BOUNDARY INHOMOGENEITY MODEL OF FERROMAGNETIC THIN FILMS

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The diagonalization problem for the Hamiltonian of a thin ferromagnetic film is solved strictly within the framework of the Boundary Inhomogeneity Model. Complete generality is ensured by assuming the spin quantization axes in each layer as different. Parameters having the physical meaning of boundary spin pinning parameters are introduced, and their role in the boundary conditions is discussed.

1. Introduction

Haisenberg's model, when applied to a description of the ferromagnetic state of thin films, has proved equally fruitful as in its application to bulk materials. However, the rather simple mathematical formalism involved by it requires some amount of modification in the case of films, since the theory has now to take into account correctly the existing boundary conditions, namely those resulting from the boundedness of the dimensions of the body under consideration. In fact, since 1912, the theory of bulk bodies resorted almost exclusively to the so-called "cyclicity boundary conditions" (known as the Born — Kármán conditions) representing an idealization of the real conditions, which is justified well enough when the dimensions of body are very large (Ledermann [1], Peierls [2]). Obviously, cyclic boundary conditions could hardly be expected to lead to correct results in the theory of thin films. Thus, the earliest attempts to calculate the spontaneous magnetization of a monocrystalline film (Klein and Smith [3], Glass and Klein [4]) on the assumption of periodical boundary conditions failed to yield results in agreement with experiment, notwithstanding the fact that the discontinity of the momentum spectrum (of quasi-particles) due to the finiteness and thinness of the film had been taken into account.

Consequently, later theories could no longer ignore the true boundary conditions at the film surface *i. e.* the fact that the atoms at the surface have a neighbourhood of lower sym-

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metry (*i. e.* less neighbours) than the internal atoms. The first to take this into consideration were Döring [5] and Ferchmim [6]. Numerous papers have since appeared in which the true boundary conditions in thin films are given much attention and their influence on the physical properties of such films and the processes occuring in them is studied closely.

Döring's method (of calculating spin-wave states and their energy spectrum in thin films in Bloch's approach) underwent considerable development in the work of Abbel [7] and Jelitto [8, 9]. To Jelitto is due a highly general formulation of spin-wave theory for thin ferromagnetic films applicable to bodies with arbitrary Bravais lattice and arbitrarily oriented surface. His work is notable for a very convenient and effective method of solving the set of difference equations to which the eigenproblem of the thin film always leads, consisting in the introduction of fictitious lattice planes not physically present in the film. Our paper is aimed at a further generalisation of Jelitto's theory. In order to explain our intention, we have to make some digressions.

The surfaces constituting the boundary of a finite body constitute a specific defect of its structure, which can conveniently be referred to as "surface defect". In essence, this kind of defect resides in the fact that an atom at the surface interacts with fewer neighbours than an internal atom. Consequently, the situation, with regard to energy, of a surface atom differs from that of an internal atom. We shall be referring to such surface defect as "natural defect", since it results naturally from the property of boundedness.

In the theory of spin-waves in thin films, however, the use of boundary conditions involved by natural defect alone proved insufficient, primarily because a number of experimental results remained unexplained (*cf.* Davis [10]). In order to adjust the theory, it was moreover necessary to take into consideration the existence of very thin strata of chemically foreign compounds affecting the energy situation of the surface spins (and the deeper lying boundary spins, too). This is accounted for by considering a supplementary energy called "surface anisotropy energy". Thus, by applying the concept of surface anisotropy energy in the method of spin-waves, Davis [10] succeeded in explaining certain discrepancies between the experimental results of various authors.

Jelitto's theory suffers from the essential limitation of using boundary conditions restricted to natural defect. When proceeding to its generalisation, our first step will be to introduce surface anisotropy or, more widely, *boundary anisotropy*. Another drawback of Jelitto's theory consists in his assumption of a collinear ferromagnetic ground state of the thin film. In other words he omits to consider the influence of surface defect on the configuration of the spins, which obviously is an arbitrary simplification. In the present approach, the spin quantisation axes will be considered to depend on the distance of a given lattice layer from the surface. Obviously, such a modification of the theory extends to its very fundamentals. As we shall show, it also affects essentially its mathematical formalism. Thirdly and lastly, the present generalisation will aim at rendering the theory applicable to non-translational structures also. In this publication, however, we shall not deal with this matter to the end; from a certain point onwards, our considerations will be restricted to lattices of the Bravais type.

Throughout, we shall be applying the Holstein-Primakoff spin-wave formalism.

2. The assumptions

Let us consider a non-conducting specimen of the shape of a thin film, of uniform crystallographical structure, extending unboundedly in the directions parallel to the surface (*i. e.* fulfilling in these directions the periodic boundary conditions of Born and Kármán). On these assumptions, the atoms lying in one and the same lattice plane parallel to the film surface will be in physically identical conditions and will thus be mutually equivalent,

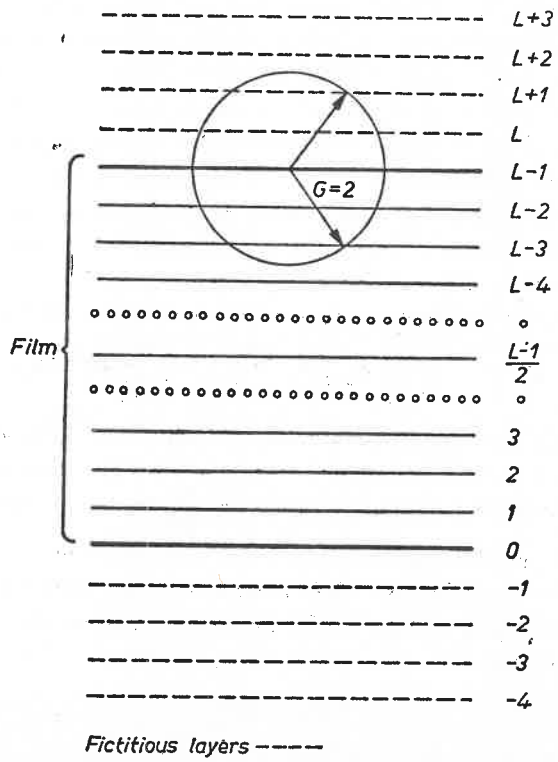

Fig. 1. Layer model of a thin ferromagnetic film

constituting a magnetic sub-lattice (Valenta [11]). Hence, the thin film can be divided into L equidistant lattice planes parallel to the surface. We shall henceforth be referring to a lattice plane *parallel* to the surface as a "layer", and shall deal with each layer as a distinct magnetic sub-lattice. We shall label these layers (beginning by the lowest layer) $l = 0, 1, 2, \ldots, L\text{-}1$ (*cf.* Fig. 1). Layers labelled $0 \leqslant l < \frac{L-1}{2}$ will be termed lower layers) and ones labelled $\frac{L-1}{2} < l \leqslant L-1$ — upper layers; the layer $l = \frac{L-1}{2}$ will be referred to as the middle layer (it exist only if L is odd). (It is sometimes of advantage, with regard to symmetry of the formulas, to label the lower and upper layers respectively as l and $L-1-l$, but this requires

imposing the restriction $0 \leqslant l \leqslant \frac{L-1}{2}$.) The position of a site will be denoted by the vector $\boldsymbol{m} = [l, \boldsymbol{j}]$, where $\boldsymbol{j} = [j_x, j_y]$ is a two-dimensional vector defining the position of the site in its layer. It is our assumption that each of the lattice layers l is a Bravais lattice and that they are all identical; for the time being, however, we refrain from assuming the set of these layers jointly as a Bravais lattice.

