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Magnons localised on surface steps: a theoretical model

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Abstract. We present the solution of the full magnetic problem arising from the absence of magnetic translation symmetry in two dimensions due to an extended magnetic surface step on the surface boundary of an insulating magnetic substrate. The calculation concerns in particular the spin fluctuation dynamics of a magnetic atomic step in the surface of a ferromagnetic simple cubic lattice, the spin order being in the direction normal to surface boundary. Only exchange interactions are considered between the spins in the model. The theoretical approach determines the evanescent spin fluctuation field in the two dimensional plane normal to the direction of the step edge. This field arises owing to the absence of magnetic translation symmetry in this plane, and is completely independent of the form of the surface defect, underlying the general character of the calculation. We show the existence of optical localised magnon modes propagating along the step, their fields being evanescent in the plane normal to the step direction.

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1 Introduction

Interest in surfaces containing defects or nanostructures has been motivated by the increasing need to refine the study of substrate surfaces on the nanometric scale, and to acquire knowledge of their associated magnetic, electronic and mechanical properties for high technology applications. Questions concerning the thermodynamic stability of vicinal 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.

There has been a growing interest, for example, in the theoretical and experimental study of the vibrational dynamics of surface nanostructures [1–4], such as atomic steps on crystal surfaces. It has been shown that these nanostructures on the surface can give rise to new vibrational modes localised in their neighbourhood [3,4], and that these can scatter bulk and surface excitations.

Interest in magnetic surfaces and ultrathin films has also increased in recent years. The study of magnons or spin waves in ultrathin films has proved to very useful, in particular, for determining magnetic anisotropy constants [5,6], using Brillouin light scattering [7,8], that provides a tool to probe these magnetic excitations in ultrathin layers and also in dot-structured permalloy layers [9]. It is normally admitted now, however, that experiments are performed on systems which lack perfectly flat atomic layers. A number of imperfections can exist including surface reconstructions and step changes in thickness [10,11], in these films. These imperfections may indeed contribute to a number of physical effects, such as changes in the thermal properties of the ultrathin film and the short lifetimes of spin waves deduced from their observed large linewidths.

The effects of localised imperfections on spin wave propagation in very 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 [12]. Another work calculates, in the framework of a quasi-one-dimensional model, the reflection and transmission coefficients for a spin wave which suffers diffraction on a step like atomic discontinuity [13].

To our knowledge little if any attention, however, has been assigned to the study of magnetic excitations localised in the neighbourhood of surface defects. The frequencies of these localised modes may provide information concerning the local magnetic anisotropy and exchange interactions in the neighbourhood of these defects. Such information will help us to understand more fully the role that such imperfections or nanostructures may play in surface phenomena, including interface instability, the growth of magnetic substrates, and surface optical properties. These systems, further, are privileged examples of a one dimensional magnetic system that breaks the magnetic translation symmetry in two dimensions.

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In this paper we will consider a simple model of a magnetic step on a magnetically ordered surface, as in Figure 1, and study the model in detail to investigate the presence of magnetic excitations localised on the step. Magnetic spin order is assumed to be in the direction of the outward normal to the surface boundary.

For an extended uniform magnetic step in the surface, the theoretical approach is to determine the evanescent magnetic modes induced in the bulk and the surface terrace domains owing to the presence of the step as an isolated nanostructure. These modes arise intrinsically because the surface and the step jointly break the translation symmetry of the magnetic order in two directions, one normal to the surface boundary of the ordered substrate, and the other in the plane of the surface boundary normal to the direction of the step. The translation symmetry of the magnetic order is preserved along only one direction, namely parallel to the step.

Though numerically based methods are at hand to treat the spin fluctuation dynamics of extended defects at surfaces, this may be computationally heavy and is nanostructure specific. The formalism 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 basic theory is presented in Section 2. In Section 3, the spin fluctuation dynamics are presented for the bulk and terrace domains, with a view to determining unique solutions for the set of evanescent modes on a two dimensional square lattice normal to the step direction. This permits the construction of the evanescent field surrounding the step in a rigourous manner. The matching procedure is applied to the spin fluctuation dynamics of the step domain, and the key theoretical results of this work concerning the magnetic excitations localised on the step, are given in Section 4. In Section 5 we present some salient numerical results as well as the conclusions.

