PHYSICALLY MEANINGFUL *VERSUS* REDUNDANT BOUNDARY EQUATIONS FOR A THIN FILM FROM THE TYABLIKOV-BOGOLYUBOV DIAGONALIZATION METHOD

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The Tyablikov-Bogolyubov method of bilinear Hamiltonian diagonalization is shown to lead to twice the number of boundary equations required by the physical aspect of the problem. Here, a procedure for selecting those boundary equations only which correspond to physically meaningful solutions of the problem is proposed and justified. With regard to the highly involved shape of the equations, certain well-founded approximations are proposed. The method is applied to a thin film of *hcp* structure and is shown to yield the same results as earlier methods.

1. General considerations

The Tyablikov and Bogolyubov [1] method of diagonalizing the full bilinear Hamiltonian was applied by one of us (Puszkarski [2]) to thin films. General boundary equations were given in [2], accounting mathematically for the influence of surface defect on the eigen-problem of the film. The present paper aims at a detailed analysis of these equations and, more practically, at a discussion of the following problem: The number of boundary equations obtained in the Tyablikov-Bogolyubov method is two times larger than that required by the "number of dimensions" of the physical problem under consideration. Some of them, in fact, "quantize" physical solutions, whereas the others concern non-physical solutions (which, as we know, always appear in this method). Hence, it will be the aim of this paper to establish a criterium for recognizing those boundary equations which correspond to physical solutions and the exclusion of the others. The criterium will then be

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tested for its correctness by applying it to the case of the *hcp* lattice, for which the boundary equations have already been derived by a different, independent method (Puszkarski [3]).

In outline, the idea of the Tyablikov-Bogolyubov method as applied to thin films consists in the following [2]: One considers the bilinear Hamiltonian in the form

$$\mathscr{H} = \sum_{l,g,\mathbf{j},\mathbf{j}'} [A_{l,\mathbf{j};\,l+g,\mathbf{j}'}\, a^{+}_{l,\mathbf{j}}\, a_{l+g,\mathbf{j}'} + \tfrac{1}{2} B_{l,\mathbf{j};l+g,\mathbf{j}'}\, a^{+}_{l,\mathbf{j}}\, a^{+}_{l+g,\mathbf{j}'} + \tfrac{1}{2} B^{*}_{l,\mathbf{j};\,l+g,\mathbf{j}'} a_{l,\mathbf{j}} a_{l+g,\mathbf{j}'}], \tag{1}$$

which, on diagonalisation, reduces to

$$\mathscr{H} = \Delta E_0 + \sum_{\vec{\varkappa},\tau} E(\vec{\varkappa}, \tau)\, \xi^{+}_{\vec{\varkappa},\tau}\, \xi_{\vec{\varkappa},\tau}, \tag{2}$$

where

$$\Delta E_0 = -\sum_{l,\mathbf{j},\vec{\varkappa}\tau} E(\vec{\varkappa}, \tau) |v_{l,\mathbf{j}}(\vec{\varkappa}, \tau)|^2. \tag{3}$$

Above, the following canonical transformation of Bose operators was used:

$$a_{l,\mathbf{j}} = \sum_{\vec{\varkappa},\tau} [u_{l,\mathbf{j}}(\vec{\varkappa}, \tau)\, \xi_{\vec{\varkappa},\tau} + v^{*}_{l,\mathbf{j}}(\vec{\varkappa}, \tau)\, \xi^{+}_{\vec{\varkappa},\tau}]. \tag{4}$$

The notation is:

$l = 0, 1, \ldots, L-1$ the number labelling a given layer (according to an idea of Valenta [4], we conceive of the film as consisting of L equidistant lattice planes parallel to the surface, each constituting an identical plane Bravais lattice; such a plane will henceforth be referred to as a "layer"),

$\mathbf{j}[j_x, j_y]$ a two-dimensional vector defining the position of a node in the layer,

g — an integer $0, \pm 1, \ldots$; we apply the convention $\mathbf{j} \in l, \mathbf{j}' \in l+g$;

$\vec{\varkappa}[\varkappa_x, \varkappa_y]$, $\tau \equiv \tau_z$ — quantum numbers depending on the boundary conditions in the X, Y, Z directions, respectively, and defining the eigen-states of the Hamiltonian,

$a_{l,\mathbf{j}}$, $\xi_{\vec{\varkappa},\tau}$ — boson operators, and

$u_{l,\mathbf{j}}(\vec{\varkappa}, \tau)$, $v_{l,\mathbf{j}}(\vec{\varkappa}, \tau)$ — as yet unknown transformation functions.

With regard to the largeness of the thin film in the directions parallel to its surface, it is usual to assume the Hamiltonian (1) as invariant with respect to operations of translation within the layers. Owing to this property, the transformation functions can be written in the form

$$\begin{aligned} u_{l,\mathbf{j}}(\vec{\varkappa}, \tau) &= N^{-\frac{1}{2}} e^{-i\vec{\varkappa}\cdot\mathbf{j}}\, u_l(\tau), \\ v_{l,\mathbf{j}}(\vec{\varkappa}, \tau) &= N^{-\frac{1}{2}} e^{-i\vec{\varkappa}\cdot\mathbf{j}}\, v_l(\tau) \end{aligned} \tag{5}$$

