

Magnetization boundary conditions at a ferromagnetic interface of finite thickness

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Abstract

We develop a systematic approach by which to derive boundary conditions at an interface between two ferromagnetic materials in the continuous medium approximation. The approach treats the interface as a two-sublattice material, although the final equations connect magnetizations outside of the interface and therefore do not explicitly depend on its structure. Instead, the boundary conditions are defined in terms of some average properties of the interface, which may also have a finite thickness. In addition to the interface anisotropy and symmetric exchange coupling, this approach allows us to take into account coupling resulting from inversion symmetry breaking in the vicinity of the interface, such as the Dzyaloshinskii-Moriya antisymmetric exchange interaction. In the case of negligible interface anisotropy and Dzyaloshinskii-Moriya exchange parameters, the derived boundary conditions represent a generalization of those proposed earlier by Barnaś and Mills and are therefore named “generalized Barnaś-Mills boundary conditions”. We demonstrate how one could use the boundary conditions to extract parameters of the interface via fitting of appropriate experimental data. The developed theory could be applied to modeling of both linear and non-linear spin waves, including exchange, dipole-exchange, magnetostatic, and retarded modes, as well as to calculations of non-uniform equilibrium micromagnetic configurations near the interface, with a direct impact on the research in magnonics and micromagnetism.

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I. Introduction

The key issue of the theory of waves propagating in non-uniform media is the nature of boundary conditions at interfaces between regions with different material properties. Owing to the unique abundance of spin-related phenomena in general and of parameters characterizing magnetic properties of materials in particular,¹⁻¹⁰ the nature of boundary conditions for spin waves¹¹⁻¹³ propagating through an interface between two magnetic media is of essential importance for magnonics and magnonic technology.^{14,15} However, despite some quite old¹⁶⁻²² and also more recent²³⁻²⁷ important results and in contrast to magnonics' sister-fields of e.g. photonics^{28,29} and phononics,^{30,31} the understanding of the nature of boundary conditions for spin waves is incomplete.³² This shortfall may hinder interpretation of experimental observations and development of theoretical models, which is unsatisfactory in view of the rapid progress observed in experimental investigations in magnonics and spintronics.³³⁻⁴¹ Indeed, the spectrum and dispersion of spin waves in planar bi-component magnonic crystals⁴² fabricated by various methods⁴³⁻⁴⁸ can now be conveniently measured e.g. using Brillouin Light Scattering (BLS),^{44-46,49} while both Ferromagnetic Resonance (FMR) and BLS characterization of thin film magnetic multilayers have long been used to extract information about interlayer exchange coupling in spintronics.⁵⁰⁻⁵⁴

The planar bi-component magnonic samples are fabricated using a combination of ion etching and lithographical tools, often exposed to air at intermediate processing steps.⁴³ Hence, it should be recognized that the interfaces in such samples might not necessarily be chemically clean and atomically sharp. Instead, they are likely to have finite thickness or even be structured at the atomic scale, which could also be done deliberately, at least in principle. This is in contrast to magnetic multilayers, which are routinely fabricated with atomic precision.^{50,51} Yet, magnetic materials can interdiffuse and / or segregate at interfaces, forming so called "magnetically dead layers".⁵⁵ Moreover, results of calculations from Ref. 56 suggest that, even when multilayer interfaces are chemically sharp, finite temperatures result in smoothing of the profiles of the magnetization magnitude and formation of magnetic "transition" layers at interfaces between the basic constituent layers in all-ferromagnetic multilayers. In addition, the itinerant nature of magnetism in transition metals and their alloys and associated spin accumulation phenomena mean that the interaction between two adjacent magnetic materials is not limited to the immediate vicinity of the geometrical (possibly, atomically sharp) interface but penetrates into their bulk regions,⁵⁷ with similar sorts of phenomena suggested to take place even at metal-dielectric interfaces.⁵⁸ These considerations show that adequate modeling of interfaces of finite thickness can be crucial for understanding and phenomenological description of micromagnetism of realistic magnonic and spintronics samples and devices.

The continuous medium theories of magnetization dynamics in samples with interfaces of finite thickness are traditionally based on solving the Landau-Lifshitz equation⁵⁹ under assumption of specific model continuous profiles for the variation of particular magnetic parameters (e.g. magnetic anisotropy) in the interface region.⁶⁰⁻⁶⁶ However, since the actual form of such profiles in realistic samples is rarely known, conclusions reached using this approach often lack generality. Thus, it would be useful to have a way of modeling interfaces of finite thickness that would be based on very general assumptions of the interface structure, thereby avoiding associated complex theoretical analyses. It is therefore tempting to account for interfacial properties via appropriate boundary conditions that would relate the magnetization on opposite sides of the interface yet outside of the transitional region in which the variation of magnetic parameters is significant. Such an approach is similar to the method of

boundary layer in fluid mechanics⁶⁷ and in fact has already been adopted in derivation of magnetization boundary conditions at boundaries of magnetic bodies.^{11,16,23,25}

In this paper, the approach proposed by Rado and Weertman for the case of *boundaries* of magnetic bodies¹⁶ is systematically developed and used to derive general boundary conditions (named “generalized Barnaś-Mills boundary conditions”, for the reasons that will become clear later) for magnetization at an *interface* of two uniaxial ferromagnetic materials. The theory is developed using the continuous medium approximation, as opposed to the often implemented discrete lattice approach,^{17,20-22,24} and is therefore mainly applicable at the mesoscale. In addition to the symmetric exchange coupling and surface anisotropy considered in this context earlier,^{11,16} we also account for the possibility of antisymmetric (Dzyaloshinskii-Moriya) exchange coupling^{68,69} in the interface region. This is accomplished by describing the interface energy as that of a two-sublattice magnetic material.¹¹ However, the resultant boundary conditions connect the magnetization defined outside of the two-sublattice interface region, i.e. in regions where magnetic parameters do not vary with coordinates. This not only allows us to use the boundary conditions without consideration of the detailed interface structure but also avoids the ambiguity in the definition of the exchange field in regions of varying exchange interaction strength pointed out in Ref. 70. The theory is developed in mind with its application to analysis of the propagation of exchange spin waves in magnonic crystals. Nonetheless, we argue that it could be adopted in a much broader range of theoretical models, as discussed below.

The paper is organized as follows. In section II, we review the key existing forms of boundary conditions and their properties. In section III, we present our theoretical approach and use it to derive boundary conditions in the most general case considered in the paper. In section IV, we offer a detailed discussion of a specific example of the proposed boundary conditions that is directly comparable to the most common results known from literature, i.e. the Hoffmann^{17,18} and Barnaś-Mills^{20,22} boundary conditions, and demonstrate how it could be used to extract parameters of the interface from experimental data analysis. Section V is devoted to general conclusions and summary.

II. Natural, Hoffmann, and Barnaś-Mills forms of magnetization boundary conditions

We begin by reviewing the derivation of the boundary conditions that naturally follow from the equation of motion of the magnetization \mathbf{M} , i.e. the Landau-Lifshitz equation,⁵⁹ in the continuous medium approximation. In the absence of dissipation, the Landau-Lifshitz equation reads

$$\frac{\partial \mathbf{M}}{\partial t} = g[\mathbf{M} \times \mathbf{H}_{\text{eff}}] \quad (1)$$

where g is the gyromagnetic ratio. The effective magnetic field \mathbf{H}_{eff} is given by¹¹

$$\mathbf{H}_{\text{eff}} = -\frac{\delta w}{\delta \mathbf{M}} = -\frac{\partial w}{\partial \mathbf{M}} + \frac{\partial}{\partial \mathbf{r}} \frac{\partial w}{\partial \left(\frac{\partial \mathbf{M}}{\partial \mathbf{r}} \right)} \quad (2)$$

where w is the magnetic energy density and \mathbf{r} is the radius vector.