2 The model

We begin by introducing the notation used in this paper and the definition of the step. Figure 1 shows the schematic configuration of the magnetic step on the surface of a simple cubic lattice. Note otherwise that it is possible to imagine a case where the *magnetic* surface boundary and *magnetic* step do not correspond to the geometric surface boundary and geometric step. On each lattice site is attributed a magnetic ion and its spin vector variable $\mathbf{S}_{(n,s,m)}$. The indices $(n, s, m) \equiv p$, are integer numbers counting the sites respectively along the x, y, z Cartesian directions of the cubic lattice. The system is assumed to be an insulating ferromagnetic lattice with no free electrons. The z-axis and the z spin component S_{pz} are assumed normal to the surface boundary, the y-axis parallel to the step edge, and the x-axis normal to the step edge.

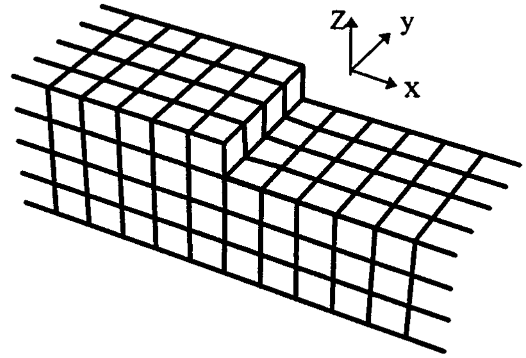

Fig. 1. A schematic representation of an isolated surface step that is infinite and symmetric along a given direction in the surface of a simple cubic crystal. The magnetic step is equivalent to this representation with equal spins on all the sites. The magnetic interactions in a Heisenberg Hamiltonian between nearest neighbour sites is J and between next nearest neighbours is $J' = \delta J$. The z axis is normal to the surface boundary, whereas the y and x axes are respectively parallel and normal to the step edge.

The magnetic step on the surface is depicted *via* a representation of a semi-infinite plane of ordered spins situated at $m = 0$, adjacent to an infinite plane of ordered spins situated at $m = 1$. The x and z axes are indexed respectively by the integers n and m. A reference cross sectional cut of the magnetic step is taken geometrically at the plane $s = 0$, and a top corner site is chosen as the reference spin site at $\mathbf{a}(0, 0, 0)$. The translation symmetry of the ordered spins for the system is broken in the x and z directions, owing respectively to the presence of the step and the surface. The y axis, in contrast, has translation symmetry for the ordered spins and Bloch's theorem may be used along its direction. Three main domains may be identified. The first consists of the bulk spin sites relatively removed from the step, the second corresponds to surface terrace sites also relatively removed from the step, referred to as terrace sites, and the last domain corresponds to spin sites belonging strictly to the step.

To illustrate the method that will be employed, consider a one dimensional insulating linear atomic chain of ordered spins, indexed with the variable p, and two nearest neighbours. For the pth spin fluctuation variables $\sigma_p^{\pm}(t)$

$$\sigma_p^{\pm}(t) = \sigma_{px}(t) \pm \mathrm{i}\sigma_{py}(t) \tag{1}$$

where $\sigma_{p\alpha}(t) = S_{p\alpha}(t) - \langle S_{p\alpha}\rangle$, we may write the following Bloch equation of motion

$$\mathrm{i}\hbar \frac{\mathrm{d}\sigma_p^{+}(t)}{\mathrm{d}t} = -2J\langle S_{pz}\rangle \left(\sigma_{p-1}^{+}(t) - \sigma_p^{+}(t) + \sigma_{p+1}^{+}(t)\right) \tag{2}$$

where J is a magnetic exchange interaction between nearest neighbour spins on the chain. Equation (2) is equivalent to the equation of motion of this variable using a Heisenberg Hamiltonian approach [14].

The z-axis, when referring to the spin component S_{pz}, is a privileged direction for the spin order. Separating the time dependence of the $\sigma_p^+(t)$ variable, by putting

$$\sigma_p^+(t) = \sigma_p^+ z^p \mathrm{e}^{-\mathrm{i}\omega t}$$

where z under z^p is a spatial phase factor along the direction of the chain, equation (2) may be recast in the form of

$$z^2 + (\Omega - 2)z + 1 = 0. \tag{3}$$

At relatively low temperatures, in comparison with the order-disorder transition temperature, the z component of the spin may be approximated as $\langle S_z \rangle \approx S$, and we may write $\Omega = \hbar\omega/2JS$, for the normalised energy of the propagating magnetic excitation. Note in this case that z in equation (3) corresponds to the phase factor of a wave for a propagating mode (not to be confused with the z-axis). An evanescent magnetic excitation is characterised, in contrast, by a phase factor satisfying the requirement that $|z| < 1$. It is worth noting that the roots of equation (3) determine when the mode is $|z| < 1$, and when it is propagating $|z| = 1$.