(N — number of nodes in the layer). The functions $u_l(\tau)$ and $v_l(\tau)$ have to satisfy the Tyablikov-Bogolyubov set of equations

$$\begin{aligned} E(\vec{\varkappa}, \tau)\, u_l(\tau) &= \sum_g [P_{l,l+g}(\vec{\varkappa}) u_{l+g}(\tau) + Q_{l,l+g}(\vec{\varkappa})\, v_{l+g}(\tau)], \\ -E(\vec{\varkappa}, \tau)\, v_l(\tau) &= \sum_g [P_{l,l+g}(\vec{\varkappa})\, v_{l+g}(\tau) + Q_{l,l+g}(\vec{\varkappa})\, u_{l+g}(\tau)], \end{aligned} \tag{6}$$

where we have used the notations:

$$P_{l,l+g}(\vec{\varkappa}) = \sum_{j'} A_{l,j;\,l+g,j'}\, e^{i\vec{\varkappa}\cdot(j-j')}, \tag{7}$$

$$Q_{l,l+g}(\vec{\varkappa}) = \sum_{j'} B_{l,j;\,l+g,j'}\, e^{i\vec{\varkappa}\cdot(j-j')}. \tag{8}$$

2. The case of hcp structure with uniaxial magnetic anisotropy

As an example of the above method, let us consider a thin ferromagnetic film cut from a crystal with *hcp* structure perpendicularly to its hexagonal axis. It will be remembered that, in such a crystal, one can distinguish two sublattices (consisting of nodes of types B or C). We agree to label the layers containing nodes from, say, sublattice B with even indices l and layers belonging to sublattice C with odd indices. We moreover shall assume that the ferromagnet is accessible to description by means of the Heisenberg model, and shall take into consideration interactions between nearest neighbours only. For the assumed surface orientation [0001], the nearest neighbours of a node are all situated in the same layer and in the two closest-lying layers, *i. e.* $g = 0, \pm 1$. We chose the hexagonal axis as the Z-direction and lay the X and Y axes in the plane of the film. In addition to the standard isotropic exchange and Zeeman terms (the external field $\boldsymbol{H}$ is directed arbitrarily with respect to the surface of the film) we take into consideration in the Hamiltonian of the system of spins an anisotropic term accounting for the energy of uniaxial anisotropy with privileged Z-axis:

$$\mathcal{H} = -\sum_{l,g\boldsymbol{j},\boldsymbol{j}'} J_g \boldsymbol{S}_{l,\boldsymbol{j}} \boldsymbol{S}_{l+g,\boldsymbol{j}'} - g\mu_B \sum_{l,\boldsymbol{j}} \boldsymbol{H}\boldsymbol{S}_{l,\boldsymbol{j}} + \sum_{l,g,\boldsymbol{j},\boldsymbol{j}'} K_g S^z_{l,\boldsymbol{j}} S^z_{l+g,\boldsymbol{j}'}. \tag{9}$$

The notation is:
J_g — isotropic exchange integral, $\boldsymbol{S}_{l,\boldsymbol{j}}$ — spin vector operator at node l; $\boldsymbol{j}$; g — spectroscopic Landé factor, K_g — anisotropic interaction coefficient.

Taking into consideration the difference between the ideal and real *hcp* structure, we assume the exchange integral as taking the two values:

$$J_g = \begin{cases} J_0 & \text{for nearest neighbours belonging to the same sublattice,} \\ J_1 (= J_{-1}) & \text{for nearest neighbours from other sublattices.} \end{cases} \tag{10}$$

We shall distinguish anisotropy coefficients K_g according to whether two neighbouring nodes denoted by vectors $l, \boldsymbol{j}$ and $l+g, \boldsymbol{j}'$ lie on the film surface or within the film, thus:

$$K_g = \begin{cases} K' & \text{if the two nodes lie on the film surface,} \\ K & \text{otherwise.} \end{cases} \tag{11}$$

In order to express the Hamiltonian (9) in the representation of second quantization, we perform two consecutive transformations. The first [1] transforms the spin operators from "crystallographical" coordinates XYZ to coordinates $X'Y'Z'$ with Z'-axis directed

along the versor $\vec{\gamma}$ of spin quantization (the Y'-axis lies in the XOY-plane). This transformation is of the form[1]:

$$\boldsymbol{S}_{l,j} = \vec{\gamma} S^{z'}_{l,j} + \frac{1}{\sqrt{2}} (\boldsymbol{A} S'^{+}_{l,j} + \boldsymbol{A}^* S'^{-}_{l,j}),$$

$$S'^{\pm}_{l,j} = S'^{x}_{l,j} \pm i S'^{y}_{l,j} \tag{12}$$

with

$$A_x = -\frac{1}{\sqrt{2}} (\gamma_x^2+\gamma_y^2)^{-1/2} (\gamma_x\gamma_z + i\gamma_y),$$

$$A_y = -\frac{1}{\sqrt{2}} (\gamma_x^2+\gamma_y^2)^{-1/2} (\gamma_y\gamma_z - i\gamma_x),$$

$$A_z = \frac{1}{\sqrt{2}} (\gamma_x^2+\gamma_y^2)^{1/2}. \tag{13}$$

The vectors $\boldsymbol{A}$ and $\vec{\gamma}$ fulfil the relations:

$$\vec{\gamma} = \vec{\gamma}^*, \quad \vec{\gamma}\cdot\vec{\gamma} = 1, \quad \boldsymbol{A}^*\cdot\boldsymbol{A} = 1,$$

$$\boldsymbol{A}\cdot\vec{\gamma} = 0, \quad \boldsymbol{A}\cdot\boldsymbol{A} = 0,$$

$$\vec{\gamma}\times\boldsymbol{A} = i\boldsymbol{A}, \quad \boldsymbol{A}\times\boldsymbol{A}^* = i\vec{\gamma}.$$

