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Localized spin modes on the insulating antiferromagnetic stepped surface model

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Abstract. We present a numerical method to calculate the spin fluctuation dynamics on a stepped surface. The model discussed here consists of an extended antiferromagnetic surface step at the surface boundary of an insulating antiferromagnetic substrate. The stepped surface is formed by two straight steps dropped randomly and the spins moments of the steps and the substrate are considered as local with no electronic effects. The full magnetic problem arising from the absence of translational symmetry due to the presence of a magnetic surface and steps is considered and studied. The calculations concern in particular the energies of localized spin-wave modes near the surface steps and employ the matching procedure in the random-phase approximation and mean field approximation. Only the nearest-neighbor exchange interactions are considered between the spins in the model. The analytical formalism presented here is adapted from an earlier work on the vibrational spectra of two isolated steps, a structure that can be considered as a low dimensional system and solved for the three dimensional evanescent crystal spin field in the bulk and the surface domains around the steps. This spin field arises from the breakdown of the magnetic translation symmetry of the system. The results are used to calculate the spin mode energies associated with the steps and surface terraces. We show the presence of localized acoustic and optical spin wave modes propagating along the surface and the steps as well as the interface surface-steps, their fields are also described as evanescent in the plane normal to the surface step layers and depend on the nature of the exchange interaction near the steps.

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1 Introduction

The study of film growth has been increasingly characterized by the application of surface science methods to understand growth at the atomic level. Work in this field has been motivated by the ever more stringent requirements on the quality of thin films needed for developing advanced microelectronic, optical, and magnetic devices, as well as the thrust toward nanometer-scale structures. As device miniaturization reaches submicrometer and nanometer length regimes, atomic level control of the fabrication processes for both novel materials and new devices have become of great importance. The presence of nanostructures such as random steps, kinks and other defects on crystal surfaces is important to their equilibrium topography as well as to a number of other surface properties. As for the role of steps, it is known, for instance, that their presence can modify the growth modes of surfaces. Questions concerning the thermodynamic stability of surfaces and the modes of their kinetic growth are also becoming important, which implies a need for a better understanding of the role of surface nanostructures and their particular properties.

Most earlier studies on surface magnetism are based on the assumption that the magnetic surface is morphologically perfectly smooth (ideal bulk termination). Real films, however, have a rough surface. The atomic heights of surface atoms can differ by a few atomic spacings because of the formation of a variety of surface defects including diffusional disorder, surface reconstruction, vacancies and step changes in the height of the film [1,2]. Such surface roughness is expected to affect magnetism. Therefore, establishing the relationship of surface/interface magnetic properties to surface/interface roughness is not only of fundamental interest but is also essential for the development of new magnetic devices using magnetic multilayers. Let us note that these imperfections may lead to a number of effects including changes in the thermal properties

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of the film and short lifetimes for spin-waves as evidenced by large linewidths in Brillouin scattering experiments.

During the last decade, an increasing interest from the theoretical and experimental points of view has been devoted to study the dynamics of disordered surfaces [3–6]. The study of magnons or spin-waves in ultrathin films has proved to be very useful, in particular, for determining the magnetic anisotropy constant [7,8] using Brillouin light scattering [9,10], that provides a tool to probe these magnetic excitations in ultrathin layers. It is normally admitted now, however, that experiments are performed on systems which lack perfectly flat atomic layers. Previous studies have shown that there is a strong reflection of the spin-waves at monoatomic steps and that spin-wave modes localized at the step edge occur at a single step. Breaking of the translational symmetry in one direction may result in new localized modes as compared to the smooth film case. The effects of localized imperfections on the spin-wave propagation in thin ferromagnetic films have been examined, where these imperfections are assumed to be materially confined to a few lattice sites causing local changes in anisotropy and exchange fields [11]. Another study has calculated, in the framework of a quasi-one-dimensional model, the reflection and transmission coefficients for a spin-wave which suffers diffraction at a step like atomic discontinuity [12]. Recently, it was demonstrated that there are spin wave localized modes which occur at a single step in the ferromagnetic films models [13] and at the monolayer Fe films on stepped W surfaces [14]. Breaking of the translational symmetry in one direction may result in new localized modes as compared to the smooth film case. The case of a antiferromagnet isolated step has been recently examined [15]. The case of two isolated steps, to our knowledge, has not been treated yet. In this paper we study the full problem arising from the absence of translational symmetry in two directions due to surface steps. We present a precursor model system with the intention of studying the surface dynamics due to extended magnetic surface steps at the surface boundary of an insulating magnetic substrate. Such studies are important because surfaces are never perfectly flat in reality and atomic steps, for example, on vicinal surfaces, are known to occur [16].

The study of magnetic excitation phenomena at disordered surfaces by completely ab-initio techniques is still a difficult exercise and is nanostructure specific. Owing to the complexity of the phenomena, even though some empirical many-body approximations are available [17,18], and can lead to refinements in the numerical values attributed to exchange interactions values in the neighborhood of surface defects, and to the relaxed positions of the magnetic atoms in vicinal surfaces. The theoretical approach presented here in contrast is an analytical approach which is independent of the geometry of the nanostructure in the surface. This makes it easy to extend to a variety of real problems. It can also give in a direct manner the real space Green's functions for the spin fluctuation dynamics of an isolated nanostructure with the help of finite matrices.

The paper is organized as follows: the explicit theoretical model for a stepped surface is presented in Section 2. In Section 3, the main stages of calculations are given in detail: the spin fluctuation dynamics are presented for the bulk and terrace domains to determine unique solutions for the evanescent modes induced by the presence of a surface step. This permits the rigorous construction of the evanescent spin field surrounding the steps. The analytic approach has the advantage of presenting this field as a characteristic of a thin film lattice but remains independent of the size and the configuration of the surface steps, underlying the general character of the calculation. Section 4 is devoted to describing the numerical procedure based on the matching procedure with an application to the spin fluctuation dynamics of the steps domain. Salient numerical results and discussion are presented in Section 5 whereas the conclusions are summarized in Section 6.

2 The stepped surface model

Let us consider the schematic configuration of the semi-infinite antiferromagnetic surface and steps in the case of simple cubic lattice as illustrated in Figures 1a and 1b. The stepped surface is formed by two straight steps dropped randomly and the spin moments of the steps and the insulating substrate are considered as local with no electronic effects. The spin order is considered in the direction normal to the surface boundary (z-direction), with no loss of generality, and the spin interact via magnetic exchange. The site position perpendicular to the step is indexed by n, whereas the layer number is labeled by m. The two-dimensional reference cross section of the magnetic steps is taken geometrically at the plane indexed by the integer $s = 0$. The geometry of the model showing the different exchange parameters is illustrated in Figure 1b. Only the nearest neighbor exchange interactions are considered. In the model for that purpose, there is translational invariance parallel to the steps in the one dimensional (1D) direction defined as the y-axis. To each lattice site is attributed a spin vector variable $S_{n,s,m}(t)$ where the integer indices (n, s, m) count, respectively, the position site along the x, y, z directions. The two magnetic steps on the surface are illustrated by the semi-infinite planes of ordered spins located at $m = -1$ and $m = 0$, respectively, adjacent to an infinite plane of ordered spins labeled by $m = 2$. Each bulk spin site for which $m \geq 2$ has the position vector $\vec{r} = n\vec{a} + s\vec{b} + m\vec{c}$. The matching technique and its implementation requires the crystal to be divided into three main regions all having the same two-dimensional (2D) periodicity along the direction normal to the surface and step. *(i)* a bulk spin site region ($m \geq 2$) relatively removed from the steps having three-dimensional (3D) periodicity where the magnon dispersion curves are first worked out. Here, the exchange constants are taken equal to J. *(ii)* The surface terrace sites ($m = 1$) consisting of an arbitrary reconstructed or relaxed layer inside which translational symmetry is lost along that direction not contained in the surface plane. *(iii)* the steps

