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# Theory of bulk and surface magnons in Heisenberg ferromagnetic superlattices

L. Dobrzynski\* and B. Djafari-Rouhani†

*Laboratoire de Dynamique des Cristaux Moléculaires, Unité d'Enseignement et de Recherche de Physique Fondamentale, Université de Lille I, 59655 Villeneuve d'Ascq Cédex, France*

H. Puzkarski

*Physics Institute, A. Mickiewicz University, Poznan PL-60-679, Poland*

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We present a theoretical study of the bulk and surface magnons of a semi-infinite stack of two different ferromagnetic films. Each film is modeled by a simple-cubic lattice of spins coupled via nearest-neighbor exchange (Heisenberg ferromagnet). The superlattice has a larger periodicity in the direction perpendicular to the slabs and therefore many magnon branches in the folded Brillouin zone. In the gaps existing between these magnon branches appear the surface-localized magnons. The simplicity of our model allows one to obtain in closed form the bulk and (001) surface Green's functions for this magnetic superlattice. The analytic knowledge of these functions enables us to study easily all the bulk and surface magnetic properties of a ferromagnetic superlattice. We give here the analytic expression we obtained for the folded bulk magnons and also the expression that gives the surface-localized modes, which may appear within the extra gaps which exist between the folded bulk bands. One figure for a specific case illustrates these results.

## I. INTRODUCTION

An exciting development in materials science is the appearance of new samples of alternating thin layers of two different materials, with the thickness and composition of each element subject to precise control. The resulting entity may possess new physical properties. Most particularly, by means of a sputtering technique, one may prepare specimens from two metals, each of which is present as a layer with thickness from a few angstroms to several hundred angstroms.<sup>1-6</sup>

In the recent literature such samples have been prepared in which one of the two materials is a ferromagnetic metal and the second is a nonmagnetic one. The nature of the spin-wave spectrum of such a system was recently studied theoretically<sup>2,3,7-9</sup> and experimentally by light scattering.<sup>10</sup> The theoretical study was done within the framework of a description valid for modes whose eigenfunctions vary slowly on the scale of the lattice constant. In this approach the dominant contribution to the spin-wave energy comes from dipolar and Zeeman energy, and exchange effects were ignored.

In the present work, we address ourselves to a different system, namely, a superlattice made from two different ferromagnetic materials. We study this material within an atomic model, the Heisenberg model, including exchange effects between first-nearest neighbors and neglecting dipolar and Zeeman energies. Of course, a more complete study will also have to include these effects; but here, for a first (to our knowledge) study of this type of a ferromagnetic system, we use only the simplest Heisenberg model.

Let us note that the present model of a ferromagnetic superlattice is, from a mathematical point of view, an easy transposition of a model previously used for the study of

surface phonons in superlattices.<sup>11</sup> The superlattice under study here is also built up from alternately  $L_1$  and  $L_2$  (001) atomic planes of two different simple-cubic lattices having the same lattice parameter  $a_0$  and characterized by their Heisenberg exchange interactions ( $J_1$  and  $J_2$ ) between first-nearest-neighbor atoms. The alternating thin layers are bound together by an exchange interaction  $J$  between the interface atoms. This simple model enables one to obtain in closed form the bulk and (001) surface Green's function for this superlattice. The analytic knowledge of these functions enables us to study easily all the bulk and surface magnetic properties of this superlattice.

We will give here the analytic expressions we obtained for the Green's functions, for the folded bulk magnon dispersion curves, and also for the surface-localized modes, which may appear within the extra gaps that exist between the folded bulk bands. These expressions enable us to discuss easily the effect of the physical parameters defined above. These surface magnons also depend on the kind of layer (1 or 2) being near the (001) surface of the superlattice.

In Sec. II we obtain the bulk magnetic Green's function for the superlattice defined above. In Sec. III we give the corresponding surface Green's function. In Secs. IV and V these results are used for the calculation of the bulk and surface magnons.

## II. BULK MAGNETIC GREEN'S FUNCTION FOR A SUPERLATTICE

We start from an infinite simple-cubic lattice described by the Heisenberg Hamiltonian

$$H_{01} = - \sum_{I,I'} J_1 \mathbf{S}_I \cdot \mathbf{S}_{I'} , \quad (1)$$

where we retain only the exchange interactions  $J_1$  between the spins  $S_I$  and  $S_{I'}$  situated on nearest-neighbor atoms. The linearized Holstein-Primakoff transformation enables to rewrite this Hamiltonian in the following form:

$$H_{01} = -S \sum_{I,I'} J_1 (b_I^\dagger b_{I'} + b_I^\dagger b_I + b_I^\dagger b_I + b_I^\dagger b_{I'}) + Cte, \quad (2)$$

where  $b_I^\dagger$  and  $b_I$  are the usual creation and annihilation operators and  $S$  the spin amplitude.

