Magnons plane by plane contribution to super-lattice magnetic properties

A. Fahmi and A. Qachaou
Laboratoire de Physique de la matière condensée, Faculté des sciences, Kénitra

The paper presents a contribution to the study of super-lattice magnetic properties in the linear spin-wave theory framework. The super-lattice is represented by a Heisenberg ferromagnet with N atomic planes. The excitation spectrum and the magnetization are calculated using Green's functions method. Their expressions are obtained analytically for N=3,5 and 10 atomic planes. The effects of both surface anisotropy and dipolar interaction are studied numerically.

I- INTRODUCTION

Recently, magnetic thin films and multi-layer materials have known wide technological applications. Their magnetic behaviour is different from that observed in bulk systems. This is mainly due to the dimensionality reduction. Several theoretical approaches, in particular spin wave theory, were proposed to study their magnetic properties. Generally, the treatment of these systems as being quasi-two-dimensional gives results consistent with experiment [1,2,3].

In this work we are interested in studying a magnetic super-lattice of bcc structure such as $[Co(t_m)/Cu(t_{nm})]_N$, using the spin-wave theory. The super-lattice is represented by a ferromagnetic Heisenberg model of localized spins with different interactions: the nearest-neighbour (NN) and next-nearest-neighbour (NNN) exchange interactions (J_1 and J_2) contributing to the long-range order [4], the surface anisotropy playing an important role in the magnetic stability of this kind of system [5,6,7,8], and the dipolar interaction are taken into account. Furthermore, we suppose that the super-lattice consists of a succession of N ferromagnetic planes alternating with a nonmagnetic layer. The interactions between the planes are also ferromagnetic.

Analytical expressions of the excitation spectrum and magnetization are obtained for N=3, 5 and 10 atomic planes when only the exchange interactions are present. In the presence of the dipolar interaction and surface anisotropy, the calculations are carried out numerically.

II- THE SPIN HAMILTONIAN

The ferromagnetic film plane is taking as the (*xz*) plane. In the presence of the external magnetic field H, the spin Hamiltonian is written as:

$$
\begin{aligned}
H = & -J_1 \sum_{<ij>} (S^x S_j^x + S_i^y S_j^y + \delta S_i^z S_j^z) - J_2 \sum_{<i'j'>} S_{i'} S_{j'} \\
& - J_\perp \sum_{<ii'>} S_i S_{i'} - \alpha \sum_i (S_i^y)^2 - g\mu_B H \sum_i S_i^z \\
& + \frac{g^2 \mu_B^2}{2} \sum_{<ij>} \frac{1}{r_{ij}^3} \left\{ S_i S_j - 3 \frac{(S_i r_{ij})(S_j r_{ij})}{r_{ij}^2} \right\} \qquad (1)
\end{aligned}
$$

J_1 and $J_2 > 0$ are respectively the NN and NNN exchange integrals in the same atomic plane. $J_\perp$ corresponds to the NN belonging to two successive planes. δ and $\alpha>0$ represent the surface magnetocrystalline anisotropy, with α acting only on the surface spins (plane 1 and N). The last term in (1) describes the NN dipolar interaction in the same plane ($r_{ij} = |r_i - r_j|$).
The treatment of (1) is carried out using the Holtstein-Primakoff [9] and Fourier [10] transformations. Taking account of the symmetry translation in the (*xz*) plane, while this symmetry is broken along the *y* axis, one gets

$$
\mathcal{H} = \sum_{l,m}^{N} \sum_{k_{//}} \left\{ A_{lm}(k) a^+_{k_{//},l} a_{k_{//},m} + \frac{1}{2} B_{lm} \left(a^+_{k_{//},l} a^+_{-k_{//},m} + a_{k_{//},l} a_{-k_{//},m} \right) \right\} \qquad (2)
$$

where:

$$
\begin{aligned}
A_{lm}(k) = & \left[8SJ_1 \left(\delta - \cos\frac{k_x a}{2} \cos\frac{k_z a}{2} \right) + 4SJ_2 \left(2 - \cos k_x a \cos k_z a \right) + 2SJ_\perp - h + DS \left(2 + \cos\frac{k_x a}{2} \cos\frac{k_z a}{2} \right) \right] \delta_{lm} \qquad \text{(3-a)} \\
& + \left(4\alpha S \cos\frac{k_x a}{2} \cos\frac{k_z a}{2} \right) \left(\delta_{l,1} + \delta_{l,N} \right) - 2SJ_\perp \left(\delta_{l,m+1} + \delta_{l,m-1} \right) + 2SJ_\perp \left(1 - \delta_{l,1} + \delta_{l,N} \right)
\end{aligned}
$$

$$
B_{lm}(k) = \left[-3SD \cos\frac{k_x a}{2} \cos\frac{k_z a}{2} \right] \delta_{l,m} - \left[2S\alpha \cos\frac{k_x a}{2} \cos\frac{k_z a}{2} \right] (\delta_{l,1} + \delta_{l,N}) \qquad \text{(3-b)}
$$

with $D = \frac{g^2 \mu_B^2}{(a/\sqrt{2})^3}$; h = $g\mu_B H$ and a is a lattice parameter.