We lay the reference axes as follows: the axes x and y lie in the plane parallel to the surface of the film, with the z-axis perpendicular. Also, we introduce in each site of the lattice a local reference system x', y', z' with the positive direction of the z'-axis defined by a unit vector γ_{lj} which is the versor of quantisation of the spin situated at this site. We moreover assume that, in each site, the spin is acted on by a local effective magnetic field $\boldsymbol{H}_{lj}^{\mathrm{eff}} \equiv \boldsymbol{H}_{l}^{\mathrm{eff}}$ (the sum of the external, demagnetizing and anisotropy fields), which depends on the number l labelling the layer only. With this assumption each of the layers l continues to be a sub-lattice consisting of mutually equivalent spins, and we can write $\vec{\gamma}_{lj} \equiv \vec{\gamma}_{l}$. Thus, the classical spin can be written in the form (we restrict ourselves to the case when $S_{lj} \equiv S$, with S in $\hbar$ units): $\boldsymbol{S}_{lj} = S\vec{\gamma}_{l}$.

The Hamiltonian of the system of spins in Heisenberg's model is assumed in the form:

$$\hat{\mathscr{H}} = -2 \sum_{(lj,l'j')} J_{lj,l'j'} \hat{\mathbf{S}}_{lj} \cdot \hat{\mathbf{S}}_{l'j'} - g\mu_B \sum_{lj} \boldsymbol{H}_{l}^{\mathrm{eff}} \cdot \hat{\mathbf{S}}_{lj}, \tag{1}$$

where $J_{lj,l'j'}$, g and μ_B have the meaning, respectively, of the isotropic exchange integral, the gyromagnetic factor, and Bohr's magneton, and where $\boldsymbol{j}$ is taken to belong to the layer l ($\boldsymbol{j} \in l$) and $\boldsymbol{j}'$ to the layer l' ($\boldsymbol{j}' \in l'$); the symbol $\sum_{(\cdot)}$ denotes a sum containing each pair of spins once only. We shall be resticting our considerations to interactions between nearest neighbours; for more generality, we shall assume that the exchange interaction integral between two neighbouring spins $\mathbf{S}_{lj}$ and $\mathbf{S}_{l'j'}$ depends on the numbers labelling the layers to which the spins belong:

$$J_{lj,l'j'} \equiv J_{ll'}. \tag{2}$$

The Hamiltonian (1) can now be re-written in the form:

$$\hat{\mathscr{H}} = -\sum_{lj \neq l'j'} J_{ll'} \hat{\mathbf{S}}_{lj} \cdot \hat{\mathbf{S}}_{l'j'} - g\mu_B \sum_{lj} \boldsymbol{H}_{l}^{\mathrm{eff}} \cdot \hat{\mathbf{S}}_{lj}. \tag{3}$$

(Summation now extends over closest neighbouring spins.)

Nearest neighbours of a site of layer l can lie in the same layer or in several other layers. The question of how numerous these layers can be depends on the orientation of the surface of the thin film with respect to the crystallographical axes (a problem already discussed by Jelitto [9] for Bravais lattices). Henceforth, we shall denote summation over nearest neighbours of a given site by $\sum'$, whereas $\sum_{l'}'$ will denote summation over the neighbouring layers of layer l including this latter layer (*i.e.* admitting of $l' = l$). We denote the number of nearest neighbours (of a site of layer l) situated in a layer l' as $z_{ll'}$ (since all the layers are identical, we obviously have $z_{ll'} = z_{l'l}$). We furthermore denote the total number of spins contained in the plane XOY by N.

For the sake of convenience, we shall moreover resort to a terminology which we now proceed to define. A spin which, owing to its position near the surface, has (in the model of interaction with nearest neighbours, as assumed here) fewer *active neighbours* (*i.e.* ones with which it interacts) than a spin lying in the interior of the film will be referred to as a *boundary spin*. Obviously, at certain orientations of the surface, the spins which "feel" a deficit of neighbours will all lie on the surface *(surface spins)*, whereas at other orientations such spins will exist within the bulk of the body, in several consecutive lattice planes parallel to the surface. We shall refer to lattice planes of this kind as *boundary layers*. From Jelitto's work [8, 9], it is in some cases convenient to introduce spins which in reality are absent owing to the boundedness in dimensions of the body. Such spins will be referred to as fictitious, and layers consisting of such spins as *fictitious layers*. Finally, we shall term spins lying in the bulk of the body and subject to no deficit of their active neighbourhood *internal spins*, and the respective planes *internal layers*. The number of fictitious layers required for our considerations will always be equal to that of the boundary layers. It should be stated clearly, that, here, the notions "surface layer" and "boundary layer" cease to be equivalent.

We shall now assume that the nearest neighbours of a given site of the layer l lie in $2G+1$ layers, which we shall label as follows: $l' = l+g$, $g = 0, \pm 1, \pm 2, \ldots \pm G$. Thus, G defines the number of layers intersected by the radius of the first sphere (*cf.* Fig. 1). Labelling of the layers is, consequently, as follows:

$l = -G, -G+1, \ldots, -1$	— lower fictitious layers,
$l = 0, 1, \ldots, G-1$	— lower boundary layers,
$l = G, G+1, \ldots, L-G-1$	— internal layers,
$l = L-G, L-G+1, +, L-1$	— upper boundary layers,
$l = L, L+1, \ldots, L+G-1$	— upper fictitious layers.

We now introduce the following convention concerning the sum $\sum_{l'}'$:

$\sum_{g}^{\pm G}$ — summation over the neighbouring layers of an arbitrary internal layer,
$\sum_{g}^{l}$ — summation over the neighbouring layers of layer l,
$\sum_{g}^{f(l)}$ — summation over fictitious neighbouring layers of layer l,

with g running from -1 and from $+1$ (if the sum is to include $g = 0$ as well, this will be indicated explicitely). Clearly, the following identities hold $\left(\text{provided } 0 \leqslant l \leqslant \frac{L-1}{2}\right)$:

1) $\sum_{g}^{l} + \sum_{g}^{f(l)} \equiv \sum_{g}^{\pm G}$;

2) $\sum_{g}^{f(l)} \equiv \sum_{g=-(l+1)}^{-G}$, $\quad \sum_{g}^{f(L-1-l)} \equiv \sum_{g=l+1}^{+G}$;

3) $\sum_{g}^{l} \equiv \sum_{g=1}^{+G} + \sum_{g=-1}^{-l}$, $\quad \sum_{g}^{L-1-l} \equiv \sum_{g=-1}^{-G} + \sum_{g=1}^{l}$.

Let us still draw attention to the nature of the model stated in the title of this paper. Valenta's model, where a physical "individuality" is attributed to each layer, can well be said to represent a Volume Inhomogeneity (VI) Model. Its extreme opposite is the Surface Inhomogeneity (SI) Model, which distinguishes surface layers and considers all the other layers as mutually equivalent. The Boundary Inhomogeneity Model is in fact intermediate between the VI and SI models, in that here boundary layers are considered as "individual" sub-lattices whereas all internal layers are considered as mutually equivalent. Hence, the number of sub-lattices is the largest (amounting to L) in the VI Model, smaller (amounting to $2G+1$) in the BI Model, and smallest in the SI Model (where it amounts to $2+1$).