The equations of motion of the  $b_I^\dagger$  operators can be written in the following matrix form:

$$(\vec{H}_{01} - \omega \vec{I}) \cdot \mathbf{u} = 0, \quad (3)$$

where  $\mathbf{u}$  is a column vector having as many rows as we have atoms in the crystal and representing the ensemble of the operators  $b_I^\dagger$ .

The diagonalization of this Hamiltonian provides the bulk magnon dispersion relation,

$$\omega = 4S_1 J_1 [3 - \cos(k_1 a_0) - \cos(k_2 a_0) - \cos(k_3 a_0)], \quad (4)$$

where  $\mathbf{k}$  is the propagation vector.

We now construct out of this lattice a film of  $L_1$  layers bounded by a pair of (001) free surfaces. Each (001) atomic plane of this slab is labeled by

$$1 \leq l_3 \leq L_1. \quad (5)$$

The equation of motion of the  $b_I^\dagger$  operators of this film can be written as

$$(\vec{H}_1 - \omega \vec{I}) \cdot \mathbf{u} = 0, \quad (6)$$

and a Green's function  $\vec{U}_1$  can be defined as

$$(\vec{H}_1 - \omega \vec{I}) \cdot \vec{U}_1 = \vec{I}. \quad (7)$$

$\vec{I}$  is a unit matrix with elements  $\delta_{II'}$ .

$$U_1(k_{||}, \omega; l_3, l'_3) = \frac{1}{2SJ_1} \frac{t_1^{|l_3 - l'_3| + 1}}{t_1^2 - 1} + \frac{1}{2SJ_1} \frac{t_1^{l_3 + l'_3}}{t_1^2 - 1} + \frac{1}{2SJ_1} \frac{t_1}{t_1^2 - 1} \frac{t_1^{2L_1}}{1 - t_1^{2L_1}} (t_1^{-l_3 - l'_3 + 1} + t_1^{-l_3 + l'_3} + t_1^{l_3 - l'_3} + t_1^{l_3 + l'_3 - 1}). \quad (13)$$

In the same manner we construct another film of  $L_2$  (001) layers. In order to distinguish these two films one from the other, we will use an index  $\kappa = 1$  or 2. The corresponding Green's function  $U_2(k_{||}, \omega; l_3, l'_3)$  can be obtained from the above equations<sup>11-13</sup> by changing all indices 1 to 2. Let us also remark that for this  $\kappa = 2$  film one has

$$1 \leq l_3 \leq L_2. \quad (14)$$

Let us now set this  $\kappa = 2$  film in epitaxy with the  $\kappa = 1$  film; we characterize this double film by another integer  $n$ . An infinite repetition  $-\infty < n < +\infty$  of this double film gives us our starting point for our model of a ferromagnetic superlattice. We couple all these alternating  $\kappa = 1$  and  $\kappa = 2$  films by exchange interactions  $J$  between the interface atoms facing each other. This creates the infinite superlattice we will study. In the same manner as for the slab [Eq. (7)] we define a Green's function  $\vec{D}$  for

The advantage of this model is that this film Green's function  $\vec{U}_1$  can be worked out in closed form, once the corresponding surface Green's function is known.<sup>11</sup> The mathematical procedure is very similar to the one used before for a similar vibrational model of surfaces<sup>12,13</sup> and slabs.<sup>14</sup> We will therefore simply give the results here.

Taking advantage of the periodicity of the film in directions parallel to the surfaces, we introduce a two-dimensional position vector

$$\mathbf{X}_{||}(l) = a_0(l_1 \hat{\mathbf{X}}_1 + l_2 \hat{\mathbf{X}}_2), \quad (8)$$

a two-dimensional wave vector parallel to the surfaces

$$\mathbf{k}_{||} = k_1 \hat{\mathbf{X}}_1 + k_2 \hat{\mathbf{X}}_2, \quad (9)$$

and

$$U_1(l, l'; \omega) = \frac{1}{N^2} \sum_{\mathbf{k}_{||}} U_1(k_{||}, \omega; l_3, l'_3) \times \exp\{i \mathbf{k}_{||} \cdot [\mathbf{X}_{||}(l) - \mathbf{X}_{||}(l')]\}, \quad (10)$$

where  $N^2$  is the number of atoms in a (001) plane.