The description given above for a one dimensional linear chain will be generalised to study the magnetic excitations localised on the surface step, using the matching method [15]. To do this, the first stage consists of determining unique solutions for the set of evanescent magnetic modes, that determine in turn the magnetic evanescent field on the two dimensional square lattice normal to the step direction. This field is independent of the type of the surface nanostructure considered, depending only on the structure of the square lattice and on the nature of the magnetic interactions proposed between its sites.

The second stage aims at matching the dynamics of the step domain to the evanescent fluctuation spin field on the two dimensional square lattice surrounding the step. This generalization to two dimensions permits the calculation of the energies of the magnetic excitations that are travelling along the step but localised in the plane normal to it, as in a waveguide.

Nearest neighbour magnetic exchange interactions J, are physically sufficient in a model Heisenberg Hamiltonian to depict the magnetic ground state, since these interactions are related to the rapidly decaying electronic wavefunction overlap integrals between the sites. For *mathematical* interest, next nearest neighbour magnetic interactions $J' = \delta J$ ($\delta \ll 1$), are also considered at first, although we drop this in the numerical work. The model is consequently centred on the analysis of exchange-dominated spin waves, neglecting for the time being other forms of magnetic interactions. The exchange interactions are considered to be the same everywhere in the magnetically ordered system. In the present calculation the softening or hardening of the magnetic interactions on the step and the terrace domains is not considered. These considerations may be introduced in the model in a relatively direct manner.

3 The dynamics of spin fluctuations

To determine unique solutions for the evanescent magnetic modes in the two dimensional square lattice, we need to calculate the fluctuation spin dynamics in the bulk as well as in the surface terraces to the left and to the right of the step, for the considered magnetic system.

3.1 Bulk spin fluctuation dynamics

The equations of motion of the spin fluctuation field for any site (n, s, m) in the bulk domain removed from the step, may be written, dropping the + sign on the σ variables for convenience, in the form

$$\begin{aligned}
\Omega\sigma_{n,s,m} = &-(\sigma_{n-1,s,m} - 2\sigma_{n,s,m} + \sigma_{n+1,s,m}) \\
&-(\sigma_{n,s-1,m} - 2\sigma_{n,s,m} + \sigma_{n,s+1,m}) \\
&-(\sigma_{n,s,m-1} - 2\sigma_{n,s,m} + \sigma_{n,s,m+1}) \\
&-\delta(\sigma_{n-1,s,m+1} - 2\sigma_{n,s,m} + \sigma_{n+1,s,m+1}) \\
&-\delta(\sigma_{n-1,s,m-1} - 2\sigma_{n,s,m} + \sigma_{n+1,s,m-1}) \\
&-\delta(\sigma_{n,s-1,m+1} - 2\sigma_{n,s,m} + \sigma_{n,s+1,m+1}) \\
&-\delta(\sigma_{n,s-1,m-1} - 2\sigma_{n,s,m} + \sigma_{n,s+1,m-1}) \\
&-\delta(\sigma_{n-1,s-1,m} - 2\sigma_{n,s,m} + \sigma_{n+1,s-1,m}) \\
&-\delta(\sigma_{n-1,s+1,m} - 2\sigma_{n,s,m} + \sigma_{n+1,s+1,m}).
\end{aligned} \tag{4}$$

The generalised spatial phase factors along the x, y, z axes are now referred to as z_1, z_2, z_3. Since the step is considered infinite along the y-axis, we use Bloch's theorem and write for z_2 its wave like representation, so that

$$\sigma_{n,s\pm1,m} = \mathrm{e}^{\pm\mathrm{i}k_2 a}\sigma_{n,s,m}. \tag{5}$$

The $\exp(\pm\mathrm{i}k_2 a)$ in equation (5) are the phase factors of propagating modes, where k_2 is the magnon wavevector along the y-axis, and a the interatomic distance between nearest neighbour spins. We describe the evanescent field of the spin fluctuation variables in the bulk of the square lattice normal to the step direction and sufficiently removed from it, by the spatial phase factors $(z_1,\, z_1^{-1})$ and $(z_3,\, z_3^{-1})$, going from one site to its nearest neighbour in either sense, along high symmetry axes of the cubic lattice. The following relations may then generically define these phase factors

$$\begin{aligned}
\sigma_{n\pm1,s,m} &= z_1^{\pm}\sigma_{n,s,m} \\
\sigma_{n,s,m\pm1} &= z_3^{\pm}\sigma_{n,s,m}.
\end{aligned} \tag{6}$$

