GENERALIZATION OF WALLACE'S STATISTICAL PERTURBATION METHOD AND ITS APPLICATION TO UNIAXIAL FERROMAGNETS WITH FIELD

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Wallace's statistical perturbation method is generalized and applied to uniaxial ferromagnets for arbitrary temperatures and fields. With an approximation analogous to Callen's decoupling a first-order renormalization of the spin-wave energy is carried out. It is shown under which conditions can the first-order energy corrections be considered reasonable.

1. Introduction

In [1, 2] Wallace has worked out two simple and efficient methods for treating many-particle problems: the Hamiltonian perturbation method [1] and the statistical perturbation method [2]. In application to the isotropic ferromagnet both methods were shown to lead in a simpler way to results for low and high temperatures obtained by other methods [1, 2, 3, 4] in a more laborious way.

The aim of the present paper is to employ the statistical perturbation method to uniaxial ferromagnets for arbitrary temperatures and fields. To do this, it is necessary to generalize Wallace's considerations to Hamiltonians which obey the following commutator equations:

$$[H, A_i^+]_- = L_i^0 A_i^+ + M_i^0 A_{-i} + P_i^+. \tag{1.1}$$

The A_i^+, A_i are basic operators of which the Hamiltonian is constructed. They need not obey Boson or Fermion commutation relations. The remainder operators P_i^+ consist in general of higher products of the operators A_i^+, A_i. L_i^0, M_i^0 are c-numbers. We shall call the Hamiltonian commutator equations (1.1) "anomalous", in contrast to the "normal" ones considered by Wallace ($M_i^0 = 0$). For convenience, the respective Hamiltonians or the corresponding systems shall also be called normal or anomalous (with respect to the operators A_i^+, A_i).

In Sec. 2, Wallace's statistical perturbation method and first-order energy renormaliza-

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tion are extended to general Hamiltonians obeying commutator equations of the type (1.1). In Sec. 3, 4 we apply the first-order energy renormalization to a uniaxial ferromagnet with arbitrary field. Zeroth-order results obtained in [5] by the same method and in [6] by the Green's function approach follow after specification of our first-order formulae. Various approximations within the first-order energy renormalization turn out to be equivalent to different decoupling procedures of higher Green's functions employed by other authors to isotropic ferromagnets. By means of an approximation similar to Callen's [7] decoupling we carry through explicitly the first-order energy renormalization for $S = \frac{1}{2}$. Under certain conditions this procedure is shown to give reasonable corrections to the zeroth-order results if Callen's empirical parameter is properly chosen.

2. The statistical perturbation method and energy renormalization

In this Section we shall briefly recapitulate the idea of Wallace's statistical perturbation method and generalize it to Hamiltonian commutator equations of the type (1.1). Moreover, we derive a formula for the "anomalous" thermodynamical averages of the type $\langle \theta^+ \theta^+ \rangle$ correct to first order.

Let the Hamiltonian H of a many-body system satisfy the normal Hamiltonian commutator equations

$$[H, \theta_i^+]_- = \omega_i \theta_i^+ + R_i^+ \tag{2.1}$$

and assume for simplicity the labelling i (lattice vectors, quantum numbers) and the parameters ω_i to be such that $\omega_i = \omega_{-i} > 0$. The operators θ_i^+, $\theta_i \equiv (\theta_i^+)^+$ are still arbitrary and obey certain q-number commutation relations. The basic requirement of the statistical perturbation theory resides now in a suitable choice of the operators θ_i, θ_i^+ and the parameters ω_i, so that the remainder operators R_i^+ be small, in the sense that statistical averages involving R_i^+ are to be small.

Assume that such a choice has already been made in (2.1) and consider from now on the remainder R_i^+ in (2.1) as a small perturbation. Then, in the zeroth-order perturbation step the R_i^+ are to be neglected and Eqs (2.1) reduce to

$$[H, \theta_i^+]_- = \omega_i \theta_i^+. \tag{2.2}$$

Basing on Eq. (2.2) the following formulae for zeroth-order thermodynamic averages have been derived in [2]:

$$\langle \theta_i^+ \Omega \rangle_0 = \varphi_i^{\pm} \langle [\Omega, \theta_i^+]_{\pm} \rangle_0 \tag{2.3}$$

$$\langle \Omega \theta_i \rangle_0 = \varphi_i^{\pm} \langle [\theta_i, \Omega]_{\pm} \rangle_0 \tag{2.4}$$

where Ω is any operator and

$$\varphi_i^{\pm} = (e^{\beta \omega_i} \pm 1)^{-1}, \qquad \beta = \frac{1}{kT}. \tag{2.5}$$

The symbol $\langle \ \rangle_0$ denotes canonical averages referring to the zeroth order ($R_i^+ = 0$), and $[\ ]_{\pm}$ means respectively the anticommutator or commutator. For $\Omega = \theta_i$ one obtains from (2.3) the usual Bose or Fermi distribution if θ_i, θ_i^+ obey the standard commutation relations.