The explicit expression of  $U_1(k_{||}, \omega; l_3, l'_3)$  was calculated as a function of

$$\xi_1 = 3 - \cos(k_1 a_0) - \cos(k_2 a_0) - \frac{\omega}{4SJ_1} \quad (11)$$

and

$$t_1 = \begin{cases} \xi_1 - (\xi_1^2 - 1)^{1/2}, & \xi_1 > 1 \\ \xi_1 + i(1 - \xi_1^2)^{1/2}, & -1 < \xi_1 < 1 \\ \xi_1 + (\xi_1^2 - 1)^{1/2}, & \xi_1 < -1 \end{cases} \quad (12)$$

and is

this superlattice. Its elements can be worked out explicitly in the same manner as for the corresponding vibrational model and are given as functions of the  $q_\kappa$  defined in terms of the  $t_\kappa$  of Eq. (12) by

$$t_\kappa = e^{q_\kappa}, \quad \kappa = 1 \text{ or } 2 \quad (15)$$

and a new variable  $t$  defined by

$$t = \begin{cases} \eta - (\eta^2 - 1)^{1/2}, & \eta > 1 \\ \eta + i(1 - \eta^2)^{1/2}, & -1 < \eta < 1 \\ \eta + (\eta^2 - 1)^{1/2}, & \eta < -1 \end{cases} \quad (16)$$

with

$$\begin{aligned}
\eta = & \frac{2J_1J_2}{J^2} \tanh\left[\frac{q_1}{2}\right] \tanh\left[\frac{q_2}{2}\right] \sinh(q_1L_1)\sinh(q_2L_2) \\
& + 2\frac{J_1}{2} \tanh\left[\frac{q_1}{2}\right] \sinh(q_1L_1) \frac{\cosh[q_2(L_2 - \frac{1}{2})]}{\cosh(q_2/2)} + 2\frac{J_2}{2} \tanh\left[\frac{q_2}{2}\right] \sinh(q_2L_2) \frac{\cosh[q_1(L_1 - \frac{1}{2})]}{\cosh(q_1/2)} \\
& + \frac{J_2}{J_1} \frac{\sinh[q_1(L_1 - 1)]}{\sinh q_1} \tanh\left[\frac{q_2}{2}\right] \sinh(q_2L_2) + \frac{J_1}{J_2} \frac{\sinh[q_2(L_2 - 1)]}{\sinh q_2} \tanh\left[\frac{q_1}{2}\right] \sinh(q_1L_1) \\
& + \frac{\cosh[q_1(L_1 - \frac{1}{2})]}{\cosh(q_1/2)} \frac{\cosh[q_2(L_2 - \frac{1}{2})]}{\cosh(q_2/2)}. \tag{17}
\end{aligned}$$

Let us give the explicit expressions of the elements  $D(k_{\parallel}, \omega | n, \kappa, l_3; n', \kappa', l'_3)$  of the superlattice Green's function  $\vec{D}$ . The elements of  $\vec{D}$  between different  $\kappa=1$  and  $\kappa=2$  films are

$$D(n, 1, l_3; n', 2, l'_3) = \frac{t}{t^2 - 1} [K_{12}(l_3, l'_3) t^{|n-n'|} + K_{12}(L_1 - l_3 + 1, L_2 - l'_3 + 1) t^{|n-n'-1|}], \tag{18}$$

where

$$\begin{aligned}
K_{12}(l_3, l'_3) = & \frac{1}{2JS} \frac{\cosh[q_1(l_3 - \frac{1}{2})]}{\cosh(q_1/2)} \frac{\cosh[q_2(L_2 - l'_3 + \frac{1}{2})]}{\cosh(q_2/2)} + \frac{1}{2J_2S} \frac{\cosh[q_1(l_3 - \frac{1}{2})]}{\cosh(q_1/2)} \frac{\sinh[q_2(L_2 - l'_3)]}{\sinh q_2} \\
& + \frac{1}{2J_1S} \frac{\cosh[q_2(L_2 - l'_3 + \frac{1}{2})]}{\cosh(q_2/2)} \frac{\sinh[q_1(l_3 - 1)]}{\sinh q_1} \tag{19}
\end{aligned}$$

