

# Formation of the band spectrum of spin waves in one-dimensional magnonic crystals with different types of interfacial boundary conditions

V. V. Kruglyak,<sup>1,\*</sup> C. S. Davies,<sup>1</sup> V. S. Tkachenko,<sup>2</sup> O. Yu. Gorobets,<sup>3,4</sup>  
Yu. I. Gorobets,<sup>4</sup> and A. N. Kuchko<sup>4,5,†</sup>

<sup>1</sup> *School of Physics, University of Exeter, United Kingdom*

<sup>2</sup> *Department of Physics and Technology, Donetsk National University, Ukraine*

<sup>3</sup> *National Technical University of Ukraine "Kyiv Polytechnic Institute", Ukraine*

<sup>4</sup> *Institute of Magnetism of NAS of Ukraine, Kiev, Ukraine*

<sup>5</sup> *Donetsk Physical and Technical Institute of NAS of Ukraine, Ukraine*

## Abstract

We report a theoretical study of the spin-wave band spectrum of magnonic crystals formed by stacking thin-film magnetic layers, with general assumptions about the properties of the interfaces between the layers. The use of the Barnaś-Mills magnetization boundary conditions has enabled us to systematically trace the origin of the magnonic band gaps in the spin-wave spectrum of such systems. We find that the band gaps are a ubiquitous attribute of a weakened interlayer coupling and a finite interface anisotropy (pinning). The band gaps in such systems represent a legacy of the discrete spin-wave spectrum of the individual magnetic layers periodically stacked to form the magnonic crystal rather than result from Bragg scattering. At the same time, magnonic crystals with band gaps due to the Bragg scattering can be described by natural boundary conditions (i.e. those maintaining continuity of the magnetization direction across the whole sample). We generalize our conclusions to systems beyond thin-film magnonic crystals and propose magnonic crystals based on the ideas of graded-index magnonics and those formed by Fano resonances as a possible way to circumvent the discovered issues.

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\* Corresponding author: [V.V.Kruglyak@exeter.ac.uk](mailto:V.V.Kruglyak@exeter.ac.uk)

† Corresponding author: [A.Kuchko@hotmail.com](mailto:A.Kuchko@hotmail.com)

## I. Introduction

Magnonic crystals, i.e. magnetic media or structures for spin-wave propagation with a periodic modulation of structural, compositional or micromagnetic characteristics, have been the flagship object of magnonics research for several decades.<sup>1-72</sup> The dispersion of spin waves with wavelength shorter than the lattice constant (period) of a magnonic crystal contains magnonic band gaps (frequency bands in which the propagation of spin waves is impossible). For spin waves of longer wavelength, the same magnonic crystal will represent an effectively continuous medium with properties defined not only by those of the constituent magnetic materials but also details of the geometrical and micromagnetic structure. Magnonic crystals therefore represent a class of metamaterials, often referred to as “magnonic metamaterials”,<sup>73-78</sup> which also includes systems that are not periodic, such as magnonic quasi-crystals<sup>79-85</sup> and (when considered from the point of view of their dynamic properties) magnetic composites.<sup>86-93</sup>

The nature of the interlayer magnetization boundary conditions has crucial consequences for the scattering of spin waves from interfaces between regions with different magnetic properties.<sup>94-106</sup> It is therefore of essential importance for magnonics and magnonic technology, in which spin waves are studied and exploited.<sup>28</sup> In multilayer magnonic crystals (i.e. those formed by stacking of continuous magnetic films), the scattering of spin waves from periodically located interfaces causes Bragg diffraction and formation of magnonic band gaps in their spectrum. This has led to proposals that one could characterize the nature and quality of magnetic interfaces experimentally via measurements of the spin-wave dispersion in magnonic crystals.<sup>107-110</sup> Hence, a systematic approach by which to attribute specific features in and / or the qualitative character of measured spin-wave spectra and dispersions to the nature and parameters of the magnetization boundary conditions at interfaces would be highly desirable.

Let us consider a one-dimensional (1D) multilayered magnonic crystal with a unit cell containing two magnetic layers made of “material A” and “material B” (Fig. 1). Earlier, we developed a method enabling a systematic study of the effect of a simultaneous periodic modulation of several magnetic parameters on the character of spin-wave propagation in such systems.<sup>111-114</sup> This method exploits the fact that, in the stationary case, the wave scattering from an interface is always defined by the wave numbers of the incident and scattered waves, which “hide” the wave frequency and properties of the media separated by the interface. Hence, the problem of finding the dispersion law of spin waves in a magnonic crystal (i.e. the frequency dependence of the Bloch wave number) can be factorized into two stages, as illustrated by Fig. 2. First, one finds the dependence of the Bloch wave number  $\chi$  on the wave numbers of spin waves in the constituent layers  $k_{A(B)}$ . This dependence is fully determined by the layer thicknesses  $d_{A(B)}$  and the boundary conditions at interfaces and can be represented as

$$\cos(\chi L) = F(k_A, k_B, d_A, d_B, \text{boundary conditions}), \quad (1)$$

where  $L = d_A + d_B$  is the period and  $F$  is a function depending on the structure of the magnonic crystal. The dependence of function  $F$  on  $k_A a$  and  $k_B a$ , where  $a$  is the inter-atomic distance (lattice constant) assumed to be the same in both materials, is plotted as a two-dimensional (in the case of two layers within the unit cell of the magnonic crystal) “spectral map”. Magnonic band gaps emerge whenever  $|F| \geq 1$ . Then, the character of the spin-wave dispersion in the magnonic crystal is determined (for specific parameters of the layers, which must be consistent with those used to plot the map) by the position of curves (called “lines of spectra” here) defined by the parametric dependence of  $k_{A(B)}$  upon the spin-wave frequency  $\omega$  in the space of  $k_A a$  and  $k_B a$ .

