THE SATURATION-STATE APPROXIMATION OF THE ANISOTROPIC FERROMAGNET'S GROUND STATE

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The use of saturation states in approximating the ground state of an anisotropic ferromagnet is studied on a general spin Hamiltonian with interactions of arbitrary type and order, the only conditions imposed upon the interaction tensors being (*i*) translational invariance and (*ii*) exclusion of intra-atomic interactions. The equivalence (in a limited sense) of two different methods is proven, of which the first one (A) resides in minimizing the classical counterpart of the spin Hamiltonian with respect to the direction of parallel spin alignment, and the second (B) in eliminating from the transformed Hamiltonian terms that are linear with respect to spin-wave (or spin-deviation) creation and annihilation operators. Furthermore, a refined method is developed which is based on the minimization of the transformed Hamiltonian's ground-state energy (in the approximation of non-interacting spin waves). The latter method is shown to lead (under certain conditions) to a better approximation of the spin system's true ground-state energy than method A.

1. Introduction

It is well known that the (exact) ground state of an isotropic Heisenberg ferromagnet in the presence of a homogeneous external magnetic field corresponds to the state of complete saturation (saturation state) in which all the spins are parallel to the direction of the external field [1–5]. If the latter is chosen as the x_3-axis of the coordinate system, the state of complete saturation can be represented by the so-called spin-deviation vacuum state $|0>$ defined as follows:

$$S_j^3|0\rangle = S|0\rangle, \quad S_j^+|0\rangle = 0 \tag{1}$$

for all j, where $S_j^{\pm} = S_j^1 \pm iS_j^2$ and S is the maximum spin eigenvalue. Here, S_j^a denotes the

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vector components ($a = 1, 2, 3$) of the spin operator ascribed to the lattice site j, the commutation rules being as usual

$$[S_j^a, S_k^b] = i\delta_{jk}\varepsilon_{abc}S_j^c. \tag{2}$$

Throughout the paper, we apply Einstein's summation rule to the tensor indices a, b, c, ... By applying the operators S_j^- to the vacuum state $|0>$ one obtains the complete set of orthonormal simultaneous eigenstates $|u>$ of the operators S_j^3:

$$|u> \equiv |\ldots u_j \ldots> = \left\{\prod_j \left[\frac{(2S-u_j)!}{(2S)!\,(u_j)!}\right]^{1/2} (S_j^-)^{u_j}\right\} |0>, \tag{3}$$

$$S_j^3 |u> = (S-u_j)|u>, \quad u_j = 0, 1, 2, \ldots, 2S. \tag{4}$$

Thus, the state $|u>$ ascribes to each lattice site j a definite number u_j of spin deviations.

The eigenvectors of a Heisenberg ferromagnet lie in the Hilbert space spanned by the vectors $|u>$. In the case of an isotropic ferromagnet, the vector $|0>$ represents the ground state of the system and, therefore, when applying spin-wave theory its choice as reference state (in the sence of [6]) is fully justified. If anisotropic interactions are taken into account, $|0>$ generally ceases to be an eigenstate of the system and hence cannot represent its groundstate (with the only exception of a specific uniaxial anisotropy and the magnetic field parallel to the anisotropy axis; see, *e. g.*, [5]). Since the exact ground state of an anisotropic ferromagnet is unknown, various mathematical procedures are being used — according to the problem be solved — in order to determine it at least approximately. Most widely in use are variational procedures applied to suitably chosen classes of trial states generated from $|0>$ by spatial (generally inhomogeneous) rotations [5–9]. In this way, *e. g.*, a theory of domain structures has been worked out in [9–14], although the approximate ground states derived in those papers are unstable because long-range interactions and surface effects have been neglected.