and

$$D(n, 2, l_3; n', 1, l'_3) = D(n, 1, l'_3; n', 2, l_3). \tag{20}$$

The elements of  $\vec{D}$  between the same  $\kappa$  films are

$$D(n, 1, l_3; n', 1, l'_3) = \frac{1}{2J_1S} t^{|n-n'|} \frac{\sinh[q_1(l_3 - l'_3)]}{\sinh q_1} \operatorname{sgn}[L_1(n - n') + l_3 - l'_3] + \frac{1}{2J_1S} \frac{t^{|n-n'|+1}}{t^2 - 1} K_{11}(l_3, l'_3), \tag{21}$$

where

$$\begin{aligned}
K_{11}(l_3, l'_3) = & \frac{1}{4 \cosh^2(q_1/2)} \{ \cosh[q_1(L_1 + l_3 - l'_3)] + \cosh[q_1(L_1 - l_3 + l'_3)] + 2 \cosh[q_1(L_1 - l_3 - l'_3 + 1)] \} \\
& \times \left[ \frac{2J_1J_2}{J^2} \tanh\left[\frac{q_2}{2}\right] \sinh(q_2L_2) + \frac{2J_1}{J} \frac{\cosh[q_2(L_2 - \frac{1}{2})]}{\cosh(q_2/2)} + \frac{J_1}{J_2} \frac{\sinh[q_2(L_2 - 1)]}{\sinh q_2} \right] \\
& + \frac{1}{2 \sinh q_1} \left\{ \frac{J_2}{J_1} \tanh \frac{q_2}{2} \frac{\sinh(q_2L_2)}{\sinh q_1} \{ \cosh[q_1(L_1 + l_3 - l'_3 - 1)] + \cosh[q_1(L_1 + l'_3 - l_3 - 1)] \right. \\
& \quad \left. - 2 \cosh[q_1(L_1 - l_3 - l'_3 + 1)] \right\} \\
& + \frac{2}{\cosh(q_1/2) \cosh(q_2/2)} \left[ \sinh[q_1(L_1 - \frac{1}{2})] \cosh[q_1(l_3 - l'_3)] \right. \\
& \quad \left. - \sinh\left[\frac{q_1}{2}\right] \cosh[q_1(L_1 - l_3 - l'_3 + 1)] \right] \\
& \times \left[ \frac{2J_2}{J} \sinh\left[\frac{q_2}{2}\right] \sinh(q_2L_2) + \cosh[q_2(L_2 - \frac{1}{2})] \right], \tag{22}
\end{aligned}$$

and  $D(n, 2, l_3; n', 2, l'_3)$  can be obtained from  $D(n, 1, l_3; n', 1, l'_3)$  by interchanging in  $J_{\kappa}$  and  $L_{\kappa}$  all the indices  $\kappa=1$  and 2. We now proceed to use these results for the calculation of the surface Green's functions of the ferromagnetic superlattice.

### III. SURFACE FERROMAGNETIC GREEN'S FUNCTION FOR A SUPERLATTICE

We will consider here two different cases, depending on the thickness of the last film near the free surface.

#### A. Surface film with same width as corresponding bulk films

We create two free surfaces by equating to zero all interactions between atoms in the plane ( $n=0, \kappa=2, l_3=L_2$ ) and atoms in the plane ( $n=1, \kappa=1, l_3=1$ ). We define a corresponding surface Green's function  $\vec{G}$ . The Dyson relation between  $\vec{G}$  and  $\vec{D}$  enables us to find easily,<sup>11</sup> for  $n$  and  $n' \geq 1$ ,

$$G(n, \kappa, l_3; n', \kappa', l'_3) = D(n, \kappa, l_3; n', \kappa', l'_3) + \frac{J}{\Delta_{S1}} D(1, 1, 1; n', \kappa', l'_3) [D(n, \kappa, l_3; 0, 2, L_2) - D(n, \kappa, l_3; 1, 1, 1)], \quad (23)$$

where

$$\Delta_{S1} = \frac{tA - 1}{t^2 - 1}, \quad (24)$$

with

$$A = \frac{\cosh[q_1(L_1 - \frac{1}{2})]}{\cosh(q_1/2)\cosh(q_2/2)} \left[ \cosh[q_2(L_2 - \frac{1}{2})] + 2\frac{J_2}{J} \sinh\left[\frac{q_2}{2}\right] \sinh(q_2 L_2) \right] + 2\frac{J_2}{J_1} \frac{\sinh(q_2/2)}{\cosh(q_2/2)} \sinh(q_2 L_2) \frac{\sinh[q_1(L_1 - 1)]}{\sinh q_1}. \quad (25)$$

#### B. Surface film with width smaller than corresponding bulk films

We create now two other free surfaces by equating to zero all interactions between atoms in the plane ( $n=1, \kappa=1, l_3=l_0 < L_1$ ) and atoms in the plane ( $n=1, \kappa=1, l_3=l_0+1$ ).