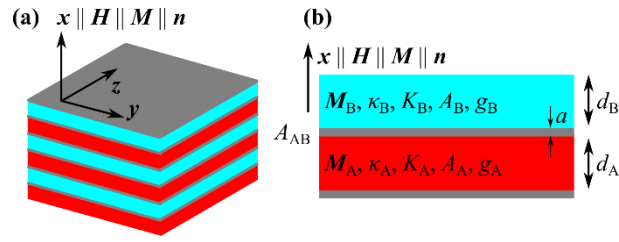


Fig. 1 (a) A multilayered thin film magnonic crystal is schematically shown together with the assumed problem geometry. The bias magnetic field  $\mathbf{H}$ , magnetisation  $\mathbf{M}$  and easy magnetisation axis (defined by unit vector  $\mathbf{n}$ ) are all parallel to the  $x$  axis and perpendicular to the planes of the constituent layers. (b) The unit cell of the magnonic crystal in (a) is schematically shown. The layers are made of materials A and B (with saturation magnetisations  $M_{A(B)}$ , uniaxial anisotropy strengths  $\kappa_{A(B)}$ , surface anisotropy strengths  $K_{A(B)}$ , exchange stiffnesses  $A_{A(B)}$  and gyromagnetic ratios  $g_{A(B)}$ ) and have thicknesses  $d_A$  and  $d_B$ . The separation between layers is  $a$  and the interlayer exchange coupling parameter is denoted as  $A_{AB}$ .

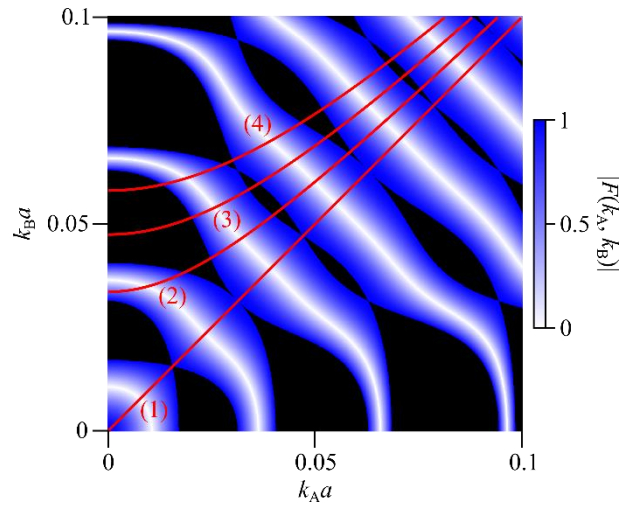


Fig. 2 A typical spectral map is shown with a set of lines of spectra for exchange spin waves, both in coordinates  $k_A a$ ,  $k_B a$ . The map is plotted using natural boundary conditions (see the text) for the magnonic crystal shown in Fig. 1 with  $A_A = A_B$  and  $d_A = d_B = 100a = 3 \times 10^{-6}$  cm. The lines of spectra are plotted for spin waves the dispersion relation of which is defined by Equation (2) with  $A_A = A_B = 2 \times 10^{-6}$  erg/cm,  $M_A = M_B$ ,  $H_A = H_B$ ,  $g_A = g_B$ , and (1)  $\kappa_A = \kappa_B = 25 \times 10^5$  erg/cm<sup>3</sup>, (2)  $\kappa_B = 2\kappa_A = 50 \times 10^5$  erg/cm<sup>3</sup>, (3)  $\kappa_B = 2\kappa_A = 100 \times 10^5$  erg/cm<sup>3</sup>, (4)  $\kappa_B = 4\kappa_A = 100 \times 10^5$  erg/cm<sup>3</sup>. Black colour corresponds to magnonic band gaps.

In Fig. 2, we assume that the materials A and B have magnetizations  $\mathbf{M}_A$  and  $\mathbf{M}_B$ , constants of the uniaxial magnetic anisotropy  $\kappa_A$  and  $\kappa_B$ , gyromagnetic ratios  $g_A$  and  $g_B$ , and parameters of the non-uniform exchange interaction (exchange stiffness parameters)  $A_A$  and  $A_B$ , respectively. The easy magnetization axis in both materials is parallel to the unit vector  $\mathbf{n}$ , which coincides with the normal to the layer planes (and therefore also to their interfaces) and parallel to which the external bias magnetic field of strength  $H$  is applied. We use a Cartesian coordinate system the  $x$  axis of which is parallel to  $\mathbf{n}$ .

Limiting the consideration to the exchange approximation, the dispersion of small amplitude plane spin waves of frequency  $\omega$  propagating along the  $x$  axis is described by

$$\omega = g_{A(B)} \left( H_{A(B)} + \frac{2\kappa_{A(B)}}{M_{A(B)}} + \frac{2A_{A(B)}}{M_{A(B)}} k_{A(B)}^2 \right), \quad (2)$$

where  $H_{A(B)}$  are the values of the static internal magnetic field in the layers, which are generally different if the magnetizations of saturation  $M_{A(B)}$  are different. Spin waves with dispersion different from that given by Equation (2) could also be studied using this method, provided the dispersion relation is justified for the choice of the implemented interface boundary conditions and more generally the model assumed in the calculation.

The map in Fig. 2 is plotted for the case when the complex wave distributions  $\mu_{A(B)}$  resulting from the interference of the forward and backward propagating waves in the adjacent layers are related at each interface via so called ‘‘natural boundary conditions’’ (note that we drop the time dependent harmonic factor here and throughout the paper, which always cancels in the linear equations)<sup>106</sup>

$$\mu_B - \mu_A = 0, \quad (3)$$

$$A_B \frac{\partial \mu_B}{\partial x} - A_A \frac{\partial \mu_A}{\partial x} = 0. \quad (4)$$

The boundary conditions (3-4) do not depend on the strength of the exchange interaction between media A and B but only require that the two media be coupled strongly enough for the equation (3) to hold. The strength of this coupling cannot therefore be extracted from comparison of a theory based on the natural boundary conditions with experiments.