Another case in point is the choice of reference states in the spin-wave theory of anisotropic ferromagnets (and antiferromagnets, ferrimagnets *etc.* as well, for that matter), particularly if the external magnetic field is not parallel to a direction of easiest magnetization. Apart from the fact that the ground state of a true ferromagnet is hardly one of uniform magnetization (domain structure), a state of complete spin alignment (in any direction) is usually not an eigenstate of a spin Hamiltonian with anisotropic interactions — even if long-range coupling and surface effects are ignored. None the less, because of serious mathematical difficulties such saturation states are commonly used as (homogeneous) reference states in the spin-wave theory of anisotropic ferromagnets [5, 7, 8]. A typical example is the uniaxial ferromagnet (or antiferromagnet) with the external magnetic field perpendicular to the anisotropy axis, in which case one uses homogeneous reference states with field-dependent direction of spin alignment. In determining this dependence (and hence the reference state), two distinctly different methods are being employed: the first one (method A) resides in minimizing the classical counterpart of the spin Hamiltonian with respect to the direction of parallel spin alignment [7, 8], the second (method B) — in eliminating from the transformed Hamiltonian terms that are linear with respect to spin-wave (or spin-devia-

tion) creation and annihilation operators [5, 15, 16]. Since the applicability of both the methods is not necessarily restricted to the quoted case, the question arises whether they ensure the best choice of a homogeneous reference state, and whether or not the results depend on the particular method used.

While answering these questions, we shall not go into the much ignored but still unsolved problem of whether the very use of homogeneous reference states is in those cases adequately justified or, in other words, of how reasonable an approximation of the anisotropic ferromagnet's ground state is the state of complete spin alignment. (Note that the departure of the reference state from the system's ground state would be immaterial, indeed, were it not for the standard approximations made in the spin-wave theory, such as the neglect of higher-order spin-wave interactions.)

In determining the homogeneous reference state for a quite general spin Hamiltonian, we use the variational method in a semi-classical approach to a class of saturation states with arbitrary direction of spin alignment, and show the methods A and B to be equivalent — in a limited sense. Furthermore, we outline a refined approach in which the reference state is determined by minimizing the ground state energy of the corresponding zeroth-order spin-wave Hamiltonian (non-interacting spin waves), and show it to lead to a better approximation of the system's true ground state than the methods A and B.

2. *Saturation-state approximation*

Using spherical coordinates, we can denote by $|0(\vartheta, \varphi)>$ the saturation state in which the spins are parallel to the direction given by the angles ϑ and φ. Such a state can be generated from $|0>$, Eq. (1), by means of a unitary transformation $U = U(\vartheta, \varphi)$,

$$|0(\vartheta, \varphi)> = U^{+}|0>, \tag{5}$$

which transforms the set (3) into the orthonormal set

$$|u(\vartheta, \varphi)> = U^{+}|u> . \tag{6}$$

Instead of using the representation (6), it is convenient to transform the Hamiltonian H (and other dynamical variables, if necessary) of the system,

$$\tilde{H} = UHU^{+} = \tilde{H}(\vartheta, \varphi), \tag{7}$$

and to work with the representation (3). In carrying out the transformation (7) we note that the operator U is equivalent to the matrix (R^{ab}) defined by (cp. [9])

$$US_j^a U^{+} = R^{ab} S_j^b. \tag{8}$$

Thus,

$$\tilde{H} = UH(\ldots S_j^a \ldots)\, U^{+} = H(\ldots\, US_j^a U^{+} \ldots) = H(\ldots R^{ab} S_j^b \ldots). \tag{9}$$

If $\vartheta = 0$ and $\varphi = 0$, $\vartheta = \pi/2$ correspond respectively to the coordinate axes x_3 and x_1, the transformation U can be specified as follows:

$$U = \prod_j U_j, \quad U_j = [\exp(i\vartheta S_j^2)]\, [\exp(i\varphi S_j^3)], \tag{10}$$

$$(R^{ab}) = \begin{pmatrix} \cos\vartheta\cos\varphi & -\sin\varphi & \sin\vartheta\cos\varphi \\ \cos\vartheta\sin\varphi & \cos\varphi & \sin\vartheta\sin\varphi \\ -\sin\vartheta & 0 & \cos\vartheta \end{pmatrix}.$$