For non-vanishing remainders R_i^+ one arrives from the Hamiltonian commutator equations (2.1) at the general formula (Eq. (2.29) in [2]):

$$\langle\theta_i^+\Omega\rangle = e^{-\beta\omega_i}\langle\Omega\theta_i^+\rangle + Z^{-1}\,\mathrm{Sp}\left\{\Omega\sum_{n=1}^{\infty}\frac{1}{n!}(-\beta)^n\times\right.$$

$$\left.\times\sum_{p=0}^{n-1}H^pR_i^+(H+\omega_i)^{n-p-1}\right\} \tag{2.6}$$

where

$$Z = \mathrm{Sp}\,e^{-\beta H}.$$

Upon specifying $\Omega = \theta_i$ and evaluating approximately the second term in (2.6) one obtains the following formula correct to first order with respect to R_i^+ (Eq. (2.33) in [2]):

$$\langle\theta_i^+\theta_i\rangle_1 = \varphi_i^{\pm}\langle[\theta_i, \theta_i^+]_{\pm}\rangle_0 \pm \beta(\varphi^{\pm}\mp 1)\langle R_i^+\theta_i\rangle_0. \tag{2.7}$$

In a similar way we shall now derive an expression for the anomalous average $\langle\theta_i^+\theta_{-i}^+\rangle|_1$.

With $\Omega = \theta_{-i}^+$ the second term of (2.6) reads:

$$Z^{-1}\,\mathrm{Sp}\sum_{n=1}^{\infty}\left\{\frac{1}{n!}(-\beta)^n\sum_{p=0}^{n=1}\theta_{-i}^+H^pR_i^+(H+\omega_i)^{n-p-1}\right\}. \tag{2.8}$$

Using (2.1) one finds by induction

$$\theta_{-i}^+H^p = (H-\omega_i)^p\theta_{-i}^+ + O(R_{-i}^+), \quad p = 0, 1, 2, \ldots \tag{2.9}$$

Thus, (2.8) takes the form

$$Z^{-1}\,\mathrm{Sp}\sum_{n=1}^{\infty}\left\{\frac{1}{n!}(-\beta)^n\sum_{p=0}^{n=1}(H-\omega_i)^p\theta_{-i}^+R_i^+(H+\omega_i)^{n-p-1}\right\} + O(R_i^+R_{-i}^+)$$

$$= Z^{-1}\,\mathrm{Sp}\sum_{n=1}^{\infty}\left\{\frac{1}{n!}(-\beta)^n\sum_{p=0}^{n=1}\theta_{-i}^+R_i^+(H+\omega_i)^{n-1}[(H-\omega_i)(H+\omega_i)^{-1}]^p\right\} + O(R_i^+R_{-i}^+). \tag{2.10}$$

In the last step we utilized the equality $\mathrm{Sp}\,AB = \mathrm{Sp}\,BA$. The sum over p in (2.10) gives

$$\sum_{p=0}^{n-1}[(H-\omega_i)(H+\omega_i)^{-1}]^p = -\frac{1}{2\omega_i}[(H+\omega_i)^{-n+1}(H-\omega_i)^n - (H+\omega_i)]. \tag{2.11}$$

The insertion of (2.11) in (2.10) and the contraction of the remaining sum to the exponential function provides[1]

$$Z^{-1}\frac{e^{-\beta\omega_i}-e^{\beta\omega_i}}{2\omega_i}\operatorname{Sp} e^{-\beta H}\theta_{-i}^{+}R_i^{+}+O(R_i^{+}R_{-i}^{+})$$

$$=\frac{e^{-\beta\omega_i}-e^{\beta\omega_i}}{2\omega_i}\langle\theta_{-i}^{+}R_i^{+}\rangle+O(R_i^{+}R_{-i}^{+}). \tag{2.12}$$

From (2.6) and (2.12) we finally get

$$\langle\theta_i^{+}\theta_{-i}^{+}\rangle_1=\varphi_i^{\pm}\langle[\theta_{-i}^{+},\theta_i^{+}]_{\pm}\rangle_0\mp\frac{1}{2\omega_i}(\varphi_i^{\mp})^{-1}\langle\theta_{-i}^{+}R_i^{+}\rangle_0. \tag{2.13}$$

In the sense of the perturbation theory the averages on the right-hand side of Eq. (2.13) have been evaluated in the zeroth order. Wallace did not derive this formula, because for the problem studied in [2] (isotropic ferromagnet) it leads to the trivial result $\langle\theta_i^{+}\theta_{-i}^{+}\rangle_1\equiv 0$. However, for anomalous Hamiltonians (*e. g.*, anisotropic ferromagnet with field of arbitrary direction) the average (2.13) will contribute [8]. Moreover, for such systems the energy renormalization carried through in [2] must be generalized. In doing it we start with Hamiltonian commutator equations of the type (1.1). The parameters L_i^0, M_i^0 can be renormalized in the following way:

$$[H,A_i^{+}]_{-}=L_iA_i^{+}+M_iA_{-i}+P_i^{+}-L_i^1A_i^{+}-M_i^1A_{-i}, \tag{2.14}$$

$$L_i=L_i^0+L_i^1,\quad M_i=M_i^0+M_i^1. \tag{2.15}$$

Now we "diagonalize" (2.14) by a suitable transformation[2]

$$(A_i^{+},A_i)\to(\theta_i^{+},\theta_i) \tag{2.16}$$

to obtain

$$[H,\theta_i^{+}]_{-}=\tilde{\omega}_i(L_i^1,M_i^1)\theta_i^{+}+R_i^{+}(L_i^1,M_i^1) \tag{2.17}$$

i. e., commutator equations of the type (2.1) with the energies and the remainders $\tilde{R}_i^{+}$ depending on L_i^1, M_i^1.