The substitutions from equations (5) and (6), in the equation of motion (4) of the field, fold to a reference site (n, s, m) and yield for the non trivial solutions of the variable $\sigma_{n,s,m}$, the following characteristic expression

$$\begin{aligned}
&\delta\big\{-12 + (z_1 + z_1^{-1})(z_3 + z_3^{-1}) + 2(z_1 + z_1^{-1} + z_3 + z_3^{-1}) \\
&\times\cos(k_2 a)\big\} + \Omega - 6 + (z_1 + z_1^{-1}) + (z_3 + z_3^{-1}) + 2\cos(k_2 a) = 0.
\end{aligned} \tag{7}$$

As has been pointed out elsewhere for the case of phonons [15], both couples (z_1, z_1^{-1}) and (z_3, z_3^{-1}) are solutions in the magnetic problem owing to the hermitian nature of the bulk spin fluctuation excitations. In practice only the evanescent solutions are however retained as physically applicable.

The frequencies of the bulk spin wave modes are obtained using equation (7), when z_1 and z_3 satisfy the propagating conditions $|z_1| = 1$ and $|z_3| = 1$. For arbitrary values of z_1 and z_3, however, equation (7) does not provide on its own the required unique solutions for either of these two generic spatial phase factors. To obtain these as a function of Ω and k_2a, one needs also to analyse the spin fluctuation dynamics for the surface terrace domains.

3.2 Surface spin fluctuation dynamics

It is necessary to specify in this instance the field equations for two types of sites, namely $(-n, s, 0)$ and $(n, s, 1)$, for spins in the surface that are somewhat removed from the step, and that are representative of respectively the topmost layers of the left and the right terraces. The equations for the dynamics of the spin fluctuation variables for terrace sites to the left of the step, $(-n, s, 0)$, are

$$\begin{aligned}\Omega\sigma_{-n,s,0} = &-(\sigma_{-n-1,s,0} - 2\sigma_{-n,s,0} + \sigma_{-n+1,s,0})\\ &-(\sigma_{-n,s-1,0} - 2\sigma_{n,s,0} + \sigma_{-n,s+1,0})\\ &-(\sigma_{-n,s,1} - 2\sigma_{-n,s,0})\\ &-\delta(\sigma_{-n-1,s,1} - 2\sigma_{-n,s,0} + \sigma_{-n+1,s,1})\\ &-\delta(\sigma_{-n,s-1,1} - 2\sigma_{-n,s,0} + \sigma_{-n,s+1,1})\\ &-\delta(\sigma_{-n-1,s-1,0} - 2\sigma_{-n,s,0} + \sigma_{-n+1,s-1,0})\\ &-\delta(\sigma_{-n-1,s+1,0} - 2\sigma_{-n,s,0} + \sigma_{-n+1,s+1,0}).\end{aligned} \tag{8}$$

For sites $(n, s, 1)$, on the terrace surface to the right of the step, one obtains the following equivalent equations

$$\begin{aligned}\Omega\sigma_{n,s,1} = &-(\sigma_{n-1,s,1} - 2\sigma_{n,s,1} + \sigma_{n+1,s,1})\\ &-(\sigma_{n,s-1,1} - 2\sigma_{n,s,1} + \sigma_{n,s+1,1})\\ &-(\sigma_{-n,s,2} - \sigma_{n,s,1})\\ &-\delta(\sigma_{n-1,s,2} - 2\sigma_{n,s,1} + \sigma_{n+1,s,2})\\ &-\delta(\sigma_{n,s-1,2} - 2\sigma_{n,s,1} + \sigma_{n,s+1,2})\\ &-\delta(\sigma_{n-1,s-1,2} - 2\sigma_{n,s,1} + \sigma_{n+1,s-1,1})\\ &-\delta(\sigma_{n-1,s+1,1} - 2\sigma_{n,s,1} + \sigma_{n+1,s+1,1}).\end{aligned} \tag{9}$$