The method A in our formulation resides in determining the angles ϑ and φ by minimizing the expectation value of H in the class (5), *i.e.*,

$$\min \langle 0(\vartheta,\varphi)|H|0(\vartheta,\varphi)\rangle = \min \langle 0|\tilde{H}(\vartheta,\varphi)|0\rangle. \tag{11}$$

Let us consider a spin Hamiltonian with exchange interactions of arbitrary type and order:

$$H = \sum_{m=1}^{M} H_m, \tag{12}$$

$$H_m = \sum_{j_1 \ldots j_m} A^{a_1 a_2 \ldots a_m}_{j_1 j_2 \ldots j_m} S^{a_1}_{j_1} S^{a_2}_{j_2} \ldots S^{a_m}_{j_m}.$$

(Note that Einstein's summation rule applies to the tensor indices $a_1, a_2, \ldots, a_m$.) The only conditions imposed upon the interaction tensors are:
(*i*) translational invariance, *i.e.*, the tensors depend only on the differences between lattice vectors:

$$A^{a_1 \ldots a_m}_{j_1 \ldots j_m} = A^{a_1 \ldots a_m}_{j_1 - j_2, j_2 - j_3, \ldots}$$

(*ii*) intra-atomic interactions are excluded, *i.e.*, $A^{a_1 \ldots a_m}_{j_1 \ldots j_m} = 0$ if $j_k = j_n$ as $k \neq n$ $(k, n \leqslant m)$. Because of these conditions, monoionic anisotropies and multipolar (*i.e.*, higher than dipolar) interactions are not accounted for.

Condition (*i*) ensures that sums like

$$\sum_{j_2 \ldots j_m} A^{a_1 a_2 \ldots a_m}_{j_1 j_2 \ldots j_m} \equiv A^{a_1 a_2 \ldots a_m} \tag{13}$$

are independent of j_1, and due to condition (*ii*) all the spin operators in the products in Eq. (12) commute.

The application of the transformation (10) to the Hamiltonian (12) is, according to (9), straightforward:

$$\tilde{H} = \sum_{m}^{M} \tilde{H}_m, \tag{14}$$

$$\tilde{H}_m = \sum_{j_1 \ldots j_m} A^{a_1 \ldots a_m}_{j_1 \ldots j_m} R^{a_1 b_1} \ldots R^{a_m b_m} S^{b_1}_{j_1} \ldots S^{b_m}_{j_m}.$$

Let us now replace the x_3-components of the spin operators with the spin-deviation operators

$$\hat{u}_j = S - S^3_j. \tag{15}$$

This permits to split the Hamiltonian in two parts,

$$\tilde{H} = \tilde{H}^0 + \tilde{H}', \quad \tilde{H}^0 = \sum_m \tilde{H}^0_m, \quad \tilde{H}' = \sum_m \tilde{H}'_m \tag{16}$$

where $\tilde{H}^0$ is a *c*-number, as

$$\tilde{H}^0_m = N S^m A^{a_1 \ldots a_m} R^{a_1 3} \ldots R^{a_m 3} \tag{17}$$

(N being the number of lattice sites), and $\tilde{H}'_m$ are operators consisting of linear combinations of products of the form

$$S^{r_1}_{j_1} \dots S^{r_p}_{j_p} \hat{u}_{j_{p+1}} \dots \hat{u}_{j_q}, \tag{18}$$

$$0 \leqslant p \leqslant q \leqslant m, \quad p+q > 0, \quad r_i = 1, 2.$$

Due to (1) and (*ii*) we have

$$\langle 0|S^{r_1}_{j_1} \dots S^{r_p}_{j_p} \hat{u}_{j_{p+1}} \dots \hat{u}_{j_q}|0\rangle = 0. \tag{19}$$