The so far arbitrary parameters L_i^1, M_i^1 can now be determined from the condition that the perturbation terms in (2.7) and (2.13) vanish:

$$\langle R_i^{+}\theta_i\rangle_0=\langle\theta_{-i}^{+}\tilde{R}_i^{+}\rangle_0=0. \tag{2.18}$$

Thus, the equations of the first order (2.7) and (2.13) become equations of zeroth order:

$$\langle\theta_i^{+}\theta_i\rangle_0=\tilde{\varphi}_i^{\pm}\langle[\theta_i,\theta_i^{+}]_{\pm}\rangle_0, \tag{2.19}$$

$$\langle\theta_i^{+}\theta_{-i}^{+}\rangle_0=\tilde{\varphi}_i^{\pm}\langle[\theta_{-i}^{+},\theta_i^{+}]_{\pm}\rangle_0 \tag{2.20}$$

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[1] In the general case $\Omega=\theta_i^{+}$ we obtain from (2.1) and (2.6) instead of (2.12) the result

$$[\exp(-\beta\omega_i)-\exp(\beta\omega_k)]\langle\theta_k^{+}R_i^{+}\rangle/(\omega_i+\omega_k)+O(R_i^{+}R_k^{+})$$

which for $k=-i$ and $\omega_i=\omega_{-i}$ leads to Eq. (2.12).

[2] For Bose or Fermi operators, *e.g.*, this can be achieved with Bogolyubov's transformation [9] which diagonalizes the bilinear part of the Hamiltonian and leads therefore automatically to commutator equations of the type (2.17).

where

$$\tilde{\varphi}_i^{\pm} = (e^{\beta\omega_i(L_i^1, M_i^1)} \pm 1)^{-1}. \tag{2.21}$$

With the zeroth-order basic equations (2.3) and (2.4) the conditions (2.18) can be written as

$$\langle [\theta_i, \tilde{R}_i^+]_{\pm} \rangle_0 = \langle [\tilde{R}_i^+, \theta_{-i}^+]_{\pm} \rangle_0 = 0. \tag{2.22}$$

Eqs (2.19), (2.20) and (2.22) represent a coupled set of equations for the quantities L_i^1, M_i^1, $\langle \theta_i^+ \theta_i \rangle$ and $\langle \theta_i^+ \theta_{-i}^+ \rangle_0$. For $M_i^0 = M_i^1 = 0$ the above results coincide with those of [2]. Because second- and higher-order terms in $\tilde{R}_i^+$, R_i^+ have been dropped in (2.7) and (2.13), the use of the zeroth-order basic equations is justified if

$$L_i^1 \ll L_i^0, \; M_i^1 \ll M_i^0. \tag{2.23}$$

Only then can the L_i^1, M_i^1 be considered as reasonable first-order corrections.

3. *The Hamiltonian commutator equations for a uniaxial ferromagnet with field*

We consider the following Hamiltonian of a uniaxial ferromagnet in a homogeneous external magnetic field of arbitrary direction:

$$H = -h_x \sum_j \tilde{S}_j^x - h_z \sum_j \tilde{S}_j^z - \sum_{j,k} I_{ik} \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_k - \sum_{j,k} G_{ik} \tilde{S}_i^z \tilde{S}_k^z. \tag{3.1}$$

The anisotropy direction is assumed to be parallel to the z-axis and the field to lie in the $x0z$-plane; $j = \boldsymbol{j}$ and $k = \boldsymbol{k}$ denote lattice *vectors*; $\tilde{\mathbf{S}}_j = (\tilde{S}_j^x, \tilde{S}_j^y, \tilde{S}_j^z)$ denotes the spin vector operator ascribed to the lattice site j; I_{jk}, G_{jk} stand respectively for the isotropic and anisotropic exchange integrals. If translational invariance of the crystal lattice is assumed the latter depend only on the distance between lattice sites:

$$I_{jk} = I(j-k) = I(f); \quad G_{jk} = G(j-k) = G(f). \tag{3.2}$$

Intra-atomic interactions (*e.g.*, crystal-field anisotropy) are excluded: $I_{jj} = G_{jj} = 0$. Furthermore, the following abbreviations are used:

$$h_x = \mu H_x, \quad h_z = \mu H_z \tag{3.3}$$

H_x, H_z being the components of the external magnetic field and μ — Bohr's magneton.

Next, we perform a homogeneous rotation of the lattice spins around the y-axis by the angle φ:

$$\begin{aligned} \tilde{S}_j^x &= \gamma_z S_j^x + \gamma_x S_j^z \\ \tilde{S}_j^y &= S_j^y \\ \tilde{S}_j^z &= -\gamma_x S_j^x + \gamma_z S_j^z, \\ \gamma_x &= \sin\varphi, \quad \gamma_z = \cos\varphi. \end{aligned} \tag{3.4}$$

The angle φ will be determined later. It is convenient to work with the three operators

$$S_j^z, \quad S_j^{\pm} = S_j^x \pm i S_j^y \tag{3.5}$$

which satisfy the commutation rules

$$[S_j^+, S_k^-]_- = 2\delta_{jk} S_j^z, \quad [S_j^\pm, S_k^z]_- = \mp \delta_{jk} S_j^\pm \tag{3.6}$$

and the operator identities

$$S_j^- S_j^+ = S(S+1) - S_j^z - (S_j^z)^2, \quad \prod_{r=-S}^{S} (S_j^z - r) = 0 \tag{3.7}$$

with S as the maximum spin eigenvalue [9].