As before,<sup>11</sup> one obtains the surface Green's function, which for  $n$  and  $n' \geq 1$  and  $l_3$  and  $l'_3 \geq l_0$ , is

$$G(n, \kappa, l_3; n', \kappa', l'_3) = D(n, \kappa, l_3; n', \kappa', l'_3) + \frac{2SJ_1}{\Delta'_{S1}} [D(n, \kappa, l_3; 1, 1, l_0) - D(n, \kappa, l_3; 1, 1, l_0+1)] D(1, 1, l_0+1; n', \kappa', l'_3), \quad (26)$$

where

$$\begin{aligned} \Delta'_{S1} = & \frac{1}{2} - \frac{t}{t^2 - 1} \frac{\sinh(q_1/2)}{\cosh^2(q_1/2)} \left[ \frac{2J_1 J_2}{J^2} \tanh\left[\frac{q_2}{2}\right] \sinh(q_2 L_2) + \frac{2J_1}{J} \frac{\cosh[q_2(L_2 - \frac{1}{2})]}{\cosh(q_2/2)} + \frac{J_1}{J_2} \frac{\sinh[q_2(L_2 - 1)]}{\sinh q_2} \right] \\ & \times \left[ \sinh\left[\frac{q_1}{2}\right] \cosh(q_1 L_1) + \sinh[q_1(L_1 - 2l_0 - \frac{1}{2})] \right] \\ & - \frac{t}{t^2 - 1} \frac{1}{\sinh q_1 \cosh(q_1/2) \cosh(q_2/2)} \left\{ 2 \sinh^2\left[\frac{q_1}{2}\right] \{ \sinh[q_1(L_1 - \frac{1}{2})] - \sinh[q_1(L_1 - 2l_0 - \frac{1}{2})] \} \right. \\ & \times \left[ \frac{2J_2}{J} \sinh\left[\frac{q_2}{2}\right] \sinh(q_2 L_2) + \cosh[q_2(L_2 - \frac{1}{2})] \right] \\ & \left. + \frac{J_2}{J_1} \sinh\left[\frac{q_2}{2}\right] \sinh(q_2 L_2) \left[ \sinh\left[\frac{q_1}{2}\right] \cosh[q_1(L_1 - 1)] \right. \right. \\ & \left. \left. - \sinh[q_1(L_1 - 2l_0 - \frac{1}{2})] \right] \right\}. \quad (27) \end{aligned}$$

We now proceed to use the results of Secs. II and III for the determination of the bulk and surface magnons in a superlattice.

#### IV. BULK AND SURFACE MAGNONS IN A SUPERLATTICE

The bulk magnons of our superlattice can be obtained from the knowledge of the bulk Green's function [Eqs. (18)–(22)]. Let us first recall that for the infinite simple-cubic lattice described above, the bulk magnon dispersion relation, Eq. (4), can be obtained from Eq. (11) and is given by

$$\xi_1 = \cos(k_3 a_0), \quad -\pi < k_3 a_0 < +\pi. \quad (28)$$

In the same manner,<sup>11</sup> for the infinite superlattice, we obtain the bulk magnons from

$$\eta = \cos[k_3(L_1 + L_2)a_0], \quad (29)$$

where  $\eta$  is given by Eq. (17); and because the periodicity in the direction  $x_3$  is now given by  $(L_1 + L_2)a_0$ , one has

$$D(\omega) = \frac{4SJ_1J_2}{J} \sinh\left[\frac{q_1}{2}\right] \sinh\left[\frac{q_2}{2}\right] \sinh(q_1L_1)\sinh(q_2L_2) + 2SJ_2 \sinh\left[\frac{q_2}{2}\right] \cosh[q_1(L_1 - \frac{1}{2})] \sinh(q_2L_2) + 2SJ_1 \sinh\left[\frac{q_1}{2}\right] \sinh(q_1L_1) \cosh[q_2(L_2 - \frac{1}{2})]. \quad (32)$$