The standard system used to derive the boundary conditions in the case of infinitely thin (sharp) interfaces is an infinite magnetic sample with magnetic properties described by some integrable (but not necessarily continuous) functions of the coordinate x . In particular, the saturation magnetization $M_S = M_S(x)$, the uniaxial anisotropy parameter $\beta = \beta(x)$, and the exchange parameter $\alpha = \alpha(x)$ are

assumed to vary without changing sign within a finite interval of x values, $(-\delta, \delta)$, referred to here as “interface region”, and to be constant in the rest of the sample. The semi-infinite parts of the sample to the left and to the right of the interface region are referred to as media A and B. The easy magnetization axis is assumed to be perpendicular to the interface, the normal to which is denoted here as \mathbf{n} and is parallel to the x -axis. \mathbf{H} is a uniform external magnetic field applied to the sample. Then, the total magnetic energy of the sample can be written as

$$W = \int w dx = \int dx \left\{ -\mathbf{H}\mathbf{M} - \frac{1}{2}\beta(\mathbf{M}\mathbf{n})^2 + \frac{1}{2}\alpha\left(\frac{\partial\mathbf{M}}{\partial x}\right)^2 \right\} \quad (3)$$

The corresponding effective magnetic fields \mathbf{H}_{eff} is given by

$$\mathbf{H}_{\text{eff}} = \mathbf{H} + \beta(\mathbf{M}\mathbf{n})\mathbf{n} + \frac{\partial}{\partial x}\left(\alpha\frac{\partial\mathbf{M}}{\partial x}\right) \quad (4)$$

The Landau-Lifshitz equation is of the second order in terms of the space derivatives, and so, two boundary conditions are required to tailor its solutions at the interface. The first of them is just the continuity of the direction of the magnetization. The second boundary condition follows from the form of the Landau-Lifshitz equation and is derived by its integration over the interface region, i.e.

$$\int_{-\delta}^{\delta} \frac{1}{g} \frac{\partial\mathbf{M}}{\partial t} dx = \int_{-\delta}^{\delta} [\mathbf{M} \times \mathbf{H}_{\text{eff}}] dx \quad (5)$$

The integration yields

$$\begin{aligned} \int_{-\delta}^{\delta} \frac{1}{g} \frac{\partial\mathbf{M}}{\partial t} dx &= \int_{-\delta}^{\delta} [\mathbf{M} \times (\mathbf{H} + \beta(\mathbf{M}\mathbf{n})\mathbf{n})] dx + \int_{-\delta}^{\delta} \frac{\partial}{\partial x} \left[\mathbf{M} \times \alpha \frac{\partial\mathbf{M}}{\partial x} \right] dx = \\ &= \int_{-\delta}^{\delta} [\mathbf{M} \times (\mathbf{H} + \beta(\mathbf{M}\mathbf{n})\mathbf{n})] dx + \left[\mathbf{M} \times \alpha \frac{\partial\mathbf{M}}{\partial x} \right]_{-\delta}^{\delta} \end{aligned} \quad (6)$$

where the vertical line $\mathbf{f}(x)_{-\delta}^{\delta}$ is used to denote the difference of values of the function \mathbf{f} at “points”⁷¹ δ and $-\delta$, i.e. $\mathbf{f}(x)_{-\delta}^{\delta} = \mathbf{f}(\delta) - \mathbf{f}(-\delta)$.

We take into account that the direction of the magnetization and its time derivative are both continuous functions of x , even when the magnetic media parameters (including the saturation magnetization) entering the Landau-Lifshitz equation are discontinuous. Then, we may use the mean value theorem for integration⁷² to obtain the following *exact* identity

$$\left[\mathbf{M} \times \alpha \frac{\partial\mathbf{M}}{\partial x} \right]_{-\delta}^{\delta} = 2\delta \cdot \left\langle \frac{M_s}{g} \right\rangle \left\{ \frac{\partial\mathbf{m}}{\partial t} \right\}_{\xi} - 2\delta \langle M_s \rangle \cdot [\{\mathbf{m}\}_{\xi} \times \mathbf{H}] - 2\delta \cdot \langle \beta M_s^2 \rangle \cdot \{\mathbf{m} \times (\mathbf{m}\mathbf{n})\mathbf{n}\}_{\xi} \quad (7)$$

where \mathbf{m} is the unit vector in the direction of the magnetization \mathbf{M} , brackets $\langle \rangle$ denote averaging over the interface region, and curly brackets $\{\mathbf{f}(x)\}_{\xi}$ are used to denote the value of function \mathbf{f} at point⁷¹ $\xi \in (-\delta, \delta)$. Points ξ at which the values of the various functions of the magnetization and its time derivative are taken are generally different for each of the terms, but the distinction is dropped here for clarity. The boundary conditions are now obtained by assuming that the thickness of the interface tends to zero. Then, the terms in the right hand side of the equation also tend to zero, except those

containing magnetic parameters the coordinate dependence of which diverges, as can be described by the Dirac delta-function, $\delta(x)$. Assuming that the latter is not the case,⁷³ the pair of the boundary conditions for sharp magnetic interfaces can be written as

$$\left[\{\mathbf{M}\}_{-0} \times \{\mathbf{M}\}_{+0} \right] = 0 \quad \left(\text{or} \quad \frac{\mathbf{M}}{M_s} \Big|_{-0}^{+0} = \mathbf{m}|_{-0}^{+0} = 0 \right) \quad (8)$$

$$\left[\mathbf{M} \times \alpha \frac{\partial \mathbf{M}}{\partial x} \right] \Big|_{-0}^{+0} = 0 \quad (9)$$

In the following, we will refer to this pair of equations as “natural boundary conditions”.

This method of derivation was originally used by Rado and Weertman in Ref. 16 to find the general form of boundary conditions imposed on the magnetization near a boundary of a magnetic sample, as

$$\alpha \left[\mathbf{M} \times \frac{\partial \mathbf{M}}{\partial x} \right] = -\mathbf{T} \quad (10)$$

where \mathbf{T} is the sum of all non-exchange contributions to the magnetic energy flux density across the boundary. The Rado-Weertman boundary condition (10) is obtained from equation (7) by assuming zero magnetization at one of the limits in its left hand side. The right hand side then gives \mathbf{T} , in which usually only the term containing the anisotropy constant is retained to yield the surface anisotropy and associated pinning of the magnetization.^{16,73} In this case, the condition of continuity of the magnetization direction (8) is irrelevant. Guslienko et al showed that the account of the demagnetizing fields leads to effective magneto-dipole pinning at the boundary of thin magnetic stripes.^{23,25} It would be interesting to see the results of Guslienko et al extended to the case of interface between two adjacent magnetic stripes.

The important feature of the natural boundary conditions (8-9) is that they do not depend on the strength of the exchange interaction between media A and B. The media do need to be coupled strongly enough for the equation (8) to hold, but the strength of this coupling does not need to be known exactly. Neither can it be extracted from comparison of a theory based on the boundary conditions with experiments. In contrast, theories based on lattice models of the ferromagnetic materials lead to so called “Hoffmann boundary conditions” that depend explicitly on the strength, A_{AB} , of exchange coupling between the two media^{17,18}

$$\frac{1}{2} A_{AB} \left[\{\mathbf{M}_A\}_{-\delta} \times \{\mathbf{M}_B\}_{\delta} \right] - \left\{ \left[\mathbf{M}_A \times \alpha_A \frac{\partial \mathbf{M}_A}{\partial x} \right] \right\}_{-\delta} = 0 \quad (11)$$

$$\frac{1}{2} A_{AB} \left[\{\mathbf{M}_B\}_{\delta} \times \{\mathbf{M}_A\}_{-\delta} \right] + \left\{ \left[\mathbf{M}_B \times \alpha_B \frac{\partial \mathbf{M}_B}{\partial x} \right] \right\}_{\delta} = 0 \quad (12)$$

Here, indices A and B denote parameters and variables characterizing materials A and B, respectively. The media are separated by distance 2δ . The separation can represent, for example, the thickness of a non-magnetic spacer layer inserted between media A and B, which generally does not prevent coupling between them.⁵⁰⁻⁵⁴ In the continuous medium approximation, the boundary conditions correspond to the following form for the energy of the interface coupling²¹

$$W_I = \int dx \{-A_{AB} \delta(x) \mathbf{M}_A(-\delta) \mathbf{M}_B(\delta)\} \quad (13)$$

Adding and subtracting the two equations, we can also write the system in the following symmetric form

$$A_{AB} [\{\mathbf{M}_B\}_\delta \times \{\mathbf{M}_A\}_{-\delta}] + \left\{ \left[\mathbf{M}_A \times \alpha_A \frac{\partial \mathbf{M}_A}{\partial x} \right] \right\}_{-\delta} + \left\{ \left[\mathbf{M}_B \times \alpha_B \frac{\partial \mathbf{M}_B}{\partial x} \right] \right\}_\delta = 0 \quad (14)$$

$$\left\{ \left[\mathbf{M}_B \times \alpha_B \frac{\partial \mathbf{M}_B}{\partial x} \right] \right\}_\delta - \left\{ \left[\mathbf{M}_A \times \alpha_A \frac{\partial \mathbf{M}_A}{\partial x} \right] \right\}_{-\delta} = 0 \quad (15)$$

We observe that the natural and Hoffman boundary conditions contain identical second equations, i.e. equations (9) and (15) respectively, which are responsible for ensuring that the magnetic energy flow across the interface is conserved.¹¹ However, the condition of continuity of the magnetization direction is broken in the case of the Hoffmann boundary conditions. Let us investigate this aspect somewhat closer.