The above equations are next applied to two inequivalent nearest neighbour spins in the terrace surface to the left of the step, namely at $(-n, 0, 0)$ and $(-n, 0, 1)$, in the planes respectively indexed by $m = 0$ and $m = 1$. The following analysis applies equally to two such sites in the terrace surface to the right of the step, *i.e.* $(n, 0, 1)$ and $(n, 0, 2)$. This yields for the sites $(-n, 0, 0)$ and $(-n, 0, 1)$, the following system of coupled equations in the spin fluctuation variables $\sigma_{-n,0,0}$ and $\sigma_{-n,0,1}$

$$\begin{aligned}&[\Omega - 5 - 8\delta + (z_1 + z_1^{-1})(1 + 2\delta\cos(k_2a))]\sigma_{-n,0,0}\\ &\quad + [1 + \delta\big(2\cos(k_2a) + (z_1 + z_1^{-1})]\sigma_{-n,0,1} = 0\\ &[1 + \delta\big(2\cos(k_2a) + (z_1 + z_1^{-1})\big)]\sigma_{-n,0,0}\\ &\quad + \big[\Omega - 6 - 12\delta + 2\cos(k_2a) + z_3 + \delta\big\{(z_1 + z_1^{-1})\\ &\quad \times \big(z_3 + 2\cos(k_2a) + 2z_3\cos(k_2a)\big)\big\}\big]\sigma_{-n,0,1} = 0.\end{aligned} \tag{10}$$

For a nontrivial solution of these coupled equations, the characteristic determinant yields an expression in terms of the phase factors z_1 and z_3, which is hermitian in z_1 but not in z_3. Since z_3 is a phase factor common to the surface and to the bulk domains, and since it is hermitian in the bulk, this property is retrieved for it in the surface domain applying symmetry considerations in the framework of the matching method [15]. As a consequence, we hence obtain the final characteristic expression

$$\begin{aligned}&[z_3^2 - 1][\delta + z_1 + \delta z_1^2 + 2\delta z_1\cos(k_2a)]\\ &\quad\times[1 + z_1(-5 - 8\delta + \Omega + z_1) + 2\delta(1 + z_1^2)\cos(k_2a)] = 0.\end{aligned} \tag{11}$$

There are three multiplying parentheses in equation (11). The first yields trivial solutions in z_3 that are not evanescent and are neglected. The two parentheses are independent, and may be analysed separately to calculate the phase factors z_1.

A first set of solutions or roots, referred to as $z_1(\pm)$, may be given from the third parenthesis as

$$z_1(\pm) = \frac{[5 + 8\delta - \Omega] \pm [(-5 + 8\delta + \Omega)^2 - 4\big(1 + 2\delta\cos(k_2a)\big)]^{1/2}}{2[1 + 2\delta\cos(k_2a)]}. \tag{12}$$

Another set of solutions for z_1, referred to as $z_1(1, 2)$, are obtained from the second parenthesis, and they read

$$z_1(1, 2) = \frac{-[1 + 2\delta\cos(k_2a)] \pm [\{1 + 2\delta\cos(k_2a)\}^2 - 4\delta^2]^{1/2}}{2\delta}. \tag{13}$$

Note that putting $\delta = 0$, corresponds to neglecting next nearest neighbour magnetic interactions on the lattice, leading in this case to a certain simplification of the equations above. The two sets of solutions for z_1, $z_1(\pm)$ and $z_1(1, 2)$, however, do not have the same behaviour in the limit as $\delta \to 0$. From equation (12) one obtains in this limit that

$$\underset{\delta\to 0}{\mathrm{Lt}}\, z_1(\pm) = \frac{[5 - \Omega] \pm [(-5 + \Omega)^2 - 4]^{1/2}}{2}. \tag{14}$$

In contrast $z_1(1)$ diverges, whereas $z_1(2)$ is vanishing, with δ

$$\begin{aligned}&\underset{\delta\to 0}{\mathrm{Lt}}\, z_1(1) = -\frac{1}{\delta}\\ &\underset{\delta\to 0}{\mathrm{Lt}}\, z_1(2) = -\delta\sin^2(k_2a).\end{aligned} \tag{15}$$

