+ a_i) - \exp(i\pi a_i^+ a_i) + \exp(i\pi a_i^+ a_i) a_i^+ a_i \\
&= -2 \sum_{n=0}^{\infty} \frac{(i\pi)^{2n}}{(2n)!} (a_i^+ a_i)^{2n} + 2 \sum_{n=0}^{\infty} \frac{(i\pi)^{2n}}{(2n)!} (a_i^+ a_i)^{2n+1}.
\end{aligned} \tag{13}$$

According to Wick's theorem,

$$(a_i^+ a_i)^n = N[(a_i^+ a_i)^{2n}] + (n-1)!N[(a_i^+ a_i)^{n-1}] + \cdots + a_i^+ a_i \tag{14}$$

where $N[AB \cdots C]$ means the normal product of operators A, B, ..., C. Then

$$\tilde{S}_i^z \exp(i\pi \tilde{S}_i^z) + \exp(-i\pi \tilde{S}_i^z)\tilde{S}_i^z = -2 + 2a_i^+ a_i + \cdots. \tag{15}$$

Other terms can be calculated similarly. After carefully calculating all the terms in (6) and (7) and keeping only the quadratic-order approximation, we obtain

$$H = H_0 + H_2 + \cdots \tag{16}$$

$$H_0 = (-JZ\cos^2 2\theta - (D/2)\sin 2\theta + D/2 - h\cos 2\theta)N \tag{17}$$

$$H_2 = -J\sum_{(i,j)}[2a_i^+ a_j - \cos^2 2\theta (a_i^+ a_i + a_j^+ a_j)$$

$$- \sin 2\theta (a_i a_j + a_i^+ a_j^+) + (\sqrt{2}/4)\sin 4\theta (a_i^2 + a_j^2 + \text{c.c.})]$$

$$+ \sum_i [(D/2 + (D/2)\sin 2\theta + h\cos 2\theta)a_i^+ a_i$$

$$\times ((\sqrt{2}/4)D\cos 2\theta - (\sqrt{2}/2)h\sin 2\theta)(a_i^2 + \text{c.c.})] \tag{18}$$

where H_0 is the Hamiltonian given in the mean-field (MF) theory.

Using the Fourier transformation of the Bose operators, we convert the Hamiltonian to the form

$$H = H_0 + \sum_k A_k a_k^+ a_k + \sum_k B_k(a_k^+ a_{-k}^+ + a_k a_{-k}) \tag{19}$$

where

$$A_k = 2JZ(\cos^2 2\theta - \gamma_k) + (D/2)\sin 2\theta + D/2 + h\cos 2\theta \tag{20}$$

$$B_k = (\sqrt{2}/2)[-JZ\sin 4\theta + (D/2)\cos 2\theta - h\sin 2\theta] + JZ\sin 2\theta\gamma_k \tag{21}$$

$$\gamma_k = (1/Z)\sum_\delta \exp(i k \cdot r_\delta) \tag{22}$$

and Z in equation (22) is the number of nearest-neighbour sites; the δ summation runs over Z nearest-neighbour sites. Hamiltonian (19) can be diagonalized by the Bogolyubov transformation:

$$H = E_0 + \sum_k \epsilon_k \alpha_k^+ \alpha_k \tag{23}$$

$$E_0 = H_0 + \sum_k [-A_k(\theta)/2 + (1/2)\sqrt{A_k^2 - 4B_k^2}] \tag{24}$$

$$\epsilon_k = \sqrt{A_k^2 - 4B_k^2}. \tag{25}$$

We understand that our CA θ_0 is the angle at which the ground-state energy $E_0(\theta_0)$ takes the minimum value. To determine it, we calculate E_0 as a function of $\sin 2\theta$ numerically with different values of the parameter $d = D/4JZ$. In any case, we are interested in finding that the CA θ_0 always satisfy the following equation:

$$\frac{\mathrm{d}}{\mathrm{d}\theta}H_0(\theta) = (JZ\sin 4\theta - (D/2)\cos 2\theta - h\sin 2\theta)N = 0. \tag{26}$$