The strength,  $\eta$ , of exchange coupling between the two media enters explicitly so called ‘‘Hoffmann boundary conditions’’.<sup>95,96</sup> For two media (layers) separated by distance  $2\delta$ , which e.g. can represent the thickness of a non-magnetic spacer layer (centered at zero), the conditions can be written as

$$\eta \left( \left\{ \mu_B \right\}_\delta - \left\{ \mu_A \right\}_{-\delta} \right) - \left\{ A_B \frac{\partial \mu_B}{\partial x} \right\}_\delta - \left\{ A_A \frac{\partial \mu_A}{\partial x} \right\}_{-\delta} = 0, \quad (5)$$

$$\left\{ A_B \frac{\partial \mu_B}{\partial x} \right\}_\delta - \left\{ A_A \frac{\partial \mu_A}{\partial x} \right\}_{-\delta} = 0, \quad (6)$$

where curly brackets  $\{f(x)\}_\xi$  are used to denote the value of function  $f$  at point  $\xi$ . The second equations in the natural and Hoffman boundary conditions, i.e. equations (4) and (8) respectively, are identical. This is because they follow from the conservation of the magnetic energy flow across the interface.<sup>115</sup> However, the Hoffmann boundary conditions do not require continuity of the magnetization direction at the interface.

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 media A and B in ‘‘direct’’ contact

$$\frac{2A_{AB}}{a} \left( \left\{ \mu_B \right\}_{\frac{a}{2}} - \left\{ \mu_A \right\}_{-\frac{a}{2}} \right) - \left\{ A_B \frac{\partial \mu_B}{\partial x} \right\}_{\frac{a}{2}} - \left\{ A_A \frac{\partial \mu_A}{\partial x} \right\}_{-\frac{a}{2}} = 0, \quad (7)$$

$$\left\{ A_B \frac{\partial \mu_B}{\partial x} \right\}_{\frac{a}{2}} - \left\{ A_A \frac{\partial \mu_A}{\partial x} \right\}_{-\frac{a}{2}} = 0. \quad (8)$$

Here, we have formally introduced a volume exchange parameter  $A_{AB}$  in place of  $\eta$  as  $A_{AB} = a\eta/2$ . It is easy to check that the direction of the magnetization is continuous only if one neglects in equation (7) terms of the order of  $\propto \frac{\partial \mu_{A(B)}}{\partial x} a \propto \frac{a}{\lambda}$ , where  $\lambda$  is the spin wave wavelength,<sup>111</sup> as expected in the continuous medium approximation, in which the natural boundary conditions (3-4) are derived.

The Hoffmann boundary conditions must only be used to connect solutions that are defined in different points,  $\delta$  and  $-\delta$  in the case of equations (5-6) or  $a/2$  and  $-a/2$  in the case of equations (7-8). If, however, they are applied formally to relate magnetization values that are defined in the same point, one could arrive to erroneous conclusions, as argued e.g. in Ref. 100. To avoid this, one needs instead to interpolate properly the Hoffman boundary conditions to the same point (the position of the interface, e.g. zero coordinate), thereby obtaining so called ‘‘Barna’s-Mills boundary conditions’’.<sup>98,100</sup> In Ref. 94,98,106, the case of a significant interface anisotropy<sup>115-123</sup> was also accounted for, leading to the following form of the Barna’s-Mills boundary conditions<sup>98,100</sup> used in our calculations

$$\frac{2A_{AB}}{a} (\mu_B - \mu_A) + A_{AB} \left( \frac{\partial \mu_B}{\partial x} + \frac{\partial \mu_A}{\partial x} \right) - A_B \frac{\partial \mu_B}{\partial x} - A_A \frac{\partial \mu_A}{\partial x} = K_A \mu_A - K_B \mu_B, \quad (9)$$

$$A_B \frac{\partial \mu_B}{\partial x} - A_A \frac{\partial \mu_A}{\partial x} = K_A \mu_A + K_B \mu_B, \quad (10)$$

where  $K_A$  and  $K_B$  are the interface anisotropies in materials A and B, respectively. The Barna’s-Mills boundary conditions (9-10) describe properly transitions to the continuous material (so called ‘‘full coupling limit’’:  $A_{AB} = A_A = A_B$  and  $K_A = K_B = 0$ ) and to the long wavelength approximation ( $\lambda \gg a$ , where  $\lambda$  is the spin-wave wavelength),<sup>98,100</sup> as we will also illustrate below for the case of magnonic crystals.

In this paper, we present a systematic generalization of the method from Refs. 111-114 to the case of 1D multilayered magnonic crystals with the Barna’s-Mills boundary conditions at interfaces.<sup>98,100</sup> The boundary conditions enable us to draw general conclusions about the effect of the strengths of the interlayer coupling and interface anisotropy (pinning) upon the spin-wave band gap spectrum in magnonic crystals. We find that, in systems with weakened interlayer coupling and/or significant interface pinning, the spectral band gaps are a rule rather than a result of the Bragg scattering associated with the periodic modulation of the magnetic properties (‘‘magnetic contrast’’). Hence, the interface anisotropy should normally be avoided in magnonic crystals, while one should also try to realise the strongest possible coupling between their constituent layers. Finally, we discuss how our findings could be extrapolated to systems beyond thin-film magnonic crystals for which the theoretical formalism is developed, while also presenting our opinion about most attractive avenues for magnonic crystals research.

## II. General spin-wave dispersion relation in magnonic crystals

We can write the space-dependent parts of the solutions and their derivatives in each layer of the magnonic crystal as

$$\mu_{A(B)} = \mu_{A(B)}^+ \exp(+ik_{A(B)}x) + \mu_{A(B)}^- \exp(-ik_{A(B)}x), \quad (11)$$

$$\frac{\partial \mu_{A(B)}}{\partial x} = ik_{A(B)}\mu_{A(B)}^+ \exp(+ik_{A(B)}x) - ik_{A(B)}\mu_{A(B)}^- \exp(-ik_{A(B)}x), \quad (12)$$

where  $\mu_{A(B)}^+$  and  $\mu_{A(B)}^-$  are amplitudes of the forward and backward propagating spin waves in the constituent layers. Substituting equations (11-12) into the boundary conditions (9-10) at interfaces and applying the Bloch theorem

$$\mu(x+L) = \mu(x)\exp(i\chi L). \quad (13)$$

at the boundaries of one period of the magnonic crystal, we obtain a system of four homogeneous algebraic equations for  $\mu_{A(B)}^+$  and  $\mu_{A(B)}^-$ . The system has non-trivial solutions if and only if its determinant is equal to zero, which (together with equations (2)) yields the sought dispersion relation of spin waves in the magnonic crystal as

