Interface-Localized Mode In Bilayer Film
Ferromagnetic Resonance Spectrum*

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ABSTRACT

Ferromagnetic resonance (FMR) in exchange-coupled bilayer films has been the subject of intensive studies in recent years. From the experimental viewpoint, a characteristic feature of this FMR is that some specimens show single resonance, whereas others show double resonance. Moreover, double resonance can exhibit a regular pattern, in which the high-field (HF) line intensity surpasses that of the low-field (LF) line, or it can exhibit an inverted pattern with the HF line less intense than the LF line. There is a general agreement that the inverted FMR pattern occurs when the HF line is an ‘optic mode’, i.e. an out-of-phase composition of individual sublayer modes, and the LF line is an ‘acoustic mode’, or an in-phase mode composition. The existing theoretical explanations of bilayer ferromagnetic resonance are, as a rule, based on phenomenological equation of motion of the magnetization vector. In this paper, we propose a theory of FMR in ultrathin bilayers based on an entirely microscopic approach, using the Heisenberg model of localized spins and assuming that the two ferromagnetic sublayers are exchange-coupled through their interface. Both the strength and the sign of this interface coupling ($J_{int}$) is arbitrary (we admit ferromagnetic or antiferromagnetic interface coupling). The Hamiltonian contains an exchange energy and a Zeeman energy terms; the external field is assumed to be applied obliquely to the film surface. We focus on the effects originating from the interface coupling, though the system is assumed to exhibit also pinning effects, originating from surface anisotropy on the outer surfaces of the film as well as from intrinsic interface anisotropy present on internal interfaces. The latter anisotropy is assumed to consist of two components: uni-directional ($\vec{K}_{int}$) and uni-axial ($D_{int}$). We show that the resonance spectrum in symmetric bilayer is completely independent of $J_{int}$, but depends strongly on the applied static field configuration with respect to the interface normal (angle $\theta$). A critical angle $\theta_{crit}$ is found to exist (as in the case of single-layer film) for which the multipeak spectrum reduces to a single-peak one. This rigorous microscopic FMR theory does explain the inverted pattern of the bilayer FMR spectrum by assuming the HF line to correspond to an in-phase mode, but of interface-localized nature. The intensity of such localized mode decreases with growing strength of its localization at the interface and, when the localization becomes sufficiently strong, becomes lower than the intensity of the other mode (which is of the bulk type). This gives a possibility to explore the HF resonance line corresponding to the interface-localized mode as a potential source of information concerning the bilayer interface.
1 Introduction

Magnetic multilayers have recently become the subject of intensive studies, both theoretical and experimental, in which special attention is paid to interface parameters, such as interface exchange coupling or interface anisotropy. This interest in interface is due to its significant effect on the properties of the multilayer system as a whole. One of the key methods of interface investigation is based on ferromagnetic resonance (FMR). The interface coupling [1–3] as well as the interface anisotropy [4, 5] in a multilayer can be studied by means of the FMR spectrum. In anisotropy studies, angle relations play an important role [6–8]. Also, FMR has been recently used in investigating magnetic particles size distribution [9].

From the experimental viewpoint, the FMR in bilayer films is characterized by the fact that some specimens show single resonance, whereas others show double resonance.
Moreover, the double resonance can exhibit a regular pattern, in which the high-field (HF) line possesses an intensity greater than that of the low-field (LF) line, or it can exhibit an inverted pattern with a HF line less intense than the LF line. According to a commonly accepted interpretation, the inverted FMR pattern occurs when the HF line is an out-of-phase composition of the individual sublayer modes ("optic mode") and the LF line is an in-phase mode composition ("acoustic mode"). Here, consensus seems to be due to the circumstance that out-of-phase modes, naturally, are associated with lower net magnetization; this is invoked as an explanation of the lower intensity of the HF resonance line in an inverted pattern. However, a perusal of the literature shows that this interpretation lacks rigorous proof; its basic assumption - that between the two lines observed always the HF line is out-of-phase and the LF line is in-phase - has never, to our knowledge, been proved. This stimulated us to take a closer look at the whole problem.

FMR spectra are commonly interpreted on the basis of macroscopic theories; in Artman-Layadi theory [10]–[15], often applied to bilayer film FMR, sublayer magnetizations are regarded as classical vectors and appear as such in the key expression for free energy of interactions between sublayer magnetizations. A microscopic theory of FMR in thin films has been developed by some authors, including Ferchmin [16], Puszkarski [17, 18] and Wojtczak [19, 20]. The Hamiltonian considered in their studies includes the exchange interaction energy, Zeeman energy and the uni-axial anisotropy energy, and is diagonalized by means of Tyablikov-Bogolyubov method [21]. The resulting eigenvalues correspond to spin-wave energies, indicating the resonance line positions, and the intensities of these resonance lines can be found from the corresponding eigenvectors. Thus, a full theoretical image of FMR spectrum is obtained by using this method.

In this study, the FMR spectrum in a magnetic bilayer film is investigated as a function of the interface coupling and the interface anisotropy, on the basis of the theory developed by Puszkarski in [17, 18]. The Hamiltonian of non-homogeneous thin film model is specified in Section 2 and diagonalized in Section 3. The Hamiltonian of ferromagnetic bilayer film is diagonalized in Section 4. Section 5 refers to the bilayer FMR spectra composed of two resonance lines, often reported in experimental studies; as we mentioned above, in the most common interpretation the low-intensity line is related to an optic mode, and the high-intensity line to an acoustic mode. However, the FMR spectra computed in our model prove this interpretation is not always right. In Section 6 we show that symmetric bilayer FMR spectrum does not depend on the interface coupling value, and the effect of the interface anisotropy on the critical angle appearance and value is studied in Section 7.

2 General planar thin film model

2.1 Assumptions

In the planar thin film model, referred to as Valenta model [22]–[23], the thin film specimen is assumed to be infinite and homogeneous in the directions parallel to its surface, but finite and generally inhomogeneous along the surface normal. In the
latter direction, the inhomogeneous thin film can be divided into a number of lattice planes parallel to the film surface (see Fig. 1). If all the lattice planes are assumed to have identical crystallographic structure (the same plane lattice type and equal lattice constant values), all atoms within a plane have identical neighbourhood, and thus are in identical physical conditions. A spin is placed in each lattice node. Its position is defined by the number of the plane to which the spin belongs \((l)\) and the site vector within this plane \((\vec{j})\); its nearest neighbours can lie not only in the same plane or a neighbouring one, but in farther planes as well (this problem is more thoroughly discussed in [24, 25, 26, 27]). The number of plane \(l'\) spins being nearest neighbours of a plane \(l\) spin shall be denoted by \(z_{ll'}\). Both the spins and the exchange interactions are assumed to be equal within a lattice plane (but they can differ from plane to plane).

Two types of coordinate system shall be used below. In the first one, \(xyz\), related to the crystal lattice, \(x\) and \(y\) axes are parallel to the film surface, the \(z\) axis being oriented along the surface normal. Another coordinate system to be used, \(x'y'z'\), is related to a single lattice site; in this local system, the positive direction of \(z'\) axis is defined by unit vector \(\vec{\gamma}_{lj}\), indicating the direction of quantization of the spin in the considered site. The direction of quantization follows that of the effective magnetic field in the spin site. Three components contribute to this effective field: the applied magnetic field, the demagnetization field and the anisotropy field, the latter usually due to the atomic magnetic moment interactions with the crystal lattice electric field (the so-called crystal field). The assumptions made within this model imply that the effective field within a
lattice plane is equal in all spin sites ($\vec{H}_{ij}^{eff} \equiv \vec{H}_{i}^{eff}$), and consequently, all the spins within a single plane have equal direction of quantization ($\vec{\gamma}_{ij} \equiv \vec{\gamma}_{i}$).

### 2.2 The Hamiltonian

We are going to consider a Heisenberg Hamiltonian of the following form:

$$\hat{H} = -2 \sum_{\vec{i},\vec{j};\vec{i}'} J_{\vec{i},\vec{j}'} \vec{S}_{\vec{i}} \cdot \vec{S}_{\vec{i}'}, - g\mu_B \sum_{\vec{i}} \vec{H}_{i}^{eff} \vec{S}_{\vec{i}} - \sum_{\vec{i}} D_i \left( \vec{S}_{i}^z \right)^2,$$

(1)

$J_{\vec{i},\vec{j}'}$ denoting the exchange integral, $g$ being the gyromagnetic ratio, and $\mu_B$ being Bohr magneton. Vector $\vec{j}$ specifies the node position in plane $l$ ($\vec{j} \in l$), and vector $\vec{j}'$ plays the same role in plane $l'$ ($\vec{j}' \in l'$). Symbol $\sum_{\vec{i},\vec{j}'}$ means the summation involves all the spin pairs, each pair being considered once only. The three terms in Hamiltonian (1) correspond to the exchange interactions energy, the Zeeman energy and the single-ion anisotropy energy, respectively. The dynamic dipolar fields shall not be taken explicitly into consideration here, since – as it has been shown by Krawczyk [28] – their effect on the localized state existence conditions is minor.