Hence, $\langle 0|\tilde{H}'|0\rangle = 0$ and

$$\langle 0|\tilde{H}|0\rangle = \tilde{H}^0 \equiv E(\vartheta, \varphi). \tag{20}$$

For further purposes, let us single out of $\tilde{H}'$ the terms with $p = q = 1$, (which are linear with respect to the operators S^r_j), and those with either $p = q = 2$, (bilinear with respect to S^r_j) or $p = 0$, $q = 1$ (linear with respect to $\hat{u}_j$). One easily verifies that these parts of $\tilde{H}'$, denoted respectively by $\tilde{H}^1$ and $\tilde{H}^2$, have the forms

$$\tilde{H}^1 = K^r \sum_j S^r_j, \tag{21}$$

$$\tilde{H}^2 = \sum_{j_1 j_2} B^{r_1 r_2}_{j_1 j_2} S^{r_1}_{j_1} S^{r_2}_{j_2} - C \sum_j \hat{u}_j \tag{22}$$

where

$$K^r = \sum_m^M S^{m-1} R^{a_1 r} R^{a_2 3} \dots R^{a_m 3} \sum_n^m A^{a_n \dots a_1 \dots a_m}, \tag{23}$$

$$B^{r_1 r_2}_{j_1 j_2} = \sum_m^M S^{m-2} R^{a_1 r_1} R^{a_2 r_2} R^{a_3 3} \dots R^{a_m 3} \times$$

$$\times \sum_{j_3 \dots j_m} \sum_{n,k}^m A^{a_n a_k \dots a_1 \dots a_2 \dots a_m}_{j_n j_k \dots j_1 \dots j_2 \dots j_m}, \tag{24}$$

$$C = \sum_{m=1}^M S^{m-1} R^{a_1 3} \dots R^{a_m 3} \sum_{n=1}^m A^{a_n \dots a_1 \dots a_m}. \tag{25}$$

In the above formulae, we use a simplified notation, according to which in (23) and (25) the indices a_1 and a_n are to be interchanged in the tensor $A^{a_1 \dots a_m}$ defined by (13), and in (24) the pairs of indices $(a_1 j_1)$, $(a_2 j_2)$ and $(a_n j_n)$, $(a_k j_k)$ are to be interchanged in the interaction tensors of the Hamiltonian (12). Note that

$$B^{r_1 r_2}_{j_1 j_2} = B^{r_1 r_2}_{j_1 - j_2} = B^{r_2 r_1}_{j_1 - j_2} \tag{26}$$

due to conditions (*i*) and (*ii*).

We can now apply the classical saturation-state approximation (11) to the Hamiltonian (12). According to (16), (20) the quantity to be minimized in the class of trial states (5) is

$$E(\vartheta, \varphi) = \sum_m^M \tilde{H}^0_m, \tag{27}$$

the conditions for E to have a minimum at ϑ_0, φ_0 being

$$[\partial E/\partial\varphi]_0 = [\partial E/\partial\vartheta]_0 = 0, \tag{28}$$

$$[(\partial^2 E/\partial\varphi^2)\,(\partial^2 E/\partial\vartheta^2) - (\partial^2 E/\partial\vartheta\partial\varphi)^2]_0 \equiv \Delta_0 > 0, \tag{29}$$

$$[\partial^2 E/\partial\varphi^2]_0 > 0 \tag{30}$$

where the symbol $[\ ]_0$ indicates the insertion of ϑ_0, φ_0.