$$\begin{aligned} \cos(\chi L) = & \cos(k_A d_A) \cos(k_B d_B) \left( 1 + \frac{4(\beta_A + \beta_B)}{A_{AB}} + \frac{8\beta_A \beta_B}{A_{AB}^2} \right) + \\ & + \cos(k_A d_A) \sin(k_B d_B) \left( \left( 1 + \frac{A_B}{A_A} - \frac{2A_B}{A_{AB}} - \frac{4A_B \beta_A}{A_{AB}^2} \right) \frac{k_B a}{2} + \right. \\ & \left. + \frac{2}{k_B a} \left( \frac{\beta_A}{A_B} + \frac{\beta_B}{A_B} \left( 1 + \frac{2(2\beta_A + \beta_B)}{A_{AB}} + \frac{4\beta_A \beta_B}{A_{AB}^2} \right) \right) \right) + \\ & + \sin(k_A d_A) \cos(k_B d_B) \left( \left( 1 + \frac{A_A}{A_B} - \frac{2A_A}{A_{AB}} - \frac{4A_A \beta_B}{A_{AB}^2} \right) \frac{k_A a}{2} + \right. \\ & \left. + \frac{2}{k_A a} \left( \frac{\beta_B}{A_A} + \frac{\beta_A}{A_A} \left( 1 + \frac{2(\beta_A + 2\beta_B)}{A_{AB}} + \frac{4\beta_A \beta_B}{A_{AB}^2} \right) \right) \right) - \\ & - \frac{1}{2} \sin(k_A d_A) \sin(k_B d_B) \left( \left( 1 + \frac{4\beta_B}{A_{AB}} + \frac{4\beta_B^2}{A_{AB}^2} \right) \frac{A_A k_A}{A_B k_B} + \left( 1 + \frac{4\beta_A}{A_{AB}} + \frac{4\beta_A^2}{A_{AB}^2} \right) \frac{A_B k_B}{A_A k_A} - \right. \\ & \left. - \left( 2 + \frac{A_A}{A_B} + \frac{A_B}{A_A} - \frac{4A_A}{A_{AB}} - \frac{4A_B}{A_{AB}} + \frac{4A_A A_B}{A_{AB}^2} \right) \frac{k_A k_B a^2}{4} - \right. \\ & \left. - \frac{4}{k_A k_B a^2} \left( \frac{(\beta_A + \beta_B)^2}{A_A A_B} + \frac{4\beta_A^2 \beta_B}{A_{AB} A_A A_B} + \frac{4\beta_A \beta_B^2}{A_{AB} A_A A_B} + \frac{4\beta_A^2 \beta_B^2}{A_{AB}^2 A_A A_B} \right) \right), \quad (14) \end{aligned}$$

where we have introduced notations  $\beta_{A(B)} = \frac{aK_{A(B)}}{2}$  and neglected  $\beta_{A(B)}$  have been in comparison to  $A_{A(B)}$  (but not  $A_{AB}$ ) as was done in the used form of the boundary conditions.<sup>98</sup>

The obtained spin-wave dispersion relation is obviously too complex to draw any direct conclusions. Hence, we consider its various limiting cases first and then apply the graphical approach from Refs. 111-114.

### III. Limits of weak coupling and strong pinning at the interface

In the limit of a weak coupling (i.e. when  $A_{AB}$  is small as compared to  $A_{A(B)}$ ) we obtain from Equation (14)

$$\begin{aligned} \cos(\chi L) = & \frac{2}{A_{AB}^2} \left( 2\beta_A \cos(k_A d_A) + \left( \frac{2\beta_A^2}{A_A k_A a} - \frac{A_A k_A a}{2} \right) \sin(k_A d_A) \right) \times \\ & \times \left( 2\beta_B \cos(k_B d_B) + \left( \frac{2\beta_B^2}{A_B k_B a} - \frac{A_B k_B a}{2} \right) \sin(k_B d_B) \right), \end{aligned} \quad (15)$$

In the limit of a strong pinning (i.e. when  $\beta_{A(B)}$  is large as compared to  $A_{AB}$ ,  $A_A$  and  $A_B$ ), we obtain

$$\cos(\chi L) = \frac{8\beta_A^2 \beta_B^2}{A_A A_B A_{AB}^2 k_A k_B a^2} \sin(k_A d_A) \sin(k_B d_B). \quad (16)$$

The right-hand sides of the dispersion relations (15) and (16) contain large pre-factors in front of the harmonic functions and are therefore expected to exceed (in absolute value) the unity in wide frequency ranges, thereby yielding large magnonic band gaps in the spin-wave spectrum.

In the limit of zero coupling, Equation (14) yields the discrete spectra of spin waves in the decoupled constituent layers of each type with mixed boundary conditions

$$\left( 1 + \left( \frac{2\beta_A}{A_A k_A a} - \frac{A_A k_A a}{2\beta_A} \right) \frac{\tan(k_A d_A)}{2} \right) \left( 1 + \left( \frac{2\beta_B}{A_B k_B a} - \frac{A_B k_B a}{2\beta_B} \right) \frac{\tan(k_B d_B)}{2} \right) = 0, \quad (17)$$

or recalling the introduced earlier notations

$$\left( 1 + \left( \frac{K_A}{A_A k_A} - \frac{A_A k_A}{K_A} \right) \frac{\tan(k_A d_A)}{2} \right) \left( 1 + \left( \frac{K_B}{A_B k_B} - \frac{A_B k_B}{K_B} \right) \frac{\tan(k_B d_B)}{2} \right) = 0. \quad (18)$$

In the limit of infinitely strong pinning, we obtain the discrete spectra of spin waves in the decoupled constituent layers of each type with Dirichlet boundary conditions

$$\sin(k_A d_A) \sin(k_B d_B) = 0 \quad (19)$$

as expected.