We now perform the Fourier transformations

$$S_j^+ = N^{-1/2} \sum_\nu e^{ij\nu} b_\nu, \quad S_j^- = N^{-1/2} \sum_\nu e^{-ij\nu} b_\nu^+ \tag{3.8}$$

$$S_j^z = \sum_\nu e^{ij\nu} a_\nu \tag{3.9}$$

where N is the total number of (magnetic) lattice atoms. Greek ondices denote reciprocal lattice *vectors*. The operators b_ν, b_ν^+, a_ν obey according to (3.6), the following commutation relations:

$$[b_\nu, b_\mu^+]_- = 2a_{\nu-\mu}, \quad [b_\nu, b_\mu]_- = [b_\nu^+, b_\mu^+]_- = 0 \tag{3.10}$$

$$[b_\nu, a_\mu]_- = -N^{-1} b_{\nu+\mu}, \quad [b_\nu^+, a_\mu]_- = N^{-1} b_{\nu-\mu}. \tag{3.11}$$

For $S = \frac{1}{2}$ the operators a_ν can be expressed by b_ν, b_ν^+:

$$a_\nu = \tfrac{1}{2}\delta_{\nu 0} - N^{-1} \sum_{\gamma,\delta} \delta(\nu+\gamma-\delta) b_\gamma^+ b_\delta. \tag{3.12}$$

This follows from (3.7), (3.8) and (3.9). By making use of Eqs (3.4), (3.5), (3.8) and (3.9) the Hamiltonian (3.1) takes the form

$$\begin{aligned} H = & -(h_x\gamma_x + h_z\gamma_z) N a_0 - \tfrac{1}{2}(h_x\gamma_z - h_z\gamma_x) \sqrt{N}\,(b_0^+ + b_0) - \\ & - \sum_\nu J(\nu)\,[b_\nu^+ b_\nu + N a_\nu a_{-\nu}] - \sum_\nu G(\nu)\,[N\gamma_z^2 a_\nu a_{-\nu} - \\ & - \gamma_x\gamma_z \sqrt{N}\,(b_\nu a_{-\nu} + b_\nu^+ a_\nu) - \tfrac{1}{4}\gamma_x^2 (b_\nu^+ b_{-\nu}^+ + 2b_\nu^+ b_\nu + b_\nu b_{-\nu})] \end{aligned} \tag{3.13}$$

where $J(\nu)$ and $G(\nu)$ denote the Fourier transforms of the exchange integrals $I(f)$ and $G(f)$

$$J(\nu) = \sum_f e^{if\nu} I(f), \quad G(\nu) = \sum_f e^{if\nu} G(\nu). \tag{3.14}$$

With (3.10) and (3.11) the Hamiltonian commutator equations following from (3.13) are

$$\begin{aligned} [H, b_\alpha^+]_- = & (h_x\gamma_x + h_z\gamma_z) b_\alpha^+ - (h_x\gamma_z - h_z\gamma_x) N^{1/2} a_{-\alpha} - \\ & - 2\sum_\nu J(\nu) b_\nu^+ a_{\nu-\alpha} + 2\sum_\nu J(\nu) a_\nu b_{\nu+\alpha}^+ + 2\gamma_z^2 \sum_\nu G(\nu) a_\nu b_{\nu+\alpha}^+ - \\ & - \gamma_x\gamma_z N^{-1/2} \sum_\nu G(\nu) b_\nu b_{\nu+\alpha}^+ + 2\gamma_x\gamma_z N^{1/2} \sum_\nu G(\nu) a_{\nu-\alpha} a_\nu - \\ & - \gamma_x\gamma_z N^{-1/2} \sum_\nu G(\nu) b_\nu^+ b_{\alpha-\nu}^+ - \gamma_x^2 \sum_\nu G(\nu) b_\nu^+ a_{\nu-\alpha} - \gamma_x^2 \sum_\nu G(\nu) b_\nu a_{\alpha-\nu}. \end{aligned} \tag{3.15}$$

4. First-order energy renormalization

In analogy to Tyablikov's decoupling [9] in the Green's function theory we introduce in (3.15) the substitution

$$a_\lambda = \langle a_\lambda \rangle + (a_\lambda - \langle a_\lambda \rangle) \tag{4.1}$$

and consider $(a_\lambda - \langle a_\lambda \rangle)$ as a small operator. Since $\langle S_j^z \rangle$ does not depend on the lattice site we get from (3.9)

$$\langle a_\lambda \rangle = \delta_{\lambda 0} \langle S_j^z \rangle = \delta_{\lambda 0} S\sigma \tag{4.2}$$

where σ is the reduced spontaneous magnetization per atom in the direction $\gamma = (\gamma_x, 0, \gamma_z)$. With (4.1) the Hamiltonian commutator equations (3.15) read

$$[H, b_\alpha^+]_- = K\delta_{\alpha 0} + L_\alpha^0 b_\alpha^+ + M_\alpha^0 b_{-\alpha}^+ + P_\alpha^+, \tag{4.3}$$

$$K = \sqrt{N}\, S\sigma[h_z\gamma_x - h_x\gamma_z + 2S\sigma G(0)\gamma_x\gamma_z], \tag{4.4}$$

$$L_\alpha^0 = h_x\gamma_x + h_z\gamma_z + 2S\sigma(J(0) - J(\alpha)) + 2S\sigma\gamma_z^2 G(0) - S\sigma\gamma_x^2 G(\alpha), \tag{4.5}$$

$$M_\alpha^0 = -S\sigma\gamma_x^2 G(\alpha). \tag{4.6}$$

The direction $\gamma = (\gamma_x, 0, \gamma_z)$ can be determined [10, 11] from the condition $K = 0$ which provides the equation

$$h_z\gamma_x - h_x\gamma_z + 2S\sigma G(0)\,\gamma_x\gamma_z = 0. \tag{4.7}$$

In the zeroth-order approximation we would have to neglect the remainder P_α^+ in (4.3). Because this approximation has been already carried out for the Hamiltonian (31) in [5] we shall at once start with the first-order energy renormalization. The zeroth-order results will be special cases of our formulae.