From (27) and (17) we have

$$(\partial E/\partial t) = \sum_m^M (\partial \tilde{H}^0_m/\partial t),\ t = \vartheta, \varphi; \tag{31}$$

$$(\partial \tilde{H}^0_m/\partial t) = NS^m A^{a_1 \ldots a_m}[\partial(R^{a_1 3} \ldots R^{a_m 3})/\partial t]$$

$$= NS^m(\partial R^{a_1 3}/\partial t)\, R^{a_2 3} \ldots R^{a_m 3} \sum_{n=1}^{m} A^{a_n \ldots a_1 \ldots a_m} \tag{32}$$

with the notation as in (25), and from (10) it follows that

$$(\partial R^{a3}/\partial\varphi) = R^{a2} \sin\vartheta,\ \ (\partial R^{a3}/\partial\vartheta) = R^{a1}. \tag{33}$$

Thus, equations (28) take the form

$$[\partial E/\partial\vartheta]_0 = NSK^1(\vartheta_0, \varphi_0) = 0, \tag{34}$$

$$[\partial E/\partial\varphi]_0 = NS \sin\vartheta_0 K^2(\vartheta_0, \varphi_0) = 0 \tag{35}$$

with K^1 and K^2 as defined by (23).

It is seen that $\sin\vartheta_0 \neq 0$ implies $K^r = 0$, and the same holds for the solutions $\sin\vartheta_0 = 0$ if Δ_0 defined by (29) is to be non-negative so that minima may exist, as in that case

$$\Delta_0 = (NS)^2 [(\partial K^1/\partial\vartheta)\,(\partial K^2/\partial\varphi) \sin\vartheta -$$

$$-\{(\partial K^2/\partial\vartheta) \sin\vartheta + K^2 \cos\vartheta\}^2]_0 = -(NS)^2 [K^2]_0^2 \leqslant 0. \tag{36}$$

Therefore, the necessary conditions for minima of E to exist are in either case $K^r = 0$. This, however, destroys in the Hamiltonian automatically the terms that are linear with respect to the spin components S^r_j, as is evident from (21). Obviously, this is equivalent to the elimination of linear terms in the Hamiltonian when passing, as usual, from the spin operators to the more convenient Bose operators a_j, a_j^+ (cp. following Section), no matter whether using the (non-unitary) Dyson-Maleyev mapping

$$S_j^+ \to \sqrt{2S}(1 - \hat{n}_j/2S)\, a_j,\quad S_j^- \to \sqrt{2S}\, a_j^+,$$

$$S_j^3 \to S - \hat{n}_j,\quad \hat{n}_j = a_j^+ a_j,\quad [a_j, a_k^+] = \delta_{jk} \tag{37}$$

or the (unitary) Holstein-Primakoff mapping

$$S_j^+ = (S_j^-)^+ \to \sqrt{2S - \hat{n}_j}\, a_j = \sqrt{2S}\,\{1 - \hat{n}_j/4S - \ldots\}\, a_j, \tag{38}$$

$$S_j^3 \to S - \hat{n}_j$$

or, for that matter, any other mapping in any approximation [17–21]. (Note that the transition from S_j^3 to $\hat{n}_j$ has actually been carried through in (15).)

It is thus seen that the method B, as applied to simple Hamiltonians and specific rotations in [15, 16] resides, generally, in determining the angles ϑ, φ from the conditions $K^r = 0$ which, as shown above, coincide with the necessary minimum conditions (28) of method A. In this sense both the methods are equivalent. However, the method A requires beside (28) the conditions (29), (30) to be satisfied, too, which permits to eliminate some of the solutions of the equations $K^r = 0$. Also, the method A has a clear physical meaning, as it aims at determining the approximate ground state of the system, whereas the method B serves purely mathematical purposes (elimination of linear terms from the mapped Hamiltonian equivalently, of constant terms in the respective Heisenberg equations; cp. [15. 16]). These arguments speak, in our opinion, in favour of method A.

One easily verifies that the semi-classical minimizing procedure used in [7] in determining the approximate ground state of an anisotropic ferromagnet in the saturation-state approximation is strictly equivalent to the method A as formulated here.