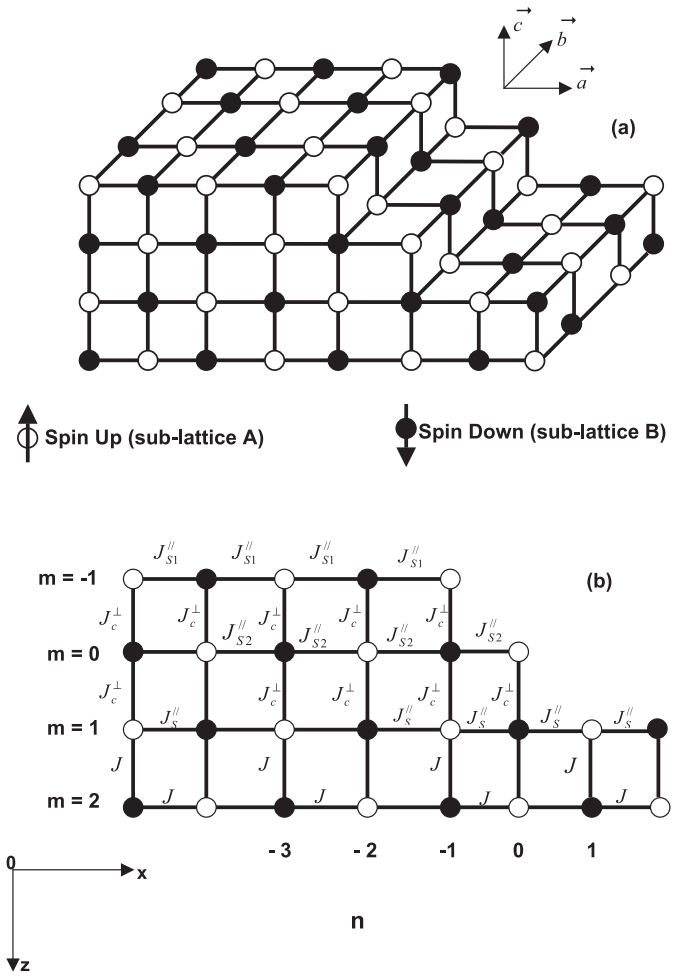

Fig. 1. (a) Schematic view of an antiferromagnetic stepped surface. The integers n, s, m count the spin site along the x-, y- and z-directions, respectively. (b) Two-dimensional cross-section of the insulating antiferromagnet model, showing the different exchange parameters. The z-axis is normal to the surface substrate, whereas the x-axis is perpendicular to the steps.

region $(-1 \leq m < 1)$ corresponding to spin sites belonging strictly to the step planes inside which translational invariance symmetry remains.

3 Bulk spin fluctuations dynamics outside the steps region

The formalism developed here and based on the matching technique is one of a number of theoretical techniques used to study surface spin-waves and resonances. It applies to ordered crystal surfaces by stipulating that the dynamics of localized surface states should conform in their decay to the evanescence dynamics of bulk modes along the direction normal and away from the surface. In the present study it is advantageous to generalize the matching method to two spatial directions, normal and parallel to the steps. To analyze the spin fluctuation dynamics on the surface and at the steps, and to calculate the frequencies of the localized modes occurring at the boundary, a formalism consisting of essentially three main stages is developed. The first consists in determining the Bloch equations of spin motions, and the set of propagating magnetic modes, that describe in turn the magnetic propagating bulk spin fluctuation field on the 2D bulk square lattice parallel to the surface step structure. This field depends only on the nature of the magnetic exchange interactions proposed between its sites. This provides a straightforward derivation of the equations of motion for any overlayer commensurate with 2D periodicity. The second defines, by introducing the 1D Fourier transform, the equation of spin fluctuation dynamics in order to deduce the precessional field on the steps as well as for the two types of spin sites in the surface that are representative of the topmost layer on the left and the right terraces. The third stage aims to match the magnetic dynamics properties of the surface and steps to the evanescent bulk spin fluctuation field. Also, the evanescent magnetic modes induced in the bulk and the surface terrace region with the existence of the steps domain which is considered as an isolated nanometer-scale structure are calculated. The formalism developed in this paper allows a study of the bulk spin fluctuations field as well as the localized modes of spin waves on the surface step region depending on the nature of the bulk-surface and surface-step coupling exchange parameters.

The problem is formulated in terms of a Heisenberg model with two equivalent sub-lattices A and B. The microscopic Hamiltonian used is a sum of an exchange, external and anisotropy magnetic fields terms:

$$H = -\sum_{\langle n,s,m\rangle}\sum_{\langle n',s',m'\rangle} J_{AB} S_{n,s,m} S_{n',s',m'} + \mu_A H_e^A \sum_{\langle n,s,m\rangle} S^Z_{n,s,m} + \mu_B H_e^B \sum_{\langle n',s',m'\rangle} S^Z_{n',s',m'}. \quad (1)$$

Primed sums indicate simultaneously $n = n'$, $s = s'$ and $m = m'$ cases are excluded, otherwise all sums range over all the lattice sites. $\mu_{A(B)}$ are the gyromagnetic ratios for ions on A or B-sites, respectively. $S_{n,s,m}$ and $S_{n',s',m'}$ are the magnitude of the corresponding local-spin operators located at the lattice sites $[\sigma] = (n, s, m)$ and $[\kappa] = (n', s', m')$, respectively. The subscripts (n, s, m) and (n', s', m') run over the sub-lattice A-sites and B-sites, respectively. J_{AB} is taken as positive in equation (1) to depict an antiferromagnetic alignment of the spin on one sub-lattice with respect to the other. Here, we consider only nearest neighbors inter-sublattices exchange interactions, allowing J_{AB} to be different from the bulk value $J\,(m \geq 2)$ and take the values $J^{\parallel}_{S1}, J^{\parallel}_{S2}, J^{\parallel}_{S}$, when the spin sites are located in the upper, lower step and surface terrace, respectively. An adjacent exchange interaction in the stepped surface domain is denoted by $J^{\perp}_c$. $H_e^{A,B} = H_o + H^a_{A,B}$ characterize the effective fields experienced by the magnetic ions on sub-lattices A and B, and are due to the externally applied field H_o and to the effective single-ion anisotropy fields $H^a_{A,B}$. They are taken to lie along the easy direction of magnetization which itself

is taken to be the direction of the z-axis, perpendicular to the substrate surface.

In treating the bulk spin fluctuation field properties outside the steps and surface regions removed from the step, it is advantageous to use the detailed form of the dispersion law and the normal modes of the bulk spin fluctuation field, so one needs to introduce the 2D periodic character of surface steps layers. This has the advantage of using the translational symmetry and transforms the site representation $\alpha^+_{n,s,m}(\beta^+_{n,s,m})$ to the spin-wave representation $\alpha^+_{\vec{k}}(\beta^+_{\vec{k}})$, where $\vec{k}$ is the corresponding wave vector, $\alpha^+_{n,s,m}(\beta^+_{n,s,m})$ are the local spin deviation at site (n,s,m). For the bulk region, only translations parallel to the surface terrace of the substrate are symmetry operations. As a result of this symmetry, the in-plane wave-vector $k_\parallel(k_x,k_y)$ is still a good quantum number. $k_\parallel$ spans the two-dimensional Brillouin zone defined by the combined substrate symmetry parallel to the surface terrace. Owing to the reduced and broken symmetries of the stepped surface problem, it is convenient to work in a mixed representation which is localized on planes parallel to the surface terrace. We define the local spin-deviation creation operators $\alpha^+_{k_\parallel}$ and $\beta^+_{k_\parallel}$ on given sites (n,s,m) and (n',s',m'), respectively, with a given transverse crystal momentum $k_\parallel$, by:

$$\alpha^+_{n,s,m}(t,k_\parallel)=\sum_{\langle n,s,m\rangle} S^+_{n,s,m}(t)e^{-ik_\parallel r_{n,s,m}}$$

and

$$S^+_{n,s,m}(t)=\sum_{\langle k_\parallel\rangle}\alpha^+_{k_\parallel}(t,k_\parallel)e^{-ik_\parallel r_{n,s,m}}, \tag{2a}$$

$$\beta^+_{n,s,m}(t,k_\parallel)=\sum_{\langle n',s',m'\rangle} S^+_{n',s',m'}(t)e^{-ik_\parallel r_{n',s',m'}}$$

and

$$S^+_{n',s',m'}(t)=\sum_{\langle k_\parallel\rangle}\beta^+_{k_\parallel}(t,k_\parallel)e^{-ik_\parallel r_{n',s',m'}}. \tag{2b}$$