In the case of $2\delta = a$, where a is the inter-atomic distance (lattice constant) at the interface, the Hoffman boundary conditions describe the interface between the media A and B in direct contact

$$\frac{2\eta}{a} \left[\{\mathbf{M}_B\}_{\frac{a}{2}} \times \{\mathbf{M}_A\}_{-\frac{a}{2}} \right] + \left\{ \left[\mathbf{M}_A \times \alpha_A \frac{\partial \mathbf{M}_A}{\partial x} \right] \right\}_{-\frac{a}{2}} + \left\{ \left[\mathbf{M}_B \times \alpha_B \frac{\partial \mathbf{M}_B}{\partial x} \right] \right\}_{\frac{a}{2}} = 0 \quad (16)$$

$$\left\{ \left[\mathbf{M}_B \times \alpha_B \frac{\partial \mathbf{M}_B}{\partial x} \right] \right\}_{\frac{a}{2}} - \left\{ \left[\mathbf{M}_A \times \alpha_A \frac{\partial \mathbf{M}_A}{\partial x} \right] \right\}_{-\frac{a}{2}} = 0 \quad (17)$$

Here, we have formally introduced a volume exchange parameter in place of the interface one as $\eta = aA_{AB}/2$. It is easy to see that the direction of the magnetization becomes continuous if one neglects in equation (16) terms of the order of $\propto \frac{\partial \mathbf{m}}{\partial x} a \propto \frac{a}{\lambda}$, where λ is the spin wave wavelength²⁴ (or any alternative appropriate quantity describing the characteristic length scale of the non-uniformity of the magnetization direction). This assumption (that the spin wave wavelength is greater than lattice constants of constituent materials) is the essence of the continuous medium approximation in magnonics, in which the natural boundary conditions (8-9) are derived. In particular, this explains why such a continuous medium approach as the plane wave method^{70,74-77} is consistent with the natural boundary conditions (8-9) but experiences difficulties adopting the notion of the interlayer exchange coupling.

In relation to the Hoffmann boundary conditions, it is important to note that, in fact, they connect solutions that are defined in different points,⁷¹ δ and $-\delta$ in the case of equations (14-15) or $a/2$ and $-a/2$ in the case of equations (16-17). Then, setting the spacer layer thickness to zero (e.g. in the long wavelength approximation) produces the natural boundary conditions, in which the information about the interlayer coupling is lost. In contrast, this limiting case is not achievable when boundary conditions of the Hoffmann form are applied formally (i.e. without taking into account the relative scales of the terms containing surface and bulk exchange parameters) to relate magnetization values that are defined in the same point,⁷¹ which can lead to erroneous conclusions as was well argued e.g. in Ref. 22. To avoid such difficulties, one needs instead to interpolate the Hoffman boundary conditions to the same point.⁷¹ For example, equations (16-17) are interpolated to $x=0$, using formulae

$$\{\mathbf{M}_B\}_{\frac{a}{2}} - \{\mathbf{M}_B\}_{+0} \approx \left\{ \frac{\partial \mathbf{M}_B}{\partial x} \right\}_{\frac{a}{2}} \approx \left\{ \frac{\partial \mathbf{M}_B}{\partial x} \right\}_{+0} \frac{a}{2} \quad \text{and} \quad \{\mathbf{M}_A\}_{-0} - \{\mathbf{M}_A\}_{-\frac{a}{2}} \approx \left\{ \frac{\partial \mathbf{M}_A}{\partial x} \right\}_{-\frac{a}{2}} \approx \left\{ \frac{\partial \mathbf{M}_A}{\partial x} \right\}_{-0} \frac{a}{2} \quad \text{and}$$

neglecting products of derivatives, to obtain^{20,22}

$$\begin{aligned} & \frac{2\eta}{a} [\{\mathbf{M}_B\}_{+0} \times \{\mathbf{M}_A\}_{-0}] + \eta \left[\left\{ \frac{\partial \mathbf{M}_B}{\partial x} \right\}_{+0} \times \{\mathbf{M}_A\}_{-0} \right] - \eta \left[\{\mathbf{M}_B\}_{+0} \times \left\{ \frac{\partial \mathbf{M}_A}{\partial x} \right\}_{-0} \right] \\ & + \left\{ \left[\mathbf{M}_A \times \alpha_A \frac{\partial \mathbf{M}_A}{\partial x} \right] \right\}_{-0} + \left\{ \left[\mathbf{M}_B \times \alpha_B \frac{\partial \mathbf{M}_B}{\partial x} \right] \right\}_{+0} = 0 \end{aligned} \quad (18)$$

$$\left\{ \left[\mathbf{M}_B \times \alpha_B \frac{\partial \mathbf{M}_B}{\partial x} \right] \right\}_{+0} - \left\{ \left[\mathbf{M}_A \times \alpha_A \frac{\partial \mathbf{M}_A}{\partial x} \right] \right\}_{-0} = 0 \quad (19)$$

In the following, we will refer to this pair of equations as ‘‘Barna’s-Mills boundary conditions’’. They are particularly useful in verifying that the limiting case of a uniform magnetic material is fulfilled.

Indeed, assuming $M_{SA} = M_{SB}$ and $\alpha_A = \alpha_B = \eta$, one can prove continuity of \mathbf{m} and $\frac{\partial \mathbf{m}}{\partial x}$ at the interface,

which is located at $x = 0$ and can now be considered as infinitely thin, in agreement with the continuous medium approximation. Once again, equation (18) demonstrate that the terms neglected in the natural boundary conditions (8-9) are of the order of $\propto \frac{a}{\lambda}$. So, the omission of the terms in the natural

boundary conditions is perfectly consistent with the continuous medium approximation, while applying the Hoffmann boundary conditions to functions defined in the one and same point⁷¹ is not. Instead, one should use Barna’s-Mills boundary conditions (18-19) if it is important to preserve the notion of the interface exchange coupling in the continuous medium theory, which is justified in the case of weak coupling. The case of a significant interface anisotropy was considered e.g. in Ref. 20.

III. Boundary conditions at diffuse interfaces between ferromagnetic media

In this section, we generalize the Barna’s-Mills boundary conditions in two aspects. Firstly, we incorporate into the boundary conditions effects associated with a broken inversion ($x \rightarrow -x$) symmetry, which is a plausible assumption at an interface between two materials even if each of them is itself centrosymmetric far from the interface. This will modify the boundary conditions to include antisymmetric exchange coupling terms,^{68,69} which are known to lead to strongly non-collinear magnetic configurations in non-centrosymmetric magnetic material. Secondly, we allow the interface to remain finite yet thin so as to formulate general boundary conditions that remove the need for assumptions of specific interface structure and thereby simplify theoretical calculations and experimental data interpretation in studies in which the structure of interfaces is a secondary topic. In the following section, we will then offer a more detailed discussion of the topic of finite thickness interfaces under some simplified assumptions. Yet, we will leave to further studies the topics of anti-symmetric interface coupling and associated non-collinear interface configurations, which are very interesting but too diverse and complex to be treated here.