3. *Quasi-saturation-state approximation*

In the spin wave approach to ferromagnetism, the spin Hamiltonian is eventually expressed in terms of Bose operators [19–21] and, upon elimination of linear terms (in case they appear), its bilinear part can be diagonalized by means of Bogolyubov's general transformation [6–8]. This procedure produces additional constant terms in the (mapped) Hamiltonian and leads to an approximate ground state energy that differs from (27). Clearly, if the conventional spin wave approach is considered to describe adequately a ferromagnet (or antiferromagnet) at low temperatures, the minimization (28)–(30) should actually be carried through after — and not before — diagonalizing the Hamiltonian. This should ensure a better approximation of the system's true ground state energy and, consequently, the best choice out of the class of homogeneous reference states (5). In the limits of non-interacting spin waves we shall show that such is the case (under certain conditions) for the Hamiltonian (12).

For this purpose, let us apply the mapping rules (37) or (38) to (21) and (22), and neglect all the terms higher than of second order with respect to the Bose operators. This yields the zeroth-order (free particles) Hamiltonian

$$\tilde{H}_{II} = E + \bar{x} \sum_j a_j + x \sum_j a_j^+ +$$

$$+ \frac{1}{2} \sum_{j_1 j_2} (P_{j_1 j_2} a_{j_1}^+ a_{j_2}^+ + 2Q_{j_1 j_2} a_{j_1}^+ a_{j_2} + \bar{P}_{j_1 j_2} a_{j_1} a_{j_2}), \tag{39}$$

where

$$x = \sqrt{S/2}(K^1 + iK^2), \tag{40}$$

$$P_{j_1 j_2} = S(B_{j_1 j_2}^{11} - B_{j_1 j_2}^{22} + 2iB_{j_1 j_2}^{12}), \tag{41}$$

$$Q_{j_1 j_2} = S(B_{j_1 j_2}^{11} + B_{j_1 j_2}^{22}) - 2C\delta_{j_1 j_2} \tag{42}$$

and the remaining symbols are defined by (23)–(25) and (27). (Note that the linear terms in (39) vanish if conditions (35) apply.)

The method A as defined by (11) amounts to minimizing $E = \langle 0|\tilde{H}_{II}|0\rangle$, whereas now we shall minimize the ground state energy of $\tilde{H}_{II}$. To eliminate the linear terms in (39) we use the transformation [6]

$$a_j = g + b_j \tag{43}$$

which leads to

$$\tilde{H}_{II} = E + N(\bar{g}x + g\bar{x}) + \frac{N}{2}(\bar{g}^2 P + 2\bar{g}gQ + g^2\bar{P}) +$$

$$+ y\sum_i b_j^+ + \bar{y}\sum_j b_j + \frac{1}{2}\sum_{j_1 j_2}(P_{j_1 j_2} b_{j_1}^+ b_{j_2}^+ + 2Q_{j_1 j_2} b_{j_1}^+ b_{j_2} + \bar{P}_{j_1 j_2} b_{j_1} b_{j_2}) \tag{44}$$

where

$$y = x + \bar{g}P + gQ, \tag{45}$$

$$P = \sum_{j_1} P_{j_1 j_2}, \qquad Q = \bar{Q} = \sum_{j_1} Q_{j_1 j_2}. \tag{46}$$

The constant g is determined from the condition

$$y = 0. \tag{47}$$

In the case of inhomogeneous fields or reference states, the constant g in (43) depends on the lattice site j, and the same holds for the coefficient y; moreover, (when higher-order terms are taken into account in (39), the coefficients y_j become non-linear functions of the constants g_j, and condition (47) converts into a set of non-linear equations.)