According to (2.15) we rewrite (4.3) with $K = 0$:

$$[H, b_\alpha^+]_- = L_\alpha b_\alpha^+ + M_\alpha b_{-\alpha}^+ + R_\alpha^+ \tag{4.8}$$

where

$$L_\alpha = L_\alpha^0 + L_\alpha^1, \quad M_\alpha = M_\alpha^0 + M_\alpha^1, \tag{4.9}$$

$$R_\alpha^+ = P_\alpha^+ - L_\alpha^1 b_\alpha^+ - M_\alpha^1 b_{-\alpha}. \tag{4.10}$$

The Hamiltonian commutator equations (4.8) can be converted into normal form by means of the transformation

$$c_\alpha = (c_\alpha^+)^+ = u_\alpha b_\alpha + v_\alpha b_{-\alpha}^+ \tag{4.11}$$

with real coefficients u_α, v_α. The reciprocal transformation of (4.11) has the form

$$b_\alpha = (b_\alpha^+)^+ = u_\alpha c_\alpha - v_\alpha c_{-\alpha}^+, \tag{4.12}$$

if the condition

$$u_\alpha^2 - v_\alpha^2 = 1 \tag{4.13}$$

is assumed (without loss of generality).

The so introduced operators c_α^+, c_α obey in general q-number commutation relations; these are not relevant for our further calculations. We multiply (4.8) by u_α and the Hermitian conjugate equation

$$[H, b_{-\alpha}]_- = -L_\alpha b_{-\alpha} - M_\alpha b_\alpha^+ - R_{-\alpha} \tag{4.14}$$

by v_α. Summation provides with regard of (4.11)

$$[H, c_\alpha^+]_- = b_\alpha^+(u_\alpha L_\alpha - v_\alpha M_\alpha) + b_{-\alpha}(u_\alpha M_\alpha - v_\alpha L_\alpha) + \tilde{R}_\alpha^+ \tag{4.15}$$

where

$$\tilde{R}_\alpha^+ = u_\alpha R_\alpha^+ - v_\alpha R_{-\alpha}. \tag{4.16}$$

If the equations

$$\begin{aligned} u_\alpha L_\alpha - v_\alpha M_\alpha &= u_\alpha \omega_\alpha, \\ u_\alpha M_\alpha - v_\alpha L_\alpha &= v_\alpha \omega_\alpha \end{aligned} \tag{4.17}$$

are satisfied the Hamiltonian commutator equations take the normal form

$$[H, c_\alpha^+]_- = \omega_\alpha c_\alpha^+ + \tilde{R}_\alpha^+. \tag{4.18}$$

Taking into account condition (4.13) the system of equations (4.17) can easily be solved:

$$\alpha_\alpha = (L_\alpha^2 - M_a^2)^{1/2}, \tag{4.19}$$

$$u_\alpha = \left(\frac{L_\alpha + \omega_\alpha}{2\omega_\alpha}\right)^{1/2}, \quad v_\alpha = \left(\frac{L_\alpha - \omega_\alpha}{2\omega_\alpha}\right)^{1/2}. \tag{4.20}$$

(The solution $\omega_\alpha = -(L_\alpha^2 - M_\alpha^2)^{1/2}$ is inadmissible on physical grounds.) According to (2.22) we determine the corrections L_α^1, M_α^1 from the conditions

$$\langle [c_\alpha, \tilde{R}_\alpha^+]_- \rangle = 0, \quad \langle [\tilde{R}_\alpha^+, c_{-\alpha}^+]_- \rangle = 0. \tag{4.21}$$

(We remind that the averages are to be calculated by the zeroth-order equations (2.19), (2.20) with the renormalized energies ω_α; for simplicity we omit the index "0".) With (4.10), (4.11), (4.16) and the abbreviations

$$X_\alpha = \langle [b_\alpha, P_\alpha^+]_- \rangle = \langle [b_\alpha, [H, b_\alpha^+]_-]_- \rangle - 2S\sigma L_\alpha^0, \tag{4.22}$$

$$Y_\alpha = [\langle P_\alpha^+, b_{-\alpha}^+]_- \rangle = \langle [[H, b_\alpha^+]_-, b_{-\alpha}^+]_- \rangle - 2S\sigma M_\alpha^0 \tag{4.23}$$

the conditions (4.21) turn into

$$\langle [c_\alpha, \tilde{R}_\alpha^+]_- \rangle = X_\alpha(u_\alpha^2 + v_\alpha^2) - 2Y_\alpha u_\alpha v_\alpha - \sigma L_\alpha^1(u_\alpha^2 + v_\alpha^2) + 2\sigma M_\alpha^1 u_\alpha v_\alpha = 0 \tag{4.24}$$

$$\langle [\tilde{R}_\alpha^+, c_{-\alpha}^+]_- \rangle = Y_\alpha(u_\alpha^2 + v_\alpha^2) - 2X_\alpha u_\alpha v_\alpha - \sigma M_\alpha^1(u_\alpha^2 + v_\alpha^2) + 2\sigma L_\alpha^1 u_\alpha v_\alpha = 0. \tag{4.25}$$

In the last formulae we utilized the relation

$$\langle [b_\alpha, b_\alpha^+]_- \rangle = 2S\sigma, \tag{4.26}$$

The solutions of (4.24) and (4.25) are:

$$L_\alpha^1 = \frac{1}{\sigma} X_\alpha, \qquad M_\alpha^1 = \frac{1}{\sigma} Y_\alpha. \tag{4.27}$$