The second is the well-known Holstein-Primakoff transformation:

$$S'^{+}_{l,j} = \sqrt{2S} f_{l,j} a_{l,j}, \quad S'^{-}_{l,j} = \sqrt{2S}\, a^{+}_{l,j} f_{l,j}, \quad S^{z'} = S - a^{+}_{l,j} a_{l,j},$$

$$f_{l,j} = \left(1 - \frac{a^{+}_{l,j} a_{l,j}}{2S}\right)^{1/2}. \tag{14}$$

On these two transformations, and resorting to the condition of magnetic quasi-saturation, the Hamiltonian (9) becomes:

$$\mathcal{H} = \sum_{l,j} [g\mu_B (H_y\gamma_y + H_z\gamma_z) + 2S \sum_{d=0}^{l} z_d (J_d - K_d\gamma_z^2)]\, a^{+}_{l,j} a_{l,j} -$$

$$-2S \sum_{l,g,j,j'} (J_g - \tfrac{1}{2} K_g \gamma_y^2)\, a^{+}_{l,j} a_{l+g,j'} + \tfrac{1}{2} S\, \gamma_y^2 \sum_{l,g,j,j'} K_g (a_{l,j} a_{l+g,j'} + a^{+}_{l,j} a^{+}_{l+g,j'}). \tag{15}$$

The preceding Hamiltonian can obviously be written in the form (1) on appropriately defining the coefficients as follows:

$$A_{l,j;\,l+g,j'} = \begin{cases} 2S \sum_{d=0}^{l} z_d (J_d - K_d\gamma_z^2) + g\mu_B H_y\gamma_y + H_z\gamma_z) \text{ for } l, j = l+g, j', \\ -2S(J_g - \tfrac{1}{2} K_g \gamma_y^2) \text{ for } l, j \neq l+g, j', \end{cases} \tag{16a}$$

$$B_{l,j;\,l+g,j'} = S\gamma_y^2 K_g \tag{16b}$$

[1] Without loss of generality, we shall henceforth assume the vector $\boldsymbol{H}$ to lie in the plane YOZ (*i. e.* $H_x = 0$); the equilibrium conditions for the system of spins now lead to $\gamma_x = 0$, simplifying considerably the expressions for the components of the vector $\boldsymbol{A}$.

($\sum_{d=0}^{l}$ stands for summation over layers $l-1, l, l+1$)

$$z_d = \begin{cases} z_0 \text{ — the number of nearest neighbours of a given node from its "own" layer,} \\ z_1 (= z_{-1}) \text{ that of its nearest neighbours in a neighbouring layer.} \end{cases}$$

The coefficients (7) and (8) now take the form:

$$P_{l,\,l+g}(\vec{\varkappa}) = -2S\,[J_g - \tfrac{1}{2}\gamma_y^2 K_g]\,\Gamma_g^{\vec{\varkappa}} + \\ + \delta_{g,0}\,[2S \sum_{d=0}^{l} z_d (J_d - K_d \gamma_z^2) + g\mu_B (H_z \gamma_z + H_y \gamma_y)], \tag{17}$$

$$Q_{l,\,l+g}(\vec{\varkappa}) = S\gamma_y^2 K_g \Gamma_g^{\vec{\varkappa}}, \tag{18}$$

where

$$\Gamma_g^{\vec{\varkappa}} = \sum_{\boldsymbol{j}'} e^{i\vec{\varkappa}\cdot(\boldsymbol{j}-\boldsymbol{j}')} \tag{19}$$

with

$$\Gamma_g^{\vec{\varkappa}} = \begin{cases} \Gamma_0^{\vec{\varkappa}} \text{ if the nodes } l, \boldsymbol{j} \text{ and } l+g, \boldsymbol{j}' \text{ lie in the same layer } (g = 0), \\ \Gamma_1^{\vec{\varkappa}} \text{ if } l, \boldsymbol{j} \text{ belongs to sublattice } B, \text{ and } l+g, \boldsymbol{j}' \text{ to sublattice } C \ (g = \pm 1, \text{ even } l), \\ \Gamma_1^{*\vec{\varkappa}} \text{ if } l, \boldsymbol{j} \text{ belongs to } C, \text{ and } l+g, \boldsymbol{j}' \text{ to } B \ (g = \pm 1, \text{ odd } l). \end{cases} \tag{20}$$

The necessity of making the distinction in $\Gamma_g^{\vec{\varkappa}} (g = \pm 1)$ according to whether the node defined by the vector $l, \boldsymbol{j}$ lies in sublattice B or C is a result of the non-translational nature of the *hcp* structure; in fact, a neighbourhood of type $C-B-C$ of a node of sublattice B is "rotated" by an angle of π with regard to a $B-C-B$ neighbourhood of a node in sublattice C. With the expressions (17) and (18), we now re-write the set of Eqs (6) in the form[2]:

$$[P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau) - p_l(\vec{\varkappa})]\,u_l(\tau) - 2S \sum_{g}^{l} [J_g - \tfrac{1}{2}\gamma_y^2 K_g]\,\Gamma_g^{\vec{\varkappa}} u_{l+g}(\tau) + \\ + [Q(\vec{\varkappa}) - q_l(\vec{\varkappa})] v_l(\tau) + S \sum_{g}^{l} \gamma_y^2 K_g \Gamma_g^{\vec{\varkappa}} v_{l+g}(\tau) = 0,$$