From the poles of this Green's function, we find the frequencies  $\omega_s$  of the surface modes localized at the free surface ( $n=1, \kappa=1, l_3=1$ ) and decaying inside the bulk situated at  $n$  and  $l_3 > 1$ . They are given by

$$D(\omega_s) = 0, \quad (33)$$

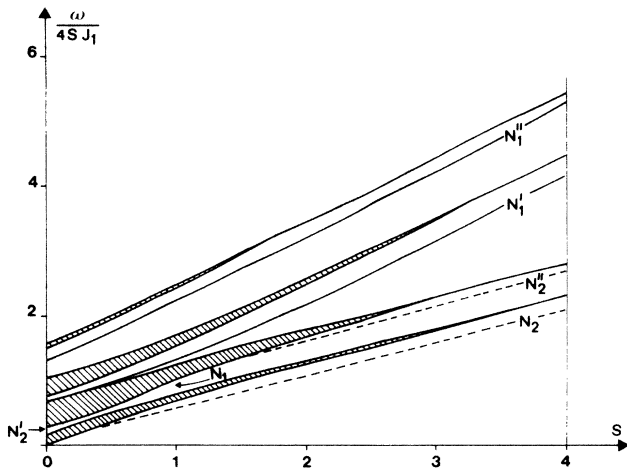


FIG. 1. Bulk (shaded areas) and surface (solid and dashed lines) magnons of a superlattice with two atomic planes in each film in function of  $S = 2 - \cos(k_1 a_0) - \cos(k_2 a_0)$ . The film labeled by the index  $\kappa=1$  is at the surface. The  $N_1', N_1''$  surface magnons are obtained for  $J_1 = 2J_2$  and the  $N_2, N_2''$  surface magnons for  $J_1 = J_2/2$ .

$$-\pi < k_3(L_1 + L_2)a_0 < +\pi. \quad (30)$$

Because of this larger periodicity in the direction  $x_3$ , one has a folding of the magnon dispersion curves in a reduced Brillouin zone specified by Eq. (30) and an opening of new gaps between these folded dispersion curves (see Fig. 1).

In the gaps, new surface magnons may appear; they can be found from the new poles in the surface Green's functions [Eqs. (23) and (26)] due to the creation of the free surface.

In particular, in the case for which the surface film has the same width as the corresponding bulk films, we worked out explicitly the diagonal element of the surface Green's function  $\vec{G}$  on the surface plane and found

$$G(1,1,1;1,1,1) = \frac{t-A}{2} \frac{\cosh(q_1/2)\cosh(q_2/2)}{D(\omega)}, \quad (31)$$

where

together with the condition

$$\frac{J_2}{J_1} \left| \frac{\sinh(q_2L_2)\tanh(q_2/2)}{\sinh(q_1L_1)\tanh(q_1/2)} \right| > 1,$$

which ensures that these modes decay inside the bulk.<sup>11</sup>

In Fig. 1 we present the results for the bulk and surface magnons of a superlattice with two atomic planes in each film ( $L_1 = L_2 = 2$ ) in functions of the parameter  $S = 2 - \cos(k_1 a_0) - \cos(k_2 a_0)$ . We assume  $J_1 = 2J_2$  or  $J_1 = J_2/2$ . The exchange at the interface is assumed to be  $J = (J_1 + J_2)/2$ . The film labeled by the index  $\kappa=1$  is at the surface. The shaded areas represent the bulk magnons (four here for each value of  $k_{||}$ ). The  $N_1', N_1''$  surface magnons (solid line) refer to  $J_1 = 2J_2$ , the  $N_2, N_2''$  surface magnons (dashed line) to  $J_1 = J_2/2$ .

#### V. DISCUSSION

In this paper we obtained for the first time surface and bulk magnons on a simple three-dimensional atomic Heisenberg model of a ferromagnetic superlattice. The simplicity of this model enables us to derive in closed form the bulk and surface magnetic Green's functions for a superlattice. From the poles of these Green's functions we obtained analytic expressions for the bulk and surface magnons of a superlattice. The surface magnons obtained here are a new feature of the superlattice, as this model has neither surface nor interface magnons<sup>15</sup> localized on

each of the two materials. One has to take into account the exchange between second-nearest neighbors, if one wants to study the superlattice effect on these surface and interface magnons. This theory will also have to be completed in the future to take into account the dipolar and Zeeman energies.<sup>7</sup>

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†Present and permanent address: Institut des Sciences Exactes et Appliquées, Université de Haute-Alsace, 4 rue des Frères Lumière, 68093 Mulhouse Cédex, France.

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