We see that the present renormalization procedure actually reduces to the evaluation of the double-commutators in (4.22) and (4.23). However, this evaluation turns out to be not unique. As an example we consider the double-commutator part in (4.22) corresponding to the third term of the Hamiltonian commutator equation (3.15). The commutator to be calculated in this case reads

$$\langle [b_\alpha, b_\nu^+ a_{\nu-\alpha}]_- \rangle. \tag{4.28}$$

We take advantage of Eqs (3.10), (3.11) and, by using Tyablikov's decoupling

$$a_\lambda \to S_\sigma \delta_{\lambda 0} \tag{4.29}$$

we obtain

$$\begin{aligned} \langle [b_\alpha, b_\nu^+ a_{\nu-\alpha}]_- \rangle &= 2\langle a_{\alpha-\nu} a_{\nu-\alpha} \rangle - N^{-1} \langle b_\nu^+ b_\nu \rangle \\ &= 2S^2\sigma^2 \delta_{\nu\alpha} - N^{-1} \langle b_\nu^+ b_\nu \rangle. \end{aligned} \tag{4.30}$$

On the other hand, according to (3.10) the operator $a_{\nu-\alpha}$ can be written as

$$a_{\nu-\alpha} = \tfrac{1}{2}(b_\nu b_\alpha^+ - b_\alpha^+ b_\nu). \tag{4.31}$$

On the basis of (4.31) we get, with the aid of Eqs (3.10) and (4.29),

$$\begin{aligned} \langle (b_\alpha, b_\nu^+ a_{\nu-\alpha}]_- \rangle &= \langle a_{\alpha-\nu} b_\nu b_\alpha^+ \rangle + \langle b_\nu^+ b_\nu a_0 \rangle - \langle a_{\alpha-\nu} b_\alpha^+ b_\nu \rangle - \\ &- \langle b_\nu^+ a_0 b_\nu \rangle = 2S\sigma\delta_{\nu\alpha} \langle a_0 \rangle = 2S^2\sigma^2\delta_{\nu\alpha}. \end{aligned} \tag{4.32}$$

Finally, in the case $S = \frac{1}{2}$ we can use formula (3.12) and obtain with (4.29)

$$\begin{aligned} \langle [b_\alpha, b_\nu^+ a_{\nu-\alpha}]_- \rangle &= \tfrac{1}{2}\delta_{\nu\alpha} \langle [b_\alpha, b_\alpha^+]_- \rangle - \\ &- N^{-1} \sum_{\gamma,\delta} \delta(\nu - \alpha + \gamma - \delta) \langle [b_\alpha, b_\nu^+ b_\gamma^+ b_\delta]_- \rangle \\ &= \tfrac{1}{2}\sigma^2 \delta_{\nu\alpha} - \sigma N^{-1} \langle b_\nu^+ b_\nu \rangle. \end{aligned} \tag{4.33}$$

The calculations in Eqs (4.22) and (4.23) for the other terms of (3.15) lead to similar discrepancies. It can be shown that in the special case of isotropic $S = \frac{1}{2}$ ferromagnets the different approximations (4.30), (4.32 and (4.33) lead to the same renormalized energies as the respective different decoupling procedures in the first-order Green's functions theory: the Hartree-Fock decoupling for the Bose-type Green's functions [12], the RPA-decoupling [9, 13], and the Hartree-Fock decoupling [12, 14] for the Pauli-type Green's functions[3]. As is well known, the first and the last approximation violate the obvious condition

$$\sigma(-H) = -\sigma(H) \tag{4.34}$$

[3] The situation is probably much the same for anisotropic ferromagnets. Unfortunately, no similarly complete Green's functions results are so far available for uniaxial ferromagnets.

and, besides, the first gives an infinite Curie temperature. Therefore, evaluations of the type (4.30) and (4.33) should be dismissed for physical reasons. On the other hand, the remaining method (4.32) provides the trivial result $L_\alpha^1 = M_\alpha^1 = 0$, *i. e.*, it leads to zeroth-order energies.

One way of overcoming these difficulties is to take advantage of the very ambiguity of the above calculations, by introducing into the theory a new parameter which, *e. g.*, can be fitted to experimental data. (In any case it has to be chosen in such a way that the condition (4.34) is fulfilled for isotropic ferromagnets.) For instance, for $S = \frac{1}{2}$ we can combine (4.32) with (4.33) and, following Callen [7], we multiply Eq. (4.32) by $(1-p)$ and Eq. (4.33) by p where p is the new parameter. Upon adding those equations we have

$$\langle [b_\alpha, b_\nu^+ a_{\nu-\alpha}]_- \rangle = \tfrac{1}{2}\sigma^2 \delta_{\alpha\nu} - p\sigma N^{-1} \langle b_\nu^+ b_\nu \rangle. \tag{4.35}$$

For $p = -1$, $p = 0$ and $p = 1$ we obtain Eqs (4.30), (4.32) and (4.33) respectively. The question of the proper choice of p will be discussed further below. The evaluation of the double-commutators in (4.22) and (4.23) according to (4.35) leads with (4.27) to the corrections

$$L_\alpha^1 = p\left[\frac{2}{N}\sum_\nu (J(\nu)-J(\nu-\alpha))\langle b_\nu^+ b_\nu\rangle - \frac{2}{N}\gamma_z^2 \sum_\nu G(\nu-\alpha)\langle b_\nu^+ b_\nu\rangle + \right.$$
$$\left. + \frac{\gamma_x^2}{N}\sum_\nu G(\nu)\langle b_\nu^+ b_\nu\rangle + \frac{\gamma_x^2}{N}\sum_\nu G(\nu)\langle b_\nu b_{-\nu}\rangle\right], \tag{4.36}$$

$$M_\alpha = p\left[\frac{2}{N}\sum_\nu (J(\nu)-J(\nu-\alpha))\langle b_\nu^+ b_{-\nu}^+\rangle - \frac{2}{N}\gamma_z^2 \sum_\nu G(\nu-\alpha)\langle b_\nu^+ b_{-\nu}^+\rangle \times \right.$$
$$\left. + \frac{\gamma_x^2}{N}\sum_\nu G(\nu)\langle b_\nu^+ b_{-\nu}^+\rangle + \frac{\gamma_x^2}{N}\sum_\nu G(\nu)\langle b_\nu^+ b_\nu\rangle\right]. \tag{4.37}$$