$$[P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau) - p_l(\vec{\varkappa})]\,v_l(\tau) - 2S \sum_{g}^{l} [J_g - \tfrac{1}{2}\gamma_y^2 K_g]\,\Gamma_g^{\vec{\varkappa}} v_{l+g}(\tau) + \\ + [Q(\vec{\varkappa}) - q_l(\vec{\varkappa})]\,u_l(\tau) + S \sum_{g}^{l} \gamma_y^2 K_g \Gamma_g^{\vec{\varkappa}} u_{l+g}(\tau) = 0, \tag{21}$$

where

$\sum_{g}^{l}$ denotes summation over layers $l-1$ and $l+1$ (*i. e.* $g = \pm 1$),

$$P(\vec{\varkappa}) = -2S[J_0 - \tfrac{1}{2}\gamma_y^2 K]\Gamma_0^{\vec{\varkappa}} + 2Sz_0[J_0 - K\gamma_z^2] + \\ + 4Sz_1[J_1 - K\gamma_z^2] + g\mu_B] H_y \gamma_y + H_z \gamma_z], \tag{22}$$

$$Q(\vec{\varkappa}) = S\gamma_y^2 K \Gamma_0^{\vec{\varkappa}}, \tag{23}$$

[2] For simplicity, the two surfaces of the thin film are assumed to present identical conditions and to belong to the same magnetic sublattice (L is odd).

$p_l(\vec{\varkappa}) = 0$ within the thin film *i.e.* for $l = 1, 2, \ldots, L-2$,

$$p_0(\vec{\varkappa}) = p_{L-1}(\vec{\varkappa}) \equiv p(\vec{\varkappa}) = -2S[J_0 - \tfrac{1}{2}\gamma_y^2 K]\Gamma_0^{\vec{\varkappa}} + $$
$$+2S[J_0 - \tfrac{1}{2}\gamma_y^2 K']\Gamma_0^{\vec{\varkappa}} + 2Sz_0[J_0 - K\gamma_z^2] -$$
$$-2Sz_0[J_0 - K'\gamma_z^2] + 2Sz_1[J_1 - K\gamma_z^2]$$
$$= S\gamma_y^2\Gamma_0^{\vec{\varkappa}}(K-K') - 2Sz_0\gamma_z^2(K-K') + 2Sz_1(J_1 - K\gamma_z^2), \tag{24}$$

$$q_0(\vec{\varkappa}) = q_{L-1}(\vec{\varkappa}) \equiv q(\vec{\varkappa}) = S\gamma_y^2 K\Gamma_0^{\vec{\varkappa}} - S\gamma_y^2 K'\Gamma_0^{\vec{\varkappa}}$$
$$= S\gamma_y^2\Gamma_0^{\vec{\varkappa}}(K-K'). \tag{25}$$

On writting out the sums occurring in Eqs (21), we get for the various l:

$$l = 0$$
$$[-p(\vec{\varkappa}) + P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)]u_0(\tau) + [-q(\vec{\varkappa}) + Q(\vec{\varkappa})]v_0(\tau) - A\Gamma_1^{\vec{\varkappa}}u_1(\tau) -$$
$$-B\Gamma_1^{\vec{\varkappa}}v_1(\tau) = 0.$$
$$[-p(\vec{\varkappa}) + P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)]v_0(\tau) + [-q(\vec{\varkappa}) + Q(\vec{\varkappa})]u_0(\tau) - A\Gamma_1^{\vec{\varkappa}}v_1(\tau) -$$
$$-B\Gamma_1^{\vec{\varkappa}}u_1(\tau) = 0; \tag{26a}$$

$l = p$ $(p = 2, 4, \ldots, L-5, L-3)$:

$$[P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)]u_p(\tau) + Q(\vec{\varkappa})v_p(\tau) - A\Gamma_1^{\vec{\varkappa}}[u_{p+1}(\tau) + u_{p-1}(\tau)] -$$
$$-B\Gamma_1^{\vec{\varkappa}}[v_{p+1}(\tau) + v_{p-1}(\tau)] = 0,$$
$$[P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)]v_p(\tau) + Q(\vec{\varkappa})u_p(\tau) - A\Gamma_1^{\vec{\varkappa}}[v_{p+1}(\tau) + v_{p-1}(\tau)] -$$
$$-B\Gamma_1^{\vec{\varkappa}}[u_{p+1}(\tau) + u_{p-1}(\tau)] = 0; \tag{26b}$$

$l = n$ $(n = 1, 3, \ldots, L-4, L-2)$:

$$[P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)]u_n(\tau) + Q(\vec{\varkappa})v_n(\tau) - A\Gamma_1^{*\vec{\varkappa}}[u_{n+1}(\tau) + u_{n-1}(\tau)] -$$
$$-B\Gamma_1^{*\vec{\varkappa}}[v_{n+1}(\tau) + v_{n-1}(\tau)] = 0,$$
$$[P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)]v_n(\tau) + Q(\vec{\varkappa})u_n(\tau) - A\Gamma_1^{*\vec{\varkappa}}[v_{n+1}(\tau) + v_{n-1}(\tau)] -$$
$$-B\Gamma_1^{*\vec{\varkappa}}[u_{n+1}(\tau) + u_{n-1}(\tau)] = 0; \tag{26c}$$

$l = L-1$

$$[-p(\vec{\varkappa}) + P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)]u_{L-1}(\tau)Q + [-q(\vec{\varkappa}) + Q(\vec{\varkappa})]v_{L-1}(\tau) -$$
$$-A\Gamma_1^{\vec{\varkappa}}u_{L-2}(\tau) - B\Gamma_1^{\vec{\varkappa}}v_{L-2}(\tau) = 0,$$
$$[-p(\vec{\varkappa}) + P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)]v_{L-1}(\tau) + [-q(\vec{\varkappa}) + Q(\vec{\varkappa})]u_{L-1}(\tau) -$$
$$-A\Gamma_1^{\vec{\varkappa}}v_{L-2}(\tau) - B\Gamma_1^{\vec{\varkappa}}u_{L-2}(\tau) = 0. \tag{26d}$$

Above, the notation is:

$$A = 2S[J_1 - \tfrac{1}{2}\gamma_y^2 K], \tag{27}$$

$$B = -S\gamma_y^2 K. \tag{28}$$

At this stage, we have again put the Tyablikov-Bogolyubov equations in general form so as to ensure the fullest generality for our further considerations, without restricting ourselves to any particular structure.