3. Transformation of spin operators to second quantization operators

We now proceed to find the eigen-states of the Hamiltonian. As a first step in the series of transformations which will be required, we perform a canonical transformation of the spin operators from the crystallographical axes x, y, z to local axes x', y', z' thus $\hat{\mathbf{S}}_{lj} \rightarrow \hat{\mathbf{S}}'_{lj}$. This transformation is of the form (Tyablikov [12]):

$$\hat{\mathbf{S}}_{lj} = \vec{\gamma}_{lj}\hat{S}^{z'}_{lj} + \frac{1}{\sqrt{2}}(\boldsymbol{A}_{lj}\hat{S}'^{+}_{lj} + \boldsymbol{A}^{*}_{lj}\hat{S}'^{-}_{lj}), \tag{4}$$

where $\vec{\gamma}_{lj}$ is the already defined local versor of the quantization axis (the z'-axis), and $\boldsymbol{A}_{lj}$ is a vector defined as follows (on the simplifying assumption that the y'-axis is taken as lying in the xy-plane):

$$\begin{aligned} A^{x}_{lj} &= -\frac{1}{\sqrt{2}}[(\gamma^{x}_{lj})^2+(\gamma^{y}_{lj})^2]^{-1/2}(\gamma^{x}_{lj}\gamma^{z}_{lj}+i\gamma^{y}_{lj}), \\ A^{y}_{lj} &= -\frac{1}{\sqrt{2}}[(\gamma^{x}_{lj})^2+(\gamma^{y}_{lj})^2]^{-1/2}(\gamma^{y}_{lj}\gamma^{z}_{lj}-i\gamma^{x}_{lj}), \\ A^{z}_{lj} &= \frac{1}{\sqrt{2}}[(\gamma^{x}_{lj})^2+(\gamma^{y}_{lj})^2]^{1/2}. \end{aligned} \tag{5}$$

The vectors $\vec{\gamma}_{lj}$ and $\boldsymbol{A}_{lj}$ satisfy the following relations:

$$\vec{\gamma}_{lj} = \vec{\gamma}^{*}_{lj}, \quad (\vec{\gamma}_{lj}, \vec{\gamma}_{lj}) = 1, \ (\boldsymbol{A}^{*}_{lj}, \boldsymbol{A}_{lj}) = 1, \tag{6a}$$

$$(\boldsymbol{A}_{lj}, \vec{\gamma}_{lj}) = 0, \quad (\boldsymbol{A}^{*}_{lj}, \vec{\gamma}_{lj}) = 0, \ (\boldsymbol{A}_{lj}, \boldsymbol{A}_{lj}) = 0, \tag{6b}$$

$$\vec{\gamma}_{lj} \times \boldsymbol{A}^{*}_{lj} = i\boldsymbol{A}_{lj}, \quad \boldsymbol{A}_{lj} \times \boldsymbol{A}^{*}_{lj} = i\vec{\gamma}_{lj}. \tag{6c}$$

We now go over from spin operators to Bose operators by way of the Holstein-Primakoff transformation:

$$\begin{aligned} \hat{S}'^{+}_{lj} &= \sqrt{2S}\,\hat{f}_{lj}\hat{a}_{lj}, \quad \hat{S}'^{-}_{lj} = \sqrt{2S}\,\hat{a}^{+}_{lj}\hat{f}_{lj}, \\ \hat{S}^{z'}_{lj} &= S - \hat{a}^{+}_{lj}\hat{a}_{lj}, \\ \hat{f}_{lj} &= \left(1 - \frac{\hat{a}^{+}_{lj}\hat{a}_{lj}}{2S}\right)^{1/2}. \end{aligned} \tag{7}$$

On inserting (7) into (4) we obtain:

$$\hat{\mathbf{S}}_{lj} = S\vec{\gamma}_{lj}\left(1-\frac{\hat{a}^{+}_{lj}\hat{a}_{lj}}{S}\right)+\sqrt{S}\,(\boldsymbol{A}_{lj}\hat{f}_{lj}\hat{a}_{lj}+\boldsymbol{A}^{*}_{lj}\hat{a}_{lj}\hat{f}_{lj}). \tag{8}$$

From this point onward our calculations will be performed in the approximation of quasi-saturation (*i.e.* restricting ourselves to low temperatures); this permits to assume $\hat{f}_{lj}=1$ and, keeping in mind the assumption $\vec{\gamma}_{lj}=\vec{\gamma}_{l}$ (which moreover involves $\boldsymbol{A}_{lj}\equiv\boldsymbol{A}_{l}$), we obtain the transformation which we shall be using throughout, in the form:

$$\hat{\mathbf{S}}_{lj} = S\vec{\gamma}_{l}\left(1-\frac{\hat{a}^{+}_{lj}\hat{a}_{lj}}{S}\right)+\sqrt{S}\,(\boldsymbol{A}_{l}a_{lj}+\boldsymbol{A}^{*}_{l}a^{+}_{lj}). \tag{9}$$

The creation and annihilation operators $\hat{a}^{+}_{lj}$ and $\hat{a}_{lj}$ satisfy boson commutation rules:

$$[\hat{a}_{lj},\,\hat{a}^{+}_{l'j'}]=\delta_{ll'}\delta_{jj'},\qquad [\hat{a}_{lj},\,\hat{a}_{l'j'}]=0. \tag{10}$$

Inserting the transformation (9) into the Hamiltonian (1), we obtain (to within terms of order 2):

$$\hat{\mathscr{H}} = E_0(\vec{\gamma}_l)+\sum_{lj,l'j'}\left(P^{jj'}_{ll'}\hat{a}^{+}_{lj}\hat{a}_{l'j'}+\frac{1}{2}Q^{jj'}_{ll'}\hat{a}_{lj}\hat{a}_{l'j'}+\right.$$

$$\left.+\frac{1}{2}Q^{*jj'}_{ll'}\hat{a}^{+}_{lj}\hat{a}^{+}_{l'j'}\right)+\sum_{lj}(R_l\hat{a}_{lj}+R^{*}_{l}\hat{a}^{+}_{lj}), \tag{11}$$

where we have introduced the notation:

$$E_0(\vec{\gamma}_l) = -NS^2\sum_{ll'}z_{ll'}J_{ll'}(\vec{\gamma}_l,\vec{\gamma}_{l'})-g\mu_B NS\sum_{l}(\boldsymbol{H}^{\mathrm{eff}}_{l},\vec{\gamma}_l), \tag{12a}$$

$$P^{jj'}_{ll'} = \begin{cases} 2S\sum\limits_{n}{}' z_{ln}J_{ln}(\vec{\gamma}_l,\vec{\gamma}_n)+g\mu_B(\boldsymbol{H}^{\mathrm{eff}}_{l},\vec{\gamma}_l) & \text{for} \quad lj=l'j', \\ -2SJ_{ll'}(\boldsymbol{A}^{*}_{l},\boldsymbol{A}_{l'}) & \text{for} \quad lj\neq l'j', \end{cases} \tag{12b}$$

$$Q^{jj'}_{ll'} = \begin{cases} 0 & \text{for} \quad lj=l'j', \\ -2SJ_{ll'}(\boldsymbol{A}_{l},\boldsymbol{A}_{l'}) & \text{for} \quad lj\neq l'j', \end{cases} \tag{12c}$$

$$R_l = -2S\sqrt{S}\sum_{n}{}' z_{ln}J_{ln}(\boldsymbol{A}_l,\vec{\gamma}_n)-g\mu_B\sqrt{S}(\boldsymbol{H}^{\mathrm{eff}}_{l},\boldsymbol{A}_l). \tag{12d}$$

With regard to the fact that $J_{ll'}=J_{l'l}$, we find immediately that the coefficients $P^{jj'}_{ll'}$ and $Q^{jj'}_{ll'}$ fulfil the relations:

$$P^{j'j}_{l'l}=\overset{*}{P}{}^{jj'}_{ll'},\qquad Q^{j'j}_{l'l}=Q^{jj'}_{ll'}, \tag{13}$$

which ensure the hermiticity of the Hamiltonian (11).

E_0 is a classical expression, to be had from the initial Hamiltonian (3) on replacing the spin operators by their classical vectors. It is found to be a function of the vectors $\vec{\gamma}_l$. This can be written symbolically as $E_0=E_0(\vec{\gamma}_l)$.