The solution of (47) reads

$$g_1 = [x_2 P_2 - x_1 (Q - P_1)]/2W, \quad g_2 = [x_1 P_2 - x_2 (Q + P_1)]/2W, \tag{48}$$

$$W \equiv Q^2 - P_1^2 - P_2^2 \neq 0$$

when splitting the complex quantities g, x and P into their real and imaginary parts,

$$g = g_1 + ig_2, \quad x = x_1 + ix_2, \quad P = P_1 + iP_2. \tag{49}$$

With that the Hamiltonian (44) takes the form

$$H_{II} = E + \delta E +$$

$$+ \frac{1}{2}\sum_{j_1 j_2}(P_{j_1 j_2} b_{j_1}^+ b_{j_2}^+ + 2Q_{j_1 j_2} b_{j_1}^+ b_{j_2} + \bar{P}_{j_1 j_2} b_{j_1} b_{j_2}) \tag{50}$$

where

$$\delta E = N[2x_1 x_2 P_2 - x_1^2 (Q - P_1) - x_2^2 (Q + P_1)]/2W$$

$$\equiv Dx_1^2 + 2Fx_1 x_2 + Gx_2^2. \tag{51}$$

If $Q > P_1$, then

$$\delta E < 0. \tag{52}$$

(Note that all the quantities are functions of ϑ, φ.)

Although $E' = E + \delta E$ is not yet the ground state energy of the Hamiltonian (39), it is instructive to write down for E' the conditions (28):

$$\partial E'/\partial t = \partial E/\partial t + \tag{53}$$
$$+x_1[x_1(\partial D/\partial t)+2D(\partial x_1/\partial t)+x_2(\partial F/\partial t)+2F(\partial x_2/\partial t)]+$$
$$+x_2[x_2(\partial G/\partial t)+2G(\partial x_2/\partial t)+x_1(\partial F/\partial t)+2F(\partial x_1/\partial t)]$$

where $t = \vartheta, \varphi$. From (34), (35), (40) and (48) it is seen that the solutions of (34), (35) are among those of equations (53), though they do not necessarily correspond to minima of E' even if they do satisfy the conditions (29), (30). In fact, for the case of a uniaxial ferromagnet with perpendicular external field it can be shown [22] that the minima of E correspond to maxima or inflection of points E'.

The exact ground state energy of $\tilde{H}_{II}$ is obtained upon diagonalizing (50) by means of Bogolyubov's linear transformation

$$b_j = \sum_k (u_{jk} c_k + \bar{v}_{jk} c_k^+), \qquad [c_k, c_{k'}^+] = \delta_{kk'} \tag{54}$$

which leads to

$$\tilde{H}_{II} = E'' + \sum_k E_k c_k^+ c_k,$$
$$E'' = E + \delta E + \Delta E, \quad \Delta E = -\sum_{jk} |v_{jk}|^2 E_k. \tag{55}$$

The coefficients u_{jk}, v_{jk} are determined by a set of homogeneous linear equations, and the quasi-particle (spin wave) energies E_k are obtained from the corresponding secular equation (see [6, 7] for details).

E'' is the ground state energy of $\tilde{H}_{II}$ if $E_k \geqslant 0$. The minimization of E'' with respect to ϑ, φ ensures a better approximation of the spin system's exact ground state energy E_0 than the minimization of E if

$$E_k \geqslant 0, \quad Q > P_1, \quad \langle 0_{II}|\tilde{H}|0_{II}\rangle < E'' \tag{56}$$

where $|0_{II}\rangle$ denotes the ground state of H_{II}. In that case, namely, we have

$$E_0 \leqslant E''(\vartheta, \varphi) < E(\vartheta, \varphi), \tag{57}$$

hence,

$$E_0 \leqslant \min \min E'' < \min \min E. \tag{58}$$

One easily proves that $|0_{II}>$ does not correspond to a state of complete saturation in the direction given by the angles $\vartheta_0'', \varphi_0''$ obtained from the minimization of E''. Let us express the operators S_j^3 (strictly speaking: their mapped counterparts $S - \hat{n}_j$) through the operators c_k, c_k^+. According to (38), (43) and (54) we have

$$S_j^3 \to S - a_j^+ a_j = S - |g|^2 - \bar{g} b_j - g b_j^+ - b_j^+ b_j$$
$$= S - |g|^2 - \sum_k |v_{jk}|^2 - \sum_h [(\bar{g} u_{jk} + g v_{jk}) c_k + h.\,c.] -$$
$$- \sum_{kk'} (u_{jk} v_{jk'} c_k c_{k'} + h.\,c.) - \sum_{kk'} (\bar{u}_{jk} u_{jk'} + \bar{v}_{jk} v_{jk'}) c_k^+ c_{k'}. \tag{59}$$