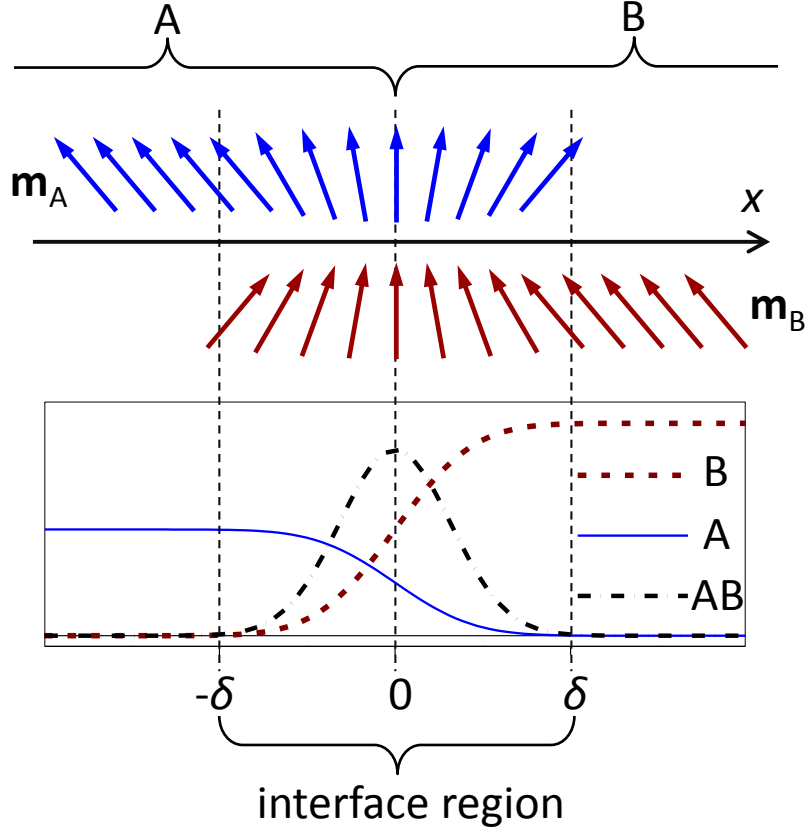


Figure 1

(Color online) The top panel shows the main idea of the two-sublattice model of the interface. The bottom panel shows schematically the assumed coordinate dependence of the magnetic parameters characterizing materials A and B, and the two-sublattice material AB of the interface region.

Thus, let us consider the interface between two semi-infinite ferromagnetic media with magnetizations \mathbf{M}_A and \mathbf{M}_B . We write the total energy of the sample in the form that takes into account the interface interaction energy as that of a two-sublattice material^{11,28}

$$\begin{aligned}
 W &= \int w dx = \\
 &= \int dx \left\{ \begin{aligned}
 &-\mathbf{H}(M_{SA}\mathbf{m}_A + M_{SB}\mathbf{m}_B) - \frac{1}{2}\beta_A M_{SA}^2 (\mathbf{m}_A \mathbf{n}_A)^2 - \frac{1}{2}\beta_B M_{SB}^2 (\mathbf{m}_B \mathbf{n}_B)^2 \\
 &+ \frac{1}{2}\alpha_A M_{SA}^2 \left(\frac{\partial \mathbf{m}_A}{\partial x}\right)^2 + \frac{1}{2}\alpha_B M_{SB}^2 \left(\frac{\partial \mathbf{m}_B}{\partial x}\right)^2 \\
 &- \beta_{AB} M_{SA} M_{SB} (\mathbf{m}_A \mathbf{n}_A)(\mathbf{m}_B \mathbf{n}_B) - A_{AB} M_{SA} M_{SB} \mathbf{m}_A \mathbf{m}_B + \alpha_{AB} M_{SA} M_{SB} \frac{\partial \mathbf{m}_A}{\partial x} \frac{\partial \mathbf{m}_B}{\partial x} \\
 &+ d_{AB} M_{SA} M_{SB} [\mathbf{m}_A \times \mathbf{m}_B] \mathbf{n} + \sigma_{AB} M_{SA} M_{SB} \mathbf{m}_A \frac{\partial \mathbf{m}_B}{\partial x} + \sigma_{BA} M_{SA} M_{SB} \mathbf{m}_B \frac{\partial \mathbf{m}_A}{\partial x}
 \end{aligned} \right\} =
 \end{aligned}$$

$$= \int dx \left\{ \begin{aligned} & -\mathbf{H}(M_{SA} \mathbf{m}_A + M_{SB} \mathbf{m}_B) - \frac{1}{2} \tilde{\beta}_A (\mathbf{m}_A \mathbf{n}_A)^2 - \frac{1}{2} \tilde{\beta}_B (\mathbf{m}_B \mathbf{n}_B)^2 \\ & + \frac{1}{2} \tilde{\alpha}_A \left(\frac{\partial \mathbf{m}_A}{\partial x} \right)^2 + \frac{1}{2} \tilde{\alpha}_B \left(\frac{\partial \mathbf{m}_B}{\partial x} \right)^2 \\ & - \tilde{\beta}_{AB} (\mathbf{m}_A \mathbf{n}_A) (\mathbf{m}_B \mathbf{n}_B) - \tilde{A}_{AB} \mathbf{m}_A \mathbf{m}_B + \tilde{\alpha}_{AB} \frac{\partial \mathbf{m}_A}{\partial x} \frac{\partial \mathbf{m}_B}{\partial x} \\ & + \tilde{d}_{AB} [\mathbf{m}_A \times \mathbf{m}_B] \mathbf{n} + \tilde{\sigma}_{AB} \mathbf{m}_A \frac{\partial \mathbf{m}_B}{\partial x} + \tilde{\sigma}_{BA} \mathbf{m}_B \frac{\partial \mathbf{m}_A}{\partial x} \end{aligned} \right\} \quad (20)$$

where all magnetic parameters are assumed to vary within the interface but to be constant in the media A and B, as summarized in Table 1 and also schematically shown in Figure 1. As in the previous section, the interface, its thickness, 2δ , and location are defined by the range of variation of the saturation magnetizations, i.e. $-\delta \leq x \leq \delta$. Naturally, the values of the magnetic parameters of a particular material cannot be defined in regions in which its saturation magnetization is equal to zero. In such cases, we assume those magnetic parameters to have zero values, too. The axes of the easy magnetization characterized by unit vectors \mathbf{n}_A and \mathbf{n}_B are allowed to have different directions in the two media. In addition, the term with coefficient $\beta_{AB}(x)$ takes into account the anisotropy energy of the interface as a two-sublattice magnetic material. d_{AB} is the parameter of the antisymmetric (Dzyaloshinskii-Moriya) exchange interaction,^{68,69} which usually does not contribute to the energy density (since the great majority of magnetic materials are centrosymmetric) but has to be taken into account near the interface where the inversion symmetry is broken. As we will show later, the phenomenological terms with coefficients $\sigma_{AB}(x)$ and $\sigma_{BA}(x)$ are responsible for non-local exchange coupling within the interface region but can be of more general nature. This is in contrast to the term containing the non-uniform exchange constant α_{AB} , which will be shown not to contribute to the energy density but is invariant and is taken into account here for the sake generality.

As before, we integrate the coupled Landau-Lifshitz equations for the two magnetizations over the interface region, and require that the integrals be equal to zero

$$\begin{aligned} \int_{-\delta}^{\delta} \left(\frac{M_{SA}}{g_A} \frac{\partial \mathbf{m}_A}{\partial t} - [M_{SA} \mathbf{m}_A \times \mathbf{H}_{\text{effA}}] \right) dx &= 0, \\ \int_{-\delta}^{\delta} \left(\frac{M_{SB}}{g_B} \frac{\partial \mathbf{m}_B}{\partial t} - [M_{SB} \mathbf{m}_B \times \mathbf{H}_{\text{effB}}] \right) dx &= 0 \end{aligned} \quad (21)$$

Table 1. The character of variation of the magnetic parameters in the vicinity of the interface is described.