In other words,

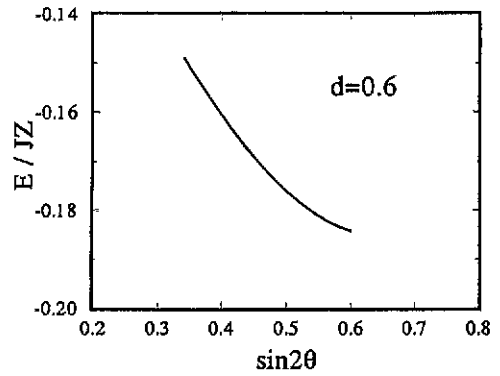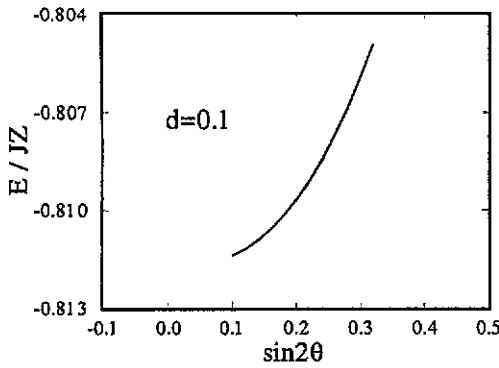$$\sin 2\theta_0 = d = D/4JZ. \tag{27}$$

Figure 1. Energy as a function of $\sin 2\theta$ for $d = 0.1$.

Figure 2. Energy as a function of $\sin 2\theta$ for $d = 0.6$.

As an example, the cases of $d = 0.1$ and $d = 0.6$ are shown in figure 1 and figure 2; the values of $\sin 2\theta_0$ are found to be 0.1 and 0.6, respectively.

We will now give a rough explanation.

Let us define:

$$\Delta(\theta) = (1/2JZ)^2 [A_k^2(\theta) - 4B_k^2(\theta)]|_{k=0}$$
$$= (d + \sin 2\theta(d - \sin 2\theta))^2 - (\sin 2\theta + \sqrt{2}\cos 2\theta(d - \sin 2\theta))^2. \quad (28)$$

From equation (25), we find

$$\epsilon_0 = 2JZ\sqrt{\Delta(\theta)}. \tag{29}$$

Obviously,

$$\Delta(\theta) \geqslant 0 \tag{30}$$

is a restriction for our calculations.

Now differentiate $\Delta(\theta)$ and $\frac{1}{2}JZ)E_0(\theta)$ with respect to θ and substitute θ with $\theta_0 = \frac{1}{2}\sin^{-1} d$, we get

$$D(d) = \frac{d}{d\theta}\Delta(\theta)|_{\theta_0}$$
$$= -2d(d + 1)\sqrt{1 - d^2} + 2\sqrt{2}d(1 - d^2) \tag{31}$$

$$F(d) = (1/2JZ)\frac{d}{d\theta}E_0(\theta)|_{\theta_0}$$
$$= (1/2N)\sum_k \left[2d\sqrt{1 - d^2} + \frac{-2d\sqrt{1 - d^2}(1 - \gamma_k + d - \sqrt{2(1 - d^2)}\gamma_k + \gamma_k^2)}{\sqrt{(1 - \gamma_k + d)^2 - (d\gamma_k)^2}} \right].$$
$$\tag{32}$$