The Green's function method [11] allows us to diagonalise the Hamiltonian (2) where we kept only the quadratic terms corresponding to the elementary excitations. The equations of motion of the retarded Green's functions:

$G_{l,m} = \ll a_{k_{//},l}, a^{+}_{k_{//},m} \gg$ and $G'_{l,m} = \ll a^{+}_{k_{//},l}, a^{+}_{k_{//},m} \gg$ enabled us to obtain a 2N equations system represented in the matrix form as:

$$\underline{M}\,\underline{G} = \begin{pmatrix} \underline{A} & \underline{B} \\ -\underline{B} & -\underline{A} \end{pmatrix} \begin{pmatrix} \underline{G} & 0 \\ \underline{G'} & 0 \end{pmatrix} = \frac{-1}{2\pi}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (4)$$

$\underline{A}$ and $\underline{B}$ are N-order matrices. Their elements $A_{lm}(k)$ and $B_{lm}(k)$ are given by (3-a) and (3-b). The elementary excitations energies are obtained from the poles of the matrix $\underline{G}$ as the (2N×2N) matrix $\underline{M}$ eigenvalues. In the following, we start by finding an analytical solution to (4) in the absence of the dipolar interactions and surface anisotropy. A numerical solution will be found when various interactions are included.

III- ANALYTICAL RESOLUTION

In the case of a super-lattice with transition metals, the exchange effect is more important. So an exact solution is possible when omitting the α and D contributions ($D=\alpha=0$). The magnetic field ($h=g\mu_B H$) has a simple effect that consists of moving the frequency modes. Thus,

$$\mathcal{H} = \sum_{lm} \sum_{k_{//}} A_{lm}(k_{//}) a^{+}_{k_{//},l} a_{k_{//},m} . \quad (5)$$

$A_{lm}(k)$ are deduced from (3-a) with $D=\alpha=0$.

3.1-Excitation spectra :

The spin wave excitation spectrum E(k) are calculated by solving the equation system according to:

$Det[\underline{A}-E\underline{I}]=0$ (6)

The matrix $\underline{A}$-$E\underline{I}$ is tridiagonal. It is decomposable into a product of two triangular matrices. The determination of diagonal elements allows us to calculate (6). For a super-lattice with N=3; 5 and 10 planes, we have obtained respectively 3, 5 and 10 distinct solutions $E_i^N(k)$, such as:

$E_i(k) = A(k) + \varepsilon_i^N W$ with:

$\varepsilon_i^3 = \{-1\ ;\ 0\ ;\ 2\}$;

$\varepsilon_i^5 = \left\{(1 \pm \sqrt{5})/2\ ;\ -1\ ;\ (3 \pm \sqrt{5})/2\right\}$;

$\varepsilon_i^{10} = \left\{(2 \pm \sqrt{10 \pm 2\sqrt{5}})/2\ ;\ \pm 1\ ;\ (2 \pm \sqrt{6 \pm 2\sqrt{5}})/2\right\}$

; $A(k)=A_{11}$ and $W=-A_{12}$ (7)

3.2- Magnetization by spin:

3.2- Magnetization by spin: The general reduced super-lattice magnetization expression is:

$$\frac{M^z}{NLS} = 1 - \frac{1}{S}\frac{1}{N}\frac{v}{(2\pi)^2}\sum_{l=1}^{N} \int_{BZ} < a^{+}_{k,l}, a_{k,l} > dk_x dk_z \quad (8)$$

where v is the unit-cell surface and $< a^{+}_{k,l}, a_{k,l} >$ is the spin wave average occupation number:

$$< a^{+}_{k,l}, a_{k,l} > = \left[\exp\left(\frac{E_l(k)}{kT}\right) - 1\right]^{-1} \quad (9)$$

Since, only the low-frequency spin waves are excited at low temperatures, we have developed $E_l(k)$ expressions in the vicinity of $k=(0,0)$. So:

$$E_l(k) = 8J_1 S(\delta - 1) + (J_1 S + 2J_2 S)\rho^2 + 2J_\perp S(1+\varepsilon_l) + h$$

with $\rho^2=(k_x a)^2+(k_z a)^2$. (10)

Then, in the polar coordinates, and after integration of (8), we have:

$$\frac{M^z}{NLS} = 1 + \frac{1}{4\pi}\frac{1}{N}\frac{kT}{2(J_1 S + 2J_2 S)}\sum_{i=1}^{N} Ln\left\{1 - \exp\left[-(8J_1 S(\delta-1) + h + 2J_\perp S(1+\varepsilon_i))/kT\right]\right\} \quad (11)$$

Otherwise, for N $\to \infty$ (semi infinite super-lattice), the N planes system becomes continuous, then:

$$\frac{1}{N}\sum_{i=1}^{N} \to \frac{a}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dk_y \quad \text{and}$$

$$2J_\perp S(1+\varepsilon_i) \to 4SJ_\perp(1-\cos k_y a) = 4SJ_\perp(1-\xi^2/2)$$