Magnetic parameter	Notations			Corresponding contributions to the total energy density
	material A $x \leq -\delta$	interface $-\delta \leq x \leq \delta$	material B $x \geq \delta$	
Saturation magnetization	M_{SA}	$M_{SA}(x)$	0	
	0	$M_{SB}(x)$	M_{SB}	
Gyromagnetic ratio	g_A	$g(x)$	g_B	
Uniform exchange between sublattices	0	$A_{AB}(x)$	0	$-A_{AB}M_{SA}M_{SB}\mathbf{m}_A\mathbf{m}_B$
Non-uniform exchange between sublattices	0	$\alpha_{AB}(x)$	0	$\alpha_{AB}M_{SA}M_{SB}\frac{\partial\mathbf{m}_A}{\partial x}\frac{\partial\mathbf{m}_B}{\partial x}$
Non-uniform exchange	α_A	$\alpha_A(x)$	0	$\frac{1}{2}\alpha_A M_{SA}^2\left(\frac{\partial\mathbf{m}_A}{\partial x}\right)^2$
	0	$\alpha_B(x)$	α_B	$\frac{1}{2}\alpha_B M_{SB}^2\left(\frac{\partial\mathbf{m}_B}{\partial x}\right)^2$
Uniaxial magnetic anisotropy (two-sublattice contribution), value	0	$\beta_{AB}(x)$	0	$-\beta_{AB}M_{SA}M_{SB}(\mathbf{m}_A\mathbf{n}_A)(\mathbf{m}_B\mathbf{n}_B)$
Uniaxial magnetic anisotropy, values	β_A	$\beta_A(x)$	0	$-\frac{1}{2}\beta_A M_{SA}^2(\mathbf{m}_A\mathbf{n}_A)^2$
	0	$\beta_B(x)$	β_B	$-\frac{1}{2}\beta_B M_{SB}^2(\mathbf{m}_B\mathbf{n}_B)^2$
Uniaxial magnetic anisotropy, axes	\mathbf{n}_A	$\mathbf{n}_A(x)$	not defined	$-\frac{1}{2}\beta_A M_{SA}^2(\mathbf{m}_A\mathbf{n}_A)^2$
	not defined	$\mathbf{n}_B(x)$	\mathbf{n}_B	$-\frac{1}{2}\beta_B M_{SB}^2(\mathbf{m}_B\mathbf{n}_B)^2$
Antisymmetric (Dzyaloshinskii-Moriya) exchange interaction, value	0	$d_{AB}(x)$	0	$d_{AB}M_{SA}M_{SB}[\mathbf{m}_A \times \mathbf{m}_B] \mathbf{n}$
Phenomenological non-local exchange coupling terms	0	$\sigma_{AB}(x)$	0	$\sigma_{AB}M_{SA}M_{SB}\mathbf{m}_A\frac{\partial\mathbf{m}_B}{\partial x}$
	0	$\sigma_{BA}(x)$	0	$\sigma_{BA}M_{SA}M_{SB}\mathbf{m}_B\frac{\partial\mathbf{m}_A}{\partial x}$

The effective magnetic fields \mathbf{H}_{effA} and \mathbf{H}_{effB} act on magnetizations \mathbf{M}_A and \mathbf{M}_B , respectively, and are calculated as

$$\mathbf{H}_{\text{effA}} = -\frac{\delta w}{M_{\text{SA}} \delta \mathbf{m}_A} = \frac{1}{M_{\text{SA}}} \left(\begin{array}{l} \mathbf{H} M_{\text{SA}} + \tilde{\beta}_A (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_A + \frac{\partial}{\partial x} \left(\tilde{\alpha}_A \frac{\partial \mathbf{m}_A}{\partial x} \right) \\ + \tilde{\beta}_{\text{AB}} (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_A + \tilde{A}_{\text{AB}} \mathbf{m}_B + \frac{\partial}{\partial x} \left(\tilde{\alpha}_{\text{AB}} \frac{\partial \mathbf{m}_B}{\partial x} \right) \\ - \tilde{d}_{\text{AB}} [\mathbf{m}_B \times \mathbf{n}] - \tilde{\sigma}_{\text{AB}} \frac{\partial \mathbf{m}_B}{\partial x} + \frac{\partial}{\partial x} (\tilde{\sigma}_{\text{BA}} \mathbf{m}_B) \end{array} \right) \quad (22)$$

$$\mathbf{H}_{\text{effB}} = -\frac{\delta w}{M_{\text{SB}} \delta \mathbf{m}_B} = \frac{1}{M_{\text{SB}}} \left(\begin{array}{l} \mathbf{H} M_{\text{SB}} + \tilde{\beta}_B (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_B + \frac{\partial}{\partial x} \left(\tilde{\alpha}_B \frac{\partial \mathbf{m}_B}{\partial x} \right) \\ + \tilde{\beta}_{\text{AB}} (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_B + \tilde{A}_{\text{AB}} \mathbf{m}_A + \frac{\partial}{\partial x} \left(\tilde{\alpha}_{\text{AB}} \frac{\partial \mathbf{m}_A}{\partial x} \right) \\ - \tilde{d}_{\text{AB}} [\mathbf{n} \times \mathbf{m}_A] + \frac{\partial}{\partial x} (\tilde{\sigma}_{\text{AB}} \mathbf{m}_A) - \tilde{\sigma}_{\text{BA}} \frac{\partial \mathbf{m}_A}{\partial x} \end{array} \right) \quad (23)$$

Isolating full derivatives in the integrands, the integrals are calculated as

$$\begin{aligned} & \int_{-\delta}^{\delta} \left(\frac{M_{\text{SA}}}{g_A} \frac{\partial \mathbf{m}_A}{\partial t} - [M_{\text{SA}} \mathbf{m}_A \times \mathbf{H}] \right) dx = \\ & = \int_{-\delta}^{\delta} \left(\begin{array}{l} \tilde{\beta}_A [\mathbf{m}_A \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_A] + \tilde{\beta}_{\text{AB}} [\mathbf{m}_A \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_A] \\ + \tilde{A}_{\text{AB}} [\mathbf{m}_A \times \mathbf{m}_B] - \tilde{d}_{\text{AB}} [\mathbf{m}_A \times [\mathbf{m}_B \times \mathbf{n}]] \\ - \tilde{\alpha}_{\text{AB}} \left[\frac{\partial \mathbf{m}_A}{\partial x} \times \frac{\partial \mathbf{m}_B}{\partial x} \right] - \tilde{\sigma}_{\text{AB}} \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_B}{\partial x} \right] - \tilde{\sigma}_{\text{BA}} \left[\frac{\partial \mathbf{m}_A}{\partial x} \times \mathbf{m}_B \right] \end{array} \right) dx \\ & + \left[\mathbf{m}_A \times \left(\tilde{\alpha}_A \frac{\partial \mathbf{m}_A}{\partial x} + \tilde{\alpha}_{\text{AB}} \frac{\partial \mathbf{m}_B}{\partial x} + \tilde{\sigma}_{\text{BA}} \mathbf{m}_B \right) \right]_{-\delta}^{\delta} \end{aligned} \quad (24)$$

$$\begin{aligned} & \int_{-\delta}^{\delta} \left(\frac{M_{\text{SB}}}{g_B} \frac{\partial \mathbf{m}_B}{\partial t} - [M_{\text{SB}} \mathbf{m}_B \times \mathbf{H}] \right) dx = \\ & = \int_{-\delta}^{\delta} \left(\begin{array}{l} \tilde{\beta}_B [\mathbf{m}_B \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_B] + \tilde{\beta}_{\text{AB}} [\mathbf{m}_B \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_B] \\ + \tilde{A}_{\text{AB}} [\mathbf{m}_B \times \mathbf{m}_A] - \tilde{d}_{\text{AB}} [\mathbf{m}_B \times [\mathbf{n} \times \mathbf{m}_A]] \\ - \tilde{\alpha}_{\text{AB}} \left[\frac{\partial \mathbf{m}_B}{\partial x} \times \frac{\partial \mathbf{m}_A}{\partial x} \right] - \tilde{\sigma}_{\text{AB}} \left[\frac{\partial \mathbf{m}_B}{\partial x} \times \mathbf{m}_A \right] - \tilde{\sigma}_{\text{BA}} \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \end{array} \right) dx \\ & + \left[\mathbf{m}_B \times \left(\tilde{\alpha}_B \frac{\partial \mathbf{m}_B}{\partial x} + \tilde{\alpha}_{\text{AB}} \frac{\partial \mathbf{m}_A}{\partial x} + \tilde{\sigma}_{\text{AB}} \mathbf{m}_A \right) \right]_{-\delta}^{\delta} \end{aligned} \quad (25)$$