Inserting equations (2) in equation (1) and putting $E=(\hbar w-g\mu_B H_0)/JS$ and $J_{AB}=J$, the linearized equations of motion of each layer in sub-lattices A and B relating to the spin fluctuation field for any site σ in the bulk domain removed from the step are found by commuting the sub-lattice spin lowering operators with the Hamiltonian in the form $idS^\pm_{n,s,m}/dt=[S^\pm_{n,s,m},H]$. This leads to:

$$\begin{aligned}E\alpha^+_{n,s,m(r)}(k_\parallel,w)&=z_{\sigma\kappa}\sum_{\langle\sigma,\kappa\rangle}J\Big\{\langle S^Z_A\rangle\frac{1}{z_{\sigma\kappa}}\gamma_k^{\sigma\kappa(\parallel)}\beta^+_{n,s,m(r+\Delta)}\\&-\langle S^Z_B\rangle\gamma_k^{\sigma\kappa(\perp)}\alpha^+_{n,s,m(r)}\Big\}+\mu_A H^a_A\alpha^+_{n,s,m(r)},\end{aligned} \tag{3a}$$

$$\begin{aligned}E\beta^+_{n,s,m(r+\Delta)}(k_\parallel,w)&=z_{\sigma\kappa}\sum_{\langle\sigma,\kappa\rangle}J\Big\{\langle S^Z_B\rangle\frac{1}{z_{\sigma\kappa}}\gamma_k^{\sigma\kappa(\parallel)}\alpha^+_{n,s,m(r)}\\&-\langle S^Z_A\rangle\gamma_k^{\sigma\kappa(\perp)}\beta^+_{n',s',m'(r+\Delta)}\Big\}+\mu_B H^a_B\beta^+_{n,s,m(r+\Delta)},\end{aligned} \tag{3b}$$

In obtaining equations (3), we replaced $S^Z_{n,s,m}$ and $S^Z_{n',s',m'}$ by its thermal expectation value, given by $\langle S^Z_A\rangle$ and $\langle S^Z_B\rangle$, respectively, considering that at relatively low temperatures, in comparison with the order-disorder transition temperature, the z-component of the spin on either A or B may be approximated by $\langle S^Z_{n,s,m}\rangle=S_A$ and $\langle S^Z_{n',s',m'}\rangle=S_B$. Owing to the antiferromagnetic character of the model used here, we consider $S_A=-S_B$. The summation (σ,κ) is over nearest neighbors only, and $z_{\sigma\kappa}$ denotes the number of nearest neighbors sitting on $[\kappa]$ sites to an ion on a $[\sigma]$ site. We have used σ, $\kappa=$ A, B throughout. Two types of contributions occur for the first part in the second term of equation (3a). For the first type, the nearest neighbors of the spin at r are in adjacent layers. In the second, the nearest neighbors are in the same layer. Whereas for equation (3b), the opposite case is assumed. We consider that $r_{n,s,m}-r_{n\pm1,s\pm1,m\pm1}=\Delta$, for any variation of integers n,s and m. The functions $\gamma_k^{\sigma\kappa(\parallel)}$ and $\gamma_k^{\sigma\kappa(\perp)}$ are relative to the geometry of the magnetic model and result from the exponential factors when $z^{(\parallel)}_{\sigma\kappa}$ and $z^{(\perp)}_{\sigma\kappa}$ characterize the number of nearest neighbors in the same and in the adjacent layer, respectively. It may be expressed as:

$$\begin{aligned}\gamma_k^{\sigma\kappa(\parallel)}&=\left[z^{(\parallel)}_{\sigma\kappa}\right]^{-1}\sum_{\langle n,s,m\rangle}\exp ik_\parallel(r_{n,s,m}-r_{n\pm1,s\pm1,m})\\&=1/2\left[\cos(k_xa)+\cos(k_ya)\right],\\\gamma_k^{\sigma\kappa(\perp)}&=\left[z^{(\perp)}_{\sigma\kappa}\right]^{-1}\sum_{\langle n,s,m\rangle}\exp ik_\parallel(r_{n,s,m}-r_{n,s,m\pm1})=1.\end{aligned} \tag{4}$$

To give a complete description of the spin fluctuations field, the equations of motion for each domain need to be rewritten for any site (n,s,m) in the bulk domain removed from the step as well as on the surface terrace. Using equations (3a) and (3b) and owing to the translational invariance in two dimensions for the bulk region $(m\geq 2)$, the Bloch conditions may be applied in the x and y-directions, resulting in the equations of the bulk spin fluctuation dynamics which for each sub-lattice takes the recurrent form:

$$\begin{aligned}E\alpha^+_{n,s,m}&=\Big[\gamma_k^{\sigma\kappa(\parallel)}\\&\times\Big\{\beta^+_{n+1,s,m}+\beta^+_{n-1,s,m}+\beta^+_{n,s-1,m}+\beta^+_{n,s+1,m}\Big\}-\alpha^+_{n,s,m}\Big]\\&+\Big[\gamma_k^{\sigma\kappa(\perp)}\left\{\beta^+_{n,s,m+1}+\beta^+_{n,s,m-1}\right\}-\alpha^+_{n,s,m}\Big]+\mu_A H^a_A\alpha^+_{n,s,m},\end{aligned}$$

$$E\beta^{+}_{n,s,m} = \Big[\gamma_k^{\sigma\kappa(\parallel)} \times\Big\{\alpha^{+}_{n+1,s,m} + \alpha^{+}_{n-1,s,m} + \alpha^{+}_{n,s-1,m} + \alpha^{+}_{n,s+1,m}\Big\} - \beta^{+}_{n,s,m}\Big] + \Big[\gamma_k^{\sigma\kappa(\perp)}\Big\{\alpha^{+}_{n,s,m+1} + \alpha^{+}_{n,s,m-1}\Big\} - \beta^{+}_{n,s,m}\Big] + \mu_B H^a_B \beta^{+}_{n,s,m}. \tag{5}$$

The spin fluctuation motion on sites (n, s, m) and (n', s', m') outside the surface steps boundaries, may hence be expressed as:

$$\Big[E^2 I - D\left(\gamma_k^{\sigma\kappa(\parallel)}, \gamma_k^{\sigma\kappa(\perp)}, J, S_A, S_B\right)\Big] \left| \begin{matrix}\alpha^{+}_{n,s,m} \\ \beta^{+}_{n,s,m}\end{matrix} \right\rangle = 0. \tag{6}$$