Incidentally, the set of Eqs (26*a*, *b*, *c*, *d*) can be put in compact form resorting to matrix notation (see, Appendix A).

3. Energy dispersion relation

We solve the set of difference equations (26) by the method proposed by Jellitto [5] and generalized in Ref. [2] to the case now under consideration (*cf.* also Puszkarski [6]).

We introduce two fictitious layers, labelled by indices $l = -1$ and $l = L$. This enables us to write the sub-sets (26*a*) and (26*d*) in the same form as (26*b*) and (26*c*), yielding:

1) a set of equations of the "bulk body"

$$\begin{aligned}
&[P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)]u_p(\tau) + Q(\vec{\varkappa})v_p(\tau) - A\Gamma_1^{\vec{\varkappa}}[u_{p+1}(\tau) + u_{p-1}(\tau)] - \\
&\qquad - B\Gamma_1^{\vec{\varkappa}}[v_{p+1}(\tau) + v_{p-1}(\tau)] = 0, \\
&[P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)]v_p(\tau) + Q(\vec{\varkappa})u_p(\tau) - A\Gamma_1^{\vec{\varkappa}}[v_{p+1}(\tau) + v_{p-1}(\tau)] - \\
&\qquad - B\Gamma_1^{\vec{\varkappa}}[u_{p+1}(\tau) + u_{p-1}(\tau)] = 0,
\end{aligned}$$

$p = 0, 2, 4, \ldots, L-3, L-1;$

$$\begin{aligned}
&[P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)]u_n(\tau) + Q(\vec{\varkappa})v_n(\tau) - A\Gamma_1^{*\vec{\varkappa}}[u_{n+1}(\tau) + u_{n-1}(\tau)] - \\
&\qquad - B\Gamma_1^{*\vec{\varkappa}}[v_{n+1}(\tau) + v_{n-1}(\tau)] = 0, \\
&[P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)]v_n(\tau) + Q(\vec{\varkappa})u_n(\tau) - A\Gamma_1^{*\vec{\varkappa}}[v_{n+1}(\tau) + v_{n-1}(\tau)] - \\
&\qquad - B\Gamma_1^{*\vec{\varkappa}}[u_{n+1}(\tau) + u_{n-1}(\tau)] = 0,
\end{aligned} \tag{29}$$

$n = 1, 3, 5, \ldots, L-4, L-2;$

and, associated to it,

2) the set of boundary equations

$$\begin{aligned}
A\Gamma_1^{\vec{\varkappa}}u_{-1}(\tau) + B\Gamma_1^{\vec{\varkappa}}v_{-1}(\tau) &= p(\vec{\varkappa})u_0(\tau) + q(\vec{\varkappa})v_0(\tau), \\
A\Gamma_1^{\vec{\varkappa}}v_{-1}(\tau) + B\Gamma_1^{\vec{\varkappa}}u_{-1}(\tau) &= p(\vec{\varkappa})v_0(\tau) + q(\vec{\varkappa})u_0(\tau), \\
A\Gamma_1^{\vec{\varkappa}}u_L(\tau) + B\Gamma_1^{\vec{\varkappa}}v_L(\tau) &= p(\vec{\varkappa})u_{L-1}(\tau) + q(\vec{\varkappa})u_{L-1}(\tau), \\
A\Gamma_1^{\vec{\varkappa}}v_L(\tau) + B\Gamma_1^{\vec{\varkappa}}u_L(\tau) &= p(\vec{\varkappa})v_{L-1}(\tau) + q(\vec{\varkappa})u_{L-1}(\tau).
\end{aligned} \tag{30}$$

By associating the boundary equations (30) required to account for the two previously introduced fictitious layers, we have made the set of equations (29) fully equivalent to the set (26*a–d*). The quantity $\Gamma_1^{\vec{\varkappa}}$ is in general complex and thus can be written as:

$$\Gamma_1^{\vec{\varkappa}} = |\Gamma_1^{\vec{\varkappa}}| e^{i\varphi}, \quad (\varphi \text{ — real}). \tag{31}$$

We assume the functions $u_l(\tau)$ and $v_l(\tau)$ with even indices to be shifted in phase (Wojtczak [7]) by φ with respect to the functions with odd indices:

$$\begin{aligned} u_n(\tau) &= U_n(\tau), \qquad v_n(\tau) = V_n(\tau), \\ u_p(\tau) &= U_p(\tau) e^{i\varphi}, \quad v_p(\tau) = V_p(\tau) e^{i\varphi}. \end{aligned} \tag{32}$$