Again taking into account that the direction of the magnetization and its time derivative are both continuous functions of x , even when the magnetic parameters entering the Landau-Lifshitz equation are discontinuous, we use the mean value theorem for integration to obtain the following *exact* identities

$$\begin{aligned}
& \left(\left\langle \frac{M_{SA}}{g_A} \right\rangle \left\{ \frac{\partial \mathbf{m}_A}{\partial t} \right\}_{\xi} - [\langle \mathbf{m}_A M_{SA} \rangle \times \mathbf{H}] \right) 2\delta = \\
& \left(\begin{aligned} & \langle \tilde{\beta}_A \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_A] \}_{\xi} + \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_A] \}_{\xi} \\ & + \langle \tilde{A}_{AB} \rangle \{ [\mathbf{m}_A \times \mathbf{m}_B] \}_{\xi} - \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_A \times [\mathbf{m}_B \times \mathbf{n}]] \}_{\xi} \\ & - \langle \tilde{\alpha}_{AB} \rangle \left\{ \left[\frac{\partial \mathbf{m}_A}{\partial x} \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_{\xi} - \langle \tilde{\sigma}_{AB} \rangle \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_{\xi} - \langle \tilde{\sigma}_{BA} \rangle \left\{ \left[\frac{\partial \mathbf{m}_A}{\partial x} \times \mathbf{m}_B \right] \right\}_{\xi} \end{aligned} \right) 2\delta \quad (26) \\
& + \left[\mathbf{m}_A \times \left(\tilde{\alpha}_A \frac{\partial \mathbf{m}_A}{\partial x} + \tilde{\alpha}_{AB} \frac{\partial \mathbf{m}_B}{\partial x} + \tilde{\sigma}_{BA} \mathbf{m}_B \right) \right]_{-\delta}^{\delta}
\end{aligned}$$

$$\begin{aligned}
& \left(\left\langle \frac{M_{SB}}{g_B} \right\rangle \left\{ \frac{\partial \mathbf{m}_B}{\partial t} \right\}_{\xi} - [\langle \mathbf{m}_B M_{SB} \rangle \times \mathbf{H}] \right) 2\delta = \\
& \left(\begin{aligned} & \langle \tilde{\beta}_B \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_B] \}_{\xi} + \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_B] \}_{\xi} \\ & + \langle \tilde{A}_{AB} \rangle \{ [\mathbf{m}_B \times \mathbf{m}_A] \}_{\xi} - \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_B \times [\mathbf{n} \times \mathbf{m}_A]] \}_{\xi} \\ & - \langle \tilde{\alpha}_{AB} \rangle \left\{ \left[\frac{\partial \mathbf{m}_B}{\partial x} \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{\xi} - \langle \tilde{\sigma}_{AB} \rangle \left\{ \left[\frac{\partial \mathbf{m}_B}{\partial x} \times \mathbf{m}_A \right] \right\}_{\xi} - \langle \tilde{\sigma}_{BA} \rangle \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{\xi} \end{aligned} \right) 2\delta \quad (27) \\
& + \left[\mathbf{m}_B \times \left(\tilde{\alpha}_B \frac{\partial \mathbf{m}_B}{\partial x} + \tilde{\alpha}_{AB} \frac{\partial \mathbf{m}_A}{\partial x} + \tilde{\sigma}_{AB} \mathbf{m}_A \right) \right]_{-\delta}^{\delta}
\end{aligned}$$

Again, we note that points ξ at which the values of the various functions of the magnetization and its time derivatives are taken are generally different for each of the terms. The distinction has however been lost here for clarity.

Let us assume that the magnetization directions vary slowly in space on the interval $(-\delta, \delta)$, so that we can neglect terms containing products of space derivatives (e.g. $\propto \left[\frac{\partial \mathbf{m}_A}{\partial x} \times \frac{\partial \mathbf{m}_B}{\partial x} \right]$). Next, to obtain the boundary conditions, we assume that the thickness of the boundary 2δ is small enough to neglect the left hand side of the equations in comparison to their right hand sides. Indeed, the last terms on the right of each of the equations remain finite even if $\delta = 0$. As to the terms containing products $\langle \tilde{\beta}_A \rangle \delta$, $\langle \tilde{\beta}_B \rangle \delta$, $\langle \tilde{\beta}_{AB} \rangle \delta$, $\langle \tilde{A}_{AB} \rangle \delta$, $\langle \tilde{d}_{AB} \rangle \delta$, $\langle \tilde{\sigma}_{AB} \rangle \delta$, and $\langle \tilde{\sigma}_{BA} \rangle \delta$, it is the aim of this derivation to consider the case when they remain finite. Also, we have to take into account the spatial dependence of parameters $\tilde{\alpha}_A$, $\tilde{\alpha}_B$, $\tilde{\alpha}_{AB}$, $\tilde{\sigma}_{AB}$, and $\tilde{\sigma}_{BA}$, and therefore to note that only parameters $\tilde{\alpha}_A$ and $\tilde{\alpha}_B$ remain finite at the limits of integration, i.e. at points $-\delta$ and δ , respectively. Then we obtain

$$\left(\begin{array}{l} \langle \tilde{\beta}_A \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_A] \}_\xi + \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_A] \}_\xi \\ + \langle \tilde{A}_{AB} \rangle \{ [\mathbf{m}_A \times \mathbf{m}_B] \}_\xi - \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_A \times [\mathbf{m}_B \times \mathbf{n}]] \}_\xi \\ - \langle \tilde{\sigma}_{AB} \rangle \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\xi - \langle \tilde{\sigma}_{BA} \rangle \left\{ \left[\frac{\partial \mathbf{m}_A}{\partial x} \times \mathbf{m}_B \right] \right\}_\xi \end{array} \right) 2\delta = \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-\delta} \quad (28)$$

$$\left(\begin{array}{l} \langle \tilde{\beta}_B \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_B] \}_\xi + \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_B] \}_\xi \\ + \langle \tilde{A}_{AB} \rangle \{ [\mathbf{m}_B \times \mathbf{m}_A] \}_\xi - \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_B \times [\mathbf{n} \times \mathbf{m}_A]] \}_\xi \\ - \langle \tilde{\sigma}_{AB} \rangle \left\{ \left[\frac{\partial \mathbf{m}_B}{\partial x} \times \mathbf{m}_A \right] \right\}_\xi - \langle \tilde{\sigma}_{BA} \rangle \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_\xi \end{array} \right) 2\delta = -\tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\delta \quad (29)$$

By subtracting and adding the two equations, the system can also be written as

$$\begin{aligned} & 4\delta \cdot \langle \tilde{A}_{AB} \rangle \{ [\mathbf{m}_B \times \mathbf{m}_A] \}_\xi - 4\delta \cdot \langle \tilde{\sigma}_{AB} \rangle \left\{ \left[\frac{\partial \mathbf{m}_B}{\partial x} \times \mathbf{m}_A \right] \right\}_\xi - 4\delta \cdot \langle \tilde{\sigma}_{BA} \rangle \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_\xi \\ & + \tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\delta + \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-\delta} = \\ & = \left(\begin{array}{l} \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_B \times [\mathbf{n} \times \mathbf{m}_A]] \}_\xi - \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_A \times [\mathbf{m}_B \times \mathbf{n}]] \}_\xi \\ + \langle \tilde{\beta}_A \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_A] \}_\xi - \langle \tilde{\beta}_B \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_B] \}_\xi \\ + \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_A] \}_\xi - \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_B] \}_\xi \end{array} \right) 2\delta \end{aligned} \quad (30)$$

$$\begin{aligned} & \tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\delta - \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-\delta} = \\ & = \left(\begin{array}{l} \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_B \times [\mathbf{n} \times \mathbf{m}_A]] \}_\xi + \langle \tilde{d}_{AB} \rangle \{ [\mathbf{m}_A \times [\mathbf{m}_B \times \mathbf{n}]] \}_\xi \\ - \langle \tilde{\beta}_A \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_A] \}_\xi - \langle \tilde{\beta}_B \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_B] \}_\xi \\ - \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_A \times (\mathbf{m}_B \mathbf{n}_B) \mathbf{n}_A] \}_\xi - \langle \tilde{\beta}_{AB} \rangle \{ [\mathbf{m}_B \times (\mathbf{m}_A \mathbf{n}_A) \mathbf{n}_B] \}_\xi \end{array} \right) 2\delta \end{aligned} \quad (31)$$

Finally, the sought boundary conditions are obtained using one of the following approaches. In the first of them, identities $\mathbf{m}_B(\delta) - \mathbf{m}_B(\xi) \approx \left\{ \frac{\partial \mathbf{m}_B}{\partial x} \right\}_\delta (\delta - \xi) \approx \left\{ \frac{\partial \mathbf{m}_B}{\partial x} \right\}_\xi (\delta - \xi)$ and $\mathbf{m}_A(\xi) - \mathbf{m}_A(-\delta) \approx \left\{ \frac{\partial \mathbf{m}_A}{\partial x} \right\}_{-\delta} (\xi + \delta) \approx \left\{ \frac{\partial \mathbf{m}_A}{\partial x} \right\}_\xi (\xi + \delta)$ are used to express quantities defined at intermediate points ξ in terms of the values of either \mathbf{m}_B and $\frac{\partial \mathbf{m}_B}{\partial x}$ defined at point δ and \mathbf{m}_A and $\frac{\partial \mathbf{m}_A}{\partial x}$ defined at point $-\delta$.⁷¹ All terms containing products of derivatives are neglected, as we have already done once. The resultant boundary conditions can be used to connect the solutions defined on

the opposite sides of the interface of finite thickness, i.e. in the same way as Hoffmann boundary conditions are defined and used.