To describe the evanescent field of the bulk spin fluctuation variables on the square lattice parallel to the surface step region, we introduce the spatial phase factors which describe the evanescent modes. This is done considering the travelling spin-wave from one site to its nearest neighbors in either sense along both the broken symmetry directions (z- and x-axis) of the cubic lattice and by introducing the static and dynamic parts of the variable $\alpha^{+}_{n,s,m}(t)$ and $\beta^{+}_{n,s,m}(t)$ given by equations (2) as follows:

$$\alpha^{+}_{n,s,m\pm1}(t) = \alpha^{+}_{n,s,m\pm1}(0) + \alpha^{+}_{n,s,m\pm1}\psi_{n,s,m\pm1}e^{-iwt}$$
$$\text{and} \quad \beta^{+}_{n,s,m\pm1}(t) = \beta^{+}_{n,s,m\pm1}(0) + \beta^{+}_{n,s,m\pm1}\psi_{n,s,m\pm1}e^{-iwt}, \tag{7a}$$

$$\alpha^{+}_{n\pm1,s,m}(t) = \alpha^{+}_{n\pm1,s,m}(0) + \alpha^{+}_{n\pm1,s,m}\psi_{n\pm1,s,m}e^{-iwt}$$
$$\text{and} \quad \beta^{+}_{n\pm1,s,m}(t) = \beta^{+}_{n\pm1,s,m}(0) + \beta^{+}_{n\pm1,s,m}\psi_{n\pm1,s,m}e^{-iwt}, \tag{7b}$$

where $\alpha^{+}_{n,s,m\pm1}(0)$ $(\alpha^{+}_{n\pm1,s,m}(0))$ and $\beta^{+}_{n,s,m\pm1}(0)$ $(\beta^{+}_{n\pm1,s,m}(0))$ are the time independent part in the direction of the magnetic order along the $z(x)$-axis, $\psi_{n,s,m\pm1}$ $(\psi_{n\pm1,s,m})$ characterizes the spatial phase factors of a wave for a propagating mode along the chain corresponding to a spin site and its nearest neighbors in $z(x)$-direction, respectively. The last terms in equations (7) depict the spin fluctuation variable from the direction of magnetic order, giving rise to spin excitations [19–21]. Since the system has the translational invariance parallel to the surface terrace, we focus our attention on determining the unique solution for the evanescent magnetic modes propagating in the direction normal to the 2D lattice extended in the x- and y-axis. Consequently, the z-direction is chosen to characterize the exponentially decay of amplitude with increasing penetration into the crystal. Inserting equations (7a) and (7b) in equation (6), we are able to give the bulk secular equation as:

$$\sum_{\eta=1}^{\eta=5} \xi_\eta \psi^{(\eta-1)}_{n,s,\pm m} = 0 \tag{8}$$

where the coefficient ξ_η are described by the following expressions with the properties:

$$\xi_1 = \xi_5 = J^2 S_A S_B,$$
$$\xi_2 = \xi_4 = 4J^2 S_A S_B(\cos k_x a + \cos k_y a),$$
$$\xi_3 = -\left[(E + JS_B z_{\sigma\kappa} + \mu_A H^A_e)(E + JS_A z_{\sigma\kappa} + \mu_B H^B_e)\right] + 2J^2 S_A S_B(1 + 2(\cos k_x a + \cos k_y a)^2).$$

The phase factor doublet $(\psi_{n,s,\pm m}(\zeta), \psi^{-1}_{n,s,\pm m}(\zeta))$ can be shown to verify symmetrically the polynomial equation (8), owing to the Hermitian nature of the bulk dynamics or time reversal symmetry in such a bulk crystalline lattice [22,23]. ζ depicts both the evanescent (n_e) and bulk (n_b) modes. The frequencies of the bulk spin fluctuations dynamics field are obtained using equation (10), when ψ satisfies the propagating condition $|\psi_{n,s,\pm m}(\zeta)| = 1$. For arbitrary values of $\psi_{n,s,\pm m}(\zeta)$, however, equation (8) does not provide on its own the required unique solution for the surface steps system. To obtain this one also needs to analyze the spin dynamics on the surface terrace and step regions. To do this, we require knowledge of the complete set of evanescent modes in the bulk region. These latter modes and their properties will be discussed in the next section. These can be characterized by complex phase factors which describe the decrease of precessional amplitude field with the distance from the surface steps domain. The latter region is specific because it constitutes strictly a surface problem with reconstruction and/or relaxed layers. Consequently, we need to describe the spin fluctuation dynamics for the topmost layer as step terrace $(n < 0, s, 0)$ and for two types of sites for spins in the surface that are somewhat removed from the step, and that are representative of the left $(n < 0, s, 1)$ and the right $(n > 0, s, 1)$ terraces, respectively.

4 Spin modes localized on the stepped surface region

In order to describe the full spin fluctuations dynamics problem in the presence of surface steps, we have not only to know the propagating modes described by their above phase factors, but also consider the evanescent solutions of the system. Explicitly, for a given energy value E, we need all the solutions $\psi_{n,s,m}(\zeta)$, including those with $|\psi_{n,s,m}(\zeta)| \neq 1$.

As regards the spin surface dynamics, it is necessary to specify in the surface boundary substrate, five elementary domains due to the broken symmetry along the x- and z-directions. The primary domain consists of the spin sites belonging strictly in the first step $(m = -1)$. The second corresponds to two domains for spin sites also relatively removed from the step belonging in the second step $(m = 0)$. The third characterizes surface terrace sites $(m = 1)$ which refers to the two regions for spin sites located to the left of the surface plane $(n < 0, s, m = 1)$ and right of the second step $(n > 0, s, m = 1)$. This representation allows us to determine the spin fluctuation field for both surface and

steps layers. Furthermore, as has been pointed out previously, Bloch's theorem may be used in the y-direction due to the existence of translational symmetry. Furthermore, we need for simplicity, to introduce the following parameters: $\varepsilon_1^{\parallel} = J_{S1}^{\parallel}/J$, $\varepsilon_2^{\parallel} = J_{S2}^{\parallel}/J$, $\varepsilon_s^{\parallel} = J_s^{\parallel}/J$, $\varepsilon_{1\parallel}^{\perp} = J_{s1}^{\parallel}/J_c^{\perp}$, $\varepsilon_{2\parallel}^{\perp} = J_{s2}^{\parallel}/J_c^{\perp}$, $\varepsilon_{S\parallel}^{\perp} = J_S^{\parallel}/J_c^{\perp}$ and $\varepsilon_c^{\perp} = J_c^{\perp}/J$. This leads to give the equations of motion for spin sites located to the left ($n < 0$, s, $m = 1$) and right of the surface substrate ($n > 0$, s, $m = 1$). These are given, respectively, by the following expressions:

$$E\alpha_{n,s,1}^{(A)} = \varepsilon_S^{\parallel}\Big[(1-\cos k_y a) \times \left\{\beta_{n+1,s,1}^{+} + \beta_{n-1,s,1}^{+} + \beta_{n,s-1,1}^{+} + \beta_{n,s+1,1}^{+}\right\} - \alpha_{n,s,1}^{+}\Big] + \Big[\left\{\varepsilon_{S\parallel}^{\perp}\beta_{n,s,0}^{+} + \varepsilon_S^{\parallel}\beta_{n,s,2}^{+}\right\} - \alpha_{n,s,1}^{+}\Big] + \mu_A H_A^a \alpha_{n,s,1}^{+},$$

$$E\beta_{n,s,1}^{+} = \varepsilon_S^{\parallel}\Big[((1-\cos k_y a) \times \left\{\alpha_{n+1,s,1}^{+} + \alpha_{n-1,s,1}^{+} + \alpha_{n,s-1,1}^{+} + \alpha_{n,s+1,1}^{+}\right\} - \beta_{n,s,1}^{+}\Big] + \Big[\left\{\varepsilon_{S\parallel}^{\perp}\alpha_{n,s,0}^{+} + \varepsilon_S^{\parallel}\alpha_{n,s,2}^{+}\right\} - \beta_{n,s,1}^{+}\Big] + \mu_B H_B^a \beta_{n,s,1}^{+}. \quad (9a)$$

$$E\alpha_{n,s,1}^{+} = \varepsilon_S^{\parallel}\Big[(1-\cos k_y a) \times \left\{\beta_{n+1,s,1}^{+} + \beta_{n-1,s,1}^{+} + \beta_{n,s-1,1}^{+} + \beta_{n,s+1,1}^{+}\right\} - \alpha_{n,s,1}^{+}\Big] + \Big[\varepsilon_S^{\parallel}\beta_{n,s,2}^{+} - \alpha_{n,s,1}^{+}\Big] + \mu_A H_A^a \alpha_{n,s,1}^{+},$$

$$E\beta_{n,s,1}^{+} = \varepsilon_S^{\parallel}\Big[(1-\cos k_y a) \times \left\{\alpha_{n+1,s,1}^{+} + \alpha_{n-1,s,1}^{+} + \alpha_{n,s-1,1}^{+} + \alpha_{n,s+1,1}^{+}\right\} - \beta_{n,s,1}^{+}\Big] + \Big[\varepsilon_S^{\parallel}\alpha_{n,s,2}^{+} - \beta_{n,s,1}^{+}\Big] + \mu_B H_B^a \beta_{n,s,m}^{+}. \quad (9b)$$