### IV. Limiting case of natural boundary conditions

A typical issue that arises in numerical calculations of the spin-wave dispersion is how to set the value of the exchange parameter at interface between two materials, e.g. when numerically computed dispersions are to be compared with analytical theories. The following considerations could ensure that the comparison is reasonable even beyond the long-wavelength limit, when the applicability of the

natural boundary conditions is guaranteed. Let us first consider the case of zero interface anisotropy. Then we obtain from Equation (14)

$$\begin{aligned} \cos(\chi L) = & \cos(k_A d_A) \cos(k_B d_B) + \\ & + \frac{k_B a}{2} \left( 1 + \frac{A_B}{A_A} - \frac{2A_B}{A_{AB}} \right) \cos(k_A d_A) \sin(k_B d_B) + \frac{k_A a}{2} \left( 1 + \frac{A_A}{A_B} - \frac{2A_A}{A_{AB}} \right) \sin(k_A d_A) \cos(k_B d_B) - \\ & - \frac{1}{2} \sin(k_A d_A) \sin(k_B d_B) \left( \frac{A_A k_A}{A_B k_B} + \frac{A_B k_B}{A_A k_A} - \left( 2 + \frac{A_A}{A_B} + \frac{A_B}{A_A} - \frac{4A_A}{A_{AB}} - \frac{4A_B}{A_{AB}} + \frac{4A_A A_B}{A_{AB}^2} \right) \frac{k_A k_B a^2}{4} \right) \end{aligned} \quad (20)$$

This dispersion relation reduces to that obtained using "natural" boundary conditions (3-4), i.e.

$$\cos(\chi L) = \cos(k_A d_A) \cos(k_B d_B) - \frac{1}{2} \left( \frac{A_A k_A}{A_B k_B} + \frac{A_B k_B}{A_A k_A} \right) \sin(k_A d_A) \sin(k_B d_B), \quad (21)$$

if and only if

$$A_{AB} = \frac{2A_A A_B}{A_A + A_B} \quad \text{or} \quad \frac{1}{A_{AB}} = \frac{1}{2} \left( \frac{1}{A_A} + \frac{1}{A_B} \right), \quad (22)$$

which is identical to the averaging law in the thin layer limit ( $\lambda \gg L$ ).<sup>124</sup> When the interface anisotropy is non-zero but the interface exchange is defined by Equation (22), we obtain

$$\begin{aligned} \cos(\chi L) = & \cos(k_A d_A) \cos(k_B d_B) + \\ & + \frac{2(\beta_A + \beta_B)}{A_B k_B a} \cos(k_A d_A) \sin(k_B d_B) + \frac{2(\beta_A + \beta_B)}{A_A k_A a} \sin(k_A d_A) \cos(k_B d_B) - \\ & - \frac{1}{2} \left( \frac{A_A k_A}{A_B k_B} + \frac{A_B k_B}{A_A k_A} - \frac{4(\beta_A + \beta_B)^2}{A_A A_B k_A k_B a^2} \right) \sin(k_A d_A) \sin(k_B d_B) \end{aligned} \quad (23)$$

The strength of the exchange interaction between different materials is defined using Equation (22) e.g. in MuMax.<sup>125</sup> Hence, an analytical theory aiming to explain observations made from micromagnetic simulations performed in MuMax could be based on the natural boundary conditions (3-4), which are arguably simpler than the Barnaś-Mills boundary conditions.

## V. Barnaś-Mills and Hoffmann boundary conditions in the full coupling limit

Let us illustrate the relation between the Barnaś-Mills and Hoffmann boundary conditions, which is best noted in the full coupling limit, or the limit of a uniform medium for a magnonic crystal. The surface anisotropy is absent in the case of a uniform medium. Then, dropping indices A and B (except in  $d_{A(B)}$ ) in the equation (20), we obtain

$$\cos(\chi L) = \cos(kL) + ka \left( \frac{A_{AB} - A}{A_{AB}} \right) \sin(kL) + \left( \frac{A_{AB} - A}{A_{AB}} \right)^2 \frac{k^2 a^2}{2} \sin(kd_A) \sin(kd_B). \quad (24)$$

In the case of  $A = A_{AB}$ , the second and third terms are strictly equal to zero, and the Bloch wave number equals that in the continuous material, satisfying the full coupling limit, as expected for the Barnaś-Mills boundary conditions. In contrast, from the Hoffmann boundary conditions, we obtain for the same case of  $A = A_{AB}$



$$\begin{aligned}\cos(\chi L) &= \cos(kL) - \frac{Aka}{A_{AB}} \sin(kL) + \frac{A^2 k^2 a^2}{A_{AB}^2} \sin(kd_A) \sin(kd_B) = \\ &= \cos(kL) - ka \sin(kL) + k^2 a^2 \sin(kd_A) \sin(kd_B)\end{aligned}\quad (25)$$

i.e. the full coupling limit is fulfilled only approximately in the long wavelength limit. This shows that the limits of applicability of the Hoffmann boundary conditions basically coincide with those of the continuous medium approximation, although a weakened exchange coupling at interfaces might increase the error associated with their use. Furthermore, the overlap between the regions of validity the exchange and continuous medium approximations is rather narrow, making errors associated with the incorrect use of the Hoffmann boundary conditions to describe exchange spin waves more likely.

## VI. Graphical analysis of the general dispersion relation

We begin our graphical analysis of the general dispersion relation (14) by considering the symmetrical case  $d_A = d_B$ ,  $A_A = A_B$  and  $\beta_A = \beta_B$ . It is useful to assume that the strengths of both the exchange interaction and of the interface anisotropy in the layers are measured in *relative* units of  $A_{AB}$ .

Hence, we replace (both in the text and figure captions)  $A_{A(B)} \rightarrow \frac{A_{A(B)}}{A_{AB}}$  and  $\beta_{A(B)} \rightarrow \frac{\beta_{A(B)}}{A_{AB}}$  in this section. Furthermore, to plot the spectra maps, we assume that  $d_A = d_B = 100a$ .