4. The ground state

The ground state of the thin film (whose energy we denote by E_0) will be determined by the semi-classical method (see, Tyablikov [12]). To this aim, $E_0(\vec{\gamma}_l)$ has to be minimalized with respect to the variables $\vec{\gamma}_l$ adjoining the L supplementary conditions:

$$E_0 = \min E_0(\vec{\gamma}_l), \quad (\vec{\gamma}_l, \vec{\gamma}_l) = 1. \tag{14}$$

The usual variational procedure leads to the following equations:

$$\begin{cases} \dfrac{\partial E_0(\vec{\gamma}_l)}{\partial \gamma_l^\alpha} - 2\lambda_l \gamma_l^\alpha = 0, & (14a) \\ \sum\limits_\alpha (\gamma_l^\alpha)^2 = 1, \quad l = 0, 1, \ldots, L-1; \quad \alpha = x, y, z, & (14b) \end{cases}$$

whence the γ_l^α and indeterminate Lagrange factors λ_l can be determined. With (12a) and the equality $z_{ll'} = z_{l'l}$, we can write Eq. (14a) in vectorial form:

$$2\lambda_l \vec{\gamma}_l + 2S^2 N \sum_{l'}{}' z_{ll'} J_{ll'} \vec{\gamma}_{l'} = -g\mu_B SN \boldsymbol{H}_l^{\text{eff}}, \tag{15}$$

$$l = 0, 1, \ldots, L-1.$$

The set (15) decomposes into 3 sets of inhomogeneous difference equations (of L equations each) containing the unknown functions $\gamma_l^\alpha (\alpha = x, y, z)$, respectively. It should be noted that these solutions have to fulfil the normalization conditions (14b). Multiplying both terms of Eq. (15) by $\vec{\gamma}_l$, we get a formula for the Lagrange factors:

$$2\lambda_l = -g\mu_B SN(\boldsymbol{H}_l^{\text{eff}}, \vec{\gamma}_l) - 2S^2 N \sum_{l'}{}' z_{ll'} J_{ll'} (\vec{\gamma}_l, \vec{\gamma}_{l'}). \tag{16}$$

From the theory of difference equations, the solutions $\vec{\gamma}_l$ of the set (15) can be written as a sum of its particular solution and the general solution of the set of homogeneous equations belonging to it (we denote this general solution by $\tilde{\vec{\gamma}}_l$). For instance, $\vec{\gamma}_l = \text{const}\ (l) \equiv \vec{\gamma}$ is a particular solution of (15). On insertion of this solution in (15) and summation of the equations, we get the relation:

$$\lambda \vec{\gamma} = -g\mu_B SN \sum_l \boldsymbol{H}_l^{\text{eff}}, \tag{17}$$

where λ is a new Lagrange factor, equal to:

$$\lambda = 2 \sum_l \lambda_l + 2S^2 N \sum_{ll'} z_{ll'} J_{ll'}. \tag{18}$$

From (17):

$$\vec{\gamma} \| (\sum_l \boldsymbol{H}_l^{\text{eff}}). \tag{19}$$

Consequently, we can write the general solution of Eqs (15) as:

$$\vec{\gamma}_l = \vec{\gamma} + \tilde{\vec{\gamma}}_l, \tag{20}$$

where $\tilde{\vec{\gamma}}_l$ fulfils the homogeneous equation:

$$2\lambda_l \tilde{\vec{\gamma}}_l + 2S^2 N \sum_{l'}{}' z_{ll'} J_{ll'} \tilde{\vec{\gamma}}_{l'} = 0. \tag{21}$$

The vector $\tilde{\vec{\gamma}}_l$ defines the deviation of the local quantization axis (in the l-th layer) from the direction $\vec{\gamma}$ due to the influence of surface defect.

In various papers (Abbel [7], Jelitto [8,9], Corciovei [13], Ferchmin [14], Wojtczak [15], Puszkarski [16]), it was a current assumption that $\vec{\gamma}_l = \vec{\gamma}$. As seen from (20), this constituted an assumption which is correct in the case $\tilde{\vec{\gamma}}_l = 0$ only. In order to determine the range of validity of an approximation of this kind, it would be necessary to proceed to a detailed discussion of Eqs (21) for each of the cases dealt with by the above-named authors.

Finally, let us note that the ground state determined by us semi-classically eliminates from the Hamiltonian (1) terms linear in the operators $\hat{a}$, $\hat{a}^+$ (Tyablikov [12], Kowalewski [17]). In fact, multiplying the right and left hand sides of (15) by $\boldsymbol{A}_l$, we find that R_l (formula 12d)) now vanishes:

$$R_l = 2\lambda_l N^{-1} S^{-1/2} (\vec{\gamma}_l, \boldsymbol{A}_l) = 0, \tag{22}$$

with regard to the equality (6b).

5. *The diagonalizing transformations*

With the aim of finding the elementary spin-wave excitations, we have to diagonalize the bilinear Hamiltonian

$$\hat{\mathscr{H}} = \sum_{ij,l'j'} \left(P^{ij'}_{ll'} \hat{a}^+_{ij} \hat{a}_{l'j'} + \frac{1}{2} Q^{ij'}_{ll'} \hat{a}_{ij} \hat{a}_{l'j'} + \frac{1}{2} Q^{*ij'}_{ll'} \hat{a}^+_{ij} \hat{a}^+_{l'j'} \right). \tag{23}$$

We note that, where we assume $\vec{\gamma}_l = \vec{\gamma}$ (entailing $\boldsymbol{A}_l = \boldsymbol{A}$ too), Eqs (12c) would result in $Q^{ij'}_{ll'} = 0$ and the Hamiltonian would contain terms $\hat{a}^+\hat{a}$ only. This was the case considered *e.g.* by Wojtczak [15]. A transformation similar to (9) was also applied by Corciovei [18] in thin films (on the assumption of $\vec{\gamma}_l = \vec{\gamma}$); however, since Corciovei's Hamiltonian contained terms accounting for anisotropic interactions, he obtained a Hamiltonian of the type (23) in spite of this simplifying assumption. Quite recently, Wojtczak[1] considered the case of different axes $\vec{\gamma}_l$ in different layers but all lying in the film plane. Our considerations will contain no restriction of this kind *i.e.* the $\vec{\gamma}_l$ can have arbitrary directions.

A general method for reducing the quadratic form (23) to its diagonal form is due to Tyablikov and Bogolyubov (*cf.* Bogolyubov [19], Tyablikov [12]). The method has been applied to thin films by Puszkarski [20]. Significantly, as soon as the Hamiltonian (23) is obtained, the problem of diagonalization of the Hamiltonian in thin films becomes much more general than in Jelitto's work, since his Hamiltonian is of a form (if one goes over to second quantization) which is equivalent to an expression involving solely terms $\hat{a}^+\hat{a}$.

[1] Private communication (to be published).

The first transformation to which we shall proceed will consist in a Fourier transformation in the xy-plane of the film; this is justified by our assumption of the periodicity conditions in the x and y directions:

$$\hat{a}_{lj} = \frac{1}{\sqrt{N}} \sum_{\vec{\varkappa}} e^{-i(\vec{\varkappa},\vec{j})} \hat{b}_{\vec{\varkappa} l}, \qquad \hat{a}^{+}_{lj} = \frac{1}{\sqrt{N}} \sum_{\vec{\varkappa}} e^{i(\vec{\varkappa},\vec{j})} \hat{b}^{+}_{\vec{\varkappa} l}, \tag{24}$$

where $\vec{\varkappa} = \vec{\varkappa}[k_x, k_y]$ is a bi-dimensional vector defined in the first Brillouin zone of the planar reciprocal lattice (in the plane xy). One checks easily that the new operators satisfy boson commutation rules:

$$[\hat{b}_{\vec{\varkappa} l}, \hat{b}^{+}_{\vec{\varkappa}' l'}] = \delta_{\vec{\varkappa}\vec{\varkappa}'}\, \delta_{ll'}, \qquad [\hat{b}_{\vec{\varkappa} l}, \hat{b}_{\vec{\varkappa}' l'}] = 0. \tag{24a}$$

