REMARK ON THE METHODS OF DETERMINING THE APPROXIMATE GROUND-STATE IN THE SPIN WAVE THEORY OF MAGNETIC CRYSTALS

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(Received April 16, 1970)

A proof is given of the limited equivalence of two different methods used in determining the approximate ground-state of magnetic crystals in the spin wave theory, for the general case of an arbitrary spin lattice with bilinear coupling and an inhomogeneous external magnetic field.

1. Introduction

When employing the spin wave formalism to the Heisenberg model of ferro- or antiferromagnetism there is usually the problem of choosing a suitable reference state (spin wave vacuum) if the spin wave interactions are to be sufficiently small to justify the standard long-wavelength low-temperature approximations [1–3]. A typical example is the case when the (homogeneous) external magnetic field is not parallel to a direction of easiest magnetization, in which case the reference state depends on the field strength and direction. As in this case there appear in the (transformed) Hamiltonian terms linear with respect to the spin wave creation and annihilation operators, one method of determining the reference state (usually in the saturation-state approximation) resides in eliminating those terms from the Hamiltonian (method B). This method is used, *e. g.*, in describing the spin-flop phase of antiferromagnets (see, *e. g.*, [4]). Another method aims at determining the approximate ground state of the spin Hamiltonian, by minimizing its expectation value in a class of trial states generated by spatial rotations from the state of complete spin alignment (saturation state). The latter (method A) is preferably used in the theory of ferromagnetism [5].

In [1], the methods A and B were shown to be equivalent in a limited sense, and the proof was given for a spin Hamiltonian with spin coupling of arbitrary type and order. However, the following restrictions have been assumed: (a) the class of reference states has been confined to "homogeneous" states corresponding to complete spin alignment (satura-

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tion states); (b) the maximum spin eigenvalue was assumed to be the same for all lattice spins; (c) intra-atomic spin coupling has been excluded, and (d) translational invariance for the interaction tensor has been assumed.

We shall show that, for a simpler Hamiltonian with spin coupling up to second order, the proof given in [1] can be generalized to the case when neither of the restrictions (a)–(d) applies. The practical implications of our proof become apparent when one notes that restriction (a) excludes, *inter alia*, helicoidal and domain structures; restriction (b) confines the proof in [1] practically to ferromagnetism, and (c) excludes, *e. g.*, mono-ionic and multipolar (*i. e.*, higher than dipolar) coupling.

2. *Method A*

We consider a spin Hamiltonian of the form

$$H = -\frac{1}{2}\sum_{ij} K_{ij}^{\alpha\beta} S_i^\alpha S_j^\beta - \sum_i L_i^\alpha S_i^\alpha \tag{1}$$

where

$$K_{ij}^{\alpha\beta} = K_{ji}^{\alpha\beta} = K_{ji}^{\beta\alpha}; \qquad L_i^\alpha = \mu_i H_i^\alpha; \qquad \mu_i = \mu g_i. \tag{2}$$

The subscripts i, j denote lattice sites, and to the tensor indices α, β $(= x, y, z)$ Einstein's summation convention applies. In (2), μ is Bohr's magneton, g_i Landé's factor, and H_i^α the external field.

The spin operators S_j^α satisfy the standard commutation rules

$$[S_j^\alpha, S_k^\beta] = \mathrm{i}\delta_{jk}\varepsilon_{\alpha\beta\gamma}S_j^\gamma \tag{3}$$

or

$$[S_k^+, S_j^-] = 2\delta_{kj}S_j^z; \qquad [S_k^-, S_j^z] = \delta_{kj}S_j^-; \qquad [S_k^z, S_j^+] = \delta_{kj}S_j^+, \tag{4}$$

where $S_j^\pm = S_j^x \pm iS_j^y$. We note the useful identities

$$S_i^\alpha S_i^\alpha = S_i(S_i+1); \qquad S_i^- S_i^+ = S_i(S_i+1) - S_i^z - (S_i^z)^2; \tag{5}$$

$$S_i^+ S_i^- = S_i(S_i+1) + S_i^z - (S_i^z)^2$$

where $S_i^\pm$ is the maximum spin eigenvalue at the lattice site i.

Let $|0>$ be the state of complete spin-alignment along the z-axis, *i. e.*,

$$S_j^z = S_j \,|\, 0> ; \qquad S_j^+ \,|\, 0> = 0. \tag{6}$$

The class of reference states (trial ground states)

$$|\tilde{0}> = U^+ \,|\, 0> \tag{7}$$

considered in [1] was confined to saturation-states, as the unitary transformation U was restricted to homogeneous rotations. To widen this class, we admit inhomogeneous rotations and specify the operator U as follows:

$$U = \prod_i U_j; \qquad U_j = [\exp(i\vartheta_j S_j^y)]\,[\exp(i\varphi_j S_j^z)]. \tag{8}$$