For the first step layer ($-\infty < n \leq -1$, s, $m = -1$), this yields:

$$E\alpha_{n,s,-1}^{+} = \varepsilon_1^{\parallel}\Big[(1-\cos k_y a) \times \left\{\beta_{n+1,s,-1}^{+} + \beta_{n-1,s,-1}^{+} + \beta_{n,s-1,-1}^{+} + \beta_{n,s+1,-1}^{+}\right\} - \alpha_{n,s,-1}^{+}\Big] + \Big[\varepsilon_{1\parallel}^{\perp}\beta_{n,s,0}^{+} - \alpha_{n,s,-1}^{+}\Big] + \mu_A H_A^a \alpha_{n,s,-1}^{+},$$

$$E\beta_{n,s,-1}^{+} = \varepsilon_1^{\parallel}\Big[(1-\cos k_y a) \times \left\{\alpha_{n+1,s,-1}^{+} + \alpha_{n-1,s,-1}^{+} + \alpha_{n,s-1,-1}^{+} + \alpha_{n,s+1,-1}^{+}\right\} - \beta_{n,s,-1}^{+}\Big] + \Big[\varepsilon_{1\parallel}^{\perp}\alpha_{n,s,0}^{+} - \beta_{n,s,-1}^{+}\Big] + \mu_B H_B^a \beta_{n,s,-1}^{+}. \quad (10)$$

For the second step layer ($m = 0$), we may write the equations of spin fluctuations variables corresponding to the quarter-infinite half spaces to the left ($-\infty < n < -1$) and to the right ($-1 \leq n \leq 0$) of the second semi-infinite step. These are expressed in the following forms:

For site spins belonging on the domain ($-\infty < n < -1$, s, $m = 0$):

$$E\alpha_{n,s,0}^{+} = \varepsilon_2^{\parallel}\Big[(1-\cos k_y a) \times \left\{\beta_{n+1,s,0}^{+} + \beta_{n-1,s,0}^{+} + \beta_{n,s-1,0}^{+} + \beta_{n,s+1,0}^{+}\right\} - \alpha_{n,s,0}^{+}\Big] + \Big[\varepsilon_{2\parallel}^{\perp}\left\{\beta_{n,s,-1}^{+} + \beta_{n,s,1}^{+}\right\} - \alpha_{n,s,0}^{+}\Big] + \mu_A H_A^a \alpha_{n,s,0}^{+},$$

$$E\beta_{n,s,0}^{+} = \varepsilon_2^{\parallel}\Big[(1-\cos k_y a) \times \left\{\alpha_{n+1,s,0}^{+} + \alpha_{n-1,s,0}^{+} + \alpha_{n,s-1,0}^{+} + \alpha_{n,s+1,0}^{+}\right\} - \beta_{n,s,0}^{+}\Big] + \Big[\varepsilon_{2\parallel}^{\perp}\left\{\alpha_{n,s,-1}^{+} + \alpha_{n,s,1}^{+}\right\} - \beta_{n,s,0}^{+}\Big] + \mu_B H_B^a \beta_{n,s,0}^{+}. \quad (11)$$

For spin sites belonging strictly on the second terrace step ($-1 \leq n \leq 0$, s, $m = 0$), we may write:

$$E\alpha_{n,s,0}^{+} = \varepsilon_2^{\parallel}\Big[(1-\cos k_y a) \times \left\{\beta_{n-1,s,0}^{+} + \beta_{n,s-1,0}^{+} + \beta_{n,s+1,0}^{+}\right\} - \alpha_{n,s,0}^{+}\Big] + \Big[\varepsilon_{2\parallel}^{\perp}\beta_{n,s,1}^{+} - \alpha_{n,s,0}^{+}\Big] + \mu_A H_A^a \alpha_{n,s,0}^{+},$$

$$E\beta_{n,s,0}^{+} = \varepsilon_2^{\parallel}\Big[(1-\cos k_y a) \times \left\{\alpha_{n-1,s,0}^{+} + \alpha_{n,s-1,0}^{+} + \alpha_{n,s+1,0}^{+}\right\} - \beta_{n,s,0}^{+}\Big] + \Big[\varepsilon_{2\parallel}^{\perp}\alpha_{n,s,1}^{+} - \beta_{n,s,0}^{+}\Big] + \mu_B H_B^a \beta_{n,s,0}^{+}. \quad (12)$$

The generalized spatial phase factors along the y-direction may be written according to equation (7). Since the steps are considered infinite along the y-axis, we use Bloch's theorem and write the operators $\alpha_{n,s\pm1,m}^{+}$ and $\beta_{n',s'\pm1,m'}^{+}$ in their wave-like representation, so that:

$$\alpha_{n,s\pm1,m}^{+}(t) = \alpha_{n,s\pm1,m}^{+}(0) + \alpha_{n,s\pm1,m}^{+} e^{\pm ik_y a} e^{-iwt}$$

and

$$\beta_{n,s\pm1,m}^{+}(t) = \beta_{n,s\pm1,m}^{+}(0) + \beta_{n,s\pm1,m}^{+} e^{\pm ik_y a} e^{-iwt}. \quad (13)$$

The quantity $\exp(\pm ik_y a)$ was chosen to depict the phase factor for the propagating mode along the y-axis by considering the travelling spin-wave from one site to its nearest neighbors in either sense.

In general, the precessional spin fluctuation field of quantum spins in the surface step domain includes both evanescent and propagating spin fluctuation dynamics. Also, it may be described by a general linear development of a complete set of the n_e and n_b modes. In order to solve for the magnetic excitations localized on the surface and steps, we need to match the propagating bulk modes to

the corresponding evanescent field near the surface and step regions using the matching procedure [15,24,25]. For spin sites somewhat removed from the first step yet on the second, to the right and left of the step, the fluctuation spin variables may be represented in terms of the evanescent field as follows:

for spins located on the domain ($-\infty < n \leq 1, s, m = 0$) we may put:

$$\alpha^{+}_{-\infty<n\leq 1,s,m=0} = \sum_{\zeta=1}^{n_e+n_b} \psi_{\zeta(-\infty<n\leq 1,s,m=0)}(E,k,\zeta),$$
$$\beta^{+}_{-\infty<n\leq 1,s,m=0} = \sum_{\zeta=1}^{n_e+n_b} \psi_{\zeta(-\infty<n\leq 1,s,m=0)}(E,k,\zeta). \tag{14}$$