By the transformation (24), the Hamiltonian (23) becomes:

$$\hat{\mathscr{H}} = \sum_{\vec{\varkappa}} \sum_{ll'} \left[P_{ll'}(\vec{\varkappa})\, \hat{b}^{+}_{\vec{\varkappa} l}\, \hat{b}_{\vec{\varkappa} l'} + \frac{1}{2} Q_{ll'}(\vec{\varkappa}) \hat{b}_{\vec{\varkappa} l} \hat{b}_{-\vec{\varkappa}, l'} + \frac{1}{2} \overset{*}{Q}_{ll'}(\vec{\varkappa}) \hat{b}^{+}_{\vec{\varkappa} l} \hat{b}^{+}_{-\vec{\varkappa}, l'} \right], \tag{25}$$

with coefficients of the form:

$$P_{ll'}(\vec{\varkappa}) = -2SJ_{ll'}(\boldsymbol{A}^{*}_{l}, \boldsymbol{A}_{l'}) \Gamma^{\vec{\varkappa}}_{ll'} + \delta_{ll'} [2S \sum_{n}{}' z_{ln} J_{ln}(\vec{\gamma}_l, \vec{\gamma}_n) + g\mu_B(\boldsymbol{H}^{\mathrm{eff}}_{l}, \vec{\gamma}_l),$$

$$Q_{ll'}(\vec{\varkappa}) = -2SJ_{ll'}(\boldsymbol{A}_{l}, \boldsymbol{A}_{l'}) \Gamma^{\vec{\varkappa}}_{ll'}, \tag{26}$$

$$\Gamma^{\pm\vec{\varkappa}}_{ll'} = \sum_{\vec{j}'}{}' e^{\pm i(\vec{\varkappa}, \vec{j}-\vec{j}')} \tag{27}$$

$$(\vec{j} \in l, \vec{j}' \in l' \text{ and } \vec{j} \text{ given}).$$

The expression $\Gamma^{\pm\vec{\varkappa}}_{ll'}$ is commonly referred to as a "structure coefficient"; it satisfies the relations:

$$\overset{*}{\Gamma}{}^{\vec{\varkappa}}_{ll'} = \Gamma^{-\vec{\varkappa}}_{ll'}, \Gamma^{\vec{\varkappa}}_{l'l} = \overset{*}{\Gamma}{}^{\vec{\varkappa}}_{ll'}, \Gamma^{0}_{ll'} = z_{ll'}. \tag{28}$$

By (26), (27) and (28), the following relations result:

$$P_{ll'}(\vec{\varkappa}) = \overset{*}{P}_{ll}(\vec{\varkappa}), \tag{29a}$$

$$Q_{ll'}(\vec{\varkappa}) = Q_{l'l}(-\vec{\varkappa}). \tag{29b}$$

We now perform the canonical Tyablikov-Bogolyubov transformation:

$$\hat{b}_{\vec{\varkappa} l} = \sum_{\tau} [u_l(\tau) \hat{\xi}_{\vec{\varkappa}\tau} + v^{*}_{l}(-\tau) \hat{\xi}^{+}_{-\vec{\varkappa}, -\tau}],$$

$$\hat{b}^{+}_{-\vec{\varkappa}, l} = \sum_{\tau} [u^{*}_{l}(-\tau) \hat{\xi}^{+}_{-\vec{\varkappa}, -\tau} + v_l(\tau) \hat{\xi}_{\vec{\varkappa}\tau}], \tag{30}$$

where τ denotes a new quantum number taking L values; this transformation finally reduces the Hamiltonian (25) to its diagonal form:

$$\hat{\mathscr{H}} = \sum_{\vec{\varkappa}\tau} E(\vec{\varkappa}, \tau) \hat{\xi}^{+}_{\vec{\varkappa}\tau} \hat{\xi}_{\vec{\varkappa}\tau} + \text{const.} \tag{31}$$

Since $\hat{\mathscr{H}}$ is hermitian, we obviously require that $E(\vec{\varkappa}, \tau) = E^*(\vec{\varkappa}, \tau)$. In order that the transformation (30) shall lead to the result (31), the transformation functions $u_l(\tau)$ and $v_l(\tau)$ have to:

(1) fulfil the orthonormality conditions (see, Tyablikov [12]):

$$\sum_l [u_l(\tau)u_l^*(\tau') - v_l(\tau)v_l^*(\tau')] = \delta_{\tau\tau'}, \tag{32a}$$

$$\sum_l [u_l(\tau)v_l(-\tau) - v_l(\tau)u_l(-\tau)] = 0, \tag{32b}$$

$$\sum_\tau [u_l(\tau)u_{l'}^*(\tau) - v_{l'}(-\tau)v_l^*(-\tau)] = \delta_{ll'}, \tag{33a}$$

$$\sum_\tau [u_l(\tau)v^*(\tau) - v_l^*(-\tau)u_{l'}(-\tau)] = 0; \tag{33b}$$

(2) satisfy the so-called Tyablikov-Bogolyubov set of equations.

To derive the latter we write, with regard to (25) and (31), the following Heisenberg equations of motion:

$$i\dot{\hat{b}}_{\vec{\varkappa}l} = [\hat{b}_{\vec{\varkappa}l}, \hat{\mathscr{H}}] = \sum_{l'} [P_{ll'}(\vec{\varkappa})\hat{b}_{\vec{\varkappa}l'} + Q_{ll'}^*(\vec{\varkappa})\hat{b}^+_{-\vec{\varkappa},l'}], \tag{34}$$

$$i\dot{\hat{\xi}}_{\vec{\varkappa}\tau} = [\hat{\xi}_{\vec{\varkappa}\tau}, \hat{\mathscr{H}}] = E(\vec{\varkappa}, \tau)\hat{\xi}_{\vec{\varkappa}\tau}, \tag{35a}$$

$$i\dot{\hat{\xi}}^+_{-\vec{\varkappa},-\tau} = [\hat{\xi}^+_{-\vec{\varkappa},-\tau}, \hat{\mathscr{H}}] = -E(-\vec{\varkappa}, -\tau)\hat{\xi}^+_{-\vec{\varkappa},-\tau}. \tag{35b}$$

Inserting (30) into (34) and applying the relations (35a) and (35b), we obtain an equality which can hold only if the coefficients of the linearly independent variables $\hat{\xi}_{\vec{\varkappa}\tau}$ and $\hat{\xi}^+_{-\vec{\varkappa},-\tau}$ vanish. This leads to the equations:

$$\begin{aligned} u_l(\tau)E(\vec{\varkappa}, \tau) &= \sum_{l'} [P_{ll'}(\vec{\varkappa})u_{l'}(\tau) + Q_{ll'}^*(\vec{\varkappa})v_{l'}(\tau)], \\ -v_l^*(-\tau)E(-\vec{\varkappa}, -\tau) &= \sum_{l'} [P_{ll'}(\vec{\varkappa})v_{l'}^*(-\tau) + Q_{ll'}^*(\vec{\varkappa})u_{l'}^*(-\tau)]. \end{aligned} \tag{36}$$

On conjugating the second of these equations and on performing therein the substitution $\vec{\varkappa} \to -\vec{\varkappa}$, $\tau \to -\tau$, we finally obtain:

$$\begin{aligned} u_l(\tau)E(\vec{\varkappa}, \tau) &= \sum_{l'} [P_{ll'}(\vec{\varkappa})u_{l'}(\tau) + Q_{ll'}^*(\vec{\varkappa})v_{l'}(\tau)], \\ -v_l(\tau)E(\vec{\varkappa}, \tau) &= \sum_{l'} [P_{ll'}^*(-\vec{\varkappa})v_{l'}(\tau) + Q_{ll'}(-\vec{\varkappa})u_{l'}(\tau)], \\ l &= 0, 1, \ldots, L-1. \end{aligned} \tag{37}$$

Eq. (37) is the Tyablikov-Bogolyubov set of equations of our problem.

We note that in accordance with a general property of these equations, their set remains unchanged under the transformation:

$$u_l(\tau) \to v_l^*(-\tau), \quad v_l(\tau) \to u_l^*(-\tau), \tag{38}$$

$$E(\hat{\varkappa}, \tau) \to -E(-\vec{\varkappa}, -\tau), \tag{39}$$

meaning that if $E(\vec{\varkappa}, \tau)$ is an eigen-values then so is $-E(-\vec{\varkappa}, -\tau)$ and the respective solutions fulfil the relation (38). These two sets of solutions (*i.e.* corresponding to eigenvalues $E(\vec{\varkappa}, \tau)$ and $-E(-\vec{\varkappa}, -\tau)$) cannot simultaneously fulfil the same normalization conditions (32a) and (33a), and only one set is selected, namely the one corresponding to positive values E. Solutions corresponding to $E > 0$ will be termed *physical* and solutions corresponding to $E < 0$ *non-physical*. Henceforth, a solution of the Tyablikov-Bogolyubov set of equations will be meant to imply a physical solution only.