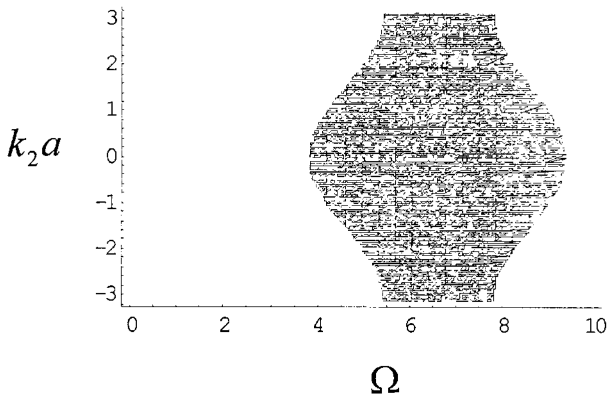

Fig. 2. The figure depicts the regions which are respectively propagating and evanescent in the phase space (Ω, k_2a), for $\delta = 0.2$. The blackened region delimits propagating bulk magnon modes. To its left and right are regions that contain evanescent bulk magnetic modes.The left region contains the evanescent $z_1(-)$ modes, and the right one the evanescent $z_1(+)$ modes.

The graphical solutions for $z_1(\pm)$, show that the $\underset{\delta\to 0}{\mathrm{Lt}}\, z_1(-)$ is evanescent for $\Omega \leq 3$, and that the $\underset{\delta\to 0}{\mathrm{Lt}}\, z_1(+)$ is evanescent for $\Omega \geq 7$. In the interval of energy, $3 < \Omega < 7$, these phase factors satisfy $|z_1(\pm)| = 1$, which condition corresponds to propagating modes. The main effect of δ is illustrated in Figure 2, in the phase space spanned by Ω and k_2a, for the particular case of $\delta = 0.2$. The division of this space into regions that correspond to propagating and evanescent modes, is presented. The black region in this figure corresponds to the propagating modes, whereas the left region corresponds to the evanescent $z_1(-)$ modes, and the right one to the evanescent $z_1(+)$ modes.

The set of nondegenerate solutions $\{z_1(i)\}$, $i = \pm, 1, 2$, where $|z_{1i}| < 1$, as a function of the energy Ω, the normalised wavevector k_2a along the step edge, and parametrically as a function of δ, determine the evanescent modes both to the right and to the left of the step edge. Given this set of $z_1(i)$ solutions, equation (7) provides in turn the set of nondegenerate solutions $\{z_3(j)\}$ that determine the evanescent modes in the direction normal to the surface boundary as one goes into the bulk.

Since the nondegenerate z_1 modes may be obtained in an unique manner, thanks to the analysis of the terrace field equations, it is next possible to obtain the solutions for the nondegenerate z_3 modes using the bulkfield equations. In order to identify these solutions, equation (7) is analysed in each situation when substituting for each of $z_1(i)$ solutions.

As pointed out previously, the case of nearest neighbour magnetic exchange interactions is sufficient to depict the ground state energy in a Heisenberg Hamiltonian, since these interactions are related to the rapidly decaying electronic wavefunction overlap integrals between crystallographic sites. The numerical work shall hence be limited to this case, for which the $z_1(1)$ solutions diverge and are not physical, whereas $z_1(2)$ is vanishing and is of no interest. The model remains relatively simple, since only one couple at a time of the z_1 and z_3 modes, in any given window of the phase space (Ω, k_2a), are sufficient to determine the evanescent magnetic field surrounding the step.The following discussion is consequently confined to considering only the two solutions $z_1(\pm)$, for which the following results are derived

$$z_3\big(\pm, z_1(-)\big) = \frac{A \pm \left[(A+B)^2[(1-2K)^2-4] + B(1-2K) - 2AK\right]^{1/2}}{2(A+B)} \quad (16)$$

$$z_3\big(\pm, z_1(+)\big) = \frac{\mp\left[(A+B)^2[(1-2K)^2-4] + (B-A)(1-2K)\right]^{1/2}}{2(B-A)} \quad (17)$$

where $A = \Omega - 5$, $B = [(\Omega-7)(\Omega-3)]^{1/2}$, and $K = \cos(k_2a)$. Note that the index j now identifies four possible $z_3(j)$ modes and refers to the four couplets, $j = \pm, z_1(\pm)$.

The following results for the domains of evanescence of the z_3 modes when $\delta = 0$, were found numerically. For the evanescent $z_1(-)$ mode, the $z_3(+)$ is evanescent in the phase space window defined by the intervals $0 \leq \Omega \leq 5$, and $2 \leq k_2a \leq \pi$, whereas the $z_3(-)$ mode is evanescent over the same interval of the Brillouin zone but for higher energies $\Omega > 5$. In contrast, substituting for the evanescent $z_1(+)$ mode in equation (7), the $z_3(+)$ and the $z_3(-)$ modes persist but interchange their domains.