Assuming that the exchange interactions occur between the nearest neighbours only, and admitting that these interactions, though equal within a lattice plane, can be different between spins lying in different planes (in this case, $J_{\vec{i},\vec{j}'} = J_{\vec{i}}$), we obtain the following form of the Hamiltonian:

$$\hat{H} = - \sum_{\vec{i},\vec{j} \neq \vec{i}'} J_{\vec{i}} \vec{S}_{\vec{i}} \cdot \vec{S}_{\vec{j}'}, - g\mu_B \sum_{\vec{i}} \vec{H}_{i}^{eff} \vec{S}_{\vec{i}} - \sum_{\vec{i}} D_i \left( \vec{S}_{i}^z \right)^2.$$

(2)

In order to find the inhomogeneous thin film eigenstates, Hamiltonian (2) must be diagonalized.

### 3 Hamiltonian diagonalization procedure

Four transformations shall be performed [29], leading to the diagonal form of Hamiltonian (2): 1) transformation to the local coordinate system, 2) transformation to the boson operators, 3) Fourier transformation in the film plane and 4) the transformation along the film surface normal.

#### 3.1 Transformation to the local coordinate system

First we shall transform Hamiltonian (2) from its form in the crystal lattice coordinate system, $xyz$, to that in the local coordinate system, $x'y'z'$. This transformation reads [21]:

$$\vec{S}_{ij} = \vec{\gamma}_{ij} \vec{S}_{ij} + \frac{1}{\sqrt{2}} \left( \vec{A}_{ij} \vec{S}_{ij}^+ + \vec{A}_{ij}^* \vec{S}_{ij}^\dagger \right),$$

(3)
$\vec{g}_l^j$, denoting the previously introduced quantization axis unit vector, and $\vec{A}_l^j$ having the following coordinates (provided that $y'$ lies in plane $xy$):

\begin{align*}
A_{l}^x &= -\frac{1}{\sqrt{2}}\sqrt{1-(\gamma_{l}^x)^2}(\gamma_{l}^x\gamma_{l}^z + i\gamma_{l}^y), \\
A_{l}^y &= -\frac{1}{\sqrt{2}}\sqrt{1-(\gamma_{l}^y)^2}(\gamma_{l}^y\gamma_{l}^z - i\gamma_{l}^x), \\
A_{l}^z &= \frac{1}{\sqrt{2}}\sqrt{1-(\gamma_{l}^z)^2}.
\end{align*} \tag{4}

Vectors $\vec{g}_l^j$ and $\vec{A}_l^j$ fulfill the following relations:

\begin{align*}
\vec{g}_l^j &= \vec{g}_l^j, \quad \vec{g}_l^j \cdot \vec{g}_l^j = 1, \quad \vec{A}_l^j \cdot \vec{A}_l^j = 1, \\
\vec{A}_l^j \cdot \vec{g}_l^j &= 0, \quad \vec{A}_l^j \cdot \vec{g}_l^j = 0, \quad \vec{A}_l^j \cdot \vec{A}_l^j = 0, \\
\vec{g}_l^j \times \vec{A}_l^j &= i\vec{A}_l^j, \quad \vec{A}_l^j \times \vec{A}_l^j = i\vec{g}_l^j. \tag{5}
\end{align*}

### 3.2 Transformation to second quantization operators

In the second step, the spin operators (expressed in $x'y'z'$ coordinates) shall be replaced with boson operators by means of Holstein-Primakoff transformation. In the resulting Hamiltonian, only quadratic terms shall be retained, and all the terms of other orders shall be omitted (however, the commutation rules should be taken into consideration, and attention paid to the sequence of boson operators when omitting the higher-order terms).

Holstein-Primakoff transformation reads \cite{21}:

\begin{align*}
\hat{S}_l^+ &= \sqrt{2S_l^z}\hat{f}_{ij}\hat{a}_{ij}, \\
\hat{S}_l^- &= \sqrt{2S_l^z}\hat{a}_{ij}^+\hat{f}_{ij}, \\
\hat{S}_l^z &= S_l^z - \hat{a}_{ij}^+\hat{a}_{ij}, \\
\hat{f}_{ij} &= \frac{1}{\sqrt{1 - \hat{a}_{ij}^+\hat{a}_{ij}/2S_l^z}}.
\end{align*} \tag{6}

with operators of creation ($\hat{a}_{ij}^+$) and annihilation ($\hat{a}_{ij}$) satisfying the following commutation rules:

\begin{align*}
[\hat{a}_{ij}, \hat{a}_{ij}^+] &= \delta_{lj}\delta_{ij}, \\
[\hat{a}_{ij}, \hat{a}_{ij'}^+] &= 0. \tag{7}
\end{align*}

Using the approximation of quasi-saturation, we obtain:

\begin{align*}
\hat{S}_l^+ &= \sqrt{2S_l^z}\hat{a}_{ij}, \\
\hat{S}_l^- &= \sqrt{2S_l^z}\hat{a}_{ij}^+, \\
\hat{S}_l^z &= S_l^z - \hat{a}_{ij}^+\hat{a}_{ij}.
\end{align*} \tag{8}

The above transformations shall be applied to the first two terms in the Hamiltonian, i.e. the exchange (bi-ion) interaction term and the Zeeman (single-ion, linear) term. The transformations to be applied to the remaining anisotropy term (single-ion, non-
linear), are as follows [30]:

\[
\begin{align*}
\hat{S}^+_{ij} \hat{S}^-_{ij} & = 2S_{ij} \hat{a}^+_{ij}, \\
\hat{S}^+_{ij} \hat{S}^-_{ij} & = 2S_{ij} + (2S_{ij} - 2) \hat{a}^+_{ij}, \\
(\hat{S}^z_{ij})^2 & = S_{ij}^2 - (2S_{ij} - 1) \hat{a}^z_{ij}, \\
\hat{S}^+_{ij} \hat{S}^-_{ij} & = \sqrt{2S_{ij}} (S_{ij} - 1) \hat{a}^z_{ij}, \\
\hat{S}^+_{ij} \hat{S}^-_{ij} & = \sqrt{2S_{ij}} S_{ij} \hat{a}^z_{ij}.
\end{align*}
\]

After transformations [3], [8] and [11] Hamiltonian [2] becomes:

\[
\hat{\mathcal{H}} = E_0(\bar{\gamma}_l) + \sum_{l,j,l'} \left( P_{ll'}^{j,j'} \hat{a}^+_l \hat{a}^-_{l'} + \frac{1}{2} Q_{ll'}^{j,j'} \hat{a}^+_l \hat{a}^-_{l'} + \frac{1}{2} Q_{ll'}^{j,j'} \hat{a}^+_l \hat{a}^-_{l'} \right) + \sum_{l} \left( R_l \hat{a}^+_l + R^*_l \hat{a}^-_l \right),
\]

where:

\[
E_0(\bar{\gamma}_l) = -N \sum_{ll'} z_{ll'} J_{ll'} S_l S_{l'} \bar{\gamma}_l \cdot \bar{\gamma}_{l'} - N g \mu_B \sum_l S_l \bar{H}_l^{\text{eff}} \cdot \bar{\gamma}_l \\
- N \sum_l D_l S_l \left( S_l \cos^2 \theta + \frac{1}{2} \cos^2 \theta - \frac{1}{2} \right),
\]

\[
P_{ll'}^{j,j'} = \begin{cases} 
2 \sum_n z_{ln} J_{ln} S_n \bar{\gamma}_l \cdot \bar{\gamma}_n + g \mu_B \bar{H}_l^{\text{eff}} \cdot \bar{\gamma}_l \\
- D_l (S_l - \frac{1}{2})(1 - 3 \cos^2 \theta) & \text{for } l_j = l_j', \\
-2 \sqrt{S_l S_{l'}} J_{ll'} A_l \cdot A_{l'} & \text{for } l_j \neq l_j',
\end{cases}
\]

\[
Q_{ll'}^{j,j'} = \begin{cases} 
- D_l \sqrt{S_l (S_l - \frac{1}{2}) (1 - \cos^2 \theta)} & \text{for } l_j = l_j', \\
-2 \sqrt{S_l S_{l'}} J_{ll'} A_l \cdot A_{l'} & \text{for } l_j \neq l_j',
\end{cases}
\]

\[
R_l = -2 \sqrt{S_l} \sum_n z_{ln} J_{ln} S_n A_l \cdot \bar{\gamma}_n - g \mu_B \sqrt{S_l \bar{H}_l^{\text{eff}} \cdot A_l} \\
- \frac{1}{2} \sqrt{2S_l (2S_l - 1)} \cos \theta \sqrt{1 - \cos^2 \theta}.
\]

Symbol \( \theta \), appearing in the above equations, denotes the angle between the film magnetization vector and the surface normal; \( z_{ll'} \), as previously defined, is the number of a plane \( l \) spin nearest neighbours in plane \( l' \). Equality \( J_{ll'} = J_{l'l} \) implies that \( P_{ll'}^{j,j'} = P_{l'l}^{j,j'} \) and \( Q_{ll'}^{j,j'} = Q_{l'l}^{j,j'} \), which means that Hamiltonian [10] is Hermitian.
3.3 Bi-linear Hamiltonian

As mentioned above, only quadratic terms shall be retained in the considered Hamiltonian:

\[
\hat{H} = \sum_{l, \vec{j}, l', \vec{j}'} \left( P_{l'w}^{\vec{j}'} \hat{a}_{l' \vec{j}'}^+ \hat{a}_{l \vec{j}} + \frac{1}{2} Q_{l'w}^{\vec{j}'} \hat{a}_{l' \vec{j}'} \hat{a}_{l \vec{j}} + \frac{1}{2} Q_{l'w}^{\vec{j}'} \hat{a}_{l' \vec{j}'}^+ \hat{a}_{l \vec{j}}^+ \right). \tag{15}
\]

The terms of order zero, shifting uniformly the energy scale, are omitted. The first-order terms vanish when the direction of \( \vec{\gamma} \) corresponds to the minimum energy \[30\]. The fourth-order terms are related to the interactions between magnons, and their omitting is justified by our previous assumptions.