In spin-wave formalism, the $\hat{\xi}^{\pm\dagger}_{\vec{\varkappa}\tau}$ are creation operators of a spin-wave and $E(\vec{\varkappa}, \tau)$ is its energy. The requirement of positive E is equivalent to considering elementary excitations of positive energies only. In this way, we satisfy the postulate that the selected ground state shall be a state of stable equilibrium of the system.

6. *The concept of layer parameters of spin pinning*

1. We now proceed to solve the set of Eqs (37). It may be worth noting that the set (37) is of more generality than the set considered by Jelitto [8]: in fact, his set of equations can be obtained from the first equation of our set (37) by putting therein $Q_{ll'}(\vec{\varkappa}) = 0$. From this Section onwards, we shall be considering only bodies of Bravais structure (an example of solving Eqs (37) for structures which are not a Bravais lattice will be given in a separate paper).

By our assumption of a translational lattice, the following quantities are independent of the index l:

$$
\begin{aligned}
&1.\ z_{l,l\pm g} = z_g,\\
&2.\ J_{l,l\pm g} = J_g,\\
&3.\ \Gamma^{\vec{\varkappa}}_{l,l\pm g} = \Gamma^{\vec{\varkappa}}_{\pm g},\ \Gamma^{\vec{\varkappa}}_{-g} = \Gamma^{*\vec{\varkappa}}_{g} = \Gamma^{-\vec{\varkappa}}_{g},\\
&\quad \Gamma^{\vec{\varkappa}}_{0} = \Gamma^{*\vec{\varkappa}}_{0},\ \Gamma^{0}_{g} = z_g.
\end{aligned}
\tag{40}
$$

Moreover, from physical considerations, it seems justified to restrict ourselves to cases in which the following relations are fulfilled:

$$
\begin{aligned}
&4.\ (\vec{\gamma}_l, \vec{\gamma}_{l\pm g}) = e_g = e^*_g,\ e_0 = 1;\\
&5.\ (\boldsymbol{A}_l, \boldsymbol{A}_{l\pm g}) = h_g,\ h_0 = 0;\\
&6.\ (\boldsymbol{A}_l, \boldsymbol{A}_{l\pm g}) = w_{\pm g},\ w_{-g} = w^*_g,\ w_0 = 1.
\end{aligned}
\tag{41}
$$

Also, without loss of generality, we can perform the separation:

$$
7.\ \boldsymbol{H}^{\mathrm{eff}}_l = \boldsymbol{H}^{\mathrm{eff}} + \boldsymbol{K}^{\mathrm{eff}}_l. \tag{42}
$$

2. We re-write the coefficients $P_{ll'}(\vec{\varkappa})$ and $Q_{ll'}(\vec{\varkappa})$ (Eqs (26)) resorting to the definitions and notation of the preceding Subsection:

$$
P_{l,l\pm g}(\vec{\varkappa}) = -2SJ_g w_{\pm g} \Gamma^{\pm\vec{\varkappa}}_{g}, \tag{43a}
$$

$$
P_{ll}(\vec{\varkappa}) = P(\vec{\varkappa}) - a_l, \tag{43b}
$$

$$P(\vec{\varkappa}) = -2SJ_0(\Gamma_0^{\vec{\varkappa}}-z_0)+g\mu_B(\boldsymbol{H}^{\text{eff}}, \vec{\gamma})+2S\sum_g^{\pm G} z_g J_g e_g, \tag{43c}$$

$$a_l = 2S\sum_g^{f(l)} z_g J_g e_g - g\mu_B(K_l^{\text{eff}}, \vec{\gamma})-g\mu_B(\boldsymbol{H}_l^{\text{eff}}, \vec{\gamma}_l), \tag{43d}$$

$$Q_{l,l\pm g}(\vec{\varkappa}) = -2SJ_g h_g \Gamma_g^{\pm\vec{\varkappa}}, \tag{44a}$$

$$Q_{ll}(\vec{\varkappa}) = -2SJ_0 h_0 \Gamma_0^{\varkappa} \equiv 0. \tag{44b}$$

We have intendedly given the diagonal terms $P_{ll}(\vec{\varkappa})$ the form (43b). The distinction of two components, $P(\vec{\varkappa})$ and a_l, only the second of which depends on the number l labelling the layer, will further on prove most useful. We shall refer to the a_l as *layer parameters*, and shall later distinguish between boundary parameters (*i.e.* parameters of the boundary layers) and internal parameters (ones relating to internal layers).

Let us note that the following relations are true:

$$P(\vec{\varkappa}) = P^*(\vec{\varkappa}),\ a_l' = a_l^*,\ P(-\vec{\varkappa}) = P(\vec{\varkappa}). \tag{45}$$

To achieve a higher degree of generality we assume, instead of (44b),

$$Q_{ll}(\vec{\varkappa}) = Q(\vec{\varkappa})-b_l, \tag{46a}$$

where we assume that

$$Q(-\vec{\varkappa}) = Q(\vec{\varkappa}). \tag{46b}$$

3. Using the preceding relations, we write the set of equations (37) in the form:

$$\begin{aligned}
&[P(\vec{\varkappa})-E(\vec{\varkappa}, \tau)-a_l]u_l(\tau)+[Q^*(\vec{\varkappa})-b_l^*]v_l(\tau)- \\
&-2S\sum_g^{l} J_g[w_g\Gamma_g^{\vec{\varkappa}}u_{l+g}(\tau)+h_g^*\Gamma_g^{*\vec{\varkappa}}v_{l+g}(\tau)] = 0, \\
&[Q(\vec{\varkappa})-b_l]u_l(\tau)+[P(\vec{\varkappa})+E(\vec{\varkappa}, \tau)-a_l]v_l(\tau)- \\
&-2S\sum_g^{l} J_g[h_g\Gamma_g^{*\vec{\varkappa}}u_{l+g}(\tau)+w_g^*\Gamma_g^{\vec{\varkappa}}v_{l+g}(\tau)] = 0, \\
&l = 0, 1, \ldots, L-1.
\end{aligned} \tag{47}$$

This is a set of difference equations in two unknown functions $u_l(\tau)$ and $v_l(\tau)$. The fact that it contains two unknown functions distinguishes (47) from the set of equations considered by Jelitto, where only one function $u_l(\tau)$ occurred. In spite of this dissimilarity, Eqs (47) can be solved by Jelitto's method, once the latter is appropriately modified.

We ask how the various equations of the set (47) differ from one another? The "diagonal" terms differ as to their layer parameters a_l and b_l. The "non-diagonal" terms, on the other hand, are the same in all equations; but the equations corresponding to the boundary layers lack certain of the non-diagonal terms in $\sum_g^{l}$ because of asymmetric neighbourhood (a consequence of natural defect). The dissimilarities between the various equations are a mathematical counterpart of the physical inequivalence of the layers. This inequivalence is obviously

a result of natural defect (and concerns the boundary layers only) as well as the differences occurring in the quantities which we have termed layer parameters. Thus, each pair of parameters a_l, b_l characterizes the specificity of the physical situation of a layer l. *The layer parameters a_l and b_l can be considered as a measure of the defect "localized" in the layer l.* From Eq. (43*d*), the parameter a_l is seen to account for the influence of natural defect ($\sum_g^{f(l)}$) as well as for the specificity of the quantization axis $\vec{\gamma}_l$ and effective field $\boldsymbol{H}_l^{\text{eff}}$.