This then completes the description of the nondegenerate evanescent modes in the bulk and the surface terrace domains, and permits the construction of the evanescent field surrounding the step domain.

4 Localised magnon modes on the step

The step domain includes, for a plane cut at $s = 0$, the following sites, $\mathbf{a}(0,0,0)$, $\mathbf{b}(0,0,1)$, $\mathbf{c}(0,0,2)$, $\mathbf{d}(-1,0,0)$, $\mathbf{e}(-1,0,1)$, $\mathbf{f}(1,0,1)$, and $\mathbf{g}(1,0,2)$. The choice of the stepdomain should preserve the intrinsic asymmetry and must contain a sufficient number of sites for completeness. When studying the spin fluctuation dynamics of this domain, it may be divided, furthermore, into an elementary domain $\{\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}, \mathbf{f}\}$ of irreducible spin sites that are strictly the intersection of the magnetic step with the magnetic boundary, and another that consists of neighbouring sites present in the surrounding bulk and terrace domains. Note that in our model, the magnetic surface boundary and its step are identical to the lattice surface and its step.

To solve for the magnetic excitations localised on the step, the next stage aims at matching the spin fluctuation dynamics of the step domain to the evanescent field surrounding the step.

For sites somewhat removed from the step yet on the terrace surfaces, 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 on the surface layer of the left terrace, up from the step, identified by the indices $-n < -1$, $s = 0$, $m = 0$, we may put

$$\sigma_{-n,0,0} = z_1^{n-1}\sigma_{-1,0,0}. \tag{18}$$

Further, for spins on the surface layer of the right terrace, down from the step, identified by the indices $n > 1$, $s = 0$, $m = 1$, the equivalent relation is

$$\sigma_{n,0,0} = z_1^{n-1}\sigma_{1,0,0}. \tag{19}$$

The two other relations for embedded sites surrounding the step in the plane $s = 0$, are the following. For $n > 0$, $m \geq 1$

$$\sigma_{-n,0,m} = z_1^n z_3^m R^{(-)} + 0R^{(+)} \tag{20}$$

whereas for $n > 0$, $m \geq 2$, it is

$$\sigma_{n,0,m} = 0R^{(-)} + z_1^n z_3^m R^{(+)}. \tag{21}$$

In this representation $R^{(-)}$ and $R^{(+)}$ depict basis unit vectors for projecting the evanescent field in respectively the quarter-infinite half spaces to the left and to the right of the magnetic step. This theoretical representation allows one to treat both the localised modes and the diffraction problems by generalising the framework of the matching method from one to two dimensions. In this work only the localised modes are treated. Note that the generic phase factors z_1 and z_3 in equations (18–21) have explicitly differing forms depending on the choice of the (Ω, k_2a) region for the purpose of the numerical calculation, as may be seen in Figure 2.

Using 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, employing equations (18–21), in the form of a square matrix $M(l, l')$ acting on a column vector V^{T}

$$M(l, l')V^{\mathrm{T}} = 0 \tag{22}$$

where

$$V^{\mathrm{T}} = [\sigma_a, \sigma_b, \sigma_c, \sigma_d, \sigma_d, \sigma_f, R^{(-)}, R^{(+)}]. \tag{23}$$

The non vanishing matrix elements of $M(l, l')$ are given in general, for $\delta = 0$, by the following expressions

$$\begin{aligned}
M(1,1) &= \Omega - 4 + 2\cos(k_2a)\\
M(1,2) &= M(1,4) = M(3,1) = M(3,3) = M(3,5)\\
&= M(4,2) = M(5,2) = 1\\
M(2,4) &= M(4,5) = \Omega - 5 + 2\cos(k_2a) + z_1\\
M(2,6) &= M(3,6) = z_1z_3\\
M(3,2) &= M(5,4) = \Omega - 6 + 2\cos(k_2a)\\
M(4,7) &= M(6,7) = z_1z_3^2\\
M(5,6) &= z_1z_3 + z_1z_3^2 + z_3z_1^2\\
M(6,5) &= M(7,4) = z_1[\Omega - 5 + 2\cos(k_2a) + z_1] + 1\\
M(6,7) &= z_1z_3^2\\
M(7,6) &= z_3z_1^2.
\end{aligned} \tag{24}$$