Next, we calculate the averages $\langle b_\nu^+ b_\nu\rangle$, $\langle b_\nu b_{-\nu}\rangle$, $\langle b_\nu^+ b_{-\nu}^+\rangle$ occurring in (4.36) and (4.37). For this purpose, we have to use the zeroth-order basic equations (2.19), (2.20) with the renormalized energies (4.19). We specify $\theta_i = c_\nu$, $\Omega = b_\nu$ or $b_{-\nu}$ and obtain

$$\langle c_\nu^+ b_\nu\rangle = \varphi_\nu \langle [b_\nu, c_\nu^+]_-\rangle,$$
$$\langle b_{-\nu} c_\nu\rangle = \varphi_\nu \langle [c_\nu, b_{-\nu}]_-\rangle \tag{4.38}$$

with

$$\varphi_\nu = (e^{\beta\omega_\nu} - 1)^{-1}. \tag{4.39}$$

Due to (4.11), (3.10) and (4.2) the relations (4.38) lead to the equations

$$u_\nu \langle b_\nu^+ b_\nu\rangle + v_\nu \langle b_{-\nu} b_\nu\rangle = \sigma u_\nu \varphi_\nu,$$
$$v_\nu \langle b_\nu^+ b_\nu\rangle + u_\nu \langle b_{-\nu} b_\nu\rangle = -\sigma v_\nu - \sigma v_\nu \varphi_\nu. \tag{4.40}$$

With (4.19) the solutions can be written as:

$$\langle b_\nu^+ b_\nu\rangle = \sigma(u_\nu^2 + v_\nu^2)\varphi_\nu + \sigma v_\nu = \frac{\sigma}{2}\left(\frac{I_\nu}{\omega_\nu} \operatorname{cth} \frac{\beta\omega_\nu}{2} - 1\right), \tag{4.41}$$

$$\langle b_{-\nu} b_\nu\rangle = \langle b_\nu^+ b_{-\nu}^+\rangle = -\sigma u_\nu v_\nu (2\varphi_\nu + 1) = -\frac{\sigma}{2}\frac{M_\nu}{\omega_\nu} \operatorname{cth} \frac{\beta\omega_\nu}{2}. \tag{4.42}$$

After insertion of (4.41) and (4.42) in (4.36) and (4.37) we encounter sums of the form

$$\sum_{\nu} J(\nu-\alpha)\varphi_{\nu}. \tag{4.43}$$

Assuming simple lattices with nearest-neighbour interaction the sum (4.43) simplifies according to Callen [7] to

$$J(\alpha)\sum_{\nu}\gamma_{\nu}\varphi_{\nu} \tag{4.44}$$

with $\gamma_{\nu}=J(\nu)/J(0)$, and the corrections (4.36), (4.37) become finally

$$L_{\alpha}^{1}=p\sigma A(J(0)-J(\alpha)-\gamma_{z}^{2}G(\alpha)+\frac{\gamma_{x}^{2}}{2}G(0))-p\sigma B\frac{\gamma_{x}^{2}}{2}G(0), \tag{4.45}$$

$$M_{\alpha}^{1}=-p\sigma B\,(J(0)-J(\alpha)-\gamma_{z}^{2}G(\alpha)+\frac{\gamma_{x}^{2}}{2}G(0))+p\sigma A\frac{\gamma_{x}^{2}}{2}G(0) \tag{4.46}$$

where

$$A=N^{-1}\sum_{\nu}\gamma_{\nu}\frac{L_{\nu}}{\omega_{\nu}}\operatorname{cth}\frac{\beta\omega_{\nu}}{2},$$

$$B=N^{-1}\sum_{\nu}\gamma^{\nu}\frac{M_{\nu}}{\omega_{\nu}}\operatorname{cth}\frac{\beta\omega_{\nu}}{2}. \tag{4.47}$$

The magnetization can easily be obtained from the relation (3.12). We have

$$\sigma=1-2N^{-1}\sum_{\nu}\langle b_{\nu}^{+}b_{\nu}\rangle. \tag{4.48}$$

With (4.41) this yields

$$\sigma^{-1}=N^{-1}\sum_{\nu}\frac{L_{\nu}}{\omega_{\nu}}\operatorname{cth}\frac{\beta\omega_{\nu}}{2}. \tag{4.49}$$

The coupled equations (4.7), (4.47), (4.49) for the quantities γ_x, γ_z, A, B, σ must be solved simultaneously. The zeroth-order approximation can be obtained by putting $p=0$. In this case the above set of equations reduces to (4.7) and

$$\sigma^{-1}=N^{-1}\sum_{\nu}\frac{L_{\nu}^{0}}{\omega_{\nu}^{0}}\operatorname{cth}\frac{\beta\omega_{\nu}^{0}}{2} \tag{4.50}$$

with

$$\omega_{\nu}^{0}=[(L_{\nu}^{0})^{2}-(M_{\nu}^{0})^{2}]^{1/2}.$$

Eqs (4.7), (4.50) have been derived in [5] by the same method and in [6] by the Green's functions approach (for arbitrary spins). On the basis of Eqs (4.7) and (4.50), second-order phase transitions in uniaxial ferromagnets with perpendicular field have been studied in [15].