Clearly, $|0_{II}>$ is neither an eigenvector of S_j^3 (*i.e.*, of $S - a_j^+ a_j$) nor of $\sum_j S_j^3$, and the mean value of S_j^3 in this state is

$$\langle 0_{II}|S_j^3|0_{II}\rangle = S - |g|^2 - \sum_k |v_{jk}|^2 < S. \tag{60}$$

Hence, there is no complete spin alignment in the direction ϑ_0'', φ_0'' in the state $|0_{II}>$, which is why we call it the quasi-saturation-state approximation.

4. *Concluding remarks*

The method A as formulated in Section 2 is termed saturation-state approximation for it resides in minimizing the mean value of the spin Hamiltonian in the class of saturation states (5). It is shown to be equivalent — in a limited sense — to method B which resides in eliminating linear terms in the mapped Hamiltonian (39). The method outlined in Section 3 is based on the minimization of the mapped Hamiltonian's ground state energy (here, in the free-particles approximation), and the corresponding ground state is shown not to represent a saturation state. Hence, it is termed the quasi-saturation-state approximation. The latter method ensures a better approximation of the system's true ground state if conditions (56) are satisfied.

The quasi-saturation-state method has been applied to a uniaxial ferromagnet with the external magnetic field perpendicular to the anisotropy axis [22], in which case the inequality (57) can be proven to hold, though the minimization of E'' cannot be carried through rigorously. From (51) and (55) it is obvious that even for simple Hamiltonians E'' is a much more complicated function of ϑ, φ than E. This leads to considerable mathematical difficulties in practical applications. By contrast, equations (34) and (35) of method A or B are relatively simple and can in simple cases be solved rigorously [7, 8, 22].

The equivalence of method A and B has been proven here for the class of saturation states (5) that correspond to homogeneous rotations, (10). One can show that the same (limited) equivalence holds for inhomogeneous reference states [23], and that for a simpler spin Hamiltonian with intra-atomic interactions included the proof can be extended to the general case of a ferri- or antiferrimagnet with arbitrary number of sublattices [24].

Finally, it should be emphasized that the conclusion drawn from (60) is actually independent of the method of determining the angles ϑ, φ. For instance, when applying the method A (or B) one does not need the transformation (43) as $x = y = 0$; this, however, does not destroy in (60) the term originating from the transformation (54). Hence, from this point of view the methods A and B are also quasi-saturation-state approximations. In fact, except for the cases when the saturation state is an eigenstate of the spin Hamiltonian (isotropic case or simple uniaxial anisotropy with field parallel to anisotropy axis) and the transformation (54) reduces to a Fourier expansion ($v_{jk} = 0$, cp. [7,25]), the state $|0_{II}\rangle$ can never correspond to a state of complete saturation, as the angles ϑ, φ would otherwise have to satisfy simultaneously the set of equations $g = v_{jk} = 0$. An instructive example is the use of the pseudo-dipolar coupling in describing anisotropic interactions, in which case there is no saturation in the ground state in the absence of an external field [26].

It may also be noted that the inequality (60) represents a criterion for the applicability of homogeneous reference states. If the departure from saturation in the ground state $|0_{II}\rangle$ becomes large, either higher-order terms (interactions) must be taken into consideration in (39), or else a wider class of reference states must be admitted (*e.g.*, the inhomogeneous reference states of [6]).

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