In the second approach, identities $\mathbf{m}_B(\delta) - \mathbf{m}_B(0) \approx \left\{ \frac{\partial \mathbf{m}_B}{\partial x} \right\}_\delta \delta \approx \left\{ \frac{\partial \mathbf{m}_B}{\partial x} \right\}_0 \delta$,
 $\mathbf{m}_A(0) - \mathbf{m}_A(-\delta) \approx \left\{ \frac{\partial \mathbf{m}_A}{\partial x} \right\}_{-\delta} \delta \approx \left\{ \frac{\partial \mathbf{m}_A}{\partial x} \right\}_0 \delta$, and $\mathbf{m}_{B(A)}(\xi) - \mathbf{m}_{B(A)}(0) \approx \left\{ \frac{\partial \mathbf{m}_{B(A)}}{\partial x} \right\}_\xi \xi \approx \left\{ \frac{\partial \mathbf{m}_{B(A)}}{\partial x} \right\}_0 \xi$

are used to express quantities defined at points δ , $-\delta$ or ξ in terms of their and their derivatives' values at $x = 0$. As before, terms containing products of derivatives are neglected. The boundary conditions defined in this way connect the solutions defined in the immediate vicinity (0 ± 0) of the same point of the sample,⁷¹ i.e. in the same way as Barnaś-Mills boundary conditions are defined and used.

The boundary conditions obtained using any of the two methods outlined above connect solutions defined on the opposite sides of the interface of finite thickness, thereby avoiding detailed consideration of the interface structure. It is important to note however that, in both approaches, the formal limit of $2\delta \equiv 0$ results in the loss of coupling between media A and B, and so, δ should remain finite. In terms of the usage, the relation between the boundary conditions defined using the two methods is the same as that between the Hoffmann boundary conditions (14-15), connecting solutions defined at distance a , and the Barnaś-Mills boundary conditions (18-19), connecting solutions in the same point.⁷¹

The form of the resulting boundary conditions is very complex in general. So, in the next section, we will discuss their properties in one specific yet very important limiting case. Firstly, we will assume that the sample is characterized by negligible anisotropy both in the bulk of the media A and B and at the interface. Secondly, we will neglect the Dzyaloshinskii-Moriya exchange interaction but will include the effects related to the loss of the inversion symmetry described by terms containing $\tilde{\sigma}_{AB}$ and $\tilde{\sigma}_{BA}$. In this approximation, the system of equations (30-31) reduces to

$$4\delta \cdot \langle \tilde{A}_{AB} \rangle \left\{ \left[\mathbf{m}_B \times \mathbf{m}_A \right] \right\}_\xi - 4\delta \cdot \langle \tilde{\sigma}_{AB} \rangle \left\{ \left[\frac{\partial \mathbf{m}_B}{\partial x} \times \mathbf{m}_A \right] \right\}_\xi - 4\delta \cdot \langle \tilde{\sigma}_{BA} \rangle \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_\xi + \tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\delta + \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-\delta} = 0 \quad (32)$$

$$\tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\delta - \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-\delta} = 0 \quad (33)$$

As a result of the approximations made, this system of boundary conditions does not account for the following two major classes of phenomena. Firstly, it does not account for any pinning at the interface due to the surface (interface) anisotropy, which could be described by ensuring that the products $\langle \tilde{\beta}_A \rangle \delta$, $\langle \tilde{\beta}_B \rangle \delta$, $\langle \tilde{\beta}_{AB} \rangle \delta$ remain significant when δ is reduced. The topic is treated e.g. in Ref. 20. Secondly, it does not describe any non-collinearity.⁷⁸ Indeed, even if the easy magnetization axes on the opposite sides of and within the interface were all parallel to each other and to the applied magnetic field, the coupling terms containing the product $\langle \tilde{d}_{AB} \rangle \delta$ could result in a non-collinear alignment of the magnetization vectors on opposite sides from the interface. Both sets of phenomena are certainly

interesting and most likely very rich (see e.g. the recent results from Refs. 79-81) but are beyond the scope of this paper. Nonetheless, using the same procedures outlined above, the corresponding boundary conditions can be obtained from equations (30-31) with all necessary terms (e.g. the those responsible for interface anisotropy and / or Dzyaloshinskii-Moriya exchange coupling) retained as required for a given model.

IV. Discussion

By performing the interpolation operations described in the previous section, we can rewrite the system of equations (32-33) as

$$A_{AB}^* \left[\{\mathbf{m}_B\}_\delta \times \{\mathbf{m}_A\}_{-\delta} \right] - \sigma_{AB}^* \left[\left\{ \frac{\partial \mathbf{m}_B}{\partial x} \right\}_\delta \times \{\mathbf{m}_A\}_{-\delta} \right] - \sigma_{BA}^* \left[\{\mathbf{m}_B\}_\delta \times \left\{ \frac{\partial \mathbf{m}_A}{\partial x} \right\}_{-\delta} \right] + \tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\delta + \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-\delta} = 0 \quad (34)$$

$$\tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_\delta - \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-\delta} = 0 \quad (35)$$

where we have denoted $A_{AB}^* = 4\delta \cdot \langle \tilde{A}_{AB} \rangle$, $\sigma_{AB}^* = 4\delta \cdot (\langle \tilde{\sigma}_{AB} \rangle + \langle \tilde{A}_{AB} \rangle (\delta - \xi))$ and $\sigma_{BA}^* = 4\delta \cdot (\langle \tilde{\sigma}_{BA} \rangle - \langle \tilde{A}_{AB} \rangle (\xi + \delta))$. ξ is the coordinate of the point in which the cross-product $[\mathbf{m}_B \times \mathbf{m}_A]$ is defined in equation (32).⁸² Here, vectors \mathbf{m}_A and \mathbf{m}_B are defined outside of the “two-sublattice” region and therefore are physically meaningful. The material parameters in equations (34-35) have physical meaning of effective values obtained by averaging over the interface region.

Alternatively, we can rewrite the system as

$$A_{AB}^* \left[\{\mathbf{m}_B\}_{+0} \times \{\mathbf{m}_A\}_{-0} \right] - \sigma_{AB}^{**} \left[\left\{ \frac{\partial \mathbf{m}_B}{\partial x} \right\}_{+0} \times \{\mathbf{m}_A\}_{-0} \right] - \sigma_{BA}^{**} \left[\{\mathbf{m}_B\}_{+0} \times \left\{ \frac{\partial \mathbf{m}_A}{\partial x} \right\}_{-0} \right] + \tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_{+0} + \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-0} = 0 \quad (36)$$

$$\tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right] \right\}_{+0} - \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right] \right\}_{-0} = 0 \quad (37)$$

where we have denoted $\sigma_{AB}^{**} = \sigma_{AB}^* - A_{AB}^* \delta = 4\delta \cdot (\langle \tilde{\sigma}_{AB} \rangle - \langle \tilde{A}_{AB} \rangle \xi)$ and $\sigma_{BA}^{**} = \sigma_{BA}^* + A_{AB}^* \delta = 4\delta \cdot (\langle \tilde{\sigma}_{BA} \rangle - \langle \tilde{A}_{AB} \rangle \xi)$. Here, in contrast to equations (34-35), vectors \mathbf{m}_A and \mathbf{m}_B do not describe directions of any real magnetization vectors defined at point $x=0$ but represent extrapolated directions of the real magnetization vectors defined just outside of the interface region.

The two systems of boundary conditions, i.e. (34-35) and (36-37) have similar form, which is also similar to that of the Barnaś-Mills boundary conditions (18-19). The boundary conditions (36-37) have fewer parameters to describe the interface, since they do not explicitly depend on its thickness, and so,

they should be preferable in use, e.g. in modelling experimental data. In particular, treating σ_{AB}^{**} , σ_{BA}^{**} , and A_{AB}^* formally as fitting parameters, one can use their values to extract important information about the magnetic interfaces. In the following, we refer to the equations (36-37) as to ‘‘generalized Barna’s-Mills boundary conditions’’.