The general method of quadratic form diagonalization was proposed by Tyablikov and Bogolyubov, and applied to thin film and bilayer film by Puszkarski \[31, 30\]. The procedure, analogical to that used by Ferchmin \[16\] and Corciovei \[32\], is based on two Fourier transformations, performed in the film plane and along the direction normal to the film surface. By these operations, boson operators \( \hat{a}_{l \vec{j}}^+ \) and \( \hat{a}_{l' \vec{j}'} \), originally expressed in the direct space, \( l \vec{j} \), are transformed into the reciprocal space, \( k||k⊥ \), in which the Hamiltonian is diagonal.

3.4 Fourier transformation in the film plane

The transformation in the film plane reads \[19, 16, 32\]:

\[
\hat{a}_{l \vec{j}} = \frac{1}{\sqrt{N}} \sum_{k||} \exp(-i\vec{k}|| \cdot \vec{j}) \hat{b}_{k||l}, \tag{16}
\]

\[
\hat{a}_{l \vec{j}}^+ = \frac{1}{\sqrt{N}} \sum_{k||} \exp(i\vec{k}|| \cdot \vec{j}) \hat{b}_{k||l}^+. \tag{17}
\]

\( N \) denoting the total number of spins in a single lattice plane parallel to the surface, and \( k|| = [k_x, k_y] \) being a vector from the two-dimensional Brillouin zone (coordinates \( k_x \) and \( k_y \) are quantized through imposing Born-Kármán cyclic boundary conditions in the \( x \) and \( y \) directions). Operators \( \hat{b}^+ \) and \( \hat{b} \) satisfy the boson commutation rules:

\[ [\hat{b}_{k||l}, \hat{b}_{k' || l'}^+] = \delta_{k|| k'} \delta_{l l'}, \quad [\hat{b}_{k||l}, \hat{b}_{k' || l'}] = 0. \tag{17}\]

By transformation \[16\] Hamiltonian \[15\] becomes:

\[
\hat{H} = \sum_{k||, l', w} \left( P_{l'w}(k||) \hat{b}_{k||l'}^+ \hat{b}_{l'w} + \frac{1}{2} Q_{l'w}(k||) \hat{b}_{k||l'} \hat{b}_{-k||l'} + \frac{1}{2} Q_{l'w}(k||) \hat{b}_{k||l'}^+ \hat{b}_{-k||l'}^+ \right), \tag{18}
\]

where:

\[
P_{l'w}(k||) = -2\sqrt{S_l S_{l'} J_{l'w} A_{l'} \cdot A_{l} \Gamma_{l'w}} \tag{19}
\]

\[ + \delta_{l'w} \left[ 2 \sum_n z_n J_{ln} S_n \vec{\gamma}_l \cdot \vec{\gamma}_n + g \mu_B \vec{H}_i \vec{f} \cdot \vec{\gamma}_l - D_l \left( S_l - \frac{1}{2} \right) \left( 1 - 3 \cos^2 \theta \right) \right], \]
Hamiltonian (24) is, by assumption, Hermitian, which implies that $E$ is real. Term $\Gamma_{ll'}$, referred to as structural sum, is defined as the following sum over spin neighbours:

$$
\Gamma^\pm_{ll'} = \sum_{\vec{j}} e^{\pm i \vec{k}} \cdot (\vec{J} - \vec{j}), \quad (\vec{j} \in l, \vec{j}' \in l'),
$$

and satisfies the following relations:

$$
\Gamma^{*\pm}_{ll'} = \Gamma^{-\pm}_{ll'}, \quad \Gamma^{\pm}_{ll'} = \Gamma^{*\pm}_{ll'}, \quad \Gamma^{0}_{ll'} = z_{ll'}.
$$

### 3.5 Transformation along the surface normal

In the last step of the diagonalization procedure, canonical Tyablikov-Bogolyubov transformation [21] (along the film surface normal) shall be applied to Hamiltonian (23):

$$
\hat{b}_{\vec{k}|l} = \sum_{k\perp} \left[ u_t(k\perp) \hat{\xi}_{\vec{k}|l}^{k\perp} + v_t^{*}(-k\perp) \hat{\xi}_{-\vec{k}|l}^{-k\perp} \right],
$$

$$
\hat{b}_{-\vec{k}|l}^{+} = \sum_{k\perp} \left[ u_t^{*}(-k\perp) \hat{\xi}_{-\vec{k}|l}^{+k\perp} + v_t(k\perp) \hat{\xi}_{\vec{k}|l}^{-k\perp} \right],
$$

where $\hat{\xi}_{\vec{k}|l}^{k\perp}$ and $\hat{\xi}_{-\vec{k}|l}^{-k\perp}$ are operators of creation and annihilation, respectively, of a spin wave with energy $E(\vec{k}|l, k\perp)$ and wave vector $\vec{k} = [\vec{k}|l, k\perp]$, components $\vec{k}|l$ and $k\perp$ being, respectively, parallel and perpendicular to the surface. When expressed by operators $\hat{\xi}_{\vec{k}|l}^{k\perp}$ and $\hat{\xi}_{-\vec{k}|l}^{-k\perp}$, the Hamiltonian becomes diagonal:

$$
\hat{\mathcal{H}} = \sum_{\vec{k}|l, k\perp} E(\vec{k}|l, k\perp) \hat{\xi}_{\vec{k}|l}^{k\perp} \hat{\xi}_{\vec{k}|l}^{-k\perp} + \text{const.}
$$

Hamiltonian (24) is, by assumption, Hermitian, which implies that $E(\vec{k}|l, k\perp) = E^{*}(\vec{k}|l, k\perp)$. For transformation (23) to result in the diagonal form of the Hamiltonian, functions $u_t(k\perp)$ and $v_t(k\perp)$ must satisfy the following conditions of orthonormality [33]:

$$
\sum_{l} \left[ u_t(k\perp) u_t^{*}(k\perp') - v_t(k\perp) v_t^{*}(k\perp') \right] = \delta_{k\perp k\perp'},
$$

$$
\sum_{l} \left[ u_t(k\perp) v_t(-k\perp) - v_t^{*}(-k\perp) u_t(-k\perp) \right] = 0,
$$

$$
\sum_{k\perp} \left[ u_t(k\perp) u_t^{*}(k\perp') - v_t^{*}(-k\perp) v_t(-k\perp') \right] = \delta_{ll'},
$$

$$
\sum_{k\perp} \left[ u_t(k\perp) v_t^{*}(k\perp') - v_t^{*}(-k\perp) u_t(-k\perp') \right] = 0,
$$

and, moreover, they must be solutions of so-called Tyablikov-Bogolyubov equations.
In order to find functions $u_t(k_\perp)$ and $v_t(k_\perp)$ in their explicit forms, we shall write the Heisenberg equations of motion for operators $\hat{b}_{k_{\parallel} l}$, $\hat{\xi}_{k_{\parallel} k_{\perp}}$ and $\hat{\xi}^+_{-k_{\parallel} l}$:

$$\hat{b}_{k_{\parallel} l} = \sum_{l'} [P_{l'}(k_{\parallel}) \hat{b}_{l'} + Q_{l'}(k_{\parallel}) \hat{b}^+_{-l'}],$$

$$i\hat{\xi}_{k_{\parallel} k_{\perp}} = [\hat{\xi}_{k_{\parallel} k_{\perp}}, \hat{\mathcal{H}}] = E(k_{\parallel}, k_{\perp}) \hat{\xi}_{k_{\parallel} k_{\perp}},$$

$$i\hat{\xi}^+_{-k_{\parallel} l} = [\hat{\xi}^+_{-k_{\parallel} l}, \hat{\mathcal{H}}] = E(k_{\parallel}, k_{\perp}) \hat{\xi}^+_{-k_{\parallel} l}.$$  