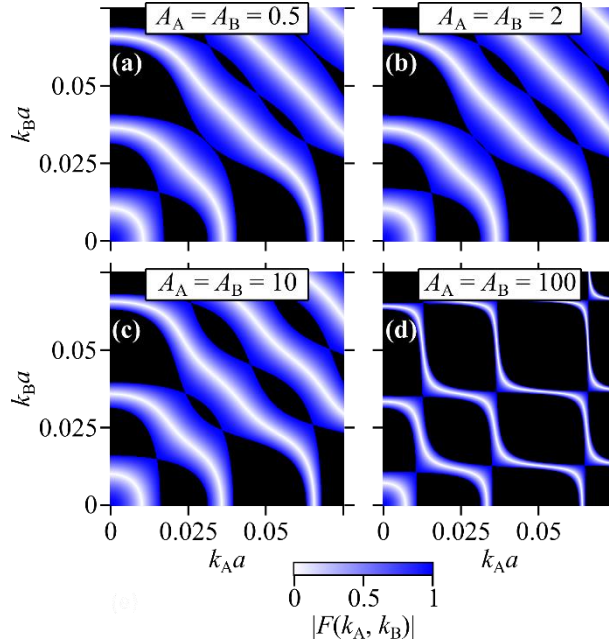


Fig. 3 Spectral maps are shown for  $\beta_{A(B)} = 0$  and different strengths of the interlayer exchange coupling (a)  $A_A = A_B = 0.5$ , (b)  $A_A = A_B = 2$ , (c)  $A_A = A_B = 10$ , and (d)  $A_A = A_B = 100$ . Black colour corresponds to magnonic band gaps.

Fig. 3 shows the spectral maps for different strengths of the interlayer exchange coupling. The map for strong coupling  $A_A = A_B = 0.5$  (Fig. 3 (a)) is virtually identical to that plotted using the natural boundary conditions in Fig. 2, with only slight deviations noticeable in the case of slightly weakened coupling  $A_A = A_B = 2$  (Fig. 3 (b)). This emphasizes the earlier made remark that the natural boundary conditions only require the coupling to be strong but do not enable quantitative analysis of the coupling strength. As the coupling strength decreases, magnonic band gaps emerge in ( $A_A = A_B = 10$ , Fig. 3 (c))

and then dominate the spectrum ( $A_A = A_B = 100$ , Fig. 3 (c)). This behaviour agrees well with the prediction made earlier based on Equation (15).

Fig. 4 shows the spectral maps for different strengths of the interface anisotropy in the layers. Again, in agreement with our earlier analytical predictions based on Equation (16), the presence of interface anisotropy leads to appearance of magnonic band gaps in the spin-wave spectrum, with the band-gap width increasing with increasing the surface anisotropy strength (i.e. pinning).

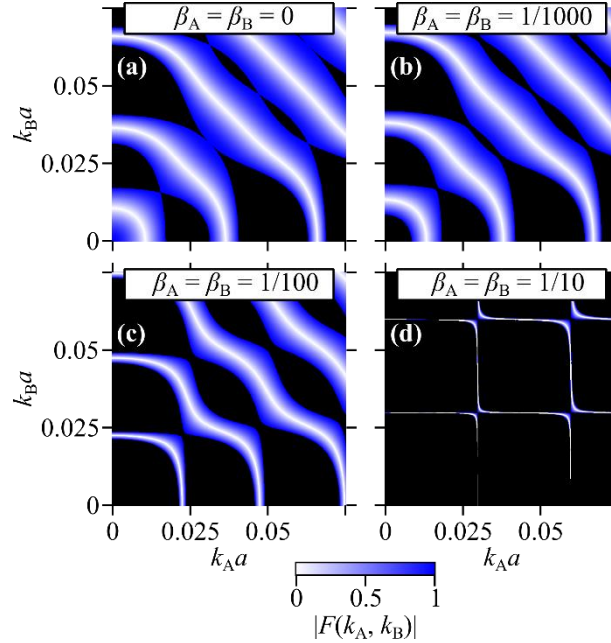


Fig. 4 Spectral maps are shown for  $A_A = A_B = 1$  and different strengths of the interface anisotropy (a)  $\beta_A = \beta_B = 0$ , (b)  $\beta_A = \beta_B = 0.001$ , (c)  $\beta_A = \beta_B = 0.01$ , and (d)  $\beta_A = \beta_B = 0.1$ . Black colour corresponds to magnonic band gaps.

It is also interesting to consider a magnonic crystal consisting of the same layers (with  $k_A = k_B = k$ ) separated by interfaces with interface anisotropy  $\beta = \beta_A = \beta_B$  and modified (relative to that in the layers) exchange coupling. This corresponds to lines of spectra in form of diagonals running from the bottom left to the top right corners in Figs. 3 and 4. The spin-wave spectra described by the lines contain magnonic band gaps. However, the band gaps emerge differently when resulting from a weakened interlayer coupling or a finite interface anisotropy, so that the low frequency (wave-number) region remains “allowed” in the former and becomes “forbidden” in the latter case. This is a result of the pinning of the magnetisation in the case of a finite strength of the interface anisotropy. For the spectral maps in this case, we could also obtain from Equation (14) keeping only leading terms in  $\beta$

$$\begin{aligned}
\cos(\chi L) = & \cos(kn_A a)\cos(kn_B a)(1 + 8\beta) + \\
& + \sin(k(n_A + n_B)a) \left( (1 - A(1 + 2\beta))ka + \frac{4\beta}{Aka} \right) - \\
& - \sin(kn_A a)\sin(kn_B a) \left( 1 + 4\beta - \frac{1}{2}(1 - A)^2(ka)^2 - \frac{8\beta^2}{A^2(ka)^2} \right)
\end{aligned} \tag{26}$$

where  $n_A$  and  $n_B$  denote the numbers of lattice constants  $a$  in the layer thicknesses  $d_A$  and  $d_B$ , respectively. Hence, we find that, for the case of  $k \approx 0$ , the leading term is

$$\cos(\chi L) \approx 1 + 4\beta \left( 2 + \frac{n_A + n_B}{A} \right) + \frac{8\beta^2 n_A n_B}{A^2} > 1, \quad (27)$$

i.e. we have a band gap if  $\beta > 0$ . If however  $\beta = 0$ , we have

$$\cos(\chi L) \approx 1 - \frac{(ka)^2 (n_A + n_B)}{2} (n_A + n_B + 2A - 2) < 1, \quad (28)$$

i.e. we have an allowed band if  $n_A + n_B > 2$ , which is always the case.