Introducing the notations:

$$A' = A|\Gamma_1^{\vec{\varkappa}}|, \quad B' = B|\Gamma_1^{\vec{\varkappa}}| \tag{33}$$

and on inserting (31) and (32) into (29), we obtain:

$$\begin{aligned} &[P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)] U_l(\tau) - A'[U_{l+1}(\tau) + U_{l-1}(\tau)] + Q(\vec{\varkappa}) V_l(\tau) - \\ &\quad - B'[V_{l+1}(\tau) + V_{l-1}(\tau)] = 0, \\ &[P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)] V_l(\tau) - A'[V_{l+1}(\tau) + V_{l-1}(\tau)] + Q(\vec{\varkappa}) U_l(\tau) - \\ &\quad - B'[U_{l+1}(\tau) + U_{l-1}(\tau)] = 0. \end{aligned} \tag{34}$$

We search for particular solutions of the set of Eqs (34) in the form (2):

$$U_l(\tau) = \alpha e^{il\tau}, \quad V_l(\tau) = \beta e^{il\tau}. \tag{35}$$

This set of equations is seen to consist of L sub-sets, of two equations each. By inserting the functions (35) into the various, sub-sets, we eliminate from them the index l and the set of $2L$ equations goes over into a set of but two equations in the unknown amplitudes α and β:

$$\begin{aligned} &\alpha[2A' \cos\tau - P(\vec{\varkappa}) + E(\vec{\varkappa}, \tau)] + \beta[2B' \cos\tau - Q(\vec{\varkappa})] = 0, \\ &\alpha[2B' \cos\tau - Q(\vec{\varkappa})] + \beta[2A' \cos\tau - P(\vec{\varkappa}) - E(\vec{\varkappa}, \tau)] = 0. \end{aligned} \tag{36}$$

The condition for non-trivial solutions of the set (36) is that the determinant of the coefficients at the unknowns α and β shall vanish, leading to the following expression for the energy:

$$E(\vec{\varkappa}, \tau) = \{[P(\vec{\varkappa}) - 2A' \cos\tau]^2 - [Q(\vec{\varkappa}) - 2B' \cos\tau]^2\}^{\frac{1}{2}} \tag{37}$$

or explicitly for the case of the *hcp* crystal considered in subsection 2:

$$E(\vec{\varkappa}, \tau) = \{\varepsilon[\varepsilon + 2SK\gamma_y^2(\Gamma_0^{\vec{\varkappa}} + 2|\Gamma_1^{\vec{\varkappa}}| \cos\tau)]\}^{\frac{1}{2}}, \tag{38}$$

where

$$\varepsilon = g\mu_B(H_y\gamma_y + H_z\gamma_z) + 2Sz_0J_0\left[1 - \frac{K\gamma_z^2}{I_0} - \frac{\Gamma_0^{\vec{\varkappa}}}{z_0}\right] - 4Sz_1\left[1 - \frac{K\gamma_z^2}{I_0} - \frac{|\Gamma_1^{\vec{\varkappa}}|}{z_1}\cos\tau\right].$$

In the particular case of $\gamma_z = 1$ ($\gamma_y = 0$) *i.e.* for a magnetic field $\boldsymbol{H}$ oriented perpendicularly to the surface, Eq. (38) goes over into a formula derived in Ref. [3].

4. Boundary equations

The set of boundary equations (30), on inserting therein the functions (32) and with the notations (33), takes the form:

$$\begin{aligned} A'U_{-1}(\tau)+B'V_{-1}(\tau) &= p(\vec{\varkappa})U_0(\tau)+q(\vec{\varkappa})V_0(\tau),\\ A'V_{-1}(\tau)+B'U_{-1}(\tau) &= p(\vec{\varkappa})V_0(\tau)+q(\vec{\varkappa})U_0(\tau),\\ A'U_L(\tau)+B'V_L(\tau) &= p(\vec{\varkappa})U_{L-1}(\tau)+q(\varkappa)V_{L-1}(\tau),\\ A'V_L(\tau)+B'U_L(\tau) &= p(\vec{\varkappa})V_{L-1}(\tau)+q(\vec{\varkappa})U_{L-1}(\tau). \end{aligned} \tag{39}$$

It should be noted that, once the energy is given by Eq. (37), the two equations of each of the L sub-sets (34) are mutually equivalent. In other words, the one can be derived from the other by way of simple transformations on resorting to the relation (37). Consequently, once the energy of the elementary excitations has been determined, each sub-set can be replaced by a single equation (rejecting the other). Since the preceding holds for all of the sub-sets (34), it is also true for the first and last (*i.e.* for the ones with $l=0$ and $l=L-1$). Now, it should be kept in mind that these two particular sets were introduced by adjoining the boundary equations (30) to the set of Eqs (29). It thus results from the preceding that only two of the four equations (39) have to be taken into consideration (those deriving *either* from the two equations with $-E$ in the sets (26a) and (26d), *i.e.* the first and third of the set (39), *or* the second and fourth of (39), which derive from those with $+E$ in (26a) and (26d)), whereas the other two have to be rejected. Thus, either the equations

$$\begin{aligned} A'U_{-1}(\tau)+B'V_{-1}(\tau) &= p(\vec{\varkappa})U_0(\tau)+q(\vec{\varkappa})V_0(\tau),\\ A'U_L(\tau)+B'V_L(\tau) &= p(\vec{\varkappa})U_{L-1}(\tau)+q(\vec{\varkappa})V_{L-1}(\tau), \end{aligned} \tag{40a}$$

or the equations

$$\begin{aligned} A'V_{-1}(\tau)-B'U_{-1}(\tau) &= p(\vec{\varkappa})V_0(\tau)+q(\vec{\varkappa})U_0(\tau),\\ A'V_L(\tau)+B'U_L(\tau) &= p(\vec{\varkappa})V_{L-1}(\tau)+q(\vec{\varkappa})U_{L-1}(\tau) \end{aligned} \tag{40}$$

should be taken.