By inserting (23) into (26), and using (27), the following equation is obtained:

$$\sum_{k_{\perp}} \left[ u_t(k_{\perp}) E(k_{\parallel}, k_{\perp}) \hat{\xi}_{k_{\parallel} k_{\perp}} - v_t^*(-k_{\perp}) E(-k_{\parallel}, -k_{\perp}) \hat{\xi}^+_{-k_{\parallel} k_{\perp}} \right] =$$

$$\sum_{k_{\perp}} \sum_{l'} \left[ P_{l'}(k_{\parallel}) \left( u_{l'}(k_{\parallel}) \hat{\xi}_{k_{\parallel} k_{\perp}} + v_{l'}^*(-k_{\perp}) \hat{\xi}^+_{-k_{\parallel} k_{\perp}} \right) +
Q_{l'}(k_{\parallel}) \left( u_{l'}^*(-k_{\perp}) \hat{\xi}^+_{-k_{\parallel} k_{\perp}} + v_{l'}(k_{\perp}) \hat{\xi}_{k_{\parallel} k_{\perp}} \right) \right],$$

equivalent to a set of $2L$ equations, if $\hat{\xi}_{k_{\parallel} k_{\perp}}$ and $\hat{\xi}^+_{-k_{\parallel} k_{\perp}}$ are linearly independent:

$$u_t(k_{\perp}) E(k_{\parallel}, k_{\perp}) = \sum_{l'} \left[ P_{l'}(k_{\parallel}) u_{l'}(k_{\perp}) + Q_{l'}(k_{\parallel}) v_{l'}(k_{\perp}) \right],$$

$$-v_t^*(-k_{\perp}) E(-k_{\parallel}, -k_{\perp}) = \sum_{l'} \left[ P_{l'}(k_{\parallel}) v_{l'}^*(-k_{\perp}) + Q_{l'}(k_{\parallel}) u_{l'}^*(-k_{\perp}) \right].$$

Reversing the direction of $\vec{k}$ in the second equation ($k_{\parallel} \rightarrow -k_{\parallel}, k_{\perp} \rightarrow -k_{\perp}$) finally leads to:

$$u_t(k_{\perp}) E(k_{\parallel}, k_{\perp}) = \sum_{l'} \left[ P_{l'}(k_{\parallel}) u_{l'}(k_{\perp}) + Q_{l'}(k_{\parallel}) v_{l'}(k_{\perp}) \right],$$

$$-v_t(k_{\perp}) E(k_{\parallel}, k_{\perp}) = \sum_{l'} \left[ P_{l'}(-k_{\parallel}) v_{l'}(k_{\perp}) + Q_{l'}(-k_{\parallel}) u_{l'}(k_{\perp}) \right].$$

This is the set of Tyablikov-Bogolyubov equations corresponding to our problem. The spin wave energy, $E(k_{\parallel}, k_{\perp})$, as well as functions $u_t(k_{\perp})$ and $v_t(k_{\perp})$, describing the spin wave precession, can be deduced from its solution.

4  The particular case: ferromagnetic bilayer film

4.1  General form of the bilayer Hamiltonian

Let us consider now a magnetic bilayer film, composed of two homogeneous sub-layers A and B having identical crystallographic structure; each sublayer is assumed to contain a number of lattice planes, $N_A$ and $N_B$, respectively (Fig. 2). Moreover,
the spins in the lattice nodes, as well as the exchange interactions between the nearest neighbours, are assumed to be equal within each sublayer, though they can differ between the sublayers. The same rule applies to the other parameters, such as the bulk anisotropy constant and the effective field. Besides the standard notion of bulk anisotropy, $D_{A(B)}$, two other quantities shall be used: surface anisotropy $D_s^{A(B)}$ and interface anisotropy $D_{int}^{A(B)}$.

The exchange interaction through the interface shall be described by introducing the interface exchange integral, $J_{AB}$, positive for ferromagnetic interface coupling, negative for antiferromagnetic interface coupling, and zero in the case where no coupling is present between the sublayers. In practice, a thin non-magnetic interlayer is inserted between the ferromagnetic thin films $A$ and $B$, and the interface properties ($D_{int}^{A(B)}$, $J_{AB}$) are determined by the interlayer thickness and material.
With these assumptions, the matrix form of (28) is:

\[
\begin{pmatrix}
X_A & X_{AB} & Y \\
X_{AB}^\dagger & X_B & Y \\
Y & X_A & X_{AB}
\end{pmatrix}
\begin{pmatrix}
U \\
V
\end{pmatrix}
= E
\begin{pmatrix}
U \\
-V
\end{pmatrix},
\]

(29)

\(U\) and \(V\) being defined as follows:

\[
U = \begin{bmatrix}
U_1 \\
U_2 \\
\vdots \\
U_{L_A} \\
U_{L_A+1} \\
\vdots \\
U_{L-1} \\
U_L
\end{bmatrix},
V = \begin{bmatrix}
V_1 \\
V_2 \\
\vdots \\
V_{L_A} \\
V_{L_A+1} \\
\vdots \\
V_{L-1} \\
V_L
\end{bmatrix}
\]

(30)

In films obtained from cubic crystal surface cuts (001), (110) or (111), the nearest neighbours of a plane \(l\) spin lie in planes up to \(l + 3\), so the general form of matrices \(X\) and \(Y\) is seven-diagonal:

\[
X_A = \begin{bmatrix}
R_A - a_0 & C_A & D_A & F_A \\
C_A^* & R_A - a_1 & C_A & D_A & F_A \\
D_A^* & C_A^* & R_A - a_2 & C_A & D_A & F_A \\
F_A^* & D_A^* & C_A^* & R_A & C_A & D_A & F_A \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
F_A^* & D_A^* & C_A^* & R_A - b_2 & C_A & D_A & F_A \\
F_A^* & D_A^* & C_A^* & R_A - b_1 & C_A & D_A & F_A \\
F_A^* & D_A^* & C_A^* & R_A - b_0 & C_A & D_A & F_A
\end{bmatrix}_{L_A \times L_A}
\]

(31)

\[
X_B = \begin{bmatrix}
R_B - c_0 & C_B & D_B & F_B \\
C_B^* & R_B - c_1 & C_B & D_B & F_B \\
D_B^* & C_B^* & R_B - c_2 & C_B & D_B & F_B \\
F_B^* & D_B^* & C_B^* & R_B & C_B & D_B & F_B \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
F_B^* & D_B^* & C_B^* & R_B - d_2 & C_B & D_B & F_B \\
F_B^* & D_B^* & C_B^* & R_B - d_1 & C_B & D_B & F_B \\
F_B^* & D_B^* & C_B^* & R_B - d_0 & C_B & D_B & F_B
\end{bmatrix}_{L_B \times L_B}
\]

(32)
\[ X_{AB} = \begin{bmatrix} \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ F_{AB} & 0 & 0 \\ D_{AB} & F_{AB} & 0 \\ C_{AB} & D_{AB} & F_{AB} \end{bmatrix}_{L_A \times L_B} \] (33)

\[ Y = \begin{bmatrix} R_{A,s}^y & R_A^y \\ \vdots & \vdots \\ R_A^y & 0 & 0 & F_A^y \\ 0 & R_A^y & 0 & D_A^y & F_A^y \\ 0 & 0 & R_{A,int}^y & C_A^y & D_A^y & F_A^y \\ (F_A^y)^* & (D_A^y)^* & (C_A^y)^* & R_{A,int}^y & 0 & 0 \\ (F_A^y)^* & (D_A^y)^* & 0 & R_B^y & 0 \\ (F_A^y)^* & 0 & 0 & R_B^y \end{bmatrix}_{L \times L} \] (34)