For spin sites below the step labeled by the indices ($-1 \leq n \leq 0, s, m = 0$), the equation (14) may be written as

$$\alpha^{+}_{-1\leq n\leq 0,s,m=0} = \sum_{\zeta=1}^{n_e+n_b} \psi_{\zeta(-1\leq n\leq 0,s,0)}(E,k,\zeta),$$
$$\beta^{+}_{-1\leq n\leq 0,s,m=0} = \sum_{\zeta=1}^{n_e+n_b} \psi_{\zeta(-1\leq n\leq 0,s,0)}(E,k,\zeta). \tag{15}$$

where as for embedded sites surrounding the first step, the equations describing the matching of bulk spin fluctuation variables with the localized modes on steps may be written in the following forms:

$$\alpha^{+}_{n,s,\pm m} = \sum_{\zeta=1}^{n_e+n_b} R_{r\zeta(n<0,s,m)} C\left(A, \psi_{\zeta(n,s,m>1)}\right) \times \psi^{m-1}_{\zeta(n,s,m>2)}(E,k,\zeta), \tag{16a}$$

$$\beta^{+}_{n,s,\pm m} = \sum_{\zeta=1}^{n_e+n_b} R_{l\zeta(n>0,s,m)} C\left(B, \psi_{\zeta(n,s,m>1)}\right) \times \psi^{m-1}_{\zeta(n,s,m>1)}(E,k,\zeta). \tag{16b}$$

This mathematical framework of evanescent magnetic modes in a two-dimensional square lattice in the neighborhood of extended inhomogeneities such as a surface step layer allows us to uncouple the equation of motion of the steps and surface terrace at the boundary from the bulk domain. The weighting coefficients $R_{r\zeta(n<0,s,m)}$ and $R_{l\zeta(n>0,s,m)}$ characterize the contributions of different modes in the bulk precessional amplitude field for projecting the evanescent field in respectively the quarter-infinite half spaces to the left and to the right of the two magnetic steps. Also, the equations (14), (15) and (16) characterize the matching relations for describing the surface and step spin wave branches from the bulk spin precessional field equations. $C(A(B), \psi_{\zeta(n,s,m\geq 2)})$ are the normalized corresponding polarization vectors of spin-waves which represent the cofactor of the dynamical matrix given in equation (6).

The evanescent spin fluctuation amplitude in the z-direction away from the surface step region, is described by the phase factor doublet $(\psi_{\zeta(n,s,m)}, \psi^{-1}_{\zeta(n,s,m)})$, going from one site to its nearest neighbors or vice-versa along the direction normal to the step terrace. The subscript ξ is carried out over all 3D travelling ($|\psi_{\zeta(n,s,m)}| = 1$ and $|\psi^{-1}_{\zeta(n,s,m)}| = 1$) and exponential-like ($|\psi_{\zeta(n,s,m)}| < 1$ and $|\psi^{-1}_{\zeta(n,s,m)}| > 1$) Bloch waves. Explicitly, we consider that an evanescent magnetic excitation from the surface step layer is characterized by a phase factor satisfying the requirement that $|\psi_{\zeta(n,s,m)}| < 1$ given by the evanescent solutions of the equations of motion, whereas the propagating mode is described when $|\psi_{\zeta(n,s,m)}| = 1$. In practice only the evanescent and propagating modes are retained as physically applicable.

By considering the above matching procedure in two dimensions, it is finally possible to recast the equations for the dynamics of the spin fluctuation variables in the step domain by using equations (6), (14), (15) and (16). This leads to the matrix form described as:

$$\left[E^2 I - M_S(\upsilon, \theta, \{\psi_\zeta\})\right] |V\rangle = |0\rangle\,, \tag{17}$$

where $|V\rangle = [\alpha^{+}_{-\infty<n\leq -1,s,-1}, \beta^{+}_{-\infty<n\leq -1,s,-1}, \alpha^{+}_{n\leq 0,s,0}, \beta^{+}_{n\leq 0,s,0}, \alpha^{+}_{n,s,1}, \beta^{+}_{n,s,1}, \alpha^{+}_{n,s,2}, \beta^{+}_{n,s,2}, R_{r\zeta}, R_{l\zeta}]^T$. I is the unit matrix and $M_S(\vartheta, \theta, \{\psi_\zeta\})$ with $\vartheta, \theta = \phi(E, \varepsilon^{\parallel}_{1(2)}, \varepsilon^{\perp}_{c}, \varepsilon^{\perp}_{\parallel}, \gamma^{\sigma\kappa(\parallel,\perp)}_{k}(k_\parallel, \psi_\xi), C(A(B), \psi_\xi), H^{a}_{A,B})$ denotes the square (10×10) mean dynamical matrix which describes the localized spin waves on the surface step layers and $\{\psi\}$ is a set of $\zeta = 1, 2, \ldots, (n_e + n_b)$ roots of the ψ-secular equation (8), in the $(E, k_\parallel)$ space. To obtain non trivial solutions for the spin fluctuation variables $\alpha^{+}_{n,s,m}$ and $\beta^{+}_{n',s',m'}$, the determinant system given by equation (17) must vanish, which defines an algebraic equation in E, whose real and positive solutions $E_S(k_\parallel)$ yield the mean surface step spin wave branches in the n_b zones, and the surface step resonances in the regions where $n_b \neq 0$. The non-vanishing matrix elements M_S are given in the appendix.

5 Numerical results and discussions

Salient numerical examples are presented to demonstrate the essential features of the surface and step spin-wave modes and the influence of bulk-surface and bulk-step exchange parameters on the localized spin modes. It is important to note that in the present calculations, due to the lack of experimental data, we neglect in our numerical results both bulk and surface anisotropy fields as well as the applied magnetic field. Their eventual inclusion into the model poses no difficulty at all from a mathematical point of view. Furthermore, let us quote that for any thorough surface study, we must include surface relaxation or reconstruction effects which can influence the exchange constants. It is quite possible that other kinds of magnetic interactions also play a role in the behavior and frequencies of the spin waves localized on the surface and step in which case these interactions should be considered in the

spin fluctuation field calculations. Consequently, we could also consider variations in the exchange constants from side to side and the step-step interactions, but we will not explore this further in this work considering the degree of complexity of problem examined here. Consequently, only the case where $\varepsilon_c^{\perp} = 1$ and $\varepsilon_1^{\parallel} = \varepsilon_2^{\parallel} = \varepsilon_s^{\parallel} = \varepsilon_{1\parallel}^{\perp} = \varepsilon_{2\parallel}^{\perp} = \varepsilon_{s\parallel}^{\perp}$ is investigated.

The set of propagating spin-wave modes energies localized in the bulk domain are obtained after inserting equations (7a) and (7b) in equation (6) and using equation (8) with the conditions $|\psi_{\pm n,s,m}| = 1$ and $|\psi_{n,s,\pm m}| = 1$. The only region where the latter conditions are verified corresponds effectively to the propagating modes for the bulk region referred to as the bulk continuum in the figures. The surface step fluctuation field amplitude decays exponentially with increasing penetration into the insulating antiferromagnetic layer. The numerical calculations, in the form of points E versus $k_y a$, gives the dispersion curves for a model of magnetic exchange interactions for that purpose.

The satisfying condition $\det(M_s) = 0$ in equation (17) leads to a non linear expression in E and $k_{\parallel}a$. The numerical solution gives the dispersion curves which depict the surface and step spin mode energies. These curves depict magnons propagating along the direction normal to the surface steps that are however effectively localized in the sense that their spin fluctuation field is evanescent in the plane normal to the step terrace. The amplitude of the localized spin-waves decreases as one goes from one site to another further and further away from the step into the bulk domain.