In figure 3, $D(d)$ and $F(d)$ are drawn together. It is easy to show that the two differentials always have the same sign, which means $\Delta(\theta)$ and $E_0(\theta)$ always have the same varying tendency at a point θ_0. In the case where two differentials are both positive, $\Delta(\theta)$ will increase when θ becomes larger. Noticing that in equation (28) $\Delta(\theta_0) = 0$, constraint (30) must require $\theta \geqslant \theta_0$, otherwise $\Delta(\theta)$ becomes negative. Since $E_0(\theta)$ is also an increasing function of θ at the point θ_0, the requirement $\theta \geqslant \theta_0$ tells us that $E_0(\theta_0)$ is
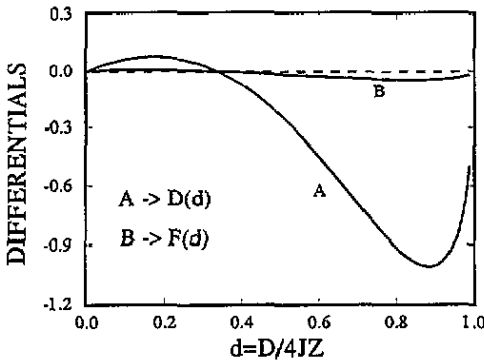
Figure 3. Comparison of two differentials.

the minimum value of $E_0(\theta)$ in the region of $\theta \sim \theta_0$. The situation is similar in the case of $F(d)$ and $D(d)$ being both negative.

Of course, this is an explanation rather than a proof, but at least we may get some general understanding of the result from the discussions above.

Applying the solution (27) to (23)–(25) for $h = 0$, we obtain the ground-state energy E_0, the magnetization M and the magnon dispersion relation ϵ_k,

$$E_0 = JZ \sum_k [-2 + d - d^2 + \gamma_k + \sqrt{(1 + d - \gamma_k)^2 - (d\gamma_k)^2}] \tag{33}$$

$$M = -\frac{1}{N}\frac{d}{dh}E_0(h)|_{h=0} = M^{MF} + \Delta M \tag{34}$$

$$\epsilon_k = 2JZ\sqrt{(1 + d - \gamma_k)^2 - (d\gamma_k)^2} \tag{35}$$

where M^{MF} is the result of the mean-field calculation

$$M^{MF} = \sqrt{1 - d^2} \tag{36}$$

and

$$\Delta M = \frac{1}{2\sqrt{1 - d^2}} - (1/2N)\sum_k \frac{d + 1 - \gamma_k + (d\gamma_k)^2}{\sqrt{(1 - d^2)((1 + d - \gamma_k)^2 - (d\gamma_k)^2)}}. \tag{37}$$

It is easy to show that the excitation energy $\epsilon_k \to 0$ as $k \to 0$.

Equations (33)–(37) are the analytical results of our method. However, the MME method gave [2]

$$E_0 = JZ \sum_k [-2 + d + \gamma_k + \sqrt{(1 + d - \gamma_k)^2 - (d\gamma_k)^2}] \tag{38}$$

$$M = \frac{3}{2} - (1/2N)\sum_k \frac{d + 1 + (\sqrt{2}d^2 - 1)\gamma_k}{(1 + d - \gamma_k)^2 - (d\gamma_k)^2} \tag{39}$$

$$\epsilon_k = 2JZ\sqrt{(1 + d - \gamma_k)^2 - (d\gamma_k)^2}. \tag{40}$$

In figure 4, the numerical result (M^{MF}, M^{CA}) obtained by our method and M^{MME} as a function of d are shown together for simple cubic lattice. Comparing our method with the MME method and the numerical result, we find:

(1) our ground-state energy E_0^{CA} is lower than E_0^{MME},

(2) our magnetization M^{CA} is much better than M^{MME} (figure 4). Except in the vicinity of the phase transition point, our M^{CA} is very close to the numerical result although M^{MME} is not,
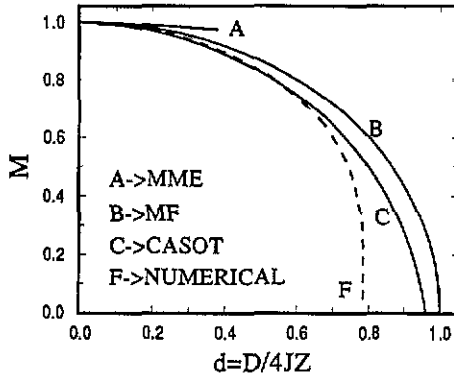
Figure 4. Magnetizations of easy-plane spin-one ferromagnetic simple cubic lattice system as a function of $D/4JZ$.