Hence, the state $|\tilde{0}\rangle = |\ldots \vartheta_j, \varphi_j \ldots\rangle$ depends on the parameters ϑ_j, φ_j and the quantity to be minimized is the mean value of (1) in the class (7), *i. e.*,

$$\langle\tilde{0}|H|\tilde{0}\rangle = \langle 0|UHU^{+}|0\rangle \equiv \langle 0|\tilde{H}|0\rangle \equiv \langle\tilde{H}\rangle. \tag{9}$$

The angles ϑ_j, φ_j represent spherical coordinates of the local direction of spin quantization at the lattice site j. Let $\vec{\gamma}_j$ be the unit vector along this direction (cp. Fig. 1). Then, the transformation

$$S_j^{\alpha} \to U_j S_j^{\alpha} U_j^{+} \tag{10}$$

expressed in terms of the operators $S_j^{\pm}$ takes the form [5]:

$$S_j^{\alpha} \to \gamma_j^{\alpha} S_j^{z} + A_j^{\alpha} S_j^{+} + A_j^{*\alpha} S_j^{-} \tag{11}$$

where

$$\begin{aligned} A_j^{x} &= -e^{i\varphi_j}\frac{1+\gamma_j^{z}}{4} + e^{-i\varphi_j}\frac{1-\gamma_j^{z}}{4} \\ A_j^{y} &= i\left(e^{i\varphi_j}\frac{1+\gamma_j^{z}}{4} + e^{-i\varphi_j}\frac{1-\gamma_j^{z}}{4}\right) \\ A_j^{z} &= \frac{1}{2}\sqrt{1-(\gamma_j^{z})^2};\ \operatorname{tg}\varphi_j = \frac{\gamma_j^{y}}{\gamma_j^{z}}. \end{aligned} \tag{12}$$

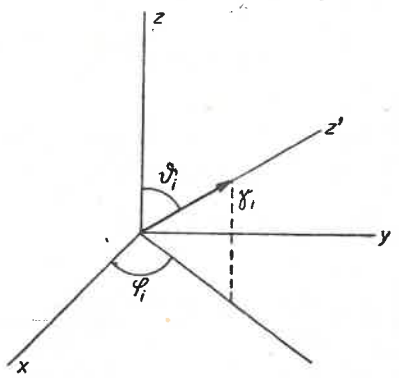

Fig. 1

The direction cosines γ_i^{α} and the coefficients A_i^{α} satisfy the following relations:

$$\begin{aligned} &\gamma_i^{\alpha}\gamma_i^{\alpha} = 1; \quad A_i^{\alpha} A_i^{*\alpha} = \tfrac{1}{2} \\ &A_i^{\alpha} A_i^{\alpha} = 0; \quad A_i^{\alpha}\gamma_i^{\alpha} = A_i^{*\alpha}\gamma_i^{\alpha} = 0 \end{aligned} \tag{13}$$

and

$$A_i^{\alpha} A_i^{*\beta} + A_i^{*\alpha} A_i^{\beta} = \tfrac{1}{2}(\delta_{\alpha\beta} - \gamma_i^{\alpha}\gamma_i^{\beta}). \tag{13'}$$

By inserting the transformation (11) into the Hamiltonian (1) we obtain

$$\tilde{H} = -\frac{1}{2}\sum_{ij}\tilde{K}_{ij}^{\xi\eta}S_i^{\xi}S_j^{\eta} - \sum_i \tilde{L}_i^{\xi}S_i^{\xi} \tag{14}$$

where

$$\xi, \eta = +, -, z$$
$$\tilde{K}_{ij}^{++} = (\tilde{K}_{ij}^{--})^* = K_{ij}^{\alpha\beta}A_i^{\alpha}A_j^{\beta}; \quad \tilde{K}_{ij}^{+-} = (\tilde{K}_{ij}^{-+})^* = K_{ij}^{\alpha\beta}A_i^{\alpha}A_j^{*\beta}$$
$$\tilde{K}_{ij}^{z+} = (\tilde{K}_{ij}^{-z})^* = K_{ij}^{\alpha\beta}\gamma_i^{\alpha}A_j^{\beta}; \quad \tilde{K}_{ij}^{z-} = (\tilde{K}_{ij}^{+z})^* = K_{ij}^{\alpha\beta}\gamma_i^{\alpha}A_j^{*\beta} \tag{15}$$
$$\tilde{K}_{ij}^{zz} = K_{ij}^{\alpha\beta}\gamma_i^{\alpha}\gamma_j^{\beta}; \quad \tilde{L}_i^{+} = (\tilde{L}^{-})^* = L_i^{\alpha}A_i^{\alpha}; \quad \tilde{L}_i^{z} = L_i^{\alpha}\gamma_i^{\alpha}.$$