Intuition would suggest for the parameters a_l the physical meaning of parameters of spin "pinning" in each layer l, and this attribution can now be made easily. Let us denote by ε_l the energy per spin $\mathbf{S}_l$ in the ground state of the system:

$$\varepsilon_l = -2\sum_{g=0}^{l} z_g J_g(\mathbf{S}_l, \mathbf{S}_{l+g}) - g\mu_B(\boldsymbol{H}_l, \mathbf{S}_l) = \text{const}\,(l) + Sa_l, \tag{48a}$$

where we have used the notation:

$$\text{const}\,(l) = -2S^2 \sum_{g=0}^{\pm G} z_g J_g e_g - g\mu_B S(\boldsymbol{H}, \vec{\gamma}). \tag{48b}$$

The energy ε_l is a measure of the "pinning" of a spin $\mathbf{S}_l$ to the local quantization axis of layer l. We now calculate the difference:

$$\Delta\varepsilon_{lm} = \varepsilon_l - \varepsilon_m = S(a_l - a_m). \tag{48c}$$

Hence, the difference between the parameters a_l and a_m of any two layers expresses the amount by which spin pinning differs between these two layers (l and m), and one is justified in referring to a_l and b_l as *spin pinning parameters*. Eq. (48a) states that the larger is a_l the weaker is the pinning of spins of the layer l — in other words, that they are the more easily "diverted" from the direction $\vec{\gamma}_l$. This means that the larger a_l the easier it is to "create" a spin-wave (a magnon) in layer l. Accordingly, the quantity $V_l = -\varepsilon_l$ can be regarded as a magnon potential, *i.e.* the potential "felt" by a magnon moving in the thin film. One notes that $-const\,(l)$ defines a constant value of this potential, and $-Sa_l$ the magnon potential increment for the layer l. The magnon potential becomes infinite outside the film, at a distance from its surface which depends on the value of the layer parameters.

For the internal layers, the first component of (43d) is zero. We restrict our further considerations to cases in which the remaining components, too, vanish for internal layers *i.e.* in which $\boldsymbol{K}_l = 0$ and when $\vec{\gamma}_l (\approx 0)$ can be neglected; consequently,

$$a_l = 0,\ b_l = 0 \quad \text{for} \quad l = G, G+1, \ldots, L-G-1. \tag{48d}$$

The preceding assumption will contribute towards simplifying the formalism of solving the set (47). Its physical meaning is that we shall be considering the internal layers as physically equivalent to one another. In other words, *the internal layers will form a single sublattice*. As a consequence, all equations corresponding to internal layers will become of the same form. The model constructed on the assumption (48d) has been termed by us the Boundary Spin Pinning (BSP) or *Boundary Inhomogeneity (BI) Model*.

As stated previously, the equations of the boundary layers differ from one another because of (*i*) different "lacunes" in the sum $\sum_g^l$ over neighbouring layers, (*ii*) different

parameters a_l and b_l. The fundamental idea of Jelitto which we shall apply here consists in the introduction of fictitious layers in a manner to bring the equations of the boundary layers to the same form as those of the internal layers. The introduction of new (fictitious) variables implies the adjunction of one new equation for each fictitious layer. The meaning of these new equations will be that of boundary conditions imposed on the required solution[2].

Owing to the introduction of layer parameters (which do not occur in Jelitto's work) the physical meaning of the present method gains in clarity.

4. Thus, the set of Eqs (47) is replaced by two sets: a set of equations of the "*bulk body*" (all these equations are identical in shape):

$$\begin{aligned}
&[P(\vec{\varkappa})-E(\vec{\varkappa},\tau)]u_l(\tau)+Q^*(\vec{\varkappa})v_l(\tau)-\\
&-2S\sum_g^{\pm G} J_g[w_g\Gamma_g^{\vec{\varkappa}}u_{l+g}(\tau)+h_g^*\Gamma_g^{*\vec{\varkappa}}v_{l+g}(\tau)]=0,\\
&Q(\vec{\varkappa})u_l(\tau)+[P(\vec{\varkappa})+E(\vec{\varkappa},\tau)]v_l(\tau)-\\
&-2S\sum_g^{\pm G} J_g[h_g\Gamma_g^{*\vec{\varkappa}}u_{l+g}(\tau)+w_g^*\Gamma_g^{\vec{\varkappa}}v_{l+g}(\tau)]=0,\qquad (49a)\\
&l=0,1,2,\ldots,L-1;
\end{aligned}$$

and a set of *boundary equations*:

$$\begin{aligned}
&-a_lu_l(\tau)-b_l^*v_l(\tau)+2S\sum_g^{f(l)} J_g[w_g\Gamma_g^{\vec{\varkappa}}u_{l+g}(\tau)+h_g^*\Gamma_g^{*\vec{\varkappa}}v_{l+g}(\tau)]=0,\\
&-b_lu_l(\tau)-a_lv_l(\tau)+2S\sum_g^{f(l)} J_g[h_g\Gamma_g^{*\vec{\varkappa}}u_{l+g}(\tau)+w_g^*\Gamma_g^{\vec{\varkappa}}v_{l+g}(\tau)]=0,\qquad (49b)\\
&l=0,1,\ldots,G-1;\ L-G,L-G+1,\ldots,L-1.
\end{aligned}$$

It should be reminded that in accordance with our convention concerning the meaning of the symbol $\sum_g^{f(l)}$, the index g can take only values satisfying the inequalities:

$$\begin{aligned}
&l+g<0 \quad &&\text{for the lower boundary,}\\
&l+g>L-1 \quad &&\text{for the upper boundary.}
\end{aligned}$$

7. *Spin-wave energy*

We derive the dispersion relation $E=E(\vec{\varkappa},\tau)$ from the set of Eqs (49a) on inserting therein a particular solution of the form:

$$u_l(\tau)=\alpha e^{i\varkappa l},\ v_l(\tau)=\beta e^{i\varkappa l}, \qquad (50)$$

[2] Born and von Kármán had the same idea when introducing so-called cyclic conditions in the linear chain (Born and von Kármán [21]). There, too, fictitious nodes were introduced with the aim of obtaining a mathematically identical form of all equations of motion of the atoms. These adjoined equations containing the new, fictitious nodes constitute the so-called boundary condition of periodicity. The latter can be shown not to correspond strictly to physical reality (see, Puszkarski [22]).

where α and β are unknown amplitudes. On insertion of (50) into Eqs (49a), we obtain (on dividing the right and left hand sides of the equations by $e^{i\tau l}$) the following two equations which permit the determination of these amplitudes:

$$[P(\vec{\varkappa})-E(\vec{\varkappa},\tau)-W_1(\vec{\varkappa},\tau)]\alpha+[Q^*(\vec{\varkappa})-T^*(\vec{\varkappa},\tau)]\beta=0,$$
$$[Q(\vec{\varkappa})-T(\vec{\varkappa},\tau)]\alpha+[P(\vec{\varkappa})+E(\vec{\varkappa},\tau)-W_2(\vec{\varkappa},\tau)]\beta=0. \tag{51}$$

Above, we have used the notation:

$$W_1(\vec{\varkappa},\tau)=2S\sum_g^{\pm G} J_g w_g \Gamma_g^{\vec{\varkappa}} e^{i\tau g}$$
$$=2S\sum_g^{+G} J_g[w_g\Gamma_g^{\vec{\varkappa}}e^{i\tau g}+w_g^*\Gamma_g^{\vec{\varkappa}}e^{-i\tau g}]=W_1^*(\vec{\varkappa},\tau), \tag{52a}$$

$$W_2(\vec{\varkappa},\tau)=2S\sum_g^{\pm G} J_g w_g^*\Gamma_g^{\vec{\varkappa}}e^{i\tau g}=W_2^*(\vec{\varkappa},\tau), \tag{52b}$$

$$T(\vec{\varkappa},\tau)=2S\sum_g^{\pm G} J_g h_g\Gamma_g^{\vec{\varkappa}}e^{i\tau g}. \tag{52c}$$

By the definitions (52) and relations (40) and (41), the following relations are found to hold:

$$W_1(-\vec{\varkappa},-\tau)=W_2(\vec{\varkappa},\tau), \tag{53a}$$
$$T(-\vec{\varkappa},-\tau)=T(\vec{\varkappa},\tau). \tag{53b}$$

On equating to zero the characteristic determinant of the set of Eqs (51), we obtain two roots $E_{1/2}(\vec{\varkappa},\tau)$. With respect to what has been said in Section 5, only the positive root is physically meaningful. We thus have finally:

$$E(\vec{\varkappa},\tau)\equiv E_1(\vec{\varkappa},\tau)=\frac{1}{2}[W_2(\vec{\varkappa},\tau)-W_1(\vec{\varkappa},\tau)]+$$
$$+\sqrt{\left\{P(\vec{\varkappa})-\frac{1}{2}[W_2(\vec{\varkappa},\tau)+W_1(\vec{\varkappa},\tau)]\right\}^2-|Q(\vec{\varkappa})-T(\vec{\varkappa},\tau)|^2}. \tag{54}$$

In $E_2(\vec{\varkappa},\tau)$, the root is preceded by the sign "—" and, as easily seen from the properties of (53), $E_2(\vec{\varkappa},\tau)=-E_1(-\vec{\varkappa},-\tau)$.