The relation between σ_{AB}^{**} , σ_{BA}^{**} , and A_{AB}^* is worthwhile a more detailed consideration. Let us assume that their values have been obtained by fitting experimental data to a theory based upon boundary conditions (36-37). Following Mills,²² we note that the continuous medium approach requires that vectors \mathbf{m}_A and \mathbf{m}_B in the energy density term $-\tilde{A}_{AB}\mathbf{m}_A\mathbf{m}_B$ be defined at the same points of space, while in reality, they are defined in different points of the magnetic lattice, e.g. x_A and x_B . So, with accuracy to terms linear in magnetization derivatives, the corresponding energy density term could be expanded as $\approx -\tilde{A}_{AB}\left(\{\mathbf{m}_A\}_{x_0}\{\mathbf{m}_B\}_{x_0} + \{\mathbf{m}_A\}_{x_0}\left\{\frac{\partial\mathbf{m}_B}{\partial x}\right\}_{x_0}(x_B-x_0) + \{\mathbf{m}_B\}_{x_0}\left\{\frac{\partial\mathbf{m}_A}{\partial x}\right\}_{x_0}(x_A-x_0)\right)$, where x_0 is some point in the magnetic unit cell. These additional terms have the same form as the terms with coefficients $\sigma_{AB}(x)$ and $\sigma_{BA}(x)$ introduced earlier into the energy density (equation (20)) phenomenologically. So, one can expect that parameters σ_{AB}^{**} and σ_{BA}^{**} of this origin should yield

$$\frac{2|\sigma_{AB}^{**} - \sigma_{BA}^{**}|}{A_{AB}^*} = \frac{2|\langle\sigma_{AB}\rangle - \langle\sigma_{BA}\rangle|}{\langle\tilde{A}_{AB}\rangle} = \frac{2|\langle\sigma_{AB} - \sigma_{BA}\rangle|}{\langle\tilde{A}_{AB}\rangle} \equiv a_{\text{eff}},$$

where a_{eff} is the effective magnetic lattice constant in the interface region. The case of $\sigma_{AB}^{**} + \sigma_{BA}^{**} = 0$ would imply the Barna’s-Mills boundary conditions. Finally, assuming that an estimate, η_{eff} , for the average volume exchange parameter for the interface is available, the effective thickness of the interface can be estimated as $2\delta_{\text{eff}} \equiv \frac{A_{AB}^* a_{\text{eff}}}{M_{SA} M_{SB} \eta_{\text{eff}}}$.

The value of η_{eff} could be derived from microscopic or ab-initio calculations, or even estimated as an arithmetic average of the corresponding parameters of materials A and B. The resulting estimate for the interface thickness cannot, of course, be smaller than the effective magnetic lattice constant, which would indicate that the volume exchange parameter, η_{eff} , and / or the saturation magnetization values, M_{SA} and M_{SB} , in the interface region are significantly reduced relative to the estimations.

It could be tempting to assume in equations (32-33) that δ tends to zero while product $\langle\tilde{A}_{AB}\rangle\delta$ remains finite, and therefore to use the following system of equations

$$A_{AB}^* \left\{ \left[\mathbf{m}_B \times \mathbf{m}_A \right]_0 \right\} + \tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right]_0 \right\} + \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right]_0 \right\} = 0 \quad (38)$$

$$\tilde{\alpha}_B \left\{ \left[\mathbf{m}_B \times \frac{\partial \mathbf{m}_B}{\partial x} \right]_0 \right\} - \tilde{\alpha}_A \left\{ \left[\mathbf{m}_A \times \frac{\partial \mathbf{m}_A}{\partial x} \right]_0 \right\} = 0 \quad (39)$$

as boundary conditions. However, as we have already noted and as it has been discussed in Refs. 20,22, this form of boundary conditions leaves questions with regard to the microscopic interpretation of the exchange coupling constant A_{AB}^* . So, either the natural boundary conditions (8-9) or the generalized Barna’s-Mills boundary conditions (36-37) should be used instead.

Let us discuss systems to which the generalized Barnaś-Mills boundary conditions could be applied. A straightforward example is an interface between two materials that can be described as Heisenberg ferromagnets, provided there are reasons to expect that some interdiffusion of the two atomic species has taken place in the interface region. Pure Heisenberg ferromagnets are relatively rare. However, fortunately, there is a plenty of other magnetic materials (notably, including many ferrimagnets and itinerant ferromagnets) that demonstrate behavior consistent with predictions of Heisenberg-type lattice models or theories based on the Landau-Lifshitz equations, which is evident e.g. from the wide use of the Hoffman boundary conditions. Hence, we believe that the generalized Barnaś-Mills boundary conditions will have a similar area of applicability. Indeed, in spite of the artificial separation of two magnetic sublattices in the interface region, the result is expressed only via magnetizations defined outside of the interface (equations (34-35)) or their extrapolations (equations (36-37)). At the same time, the excitation of antiferromagnetic resonances is excluded by neglecting the terms containing time derivatives in equations (26-27). The non-collinear static alignment of the two magnetic sublattices in the interface region is just a way of describing the magnetic ground state, while the actual distribution of the magnetization is given by the net magnetization, i.e. by $\mathbf{m}_A M_{SA} + \mathbf{m}_B M_{SA}$. Thus, to list a few topics of relevance, we expect the problems of spin wave scattering from interfaces⁸³⁻⁸⁶ (including the recently proposed magnonic Goos-Hänchen effect⁸⁷), spin wave dispersion in magnonic crystals^{24,32,44,46,47,88} and quasi-crystals,^{38,89,90} spectra and localization of defect and surface modes,^{91,92,93} and associated applications in magnonic devices^{14,40,41,94} to be revisited with the generalized Barnaś-Mills boundary conditions derived here.

As far as experimental studies of spin waves are concerned, provided that the conditions of applicability of the exchange approximation are met and all relevant energy terms and associated torques are included in equations (20) and (30-31) respectively, failure of the generalized Barnaś-Mills boundary conditions to describe experimental data could be due to two reasons. Firstly, this could imply that the interface is too thick either for the dynamical terms to be neglected in (26-27), or for the first order extrapolation to be sufficient, or both. Secondly, this could be a result of neglecting magnetic damping terms in the calculations, since dissipation could be non-negligible in the interface region.¹¹ Both cases would require a more complex interface modeling that would account for the interface regions on equal grounds with the semi-infinite materials A and B.^{60-65,95,96}

The generalized Barnaś-Mills boundary conditions proposed in this paper are not limited to linear spin wave dynamics but could equally be applied to the theory of nonlinear spin waves.^{97,98} Moreover, although the discussion above has been limited to the exchange spin waves, the boundary conditions could also be applied in the theory of magnetostatic, dipole-exchange, or even retarded spin waves.^{12,13} This would require that the magnetostatic or full Maxwell equations be solved side-by-side with the Landau-Lifshitz equation and appropriate boundary conditions for the magnetic and electric fields be applied at the interface. As a final note of this section, we note that the boundary conditions could be used to calculate static non-uniform micromagnetic configurations (e.g. magnetic domain walls^{99,100}) near the interface between material A and B. Indeed, the static calculation would only differ from the one above by that the time derivatives of the magnetizations would be equal to zero strictly rather than approximately. Moreover, this sort of calculation will always need to precede solution of any dynamic problem. Albeit beyond the scope of this paper, these applications of the theory developed here open an excellent avenue for future research.

V. Summary

Appropriate boundary conditions at interfaces separating different media represent a mandatory complement of any differential equation describing particular physical phenomena in the composite system. In this paper, we have developed a systematic approach by which to derive boundary conditions for magnetization at an interface between two ferromagnetic materials. The approach treats the interface as a two-sublattice material, although the final equations connect magnetizations outside of the interface region and therefore do not explicitly depend on the interface structure. Instead, the boundary conditions are defined in terms of some average properties of the interface, which can have a finite thickness. In addition to the interface anisotropy and symmetric exchange coupling (which can be treated using existing forms of the magnetization boundary conditions), this approach allows us to take into account coupling resulting from inversion symmetry breaking in the vicinity of the interface, including the Dzyaloshinskii-Moriya antisymmetric exchange interaction. The corresponding general result is given by equations (30-31), in which one would only need to perform the outlined interpolation to suit their specific problem. In this paper, the interpolation has been carried out only for the case of negligible interface anisotropy and Dzyaloshinskii-Moriya exchange parameters to yield boundary conditions that represent a generalization of those proposed earlier by Barnaś and Mills and are therefore named “generalized Barnaś-Mills boundary conditions”. We demonstrate how one could use the latter boundary conditions to extract parameters of the interface via fitting of appropriate experimental data. The developed theory can be applied to modeling of not only linear and non-linear spin waves, including exchange, dipole-exchange, magnetostatic, and retarded modes, but also of non-uniform equilibrium micromagnetic configurations near the interface. Finally, we have outlined the way how our results would impact the research in magnonics and micromagnetism, listing also some theoretical problems solutions of which could be generalized with help of the derived boundary conditions.

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