The symbols used above are defined as follows:

\[ C_i = -2S_i J_i \Gamma_1, \]
\[ D_i = -2S_i J_i \Gamma_2, \]
\[ F_i = -2S_i J_i \Gamma_3, \]

\[ R_i = -2S_i J_i \Gamma_0 + g\mu_B \vec{H}_{eff}^i \cdot \vec{\gamma}_i + D_i \left( S_i - \frac{1}{2} \right) \left( 3 \cos^2 \theta_i - 1 \right) + 2 \left( z_i^3 + 2 (z_i^1 + z_i^2 + z_i^3) \right) S_i J_i, \] (36)

\[ R_{i,(int,s)}^y = -D_{i,(int,s)} \sqrt{S_i \left( S_i - \frac{1}{2} \right)} \sin^2 \theta_i, \] (37)

where \( i = A; B \), and:

\[ C_{AB} = -2 \sqrt{S_A S_B} J_{AB} \vec{A}_A \cdot \vec{A}_B \Gamma_1, \]
\[ D_{AB} = -2 \sqrt{S_A S_B} J_{AB} \vec{A}_A \cdot \vec{A}_B \Gamma_2, \]
\[ F_{AB} = -2 \sqrt{S_A S_B} J_{AB} \vec{A}_A \cdot \vec{A}_B \Gamma_3, \]

\[ C_{AB}^y = -2 \sqrt{S_A S_B} J_{AB} \vec{A}_A \cdot \vec{A}_B \Gamma_1, \]
\[ D_{AB}^y = -2 \sqrt{S_A S_B} J_{AB} \vec{A}_A \cdot \vec{A}_B \Gamma_2, \]
\[ F_{AB}^y = -2 \sqrt{S_A S_B} J_{AB} \vec{A}_A \cdot \vec{A}_B \Gamma_3, \] (39)
plane (case, the nearest neighbours of a plane \( \mathbf{k} \) in which standing spin waves only are observed, we assume \( \mathbf{k} \) cut (110) in sc and bcc crystals. As our study is focused on ferromagnetic resonance, this situation takes place for surface cut (001) in all three cubic crystal types, and for same material (4.2 The effect of various surface cuts) interface (D
\[ \mathbf{A} \]
which implies \[ 20 \], this does not affect the relative
Y
throughout the bilayer film, all the diagonal elements of bulk. However, if the spin precession ellipticity is assumed approximately homogeneous within a single sublayer, but can differ between the sublayers (i.e. \( \mathbf{\gamma} = \mathbf{\gamma}_{A(B)} \), which implies \( \mathbf{A} = \mathbf{A}_{A(B)} \)).

4.2 The effect of various surface cuts

We shall henceforth consider a bilayer film whose both sublayers are made of the same material (\( S_A = S_B \equiv S \) and \( J_A = J_B \equiv J \)), possible asymmetry being due only to interface (\( D_{int} \neq D_{int}^B, \mathbf{K}_{int}^A \neq \mathbf{K}_{int}^B \) or surface (\( \mathbf{K}_s^A \neq \mathbf{K}_s^B \)) conditions. In the simplest case, the nearest neighbours of a plane \( l \) spin lie in either the same or a neighbouring plane (\( l' = l, l \pm 1 \)), which brings the Hamiltonian matrix to a three-diagonal form (34). This situation takes place for surface cut (001) in all three cubic crystal types, and for cut (110) in sc and bcc crystals. As our study is focused on ferromagnetic resonance, in which standing spin waves only are observed, we assume \( \mathbf{k}_0 = 0 \).

In order to simplify the problem, the bilayer spin precession shall be henceforth assumed to be circular. The spin precession ellipticity is allowed for in (29) through matrix \( Y \) (34), whose diagonal and out-of-diagonal elements are defined in (37) and (39), respectively. If the quantization vector \( \mathbf{\gamma} \) has the same direction in both sublayers, then \( \mathbf{A}_A = \mathbf{A}_B \), and the out-of-diagonal elements of \( Y \) vanish, since product \( \mathbf{A}_A : \mathbf{A}_B \) is zero. The diagonal elements of \( Y \) can be divided into three groups, distinguishing bulk, surface and interface elements. Their different values are due to the fact that the ellipticity of spin precession on the surface and the interface differs from that in the bulk. However, if the spin precession ellipticity is assumed approximately homogeneous throughout the bilayer film, all the diagonal elements of \( Y \) become equal; as shown in (30), this does not affect the relative intensities of the resonance lines, and thus matrix

\[
\begin{align*}
  a_0 &= 2(z_1^A + z_2^A + z_3^A)S_A J_A - g\mu_B \mathbf{K}_s^A \cdot \mathbf{\gamma}_A - (D_s^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta_A - 1), \\
  a_1 &= 2(z_2^A + z_3^A)S_A J_A, \\
  a_2 &= 2z_3^A S_A J_A, \\
  b_2 &= 2z_3^A S_A J_A - 2z_3^B S_B J_{AB} \mathbf{\gamma}_A \cdot \mathbf{\gamma}_B, \\
  b_1 &= 2(z_2^A + z_3^A)S_A J_A - 2(z_2^B + z_3^B)S_B J_{AB} \mathbf{\gamma}_A \cdot \mathbf{\gamma}_B, \\
  b_0 &= 2(z_1^A + z_2^A + z_3^A)S_A J_A - 2(z_1^B + z_2^B + z_3^B)S_B J_{AB} \mathbf{\gamma}_A \cdot \mathbf{\gamma}_B - \\
  &\quad g\mu_B \mathbf{K}_s^A \cdot \mathbf{\gamma}_A - (D_s^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta_A - 1), \\
  c_0 &= 2(z_1^B + z_2^B + z_3^B)S_B J_B - 2(z_1^A + z_2^A + z_3^A)S_A J_{AB} \mathbf{\gamma}_A \cdot \mathbf{\gamma}_B - \\
  &\quad g\mu_B \mathbf{K}_s^B \cdot \mathbf{\gamma}_B - (D_s^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta_B - 1), \\
  c_1 &= 2(z_2^B + z_3^B)S_B J_B - 2(z_2^A + z_3^A)S_A J_{AB} \mathbf{\gamma}_A \cdot \mathbf{\gamma}_B, \\
  c_2 &= 2z_3^B S_B J_B - 2z_3^A S_A J_{AB} \mathbf{\gamma}_A \cdot \mathbf{\gamma}_B, \\
  d_2 &= 2z_3^B S_B J_B, \\
  d_1 &= 2(z_2^B + z_3^B)S_B J_B, \\
  d_0 &= 2(z_1^B + z_2^B + z_3^B)S_B J_B - g\mu_B \mathbf{K}_s^B \cdot \mathbf{\gamma}_B - (D_s^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta_B - 1).
\end{align*}
\]
Y, having no effect on the resonance spectrum, can be omitted (i.e. we can assume \( Y \equiv 0 \)). Hence, in the circular spin precession approximation, set of equations (29) can be separated, and reduced to a simple eigenvalue problem with matrix \( X \) only.

With the above-specified assumptions, for cubic crystal surface cut (001) equation (29), divided by \( 2S \), equation (29), divided by \( 2S \), becomes:

\[
\begin{vmatrix}
2 - A^A_{\text{surf}} & -1 & -1 & \ldots & -1 \\
-1 & 2 & -1 & \ldots & -1 \\
-1 & 2 & -1 & \ldots & -1 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
-1 & 2 & -1 & \ldots & 2 - A^B_{\text{surf}}
\end{vmatrix}
\]

\[
U = E'U,
\]

the Hamiltonian matrix elements being defined as follows:

\[
A^A_{\text{surf}} = 1 - \frac{g\mu_B}{2S \langle \vec{r}^A \rangle} - \frac{D^A_{\text{surf}}(S - \frac{1}{2})}{2S \langle \vec{r}^A \rangle} (3 \cos^2 \theta - 1),
\]

\[
A^A_{\text{int}} = 1 - J_{\text{int}} - \frac{g\mu_B}{2S \langle \vec{r}^A \rangle} - \frac{D^A_{\text{int}}(S - \frac{1}{2})}{2S \langle \vec{r}^A \rangle} (3 \cos^2 \theta - 1),
\]

\[
J_{\text{int}} = J_{AB}/J.
\]

Properties of function \( \Gamma \) imply that \( \Gamma_{11}(\vec{k}_\parallel = 0) = z_{ll}, \) and thus

\[
E' = E/(2S \langle \vec{r}^A \rangle),
\]

where \( \langle \vec{r}^A \rangle = z_{l,l+1} \).

Considering symmetric surface or interface conditions, we shall henceforth omit indices \( A \) and \( B \) in the respective sublayer parameter symbols, e.g. \( a^A_{l0} = a^B_{l0} = a_{l0}, \) or \( A^A_{\text{surf}} = A^B_{\text{surf}} \equiv A_{\text{surf}}. \)

Equation (41) provides the basis for our further investigation. The Hamiltonian matrix corresponds to a simplified bilayer film model on which a spin-wave spectrum can be studied as a function of three essential structural magnetic parameters: the surface parameter, \( A_{\text{surf}} \), the interface parameter, \( A_{\text{int}} \), and the interface coupling, \( J_{\text{int}} \). Below, eigenvalue problem (41) shall be solved numerically only, assuming the spin value equal to one (S=1).
5 Ambiguity in existing interpretation of bilayer FMR spectra

In the ‘reversed’ double-peak FMR spectrum, reported in bilayer films, the high-intensity line is commonly interpreted as corresponding to an acoustic mode, the low-intensity line being related to an optic mode. This implies that such ‘reversed’ spectrum should appear only in bilayers with antiferromagnetic interface coupling. Fig. 3 shows examples of bilayer resonance spectra with inverse intensity arrangement, resulting from our numerical computations; (a)-(c) were obtained assuming antiferromagnetic interface coupling, while (d)-(f) correspond to bilayers in which the interface coupling is ferromagnetic. Perpendicular configuration (θ = 0), as well as the absence of the uni-directional anisotropy (a₀ = 0) were assumed in all cases. The case depicted in Fig. 3(a) corresponds to the commonly used interpretation: optic bulk mode \( n = 1 \) has lower intensity than acoustic mode \( n = 2 \). In case (b), the high-intensity mode \( n = 2 \) is still acoustic, but the low-intensity line \( n = 1 \) corresponds to an optic interface mode. Another possibility is shown in Fig. 3(c): both first modes, \( n = 1 \) and \( n = 2 \), are of ‘optic’ nature, \( n = 2 \) being an optic bulk mode and \( n = 1 \) being an optic surface mode; the low intensity of the latter is due not only to its optic character, but also to its localization at the surface (this case has already been studied in [40]). If the interface coupling is ferromagnetic, three possibilities can occur, their examples shown in Figs. 3(d)-(f). In case (d), the low-intensity peak \( n = 1 \) corresponds to an acoustic surface mode, while the high-intensity line \( n = 3 \) is related to an acoustic bulk mode. In (e), the low-intensity mode \( n = 1 \) is acoustic and localized at the surface, and the high-intensity mode \( n = 2 \) is acoustic and localized at the interface. In (f), the low-intensity mode \( n = 1 \) is acoustic and localized at the interface, while the high-intensity peak \( n = 3 \) corresponds to an acoustic bulk mode.