When the surface exchange interactions ($J_S^{\parallel}$) differ from those in the bulk (J), the behavior of the surface magnetization with changing roughness is much more complex and interesting. $J_S^{\parallel}$ may be larger or smaller than J. The reduced atomic coordination at a surface produces a narrower band width and hence a larger magnetic moment [26,27], favoring $J_S^{\parallel} > J$. On the other hand, the surface lattice spacing can be larger than the bulk lattice spacing, leading to a weaker spin-spin interaction and favoring $J_S^{\parallel} < J$. We therefore consider both possibilities. Consequently, the spin-wave dispersion curves for bulk, surface and step layers are shown in Figure 2, considering the propagating and evanescent modes along the wave-vector k_y. Let us mention that in Figures 2a and 2b, the case where the exchange parameters for both surface and step layers are weaker than in the bulk domain is considered, whereas in Figures 2c and 2e the opposite case is assumed. Figure 2d depicts the free stepped surface configuration.

Let us consider, firstly, the weak bulk-stepped surface coupling exchange ($\varepsilon_1^{\parallel} = 0.5$) as illustrated in Figure 2a. Three acoustic branches will be truncated at some value of $k_y = k_c$ (given by, $k_{c1} = 0.44$, $k_{c2} = 0.52$, $k_{c3} = 0.87$) corresponding to $E_B(k_c) = E_s(k_c)$. One optic mode (O_1) occurs tangentially with the bulk continuum with energy range 662 K $\leq E_s \leq$ 706 K. All branches are doubly degenerate. Two localized modes (A_1 and A_2) correspond to those occurring along the two steps edges, whereas the third (A_3) characterizes the surface terrace mode. When a weak bulk-stepped surface coupling exchange ($\varepsilon_1^{\parallel} = 0.8$) is considered as illustrated in Figure 2b, the two truncated acoustic modes (A_1 and A_2) occur with energies $E_{SA_1}(k_y) = E_{sA_2}(k_y)$ and the energy value for the third acoustic mode remains constant with $E_{SA_3}(k_y) \approx 355$ K.

For the "free stepped surface" case ($\varepsilon_1^{\parallel} = 1$), the surface spin-wave modes are seen to split into two branches for small enough wave vectors and they become approximately degenerate at larger wave vectors. Since the splitting of the acoustic spin-wave surface branches is most apparent for small wave vectors in the case of the free stepped surface, these surface effects in films can in principle be studied experimentally by light scattering techniques. Furthermore, the two acoustic modes localized on the two steps are practically superposed and occur in the energy range 215 K $\leq E_S \leq$ 222 K as illustrated in Figure 2c.

The strong bulk-stepped surface coupling exchange with values $\varepsilon_1^{\parallel} = 1.4$ and $\varepsilon_1^{\parallel} = 1.8$ gives the presence of optical modes. These illustrations are given in Figures 2d and 2e, respectively. No acoustic wave branches exist for $\varepsilon_1^{\parallel} \geq 1$. In Figure 2d, four modes appear, all occurring above the bulk spin-wave region so-called "optical modes". Hence, there is an energy range, approximately 188 K $\leq E_S \leq$ 319 K for which there are localized interface modes as well as surface and step modes. Two modes (O_2, O_3) will be truncated at some value of $k_y = k_c'$ (given by $k_{c2}' = 1.7$ and $k_{c3}' \approx 0.9$). One complete mode (O_4) occurs at the origin of the first Brillouin zone and becomes the magnetic cell with $E_s(k_y \to 0) \approx 242$ K. Figure 2e displays the surface and step spin wave modes. Again the shaded area corresponds to the region occupied by the bulk modes. Figure 2e is presented emphasizing the distribution of the frequencies of the localized modes and the effects of changes in the surface-step-bulk exchange parameters on the surface-step spin-wave branches that can occur. For sufficiently small values of $\varepsilon_1^{\parallel}$, the assumed antiferromagnetic ground state can become unstable, corresponding to a reorientation of spins near the surfaces. This is analogous to the type of surface reorientation phase transition discussed by Mills [28] in certain anisotropic ferromagnets.

6 Conclusions

The matching procedure is used in this work to calculate the spin-wave modes localized on a surface step for an insulating antiferromagnet model. We emphasize that the present model is simple insofar that it considers only magnetic exchange interactions between the ordered spins, yielding the exchange-dominated step localized spin-waves. Following the analytical procedure developed in this paper, it is possible to introduce other forms of magnetic interactions in the present model in a relatively direct manner.

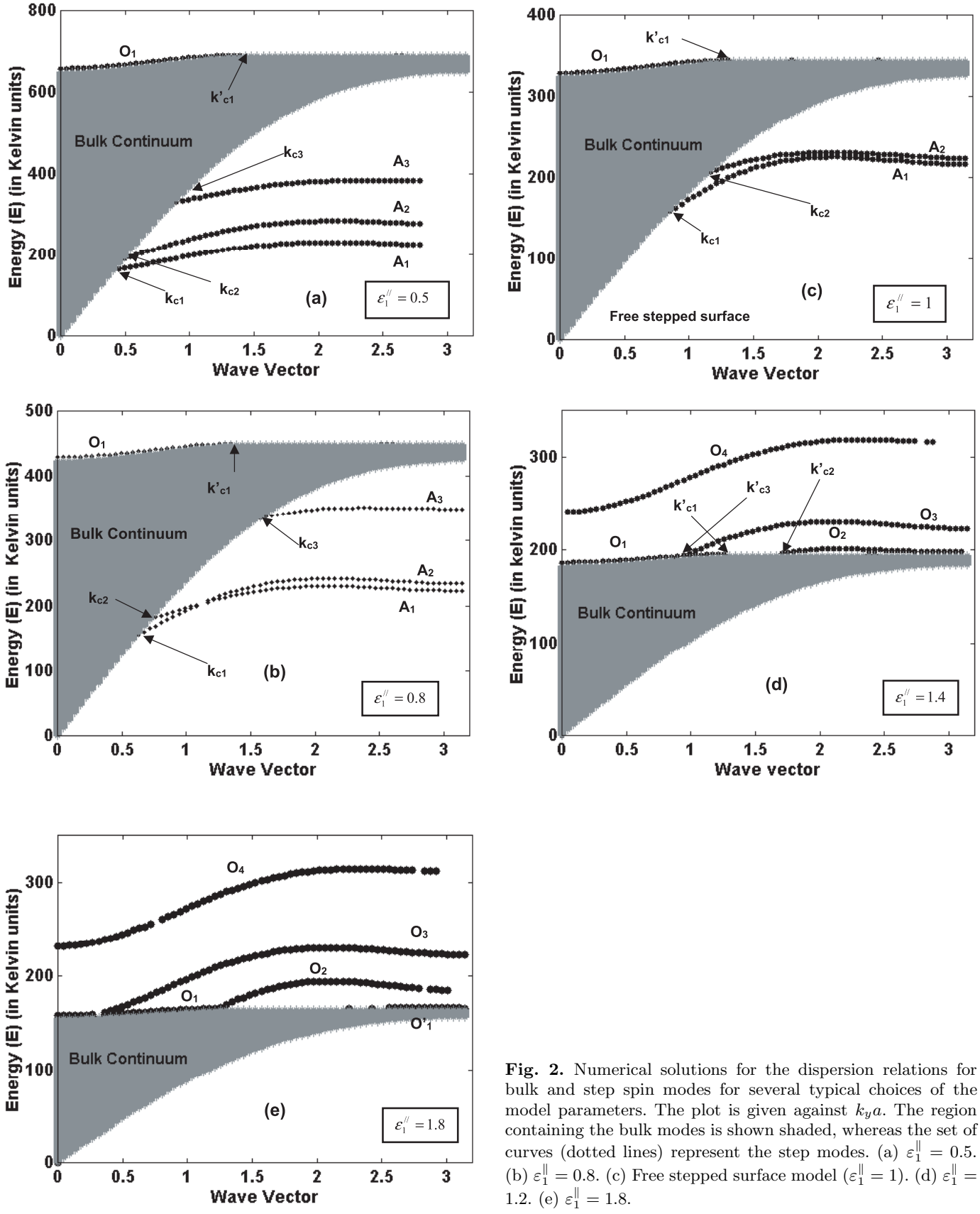

Fig. 2. Numerical solutions for the dispersion relations for bulk and step spin modes for several typical choices of the model parameters. The plot is given against $k_y a$. The region containing the bulk modes is shown shaded, whereas the set of curves (dotted lines) represent the step modes. (a) $\varepsilon_1^{\parallel} = 0.5$. (b) $\varepsilon_1^{\parallel} = 0.8$. (c) Free stepped surface model ($\varepsilon_1^{\parallel} = 1$). (d) $\varepsilon_1^{\parallel} = 1.2$. (e) $\varepsilon_1^{\parallel} = 1.8$.