The mean (expectation) value (9) of the Hamiltonian (14) is

$$\langle\tilde{H}\rangle = -\frac{1}{2}\sum_i \tilde{K}_{ij}^{zz}S_iS_j - \sum_i \tilde{K}_{ij}^{+-}S_i - \sum_i \tilde{L}_i^{z}S_i$$
$$= -\frac{1}{2}\sum_{ij} K_{ij}^{\alpha\beta}\gamma_i^{\alpha}\gamma_j^{\beta}S_iS_j - \sum_i K_{ii}^{\alpha\beta}A_i^{\alpha}A_i^{\beta}S_i - \sum_i L_i^{\alpha}\gamma_i^{\alpha}S_i. \tag{16}$$

We determine the parameters γ_i^{α} so that $\langle\tilde{H}\rangle = \min.$ with the supplementary conditions

$$\gamma_i^{\alpha}\gamma_i^{\alpha} = 1; \tag{17}$$

the necessary conditions for an extremum of $\langle\tilde{H}\rangle$ to exist have the form

$$\frac{\partial\langle\hat{H}\rangle}{\partial\gamma_k^{\sigma}} = 2\lambda_k\gamma_k^{\sigma} \tag{18}$$

with λ_k as Lagrange factors.

The left-hand side of the above equation we calculate from (16), taking into account (13′) and the symmetry of $K_{ij}^{\alpha\beta}$. In this way we immediatly obtain

$$M_k^{\sigma}S_k = 2\lambda_k\gamma_k^{\sigma} \tag{19}$$

where

$$M_k^{\sigma} = -\sum_i K_{ij}^{\alpha\sigma}S_i\gamma_i^{\alpha} + \frac{1}{2}K_{kk}^{\alpha\sigma}\gamma_k^{\alpha} - L_k^{\sigma}. \tag{20}$$

The quantities γ_k^{α} and λ_k are to be determined from the set of equations (17) and (19).

3. Method B

In showing the equivalence of the methods A and B for our Hamiltonian (1), we pass to the Bose representation by means of the Holstein–Primakoff mapping [6]

$$S_i^{-} \to \sqrt{2S_i}a_i^{+}\varphi(n_i); \quad S_i^{+} \to \sqrt{2S_i}\,\varphi(n_i)a_i; \quad S_i^{z} = S_i - n_i;$$
$$n_i = a_i^{+}a_i; \quad \varphi(n_i) = \left(1 - \frac{n_i}{2S_i}\right)^{\frac{1}{2}}; \quad [a, a_j^{+}] = \delta_{ij}. \tag{21}$$

If $\varphi(n_i)$ is expanded in a power series

$$\varphi(n_i) = 1 - \frac{n_i}{4S_i} - \ldots, \tag{22}$$

the mapped Hamiltonian $\tilde{H}$ takes the form

$$\tilde{\tilde{H}} = H_0 + H_1 + H_2 + \ldots \tag{23}$$

where H_n is a linear combination of n Bose operators.

If the latter are written in normal order, one easily verifies that

$$H_0 = \langle \tilde{H} \rangle \tag{24}$$

and

$$H_1 = \sum_j \sqrt{2S_j} M_j^\sigma (A_j^\sigma a_j + A_j^{*\sigma} a_j^+). \tag{25}$$

It thus appears that, even if intra-atomic interactions are present H_0 in the mapped Hamiltonian is equal to $\langle \tilde{H} \rangle$ provided that the products of Bose operators are written in normal order.

The terms which are linear with respect to the Bose operators vanish when γ_i^α are solutions of the equations (17) and (19). Indeed, if we substitute (19) in (25) and take into account the formulas (13) one obtains $H_1 = 0$. And *v.v.*, when demanding the linear term H_1 to vanish, *i.e.*,

$$M_j^\sigma A_j^\sigma = 0; \quad M_j^\sigma A_j^{*\sigma} = 0 \tag{26}$$

and taking into account the identity (cp. (13))

$$\gamma_i^\alpha A_i^\alpha = \gamma_i^\alpha A_i^{*\alpha} = 0 \tag{27}$$

one easily concludes that Eqs (26) are satisfied if

$$M_k^\sigma - \lambda_k' \gamma_k^\sigma = 0 \tag{28}$$

which coincides with the necessary conditions (19).

4. *Conclusions*

It is thus seen that for a Hamiltonian of the type (1) the methods A and B of determining the spin-deviation reference state are equivalent in the much wider class (7), (8) of inhomogeneous reference states, and that the restrictions assumed in [1] can be avoided. However, it should be stressed that the equivalence is limited in the same sense as in [1], *i.e.*, the method B corresponds merely to the necessary conditions of method A and therefore does not guarantee a unique determination of the reference state. For example, in case of a uniaxial two-sublattice ferrimagnet with the external magnetic field perpendicular to the anisotropy axis one obtains four different solutions for the field-dependent reference state, of which

the proper one (approximate ground state) is selected only upon application of the sufficient conditions of method A [7].

The author wishes to thank Dr W. J. Ziętek and Dr G. Kozłowski for helpful discussions. He is also grateful to Dr W. J. Ziętek for reading and correcting the manuscript.

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