These results clearly indicate that, from the theoretical point of view, the commonly used interpretation of the double-peak resonance spectra, relating the high-intensity line to an acoustic mode, and the low-intensity line to an optic mode, is not always legitimate.

6 The effect of interface coupling

In this Section we shall analyse ferromagnetic resonance spectra obtained in the so-called perpendicular configuration, i.e. for \( \theta = 0 \). For simplicity reasons, we shall assume that there is no uni-directional anisotropy on the interface \( a_0 = 0 \), and the surface spins have ‘natural’ freedom \( A_{surf} = 1 \). Thus, the only source of anisotropy

\[ A_{surf} \equiv 1 \]

This case (i.e. a bilayer with antiferromagnetic interface coupling) was also considered in our previous paper. However, as we have just recently realized, the numerical calculations performed there - for this particular case only - were incorrect due to the faulty computational program used in that paper. This resulted in misinterpretation of the energetically lowest mode as a symmetric one. Our present correct numerical calculations show that, in fact, this mode is of antisymmetric nature. This discrepancy leads to quantitatively different resonance spectra, however, it does not affect the correctness of our main hypothesis formulated in about the permissible interface-localized nature of the first resonance mode.
Figure 3: Profiles of the first (i.e. having the lowest energies) bilayer modes and the corresponding resonance spectra obtained for the parameter values specified in boxes (the values of interface parameter $A_{\text{int}}$ correspond to those assumed for $J_{\text{int}}$ and $a_{i2}$, specified on the right of the bracket). The dashed line indicates the position of a hypothetic uniform mode (UM) with $\vec{k} \equiv 0$.
(a) Asymmetric interface, antiferromagnetic interface coupling.
(b) Asymmetric interface, interface coupling still antiferromagnetic, but weaker than in (a). Note that the value of parameter $a_{i2}^B$ is negative.
Figure 3: c, d  
(c) Asymmetric surfaces, antiferromagnetic interface coupling.  
(d) Asymmetric interface, ferromagnetic interface coupling.
Figure 3: e, f
(e) Asymmetric surfaces, ferromagnetic interface coupling.
(f) Asymmetric surfaces, ferromagnetic interface coupling.
is the interface uni-axial anisotropy. Fig. 4 shows bilayer mode energies as functions of the interface coupling integral in the absence of any interface anisotropy \((a_{i2} = 0)\) (this situation was studied in [33]). If the coupling is ferromagnetic, \(J_{int}\) has no effect on the energy of the odd modes, while in the case of antiferromagnetic coupling, the modes 'insensitive' to \(J_{int}\) variations are even. This result fully corresponds to that reported in [33] and [20]. An insight into these functions is provided by the mode profiles analysed versus the interface coupling integral. Fig. 5(a) shows profiles of the six lowest modes for five different \(J_{int}\) values. In the case of ferromagnetic coupling the interface coupling integral is found to have little effect on the shape of these profiles. Mode \(n = 1\) is always a uniform mode; the even modes are antisymmetric (and as such do not appear in the resonance spectrum), and all the odd modes except \(n = 1\), though symmetric in the bilayer, are antisymmetric within each sublayer and thus do not appear in the resonance spectrum either. Hence, it is only the uniform mode that is observed in the resonance spectrum (see Fig. 5(c)). When \(J_{int} < 0\), the lowest mode is localized at the interface (the localization becoming stronger as \(J_{int}\) absolute value increases), while mode \(n = 2\) is uniform. However, also in this case only one resonance line is observed \((n = 2\), see Fig. 5(b)), as all the odd modes, including the interface mode, are antisymmetric, and thus do not appear in the resonance spectrum. Hence, the resonance spectrum is found to be insensitive to the interface coupling.
Figure 5: (a) Profiles of the six lowest modes and (b, c) the corresponding FMR spectra in a symmetric bilayer, computed assuming no interface anisotropy ($a_{i2} = 0$), the surface spins having natural freedom ($A_{surf} = 1$), for different values of interface exchange integral $J_{int}$. Each sublayer is composed of $N = 11$ lattice planes. UM denotes the resonance line corresponding to the uniform mode excitation.
integral variations (since $J_{int}$ has no effect on the symmetric modes, and affects only the antisymmetric ones).

The above conclusion can be equally deduced in a different reasoning, based on the notion of effective interface parameter, $A_{eff}$, introduced in [33]. In the considered perpendicular configuration ($\theta = 0$) this parameter is expressed as follows:

$$A_{eff} = \begin{cases} 
A^s_{eff} = 1 - 2a_i, & \text{for symmetric modes,} \\
A^a_{eff} = 1 - 2a_i - 2J_{int}, & \text{for antisymmetric modes.} 
\end{cases}$$

(46)

The above formulae directly indicate that only the antisymmetric modes depend on $J_{int}$, the symmetric modes being unrelated to it. This remains valid also when $a_i \neq 0$, as shown in Figs. 6 and 7. However, the FMR spectrum depicted there contains more than one peak, the resonance lines corresponding exclusively to either odd or even modes, for $J_{int} > 0$ or $J_{int} < 0$, respectively. In each case, as previously, the FMR spectrum does not depend on $J_{int}$ value.

7 Critical angle in bilayer resonance spectrum

The resonance spectra considered in the preceding sections were obtained for the so-called perpendicular configuration, in which the magnetization vector is oriented along the film surface normal. In this section, we are going to investigate configuration effects in resonance spectrum, due to different orientation of the magnetization vector with respect to the film surface. Our analysis shall be based on the effective interface parameter, $A_{eff}$, a concept introduced in our earlier study [33]. In a symmetric bilayer film, this parameter is expressed as follows:

$$A_{eff} = \begin{cases} 
A^s_{eff} = 1 - a_{i0} - a_{i2}(3\cos^2\theta - 1), & \text{for symmetric modes,} \\
A^a_{eff} = 1 - a_{i0} - a_{i2}(3\cos^2\theta - 1) - 2J_{int}, & \text{for antisymmetric modes.} 
\end{cases}$$

(47)

Bilayer resonance spectra are generally composed of several resonance lines (so-called spin wave resonance - SWR), though in certain conditions the spectrum reduces to a single peak. This occurs, for example, when angle $\theta$ between the magnetization vector and the surface normal takes a particular value, referred to as critical angle. The existence of the critical angle is due to the fact that the effective interface parameter (47) is a function of $\theta$. For simplicity reasons, in our investigation of the critical angle effect we shall assume that the surface parameter, $A_{surf}$, does not depend on $\theta$, and that $A_{surf} = 1$ (i.e. the spins have ‘natural’ freedom on both surfaces).

7.1 The effect of uni-axial anisotropy

In the first case to be considered, the effect of the uni-directional anisotropy shall be neglected ($a_{i0} = 0$). Figs. 8(a) and 8(c) show the intensities of mode excitations (in relation to that of the first symmetric mode, $n = 1$) as functions of angle $\theta$ in a symmetric bilayer film (composed of 22 atomic planes, 11 planes in each sublayer) with ferromagnetic interface coupling ($J_{int} = 0.3$). Graphs (a) and (c) were plotted
Figure 6: (a) Profiles of the six lowest modes and (b, c) the corresponding FMR spectra in a symmetric bilayer, computed assuming interface anisotropy $a_{12} = 0.2$, the surface spins having natural freedom ($A_{surf} = 1$), for different values of interface exchange integral $J_{int}$. Each sublayer is composed of $N = 11$ lattice planes. BM denotes a resonance line corresponding to the symmetric bulk mode excitation.
Figure 7: (a) Profiles of the six lowest modes and (b, c) the corresponding FMR spectra in a symmetric bilayer, computed assuming interface anisotropy $a_{t2} = -0.1$, the surface spins having natural freedom ($a_{surf} = 1$), for different values of interface exchange integral $J_{int}$. Each sublayer is composed of $N = 11$ lattice planes. IM denotes the resonance line corresponding to the symmetric interface mode excitation.
Figure 8: Resonance line relative intensities \textit{versus} the configuration angle in a bilayer film with symmetric interface boundary conditions and ferromagnetic coupling ($J_{\text{int}} = 0.3$). The other parameter values assumed: $N = 11$, $a_{0} = 0$, $A_{\text{surf}} = 1$. Graphs (a) and (c) show intensity ratio $I_n/I_1$ plotted \textit{versus} angle $\theta$; the corresponding profiles of the six lowest modes are shown in (b) and (d) for three different $\theta$ values.
assuming $a_{i2}^A = a_{i2}^B = -0.3$, and $a_{i2}^A = a_{i2}^B = 0.3$, respectively. The corresponding profiles of the six lowest modes are depicted in Figs. 8(b) and 8(d), for three different values of angle $\theta$: $40^o (\theta < \theta_{\text{crit}})$, $54.7^o (\theta = \theta_{\text{crit}})$ and $70^o (\theta > \theta_{\text{crit}})$. (Note that in both cases the even modes, being antisymmetric, do not appear in the resonance spectrum).