Let us now revert to the set of equations of the "bulk body". We assume the general solutions as superpositions of the following particular solutions:

$$\begin{aligned} U_l(\tau) &= \alpha e^{il\tau},\quad V_l(\tau)=\beta e^{il\tau}\\ U_l(\tau) &= \alpha e^{-il\tau},\quad V_l(\tau)=\beta^{-il\tau} \end{aligned} \tag{41}$$

The superposition constants can be determined from the set of boundary equations. Since, as already shown, only two boundary equations need be considered, we introduce only two superposition constants C_1 and C_2:

$$\begin{aligned} U_l(\tau) &= \alpha(C_1e^{il\tau}+C_2e^{-jl\tau}),\\ V_l(\tau) &= \beta(C_1e^{il\tau}+C_2e^{-il\tau}). \end{aligned} \tag{42}$$

On inserting the functions (42) into the set of boundary equations (40a) or (40b) and assuming $C_1 = C_2^*$, we get:

$$\frac{C_1}{C_2} = \pm e^{-i\tau(L-1)} \tag{43}$$

to which there correspond the following two pairs of superposition constants:

$$C_1 = Ce^{-i\frac{L-1}{2}\tau},\ C_2 = Ce^{i\frac{L-1}{1}\tau},$$
$$C_1 = iCe^{-i\frac{L-1}{2}\tau},\ C_2 = -iCe^{i\frac{L-1}{2}\tau}, \tag{44}$$

(C is real).

To the first pair correspond the symmetric solutions:

$$U_l^+(\tau) = \alpha C_+ \cos\left(\frac{L-1}{2} - l\right)\tau,$$
$$V_l^+(\tau) = \beta C_+ \cos\left(\frac{L-1}{2} - l\right)\tau \tag{45a}$$

and to the other — the antisymmetric solutions:

$$U_l^-(\tau) = \alpha C_- \sin\left(\frac{L-1}{2} - l\right)\tau,$$
$$V_l^-(\tau) = \beta C_- \sin\left(\frac{L-1}{2} - l\right)\tau. \tag{45b}$$

The constants C_+ and C_- are obtained from the normalization condition:

$$\sum_{l,j} [|u_{l,j}(\vec{\varkappa}, \tau)|^2 - v_{l,j}(\vec{\varkappa}, \tau)|^2 = 1 \tag{46}$$

yielding:

$$C_\pm = \sqrt{2}\left(L \pm \frac{\sin L\tau}{\sin\tau}\right)^{-1/2}, \tag{47a}$$

$$|\alpha|^2 - |\beta|^2 = 1. \tag{47b}$$

We derive the characteristic equations defining the quantization of τ by inserting the functions (45a) and (45b) into the boundary equations (40a) and (40b):

$$\frac{p(\vec{\varkappa}) + \frac{\beta}{\alpha} q(\vec{\varkappa})}{A' + \frac{\beta}{\alpha} B'} = \frac{\cos\frac{L+1}{2}\tau}{\cos\frac{L-1}{2}\tau} \equiv F(\tau), \qquad \frac{p(\vec{\varkappa}) + \frac{\beta}{\alpha} q(\vec{\varkappa})}{A' + \frac{\alpha}{\beta} B'} = \frac{\sin\frac{L+1}{2}\tau}{\sin\frac{L-1}{2}\tau} \equiv G(\tau), \tag{48a}$$

$$\frac{p(\vec{\varkappa}) + \frac{\alpha}{\beta} q(\vec{\varkappa})}{A' + \frac{\alpha}{\beta} B'} = F(\tau), \qquad \frac{p(\vec{\varkappa}) + \frac{\alpha}{\beta} q(\vec{\varkappa})}{A' + \frac{\alpha}{\beta} B'} = G(\tau). \tag{48b}$$

We have now to decide which of these two sets of equations has to be rejected. On closer inspection we note that they lead respectively to the following restrictions on the amplitudes α and β:

from Eqs (48a): $$\alpha \neq 0, \tag{49a}$$

from Eqs (48b): $$\beta \neq 0. \tag{49b}$$

We note immediately that the normalization condition (47b) imposes on the amplitude α the restriction (49a), whereas the restriction (49b) is obtained by normalizing the functions $u_{l,j}(\vec{\varkappa}, \tau)$ and $v_{l,j}(\vec{\varkappa}, \tau)$ to minus unity, *i.e.* by postulating

$$|\alpha|^2 - |\beta|^2 = -1. \tag{50}$$

Hence, the characteristic equations (48a) can be co-ordinated to functions which are normalized to $+1$ and the equations (48b) to functions normalized to -1. It is well know that, in the Tyablikov-Bogolyubov diagonalization method, solutions of the set of Eqs (6) which are normalized to -1 are physically meaningless as corresponding to negative energies ($E' = -E$, $E > 0$) [5]. Consequently, only Eqs (48a) correspond to physical solutions and are thus the only equations which need to be taken into consideration (a point of interest here will be raised in Appendix B).