The formalism presented here is an analytical approach which is independent of the geometry of the nanostructure in the surface. This makes it easy to extend to a variety of real problems. It can also give in a direct manner the spin fluctuation field on the surface step layer with the help of finite matrices. The theoretical formalism described for the present case can readily be generalized to other surface step problems concerning in particular the imperfect antiferromagnets films such as NiO or the perovskite structure $KNiF_3$. In both of these materials the magnetic Ni ions lie on a simple cubic lattice, and the exchange interactions are very strong making the use of Heisenberg type Hamiltonian appropriate.

To our knowledge little if any attention has been assigned to the study of magnetic excitations localized in the neighborhood of a surface step system. From the experimental point of view, we note that the lack of experimental data which are available at present to compare our results with. However, there is experimental evidence that shows the existence of step changes in the thin metastable epitaxial Fe films on Cu (100) [9] (these imperfections may lead to a number of effects including changes in the thermal properties of the film and short lifetimes for spin-waves as evidenced by the large linewidths in Brillouin scattering experiments), and the localized phonons on the step of a vicinal Ni surface [29]. With the recent theoretical work concerning these step localized phonons [30], this provides a realistic feel for such localized magnetic excitations. The phonon model, as well as the spin-wave model for that purpose, share a common theoretical approach in the harmonic approximation.

On the other hand, the frequencies of these localized modes may provide information concerning the local magnetic anisotropy and exchange interactions in the neighborhood of such a surface reconstruction and/or relaxed layers, and will contribute to understand more fully the role that surface phenomena may play such as surface steps instability, the growth of a magnetic substrate and surface optical properties. A straightforward generalization of the present calculations would be to other magnetic structures. This would allow applications to metallic films such as epitaxial fcc Fe (100) on Cu (100) films (10−17 monolayer thick) which is paramagnetic at room temperature and antiferromagnetic at low temperature [31], using Brillouin light scattering. These films have intriguing magnetic properties, making them suitable for surface reconstruction dynamics studies. Another application of these calculations may be illustrated on the monolayer Fe films grown on a stepped $W(110)$ surface. This system constitutes the only one in which growth starts with a stable Fe monolayer being formed, pseudomorphic with the W substrate. This growth mode has been observed on stepped W surfaces using scanning tunneling microscopy, where it is was seen that at 600 K the Fe films grow first along the steps, spreading across the ledges as they continue to grow [32].

It should be emphasized that the results we have found here show how sensitive the magnetic structure of a solid surface is to its atomic structure and geometry. We have to remark that our conclusions are based on a Heisenberg Hamiltonian model, with exchange reduced to nearest neighbors only, and with no inclusion of any reconstruction, pinning, step fluctuations, step-step interactions or magnetic anisotropy [33–35]. Our calculation is also restricted to a well defined model surface and to a reasonable sampling of the Brillouin zone. We believe, however, that we have uncovered some important points and that we have determined qualitatively the salient features of the spin-wave spectrum of stepped magnetic surfaces. Finally, the analytic procedure developed here for calculating the energies and intensities of the bulk and localized spin wave modes in the vicinity of two steps can be applied to other low dimensional structures and we intend to report on that elsewhere. Brillouin light scattering would provide a suitable probe of these effects.

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Appendix

The non vanishing (10×10) square matrix elements $M_s(k,l) = f(E, J^{\parallel}_{S1(S2)}, \mathrm{J}^{\parallel}_{\mathrm{S}}, J^{\perp}_c, J^{\perp}, J, C(A(B), \psi_\xi))$ are given in the following forms:

$$M_s(1,1) = E + (3J^{\parallel}_{S1} + J^{\perp}_c)S_B + \mu_A H^a_A,$$

$$M_s(1,2) = M_s(3,4) = -3J^{\parallel}_{S1}(1 - \cos k_y a)S_A,$$

$$M_s(1,4) = -J^{\perp}_c S_A,$$

$$M_s(2,1) = M_s(4,3) = -3J^{\parallel}_{S1}(1 - \cos k_y a)S_B,$$

$$M_s(2,2) = E + (3J^{\parallel}_1 + J^{\perp}_c)S_A + \mu_B H^a_B,$$

$$M_s(2,3) = M_s(4,5) = -J^{\perp}_c S_B,$$

$$M_s(3,3) = E + (3J^{\parallel}_{S1} + J^{\perp}_c)S_B + \mu_A H^a_A,$$

$$M_s(3,6) = J^{\perp}_c S_A,$$

$$M_s(4,4) = E + (3J^{\parallel}_1 + J^{\perp}_c)S_A + \mu_B H^a_B,$$

$$M_s(5,4) = M_s(5,8) = M_s(7,6) = -J^{\perp} S_A,$$

$$M_s(5,5) = E + (4J^{\parallel}_{S2} + J^{\perp}_c + J^{\perp})S_B + \mu_A H^a_A,$$

$$M_s(5,6) = -4J^{\parallel}_{S2}(1 - \cos k_y a)S_A,$$

$$M_s(6,3) = M_s(6,7) = M_s(8,5) = -J^{\perp} S_B,$$

$$M_s(6,5) = -4J^{\parallel}_{S2}(1 - \cos k_y a)S_B,$$

$$M_s(6,6) = E + (4J^{\parallel}_{S2} + J^{\perp}_c + J^{\perp})S_A + \mu_B H^a_B,$$

$$
\begin{aligned}
M_s(7,7) &= E + (5J + J^{\perp})S_B + \mu_A H_A^a, \\
M_s(7,8) &= -3JS_A, \\
M_s(7,9) &= -JS_A C(B,\psi_1), \\
M_s(7,10) &= -JS_A C(B,\psi_2), \\
M_s(8,7) &= -3JS_B, \\
M_s(8,8) &= E + (5J + J^{\perp})S_A + \mu_B H_B^a \\
M_s(8,9) &= -JS_A C(A,\psi_1), \\
M_s(8,10) &= -JS_A C(A,\psi_2), \\
M_s(9,8) &= -JS_A, \\
M_s(9,9) &= (E + 6JS_B + \mu_A H_A^a)C(A,\psi_1) \\
&\quad - 4JS_A(1-\cos k_y a)C(B,\psi_1) \\
&\quad - JS_A C(B,\psi_1)\psi_1, \\
M_s(9,10) &= (E + 6JS_B + \mu_A H_A^a)C(A,\psi_2) \\
&\quad - 4JS_A(1-\cos k_y a)C(B,\psi_2) \\
&\quad - JS_A C(B,\psi_2)\psi_2, \\
M_s(10,7) &= -JS_B, \\
M_s(10,9) &= (E + 6JS_A + \mu_A H_B^a)C(B,\psi_1) \\
&\quad - 4JS_B(1-\cos k_y a)C(A,\psi_1) \\
&\quad - JS_B C(A,\psi_1)\psi_1, \\
M_s(10,10) &= (E + 6JS_A + \mu_A H_B^a)C(B,\psi_2) \\
&\quad - 4JS_B(1-\cos k_y a)C(A,\psi_2) \\
&\quad - JS_B C(A,\psi_2)\psi_2.
\end{aligned}
$$

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