As shown in Fig. 8(b), for $a_{i2}^A = a_{i2}^B = -0.3$, mode $n = 1$, localized at the interface when $\theta < \theta_{\text{crit}}$, becomes a uniform mode for $\theta = \theta_{\text{crit}}$, and a bulk mode when $\theta > \theta_{\text{crit}}$. The other modes are of bulk nature in all $\theta$ range. The resonance intensity of the first bulk mode ($n = 3$), surpassing that of the interface mode at $\theta = 0^o$ (see Fig. 8(a)), decreases with growing $\theta$ and equals the interface mode intensity at $\theta \approx 23.4^o$. As $\theta$ continues to increase, the intensities of the bulk modes decrease still further to vanish completely at $\theta = \theta_{\text{crit}}(\approx 54.7^o)$, when mode $n = 1$ becomes uniform, and the only one to appear in the SWR spectrum. When $\theta > \theta_{\text{crit}}$, all the modes are of bulk character, the intensities of modes $n \geq 3$ being much lower than that of mode $n = 1$. Thus, the critical angle is found to separate two regions in which the relative mode intensities are radically different.

For $a_{i2}^A = a_{i2}^B = 0.3$ the situation is reversed (Figs. 8(c) and 8(d)). When $\theta < \theta_{\text{crit}}$, all the modes are of bulk character; mode $n = 1$ becomes uniform at $\theta = \theta_{\text{crit}}$ (the intensities of all other modes being zero), and localized at the interface when $\theta > \theta_{\text{crit}}$, its intensity remaining the highest in all $\theta$ range. This case is a 'mirror image' of that depicted in Figs. 8(a) and 8(b); also here, the critical angle separates two regions in which the relative mode intensities are completely different.

When the interface coupling becomes antiferromagnetic ($J_{\text{int}} = -0.3$, see Fig. 9), the angle relations of the relative mode intensities (with respect to the intensity of the first symmetric mode, $n = 2$) are in principle similar to those obtained in the case of ferromagnetic coupling, the critical angle remaining $54.7^o$.

From the numerical analysis presented above we deduce that in the case of symmetric bilayer with surface spins having natural freedom, the critical angle value is $54.7^o$ and does not depend on either the interface coupling, $J_{\text{int}}$, or the uni-axial anisotropy, $a_{i2}$. Its independence of the interface coupling is a consequence of the fact that $J_{\text{int}}$, having no effect on the symmetric modes, does not affect the bilayer resonance spectrum, as shown in Section 6. As regards the uni-axial anisotropy, its variations, though significantly modifying the SWR spectrum, do not change the $\theta_{\text{crit}}$ value, as the critical angle condition, $A^s_{\text{eff}} = 1$, is satisfied when $\cos^2 \theta - 1 = 0$ (or $\theta = 54.7^o$), $a_{i2}$ being uninvolved.

Let us now consider a bilayer film with asymmetric interface conditions. Fig. 10 shows the corresponding relative mode intensities plotted versus the configuration angle, $\theta$. In the considered asymmetric bilayer film, each sublayer is composed of 11 atomic planes, the interface coupling is antiferromagnetic ($J_{\text{int}} = -0.3$), and the assumed interface uni-axial anisotropy values in sublayers A and B are $a_{i2}^A = -0.3$ and $a_{i2}^B = 0$ or 0.2, respectively.

Asymmetric interface conditions are found to have a significant effect on the resonance spectrum. As the asymmetry becomes stronger, the relative intensities of the quasi-antisymmetric modes increase, while those of the quasi-symmetric modes decrease, but the critical angle value remains unchanged and equal to $54.7^o$, as in the
Figure 9: Resonance line relative intensities \( \text{versus} \) the configuration angle in a bilayer film with symmetric interface boundary conditions and antiferromagnetic coupling \( (J_{\text{int}} = -0.3) \). The other parameter values assumed: \( N = 11, a_{0} = 0, A_{\text{surf}} = 1 \). Graphs (a) and (c) show intensity ratio \( I_{n}/I_{2} \) plotted \( \text{versus} \) angle \( \theta \); the corresponding profiles of the six lowest modes are shown in (b) and (d) for three different \( \theta \) values.
Figure 10: Resonance line relative intensities versus the configuration angle in a bilayer film with asymmetric interface boundary conditions and antiferromagnetic coupling ($a_{i2}^A = -0.3; a_{i2}^B = 0$). The other parameter values assumed: $N = 11$, $a_{i0} = 0$, $A_{surf} = 1$. Graphs (a) and (c) show intensity ratio $I_n/I_2$ plotted versus angle $\theta$ for two different pairs $a_{i2}^A$, $a_{i2}^B$, the corresponding profiles of the six lowest modes are shown in (b) and (d) for three different $\theta$ values.
case of symmetric bilayer film. This is due to the fact that in the critical configuration a bilayer film must be fully symmetric.

Thus, in a ferromagnetic bilayer film with 'natural' surfaces and the interface properties defined by two parameters only, namely the interface coupling and the interface uni-axial anisotropy, the critical angle value is always 54.7°, for both symmetric and asymmetric interface conditions.

7.2 The effect of uni-directional anisotropy

The effect of the uni-directional anisotropy on the critical angle value in symmetric bilayer SWR spectrum is illustrated in Fig. 11. Each sublayer contains 11 atomic planes, and the coupling between them is of ferromagnetic nature ($J_{int} = 0.3$). The assumed values of interface uni-axial and uni-directional anisotropies are $a_{i2} = -0.3$ and $a_{i0} = 0.2; -0.2$, respectively.

The critical angle is found to strongly depend on the uni-directional anisotropy. The exact relation, deduced from (47), is as follows:

$$\theta_{crit} = \arccos \sqrt{\frac{1}{3} \left(1 - \frac{a_{i0}}{a_{i2}}\right)}.$$ (48)

The above relation is plotted in Fig. 12 (bold line); in the same graph, intensity ratio $I_3/I_1$ is plotted versus angle $\theta$ and uni-directional anisotropy $a_{i0}$. Function (48) follows exactly the line along which the value of function $I_3/I_1(\theta, a_{i0})$ vanishes.

Thus, a critical angle value different from 54.7°, found experimentally in a symmetric bilayer SWR spectrum, would provide evidence for co-existence of uni-axial and uni-directional anisotropies in the studied sample, the ratio of these two anisotropy types being deducible from the critical angle value (according to (48)).

8 Conclusions

The results of our theoretical investigation of bilayer FMR spectrum, presented in this study, deny the interpretation commonly used in experimental studies reporting double-peak FMR spectra in bilayer films. In this interpretation the low-intensity peak is related to an optic mode, and the high-intensity line to an acoustic mode. However, our theoretical study shows this is not always true, providing examples of double-peak spectra in which both appearing modes are acoustic or, what is more, the high-intensity peak corresponds to an optic mode. Thus, the interpretation of the observed modes cannot be unambiguous a priori, as the intensity of a resonance line depends not only on the phase shift in the sublayer magnetization precession, but also on the precession amplitude distribution, and especially on its localization.