From Eqs (51) we can determine (to within a constant) the amplitudes α and β, which are found to be functions of the variables $\vec{\varkappa}$ and τ.

It may be worth noting that already the general formula (54) provides some physically meaningfull information. If the following relation is fulfilled in the ground state of the thin film:

$$\frac{\gamma_l^x}{\gamma_l^y}=\text{const}\ (l), \tag{55}$$

i. e. if the projections of all spins onto the xy-plane lie on straight lines equally inclined to the x-axis (in other words, if the spin disposition is not "fan-wise"), then by the definitions (41) and (5)

$$h_g=h_g^* \text{ and } w_g=w_g^*$$

and

$$T(\vec{\varkappa}, \tau) = T^*(\vec{\varkappa}, \tau),\ W_2(\vec{\varkappa}, \tau) = W_1(\vec{\varkappa}, \tau) \tag{56}$$

so that the term $\frac{1}{2}(W_2 - W_1)$ vanishes in the energy of Eq. (54). This permits the conclusion that the presence of a "fan" in the ground state spin configuration necessarily involves a shift $\Delta E(\vec{\varkappa}, \tau) = \frac{1}{2}[W_2(\vec{\varkappa}, \tau) - W_1(\vec{\varkappa}, \tau)]$ in the energy spectrum and that this shift, obviously, is a function of the variables $\vec{\varkappa}$ and τ. This can prove essential *e. g.* with respect to spin wave resonance, the theory of which as yet provides no convincing explanation of the deviations of experimental spectra from the τ^2-law. The subject, however, lies beyond the field of our present considerations.

8. Spin-wave functions and boudary conditions

We now proceed to search for general solutions $u_l(\tau)$ and $v_l(\tau)$. Since (47) is a set of homogeneous equations, its general solution can be written as a superposition of particular solutions of the type (50). We note that, in its present stage, the problem presents degeneracy: to one energy value $E(\vec{\varkappa}, \tau)$ there correspond $2G$ particular values $\tau_\nu(\tau)$, with $\nu = 1, 2, \ldots, 2G$. This degeneracy is due to our having "physically equated" the $2G$ boundary layers with the internal ones on establishing the set of Eqs (49a), which served for deriving the dispersional formula. In other words: Eq. (54) was obtained on assuming the removal of boundary defect. This, in fact, was the source of degeneracy. Clearly, the latter has to vanish on re-introducing the boundary defect (as represented by the set of Eqs (49b)). Dealing with the defect as a perturbation, we can represent the general solutions in the zeroth approximation of perturbation calculus as the superposition of all "degenerate" particular solutions $u_l(\tau_\nu)$ and $v_l(\tau_\nu)$ corresponding to one and the same energy value. We accordingly write:

$$u_l(\tau) = \sum_{\nu=1}^{2G} \alpha_\nu c_\nu e^{i\tau_\nu(\tau)},\ v_l(\tau) = \sum_{\nu=1}^{2G} \beta_\nu d_\nu e^{i\tau_\nu(\tau)}. \tag{57}$$

The superposition constants c_ν and d_ν will be determined from the boundary conditions (49b) and normalization conditions (32a), (33a). On inserting (57) into (49b) and after some calculations we obtain the following $2G$ equations, permitting the determination of the c_ν and d_ν's:

$$\begin{aligned}
&\sum_{\nu=1}^{2G} \alpha_\nu e^{i\tau_\nu l}\Big[-a_l + 2S \sum_g J_g w_g \vec{\Gamma}_g^{\vec{\varkappa}} e^{i\tau_\nu g}\Big] c_\nu + \\
&+ \sum_{\nu=1}^{2G} \beta_\nu e^{i\tau_\nu l}\Big[-b_l^* + 2S \sum_g^{f(l)} J_g h_g^* \vec{\Gamma}_g^{\vec{\varkappa}} e^{i\tau_\nu g}\Big] d_\nu = 0, \\
&\sum_{\nu=1}^{2G} \alpha_\nu e^{i\tau_\nu l}\Big[-b_l + 2S \sum_g^{f(l)} J_g h_g \vec{\Gamma}_g^{\vec{\varkappa}} e^{i\tau_\nu g}\Big] c_\nu + \\
&+ \sum_{\nu=1}^{2G} \beta_\nu e^{i\tau_\nu l}\Big[-a_l + 2S \sum_g^{f(l)} J_g w_g^* \vec{\Gamma}_g^{\vec{\varkappa}} e^{i\tau_\nu g}\Big] d_\nu = 0, \\
&l = 0, 1, \ldots, G-1; L-G, L-G+1, \ldots, L-1.
\end{aligned} \tag{58}$$

The condition for the existence of non-trivial solutions of the set (58) (with regard to the fact that $\tau_\nu = \tau_\nu(\tau)$) leads to L values of the variable τ. These values obviously depend on the boundary parameters a_l and b_l as well as on the quantum number $\vec{\varkappa}$:

$$\tau = \tau(a_l, b_l, \vec{\varkappa}). \tag{59}$$

For different a_l and b_l we obtain different quantizations of the "τ-spectrum" and thus a different quantization of the energy spectrum (as $E = E(\tau)$). But the energy spectrum distribution is decisive for the behaviour of the macroscopic properties of the specimen (*e. g.* its magnetization). In this way, *the physical properties of a specimen are intimately related with the boundary parameters.* The advantage of introducing boundary parameters a_l and b_l resides precisely in their direct relation to the spectrum of the quantum number τ (Eq. (59)). The field $\boldsymbol{K}^{\text{eff}}$ occurring in the expression for a_l can comprise the field of magnetic anisotropy $\boldsymbol{K}_l^a$. Thus, the present theory enables us to discuss the influence of the local anisotropy of boundary layers on the properties of the thin film. It has to be stated, however, that the function (59) cannot be obtained in explicit form even in the simplest case of $G = 1$ (*i. e.* when the *surface* parameters only are taken into account). Nevertheless, the equations derived here are well adapted to numerical calculations.

The dependence of τ on $\vec{\varkappa}$ apparent in (59) is peculiar to the theory of thin films. As seen on inspection of the set (58), this dependence results from the terms under the summation symbol $\sum_g^{f(l)}$ there, and consequently is due to natural defect. In the case of the finite linear chain, which also privileges one direction, obviously no dependence of this kind is obtained. The existence of a functional relationship $\tau = \tau(\vec{\varkappa})$ gives rise to very considerable difficulties when proceeding to calculate *e. g.* the thermodynamical function of state. These difficulties can be circumvented only by making certain approximations.

Finally, it may be of interest to note that when non-physical solutions (thus, ones derived from (57) by way of the transformation (38)) are inserted into the boundary equations (58), the latter goes over into an identical set of equations if — for the same boundary parameters a_l, b_l and fixed $\vec{\varkappa}$ — the quantization of τ for the non-physical solutions is given, instead (59), in the form:

$$\tau = \tau(a_l, b_l, -\vec{\varkappa}). \tag{60}$$

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