Up to now we left open the question how to choose the parameter p within the first-order theory. Taking into account physical criteria Callen [7, 16] proposed

$$p=\sigma^{n}. \tag{4.51}$$

So far, for isotropic ferromagnets the cases $n = 1$ and $n = 3$ have been studied [7, 17]. (Because of the condition (4.34) the integer n must be odd.) In the following we assume $h \equiv h_x \neq 0$, $h_z = 0$. With the choice (4.51) the quantities L_ν^1, M_ν^1 are *not* reasonable first-order corrections because conditions (2.23) are in general not satisfied. Moreover, the property of the energy spectrum at the critical point [15],

$$\omega_0(T_k, h) = \omega_0(T, h_k) = 0, \tag{4.52}$$

is destroyed by choosing (4.51). On the other hand, Callen's considerations can be re-interpreted regarding σ as order-parameter. In our problem, however, the order-parameter turns out to be $\sigma^z = \gamma_z \sigma$ ($h_z = 0$; cp. [15]). With the assumption

$$p = (\sigma^z)^n \tag{4.53}$$

Eq. (4.52) holds and the conditions (2.23) are fulfilled near and far below the transition point, as well as in the paramagnetic phase. In these cases our first-order energy-renormalization method is fully justified. It can easily be shown that the first-order calculations do not change the zeroth-order results concerning the phase transitions if the first-order iteration methods of [15] are applied. For $h_x \neq 0$ and $h_z \neq 0$ hardly anything can be said about the validity of our method because in this case Eq. (4.7) cannot be solved exactly.

5. *Final remarks*

It is instructive to show briefly to what results does a straightforward application of Wallace's energy-renormalization procedure to our problem lead. Diagonalization of Eq. (4.3) (with $K = 0$) with the aid of (4.11) (with $L_\alpha = L_\alpha^0$, $M_\alpha = M_\alpha^0$) leads to

$$[H, c_\alpha^+]_- = \omega_\alpha^0 c_\alpha^+ + \tilde{P}_\alpha^+, \quad \omega_\alpha^0 = [(L_\alpha^0)^2 - (M_\alpha^0)^2]^{1/2}. \tag{5.1}$$

The renormalization procedure of [2] is based on the equality

$$[H, c_\alpha^+]_- = (\omega_\alpha^0 + \omega_\alpha^1)\, c_\alpha^+ + (P_\alpha^+ - \omega_\alpha^1 c_\alpha^+) \tag{5.2}$$

and requires the energy corrections ω_α to be determined from the conditions

$$\langle (\tilde{P}_\alpha^+ - \omega_\alpha^1 c_\alpha^+)\, c_\alpha \rangle = 0 \tag{5.3}$$

which leads to the result

$$\omega_\alpha^1 = (L_\alpha^0 X_\alpha - M_\alpha^0 Y_\alpha)/\sigma\omega_\alpha^0 \tag{5.4}$$

with X_α and Y_α as defined by Eqs (4.22) and (4.23). For $S = \frac{1}{2}$ the magnetization formula reads now

$$\sigma^{-1} = N^{-1} \sum_\alpha (L_\alpha^0/\omega_\alpha^0) \operatorname{cth} (\beta\omega_\alpha/2), \quad \omega_\alpha = \omega_\alpha^0 + \omega_\alpha^1. \tag{5.5}$$

In the case $h_z = 0$, $G(0) > 0$ the above first-order energy spectrum ω_α has the following drawbacks (cp. [15]):

with the choice (4.51) we have always $\omega_0 \to \infty$ as $T \to T_k$ or $h \to h_k$;

when choosing (4.53) and $n = 1$, the energy ω_0 is finite and positive, but the applicability condition $\omega_\alpha^1 \ll \omega_\alpha^0$ of Wallace's method is not fulfilled;

for (4.53) and $n > 1$, the result (5.4) coincides in the paramagnetic phase with that derived in Sec. 4, but in the ferromagnetic phase the agreement is only approximate and limited to the extreme cases $T \ll T_k$, $h \ll h_k$ and $T \gtrsim T_k$, $h \gtrsim h_k$.

Furthermore, the averages $\langle c_\alpha^+ c_{-\alpha}^+ \rangle$ do not vanish to first-order.

It is thus evident that our method as presented in Secs. 2–4, which actually differs from Wallace's procedure by *first* carrying out the renormalization and *thereafter* the diagonalization, leads to more satisfactory results.

Wallace's statistical perturbation method and its generalization as presented here (to first order) can be applied in two ways:

(*i*) the calculation of the perturbed averages according to formulae (2.7) and (2.13);

(*ii*) the evaluation of the unperturbed averages with renormalized energies; the renormalization resides in this case in removing the perturbation terms, and the energy corrections and the averages are coupled by transcendental equations.

In neither case is a "convenient" perturbation parameter needed. Whereas the variant (*i*) is useful for a strict treatment of limiting cases (*e. g.*, small temperatures, small fields; cp. [1–4, 8]), the variant (*ii*) is more suited for calculations over a wide range of the external parameters (cp. [2, 5] and present paper). Although the latter approach is similar to the Green's functions technique, Wallace's method clearly shows certain advantages. In contrast to the decoupling of higher Green's functions, we have in our method a reliable criterion for the quality of our approximations, Eq. (2.23). In this way, for instance, we were able to restrict the choice of the parameter p in Sec. 4.

The first-order formulae (2.7) and (2.13) are used in a subsequent paper [8] for calculating the low-temperature weak-field expansion of the magnetization of uniaxial ferromagnets with transversal field.

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