In the investigated symmetric bilayer SWR spectra both the position and the intensity of the resonance lines are found to be independent of the interface coupling integral value. The reason is that in symmetric bilayer film the effective interface parameter depends on the interface coupling integral for antisymmetric modes only, and these modes do not appear in the SWR spectrum. Hence, symmetric bilayer film seems
Figure 11: Resonance line relative intensities versus the configuration angle in a bilayer film with symmetric interface boundary conditions and ferromagnetic coupling, assuming non-zero uni-directional anisotropy ($J_{\text{int}} = 0.3$, $a_{i0} \neq 0$). The other parameter values assumed: $N = 11$, $A_{\text{surf}} = 1$. Graphs (a) and (c) show intensity ratio $I_n/I_1$ plotted versus angle $\theta$ for two different values of $a_{i0}$; the corresponding profiles of the six lowest modes are shown in (b) and (d) for three different $\theta$ values.
Figure 12: Intensity ratio $I_3/I_1$ of the two lowest symmetric modes ($n = 1, 3$) in a symmetric bilayer SWR spectrum, plotted versus the configuration angle (angle between the film magnetization and the surface normal), $\theta$, and the interface uni-directional anisotropy, $a_{i0}$. The ferromagnetic interface exchange coupling is assumed, with interface uni-axial anisotropy value $a_{i2} = -0.3$. The bold line represents the critical angle, $\theta_{\text{crit}}$, as a function of the interface uni-directional anisotropy, $a_{i0}$.
to be particularly convenient for interface anisotropy studies. However, it should be remembered that when the interface coupling is ferromagnetic the odd modes are symmetric, and the even modes are antisymmetric, while in the case of antiferromagnetic coupling the situation is reversed: the odd modes (including the first one, with the lowest energy) are antisymmetric, the even modes being symmetric.

Moreover, we show that the critical angle effect can occur in a bilayer film even in the absence of surface anisotropy. In this case, this effect is totally due to the interface, and if the interface anisotropy is purely *uni-axial*, the critical angle value is always 54.7° and does not depend on the anisotropy value. Any deviation of the critical angle value from 54.7° involves an additional source of interface anisotropy, namely the *uni-directional* anisotropy.

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Appendix: Bilayer Hamiltonian matrix elements

Below we specify the explicit form of Hamiltonian matrix elements for cubic crystal surface cuts (001) and (110). Our formulae were derived for $\vec{k}_|| = 0$, with the quantization vectors in both sublayers assumed to be identical (i.e. $\vec{\gamma}_A = \vec{\gamma}_B$, which implies $\vec{A}_A = \vec{A}_B$), and the spin precession to be circular. On these assumptions matrices (31), (32) and (33) become:

$$X_A = \begin{bmatrix}
R_A - a & C_A \\
C_A^* & R_A \\
& \ddots & \ddots & \ddots \\
& C_A^* & R_A & C_A \\
& C_A & R_A - b 
\end{bmatrix};
X_B = \begin{bmatrix}
R_B - c & C_B \\
C_B^* & R_B \\
& \ddots & \ddots & \ddots \\
& C_B^* & R_B & C_B \\
& C_B & R_B - d 
\end{bmatrix};
X_{AB} = \begin{bmatrix}
R_B - c & C_B \\
C_B^* & R_B \\
& \ddots & \ddots & \ddots \\
& C_B^* & R_B & C_B \\
& C_B & R_B - d 
\end{bmatrix};
X_{AB} = \begin{bmatrix}
R_B - c & C_B \\
C_B^* & R_B \\
& \ddots & \ddots & \ddots \\
& C_B^* & R_B & C_B \\
& C_B & R_B - d
\end{bmatrix};$$

In all the relations detailed below index $i$ denotes the sublayer label (A or B).

**sc(001) surface cut**

$$R_i = 4S_iJ_i + g\mu_\beta(\vec{H}_i^{eff} \cdot \vec{\gamma}) + D_i \left(S_i - \frac{1}{2}\right)(3\cos^2 \theta - 1),$$

$$C_i = -2S_iJ_i,$$

$$C_{int} = -2\sqrt{S_A S_B}J_{int},$$

$$a = 2S_AJ_A - g\mu_B \vec{K}_s^A \cdot \vec{\gamma} - (D_s^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1),$$

$$b = 2S_AJ_A - 2S_BJ_{int} - g\mu_B \vec{K}_s^{int} \cdot \vec{\gamma} - (D_s^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1).$$
\begin{align*}
c &= 2S_B J_B - 2S_A J_{int} - g\mu_B \vec{K}_{int}^B \cdot \vec{\gamma} - (D_{int}^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta - 1), \\
d &= 2S_B J_B - g\mu_B \vec{K}_{s}^B \cdot \vec{\gamma} - (D_s^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta - 1). \quad (49)
\end{align*}

**bcc(001) surface cut**

\begin{align*}
R_i &= 16S_i J_i + g\mu_\beta (\vec{H}_{i eff} \cdot \vec{\gamma}) + D_i \left( \frac{S_i}{2} \right) \left( 3\cos^2 \theta - 1 \right), \\
C_i &= -8S_i J_i, \\
C_{int} &= -8\sqrt{S_A S_B} J_{int}, \\
a &= 8S_A J_A - g\mu_B \vec{K}_{s}^A \cdot \vec{\gamma} - (D_s^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1), \\
b &= 8S_A J_A - 8S_B J_{int} - g\mu_B \vec{K}_{int}^A \cdot \vec{\gamma} - (D_{int}^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1), \\
c &= 8S_B J_B - 8S_A J_{int} - g\mu_B \vec{K}_{int}^B \cdot \vec{\gamma} - (D_{int}^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta - 1), \\
d &= 8S_B J_B - g\mu_B \vec{K}_{s}^B \cdot \vec{\gamma} - (D_s^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta - 1). \quad (50)
\end{align*}

**fcc(001) surface cut**

\begin{align*}
R_i &= 16S_i J_i + g\mu_\beta (\vec{H}_{i eff} \cdot \vec{\gamma}) + D_i \left( \frac{S_i}{2} \right) \left( 3\cos^2 \theta - 1 \right), \\
C_i &= -8S_i J_i, \\
C_{int} &= -8\sqrt{S_A S_B} J_{int}, \\
a &= 8S_A J_A - g\mu_B \vec{K}_{s}^A \cdot \vec{\gamma} - (D_s^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1), \\
b &= 8S_A J_A - 8S_B J_{int} - g\mu_B \vec{K}_{int}^A \cdot \vec{\gamma} - (D_{int}^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1), \\
c &= 8S_B J_B - 8S_A J_{int} - g\mu_B \vec{K}_{int}^B \cdot \vec{\gamma} - (D_{int}^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta - 1), \\
d &= 8S_B J_B - g\mu_B \vec{K}_{s}^B \cdot \vec{\gamma} - (D_s^B - D_B)(S_B - \frac{1}{2})(3\cos^2 \theta - 1). \quad (51)
\end{align*}

**sc(110) surface cut**

\begin{align*}
R_i &= 8S_i J_i + g\mu_\beta (\vec{H}_{i eff} \cdot \vec{\gamma}) + D_i \left( \frac{S_i}{2} \right) \left( 3\cos^2 \theta - 1 \right), \\
C_i &= -4S_i J_i, \\
C_{int} &= -4\sqrt{S_A S_B} J_{int}, \\
a &= 4S_A J_A - g\mu_B \vec{K}_{s}^A \cdot \vec{\gamma} - (D_s^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1), \\
b &= 4S_A J_A - 4S_B J_{int} - g\mu_B \vec{K}_{int}^A \cdot \vec{\gamma} - (D_{int}^A - D_A)(S_A - \frac{1}{2})(3\cos^2 \theta - 1),
\end{align*}

\[ \tag{52} \]
\[ c = 4S_B J_B - 4S_A J_{\text{int}} - g\mu_B \vec{K}_{\text{int}}^B \cdot \vec{\gamma} - (D_{\text{int}}^B - D_B)(S_B - \frac{1}{2})(3\cos^2\theta - 1), \]
\[ d = 4S_B J_B - g\mu_B \vec{K}_{\text{int}}^B \cdot \vec{\gamma} - (D_{\text{int}}^B - D_B)(S_B - \frac{1}{2})(3\cos^2\theta - 1). \] (52)

bcc(110) surface cut

\[ R_i = 4S_i J_i + g\mu_\beta (\vec{H}_{\text{eff}}^i \cdot \vec{\gamma}) + D_i \left( S_i - \frac{1}{2} \right) (3\cos^2\theta - 1), \]
\[ C_i = -4S_i J_i, \]
\[ C_{\text{int}} = -4\sqrt{S_A S_B} J_{\text{int}}, \]
\[ a = 4S_A J_A - g\mu_B \vec{K}_{\text{int}}^A \cdot \vec{\gamma} - (D_{\text{int}}^A - D_A)(S_A - \frac{1}{2})(3\cos^2\theta - 1), \]
\[ b = 4S_A J_A - 4S_B J_{\text{int}} - g\mu_B \vec{K}_{\text{int}}^A \cdot \vec{\gamma} - (D_{\text{int}}^A - D_A)(S_A - \frac{1}{2})(3\cos^2\theta - 1), \]
\[ c = 4S_B J_B - 4S_A J_{\text{int}} - g\mu_B \vec{K}_{\text{int}}^B \cdot \vec{\gamma} - (D_{\text{int}}^B - D_B)(S_B - \frac{1}{2})(3\cos^2\theta - 1), \]
\[ d = 4S_B J_B - g\mu_B \vec{K}_{\text{int}}^B \cdot \vec{\gamma} - (D_{\text{int}}^B - D_B)(S_B - \frac{1}{2})(3\cos^2\theta - 1). \] (53)