We have shown that a strong pinning and a weak coupling can both lead to extremely wide band gaps and narrow magnonic bands, and ultimately to a discrete spectrum of spin waves in the sample. In magnonic crystals of interest, one aims to realise the opposite situation, i.e. to make the coupling strong and the pinning weak, so that the magnetic energy flux carried by spin waves across the interfaces is as strong as possible. The magnonic band gaps are realised by increasing the depth of modulation (“contrast”) of magnetic parameters in the sample. In this practically important case, the magnonic dispersion can be calculated as

$$\begin{aligned} \cos(\chi L) = & \cos(k_A n_A a) \cos(k_B n_B a) (1 + 4(\beta_A + \beta_B)) + \\ & + \cos(k_A n_A a) \sin(k_B n_B a) \left( \left( 1 + \frac{A_B}{A_A} - 2A_B(1 + 2\beta_A) \right) \frac{k_B a}{2} + \frac{2(\beta_A + \beta_B)}{A_B k_B a} \right) + \\ & + \sin(k_A n_A a) \cos(k_B n_B a) \left( \left( 1 + \frac{A_A}{A_B} - 2A_A(1 + 2\beta_B) \right) \frac{k_A a}{2} + \frac{2(\beta_A + \beta_B)}{A_A k_A a} \right) - \\ & - \frac{1}{2} \sin(k_A n_A a) \sin(k_B n_B a) \left( \begin{aligned} & \left( (1 + 4\beta_B) \frac{A_A k_A}{A_B k_B} + (1 + 4\beta_A) \frac{A_B k_B}{A_A k_A} - \frac{4(\beta_A + \beta_B)^2}{A_A A_B k_A k_B a^2} \right) - \\ & - \left( 2 + \frac{A_A}{A_B} + \frac{A_B}{A_A} - 4(A_A + A_B) + 4A_A A_B \right) \frac{k_A k_B a^2}{4} \end{aligned} \right) \end{aligned} \quad (29)$$

Finally, Fig. 5 shows the spectral maps for the case of unequal strengths of the exchange parameter in the two layers. Expectedly, the maps become asymmetric in this case. The positions of the lines of spectra also shift (or rather get distorted) with the map. However, the possibility of tuning the positions by the parameters of the layers that do not enter Equation (14) is retained, as discussed e.g. in Ref. 112.

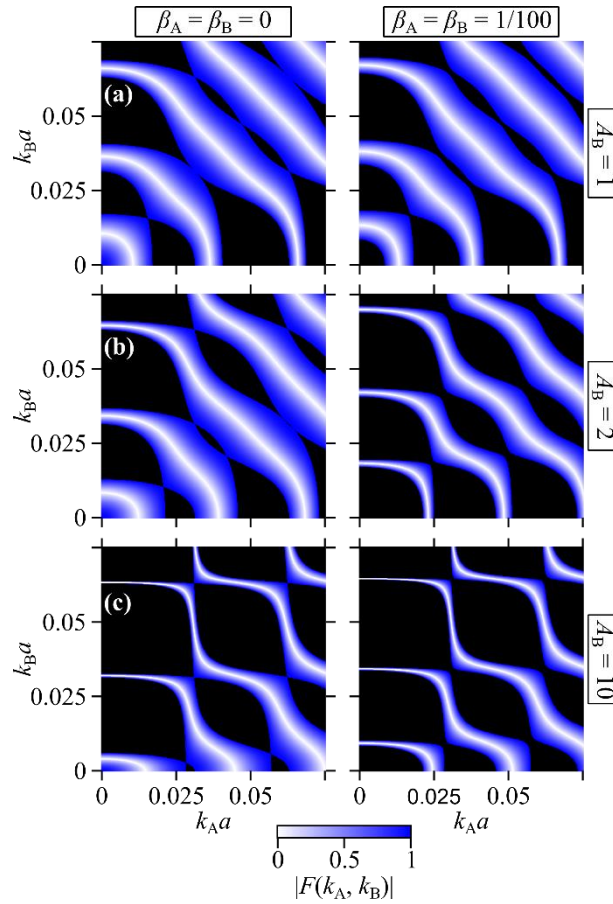


Fig. 5 Spectral maps are shown for  $A_A = 1$  and the values of  $A_B$  and  $\beta_{A(B)}$  indicated for each panel. Black colour corresponds to magnonic band gaps.

## VII. Discussion

The main take-home message of the presented analysis is that the weakened interlayer exchange coupling and finite interface anisotropy (pinning) can both lead to formation of frequency gaps (band gaps) in the spin-wave spectrum of magnonic crystals. However, the origin of such band gaps is not related to the Bragg resonance. Instead, the Bragg resonance is responsible for formation of the (quite flat) allowed bands in the systems. The bands could also be considered as splitting of the standing spin-wave resonances in the constituent layers of the magnonic crystals, in the spirit of the tight binding theory of the quantum-mechanical electron in crystals.<sup>126</sup> So, both the weakened interlayer coupling and finite interface pinning should be generally treated as imperfections and therefore avoided. Instead, in “good” magnonic crystals, magnonic band gaps are formed due to cumulative scattering from consecutive interfaces between layers with high magnetic contrast, as in the case of the nearly free electrons in crystals.<sup>126</sup> The degree to which this is achieved could be judged by the applicability of the natural boundary conditions (3-4) to the descriptions of observed magnonic band spectrum.

Strictly speaking, the formalism developed in this paper applies to the case of exchange spin waves in thin-film magnonic crystals. However, we speculate that the calculations themselves, the graphical analysis and the conclusions drawn could be extrapolated to several other systems beyond those assumed in our model. For instance, the dispersion of spin waves in the individual layers does not necessarily need to be that described by Equation (2). Indeed, the dispersion relation could be replaced by that derived using any microscopic approach, provided the approach is consistent with the Barnaś-Mills

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2 boundary conditions, given by Equations (9-10). The modification of the dispersion relation would  
3 change the shape and position of the lines of spectra but not the spectral maps.  
4