5. *Approximate form of the boundary equations*

Determinig the ratio of amplitudes $\frac{\beta}{\alpha}$ from the second equation of the set (36), we obtain:

$$\frac{\beta}{\alpha} = \frac{2B' \cos \tau - Q(\vec{\varkappa})}{E(\vec{\varkappa}, \tau) + P(\vec{\varkappa}) - 2A' \cos \tau}. \tag{51}$$

By resorting to the relations (22), (23), (27), (28), (33) and (37), we can evaluate the order of magnitude of $\frac{\beta}{\alpha}$. It results that the numerator of (51) is of the order of the anisotropy coefficient K whereas the denominator is of that of the exchange integral $J_1 (\approx J_0)$. Since $\left|\frac{K}{J}\right|$ is generally of order 10^{-3}, one can assume in good approximation that

$$\left|\frac{\beta}{\alpha}\right| \ll 1; \tag{52}$$

since moreover (for the same reason) $q(\vec{\varkappa})$ is much smaller than $p(\vec{\varkappa})$ and similarly $B' \ll A'$, the following approximation is justified:

$$\frac{p(\vec{\varkappa}) + \frac{\beta}{\alpha} q(\vec{\varkappa})}{A' + \frac{\beta}{\alpha} B'} \approx \frac{p(\vec{\varkappa})}{A'} \equiv A(\vec{\varkappa})$$

$$= \frac{z_1}{|I_1^{\vec{\varkappa}}|} \left\{ 1 + \frac{z_1 K + I_0^{\vec{\varkappa}}(K - K') - [3 z_1 K + I_0^{\vec{\varkappa}}(K - K') + 2 z_0 (K - K')] \gamma_z^2}{2 z_1 [J_1 - \tfrac{1}{2}(1 - \gamma_z^2) K]} \right\}. \tag{53}$$

The characteristic equations now takes the form:

$$A(\vec{\varkappa}) \approx F(\tau),\ A(\vec{\varkappa}) \approx G(\tau). \tag{54}$$

Since $A(\vec{\varkappa})$ does not depend on τ, these equations are much simpler than Eqs (48*a*) and are well adapted to discussion (*e.g.* graphically, *cf.* Puszkarski [6]). In the case of perpendicular configuration of the field $\boldsymbol{H}$ Eqs (54) hold strictly, since now $\frac{\beta}{\alpha} = 0$ ($\gamma_y = 0$). Precisely such characteristic equations were derived in Ref. [3] by Rutherford's determinant method. This shows that our choice of two out of the four boundary equations was the correct one.

APPENDIX A

The set of difference equations (26a, b, c, d) can be written in matrix form as follows:

$$\left[\begin{array}{cc|cc}
-p+P-E,\ -A'' & & -q+Q,\ -B'' & \\
-A^{*\prime\prime},\ P-E,\ -A^{*\prime\prime} & & -{}^{*}B'',\ Q,\ -B^{*\prime\prime} & \\
-A'',\ P-E,\ -A'' & & -B'',\ Q,\ -B'' & \\
\cdots & & \cdots & \\
 & -A'',\ -p+P-E & & -B'',\ -q+Q \\
\hline
-q+Q,\ -B'' & & -p+P+E,\ -A'' & \\
-B^{*\prime\prime},\ Q,\ -B^{*\prime\prime} & & -A^{*\prime\prime},\ P+E,\ -A^{*\prime\prime} & \\
-B'',\ Q,\ -B'' & & -A'',\ P+E,\ -A'' & \\
\cdots & & \cdots & \\
 & -B'',\ -q+Q & & A'',\ -p+P+E
\end{array}\right] \times \left[\begin{array}{c} u_0 \\ u_1 \\ u_2 \\ \cdot\cdot \\ u_{L-1} \\ \hline v_0 \\ v_1 \\ v_2 \\ \cdot\cdot \\ v_{L-1} \end{array}\right] = \left[\begin{array}{c} 0 \\ 0 \\ 0 \\ \cdot\cdot \\ 0 \\ \hline 0 \\ 0 \\ 0 \\ \cdot\cdot \\ 0 \end{array}\right]$$

where

$$A'' = A\Gamma_{\vec{1}}^{\vec{\varkappa}},\ B'' = B\Gamma_{\vec{1}}^{\vec{\varkappa}}.$$

Obviously, we have here a set of $2L$ equations in $2L$ unknowns, notwithstanding the fact that the problem under consideration is L-dimensional. The situation is typical for the Tyablikov-Bogolyubov diagonalization method which involves, beside physically meaningful solutions, non-physical solutions corresponding to negative energies. The latter are eliminated by restriction to solutions corresponding to positive energies with the normalization condition to $+1$ (47*b*). It may be of interest to note in this context that the boundary equations (40*a*), which we have shown to correspond to physical solutions, are "obtained" from the upper half of the matrix.

APPENDIX B

Incidentally, τ quantizes in the same way for the physical and unphysical solutions: from the set of Eqs (36) one obtains (we now write the dependence on the parameter E explicitly):

$$\frac{\alpha(E)}{\beta(E)} = -\frac{2B'\cos\tau - Q(\vec{\varkappa})}{2A'\cos\tau - P(\vec{\varkappa}) + E(\vec{\varkappa},\tau)} = -\frac{2A'\cos\tau - P(\vec{\varkappa}) - E(\vec{\varkappa},\tau)}{2B'\cos\tau - Q(\vec{\varkappa})}$$

or

$$\frac{\beta(E)}{\alpha(E)} = -\frac{2A'\cos\tau - P(\vec{\varkappa}) + E(\vec{\varkappa},\tau)}{2B'\cos\tau - Q(\vec{\varkappa})} = -\frac{2B'\cos\tau - Q(\vec{\varkappa})}{2A'\cos\tau - P(\vec{\varkappa}) - E(\vec{\varkappa},\tau)} = \frac{\alpha(-E)}{\beta(-E)}.$$

As a consequence, the set of boundary equations (48b) goes over into the set (48a).

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