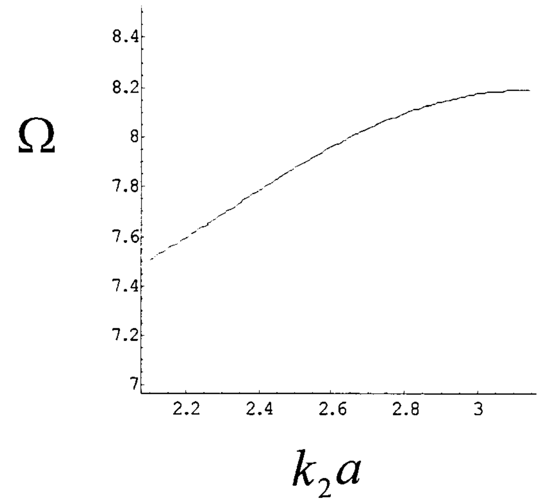

Fig. 3. The curve depicts the numerically calculated dispersion relation for the magnons localised on the step, in the region $\Omega \geq 7$ and $2.1 \leq k_2a \leq \pi$ of the phase space.

To obtain non trivial solutions for the components of the vector V^{T}, the determinant of the matrix $M(l, l')$ must vanish

$$\det M(l, l') = 0. \tag{25}$$

The determinant contains the specific expressions for the factors z_1 and z_2, which vary as a function of the selected (Ω, k_2a) region. Equation (25) yields in turn the solutions for the magnetic excitations localised in the plane normal to the step direction.

5 Numerical results and conclusions

The only regions where the couple z_1 and z_2 are simultaneously evanescent are in those determined independently by $\Omega \leq 3$ and $\Omega \geq 7$, and by the interval $2.1 \leq k_2a \leq \pi$. In other regions at least one of these modes is propagating, so that, in the search for magnetic modes that are strictly localised on the step edge, we neglect these secondary regions for the time being as being leaky.

The determinant of equation (25) leads to a non linear expression in Ω and k_2a. Its numerical solution, in the form of a set of points Ω *versus* k_2a, gives the dispersion curves of a special type of magnetic excitations. These dispersion curves depict magnons propagating along the step edge that are however effectively localised in the sense that their spin fluctuation field is evanescent in the plane normal to the step direction. The amplitude of the localised spin wave field in this plane, diminishes as one goes from one site to another further and further away from the step into the surrounding surface and bulk domains. The step plays hence the role of a wave guide for this type of magnon.

The numerical calculations yield one optical branch in the high energy region ($\Omega \geq 7$, $2.1 \leq k_2a \leq \pi$), for the dispersion curves of the spin waves localised on the step, as is presented in Figure 3. To our knowledge no experimental data is available at present to compare our results with.

In contrast, there is experimental evidence that demonstrates localised phonons on the step edges of a vicinal Ni(977) surface, observed using helium atom scattering [3]. Together with the theoretical work concerning these step localised phonons [4], this provides a realistic feel for such localised dynamic excitations. Since the phonon model, as well as the spin wave model presented here, share a common theoretical approach in the harmonic approximation, it seems to us reasonable to suppose that the calculation presented here is realistic and predicts step edge localised spin waves. These may be observed by appropriate experimental techniques, such as Brillouin light scattering and polarised HAS.

To our knowledge little if any attention has been assigned to the study of magnetic excitations localised in the neighbourhood of surface defects. The frequencies of these localised modes may provide information concerning the local magnetic anisotropy and exchange interactions in the neighbourhood of such defects, and will contribute to understand more fully the role that they may play in surface phenomena such as interface instability, the growth of magnetic substrates, and surface optical properties. These systems, further, are privileged examples of a one dimensional magnetic system that breaks the magnetic translation symmetry in two dimensions.

We emphasize that the present model is simple insofar that it considers only magnetic exchange interactions between the ordered spins, yielding hence the exchange-dominated step localised spin waves. It is quite possible that other kinds of magnetic interactions play also a role in the behaviour and frequencies of the magnons localised on the step, in which case these interactions should be considered in the equations of motion of the spin fluctuation field. As has been pointed out previously, it is feasible to introduce other forms of magnetic interactions in the present model in a relatively direct manner.

The presented model may be generalised to treat the spin fluctuation dynamics of other extended surface imperfections or nanostructures, provided they preserve the translation symmetry of the ordered spins along a direction in the surface boundary.

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