5 Surface magnetostatic waves (Damon-Eshbach modes)<sup>127</sup> in thin planar magnonic crystals could  
6 also be treated (even if approximately) using our approach. Indeed, assuming that the mode amplitude  
7 is constant across the film thickness, the dispersion relation of such modes in a magnonic crystal would  
8 be calculated by applying the Bloch theorem and requiring continuity of the magnetostatic potential and  
9 its derivative at interlayer interfaces. The latter boundary conditions have form of those considered here,  
10 perhaps with a different meaning of the parameters in the equation. The pinning would be “effective”<sup>101</sup>  
11 and have magneto-dipole origin, e.g. in samples with modulated magnetization of saturation. The  
12 strength of coupling between layers could be modified by introducing air gaps between layers.<sup>128-130</sup> Yet,  
13 any generalization to the case of dipole-exchange spin waves could be only approximate since the  
14 corresponding differential (or integro-differential equations) are of a higher order, so that a greater  
15 number of boundary conditions is required to stitch their solutions at interfaces. However, it is likely  
16 that even qualitative analysis based on the ideas presented here could prove useful in some cases.  
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22 In Ref. 106, we showed that, under certain assumptions, the Barnas-Mills boundary conditions  
23 could even be used to describe interfaces of finite (albeit small) thickness, thereby removing the need to  
24 consider the detailed structure of interfaces. In the same work, we also outlined how the boundary  
25 conditions could be derived for the case of non-collinear magnetic configurations across the interface,  
26 which could result either from non-collinearity of the easy magnetization axes in the adjacent layers, or  
27 from the antisymmetric (Dzyaloshinskii-Moriya) exchange coupling.<sup>131-134</sup> It is plausible that the spin-  
28 wave dispersion relations in one-dimensional periodic non-collinear configurations of this sort (e.g. such  
29 as that forming the domain wall magnonic crystals from Refs. 135) could be treatable using the approach  
30 developed here.  
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34 The theory presented here does not consider magnetic damping.<sup>136</sup> The spin-wave attenuation in  
35 magnonic crystals depends non-monotonically on the frequency and magnetic structure.<sup>124,137</sup> In  
36 practice, researchers face a trade-off between studying low-damping YIG magnonic crystals with periods  
37 typically greater than  $100\ \mu\text{m}$ <sup>29</sup> and relatively high damping metallic magnonic crystals with periods  
38 down to several  $100\ \text{nm}$ .<sup>30</sup> Only recently, thin (and therefore potentially patternable at the nanoscale)  
39 YIG and ultralow damping metallic ferromagnetic alloys became available,<sup>138</sup> promising to revolutionize  
40 the experimental studies of magnonic crystals. At present, however, the damping in metallic  
41 ferromagnets used so far appears to be quite high to allow formation of a magnonic band resulting from  
42 Bragg resonance of multiple spin waves scattered from successive interfaces in magnonic crystals with  
43 a strong magnetic contrast. In contrary, the wide magnonic band gaps resulting from a weakened  
44 interlayer coupling and/or a strong magnetization pinning at interfaces are not limited by damping since  
45 they originate mainly from individual layers and do not therefore require Bragg resonances to form. In  
46 this case, the damping is more relevant to the width of allowed bands. The formalism developed here  
47 might facilitate a more thorough analysis of the available experimental data to isolate the true mechanism  
48 of the magnonic band spectrum formation in metallic magnonic crystals. Yet, we note that magnonic  
49 crystals even with relatively high damping could be used as Bragg mirrors.<sup>139</sup>  
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57 In addition to mastering magnonic crystals formed on the basis of thin YIG films<sup>140</sup> and ultralow  
58 damping CoFe alloys,<sup>138</sup> we see two other main avenues for development of the magnonic crystal  
59 research in the nearest future. The first path is associated with a more extensive use of the ideas of  
60 graded-index magnonics.<sup>141</sup> This includes media with a continuously periodic modulation of the  
magnetic contrast<sup>142</sup> or applied magnetic field,<sup>143,144</sup> those with a periodic variation of the magnetic

texture (such as arrays of magnetic domain walls,<sup>145,146</sup> vortices<sup>147-149</sup> and skyrmions,<sup>150</sup> or even periodic bending of the magnetization<sup>114,151</sup>), as well as combinations of the approaches. In light of the discussion presented in this paper, this path has an obvious advantage of maintaining the full magnetic coupling between and within individual periods of the magnonic crystals, which would also be free from patterned (or otherwise defined) sharp interfaces and associated interface anisotropy and pinning.

The other path is associated with exploitation of Fano resonances<sup>25,152</sup> in binary magnonic structures, in which (presumably, metallic) magnetic resonators could be periodically formed on top of a low damping magnonic medium, such as YIG. Highly exotic effects associated with Fano resonances were observed already in the case of interaction between an isolated resonator and underlying magnonic waveguide.<sup>153,154</sup> The microwave to spin wave coupling concept from Ref. 153 was extended to an array of resonators (“nanograting coupler”) in Ref. 140,155. Both the graded-index and Fano resonance research directions lend themselves naturally to reconfigurability by altering the micromagnetic configuration of the magnonic crystals<sup>156-158</sup>, and to tuneability and dynamic modulation by the applied magnetic field,<sup>143,144</sup> which represent the perceived main attractions of the magnonic technology. Finally, we should mention here the non-reciprocity inherent to magnetism and more recently also observed in magnonic crystals,<sup>159,160</sup> which is beyond the scope of this contribution.

## VIII. Conclusions

We have investigated the origin of the band gaps in the spectrum of spin-waves propagating in thin-film magnonic crystals with general assumptions about the properties of interfaces their constituent layers, as described by the Barnaś-Mills boundary conditions.<sup>98,100</sup> Using the graphical method from Refs. 111-114, we have revealed that magnonic band gaps are a ubiquitous attribute of the spin-wave dispersion in magnonic crystals with weakened interlayer coupling and/or finite interface anisotropy (pinning). The band gaps do not result from Bragg scattering but represent a legacy of the discrete spin-wave spectrum of the individual magnetic layers periodically stacked to form the magnonic crystal. This conclusion can be generalized to the important case of arrays of dipolar-coupled magnetic elements (e.g. stripes or nanodots) since the magneto-dipole coupling between elements is usually much weaker than that within each individual element. Our conclusions lend a special attraction to magnonic crystals based on the ideas of graded-index magnonics or those formed by Fano resonances in a low damping magnetic wafer loaded by arrays of magnetic elements as they could prove free from the discovered shortcomings.

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