(3) our excitation energy ϵ_k^{CA} is the same as ϵ_k^{MME}.

To summarize, we have introduced a new method of spin-operator transformation for easy-plane spin-one ferromagnetic systems. The ground-state energy E_0, the magnetization M and the magnon dispersion relation ϵ_k are calculated analytically. A comparison with the matching of metrics elements method [3] (the MME method) and numerical calculation are given.

Appendix

In this appendix, we will prove that the transformation (3)–(5) does not affect the usual commutation relations of (S_j^+, S_j^-, S_j^z).

According to the transformation

$$S_j^+ = \cos\theta \tilde{S}_j^+ + \sin\theta \tilde{S}_j^- \exp(i\pi \tilde{S}_j^z) \tag{A1}$$

$$S_j^- = \cos\theta \tilde{S}_j^- + \sin\theta \exp(-i\pi \tilde{S}_j^z)\tilde{S}_j^+ \tag{A2}$$

$$S_j^z = \tfrac{1}{2}[S_j^+, S_j^-]_- \tag{A3}$$

the matrix forms of S_j^+ and $\tilde{S}_j^+$ in the $\tilde{S}_j^z$ representation are found to be:

$$(S^+) = \begin{pmatrix} 0 & \sqrt{2}\cos\theta & 0 \\ -\sqrt{2}\sin\theta & 0 & \sqrt{2}\cos\theta \\ 0 & \sqrt{2}\sin\theta & 0 \end{pmatrix} \tag{A4}$$

$$(\tilde{S}^+) = \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \tag{A5}$$

where the matrix elements

$$S_{mn}^+ = \langle m|S^+|n\rangle \tag{A6}$$

$$\tilde{S}_{mn}^+ = \langle m|\tilde{S}^+|n\rangle. \tag{A7}$$

in which $|m\rangle$ ($m = 1, 2, 3$) are the complete set of eigenfunctions of $\tilde{S}^z$ with eigenvalues 1, 0 and -1.

It is easy to check the truthfulness of the equation

$$S^+ = T^+ \tilde{S}^+ T \tag{A8}$$

in which

$$(T) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \tag{A9}$$

$$T^+ T = T T^+ = I. \tag{A10}$$

Equations (A8) and (A9) show that T is a unitary transformation matrix. Since operators $(\tilde{S}_j^+, \tilde{S}_j^-, \tilde{S}_j^z)$ obey the usual angular momentum commutation rules, and since a unitary transformation does not affect the matrices commutation relations, the operators (S_j^+, S_j^-, S_j^z) must obey the usual angular momentum commutation rules as well.

We have thus completed the proof that our transformation equations (A1)–(A3) do not affect the commutation relations of spin operators.

Acknowledgments

References

[1] Crow J E, Gruertin R P and Mihalisin T W (ed) 1980 *Crystalline Electric Field and Structure Effect in f-Electron Systems* (New York: Plenum)
[2] Lindgård P-A and Kowalska A 1976 *J. Phys. C: Solid State Phys.* **9** 2081
[3] Lindgård P-A and Danielsen O 1974 *J. Phys. C: Solid State Phys.* **7** 1523
[4] Cooke J F and Lindgård P-A 1977 *Phys. Rev.* B **16** 408; 1978 *J. Appl. Phys.* **49** 2136
[5] U Balucani, M G Pini, A Rettori and V Tognetti 1980 *J. Phys. C: Solid State Phys.* **13** 3895
[6] Rastelli E and Lindgård P-A 1979 *J. Phys. C: Solid State Phys.* **12** 1899
[7] Sudha Gopalan and Cottam M G 1990 *Phys. Rev.* B **42** 624
[8] Lo C F, Pan K K and Wang Y L 1991 *J. Appl. Phys.* **70** 6080