, where $k_y a=\xi<<1$, leading to:

$$\frac{M^z}{NLS} = 1 + \frac{1}{4\pi N}\frac{kT}{2S(J_1+2J_2)}\int_0^{\pi} \ln\left[1 - \exp\left(-\frac{(\Delta+h+2J_\perp S\xi^2)}{kT}\right)\right] d\xi$$

where $\Delta=8SJ_1(\delta-1)$ (12)

giving for kT<< Δ' where Δ'=Δ+h, and using the $g_{3/2}$ Bose's function

$$\frac{M^Z}{NLS} = 1 - g_{3/2}\left(e^{\frac{\Delta'}{kT}}\right)\frac{1}{8\pi^{3/2}}\frac{1}{(2SJ_\perp)^{1/2}}\frac{1}{S(J_1+2J_2)}(kT)^{3/2} \quad (13)$$

While, for kT>>Δ'; the integration of (12) gives :

$$\frac{M}{NLS}=1-\frac{1}{4\pi}\frac{1}{N}\frac{kT}{2(J_1S+2J_2S)}Ln\left\{\frac{kT}{\Delta'+4SJ_\perp}\frac{2}{1+\left[1-\left(1-4SJ_\perp/(\Delta'+4SJ_\perp)\right)^2\right]^{1/2}}\right\} \quad (14)$$

3.3- Discussion:

3.3.1- Excitation spectra:

As is shown in figure1, corresponding to N=3, 5 and 10 atomic planes, the excitation modes number is equal to the number of planes engaged in the super-lattice as obtained in previous works [13]. This reflects the existence of a coupling between these N planar modes. Furthermore, the lowest energy mode and consequently, the energy gap Δ' are N independent. So, $\Delta'=8J_1S(\delta-1)+h$ would be independent on the super-lattice thickness. For an isotropic system (δ=1) and in the external field absence, the gap vanishes reflecting the important

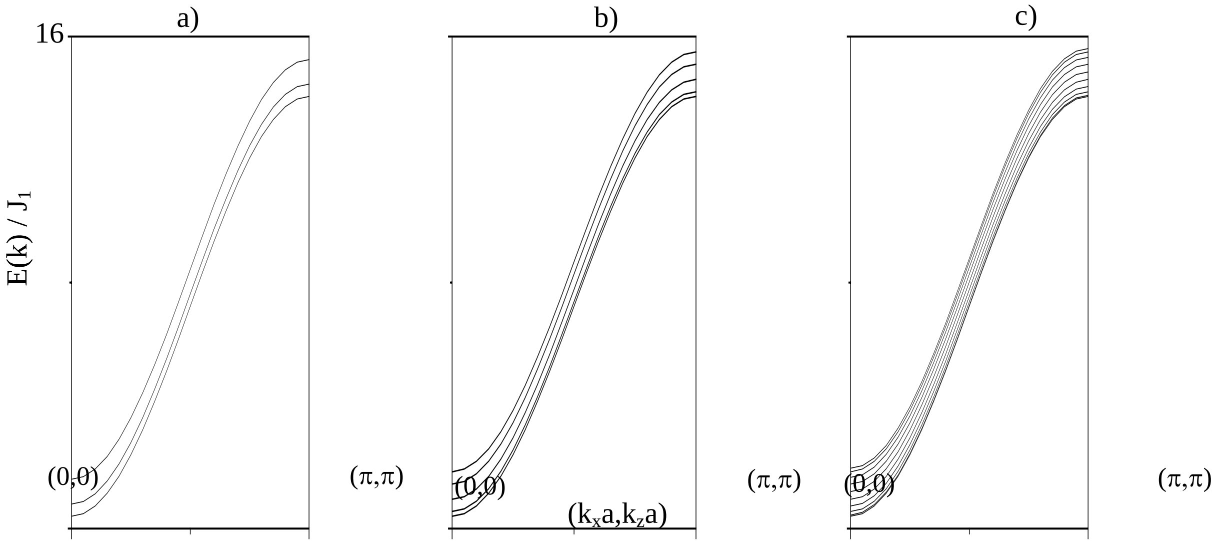

Fig.1: Excitation spectrum of a super-lattice made up of: a) 3 atomic planes, b) 5 planes and c) 10 planes. The parameters are $J_2=1/2.83\ J_1$, $J_\perp=0.2J_1$ and $\delta=0.05J_1$[11].

anisotropy effect on the quasi-two-dimensional magnetic long range order stability. This significant result agrees with existing results [3,14].

3.3.2- Magnetization:

The calculated magnetization in expressions (13) and (14) show the same behaviour in $T^{3/2}$ as in bulk samples at low temperatures, while at high temperatures the magnetization behaves as *T*log*T,* which is a characteristic of the quasi-two-dimensional systems. In the absence of anisotropy, the logarithmic factor depends only on the exchange $J_\perp$ between the planes, suggesting that it would correspond to a magnetization contribution due to the coupling between the planes. Otherwise, and as expected from expression (11), when

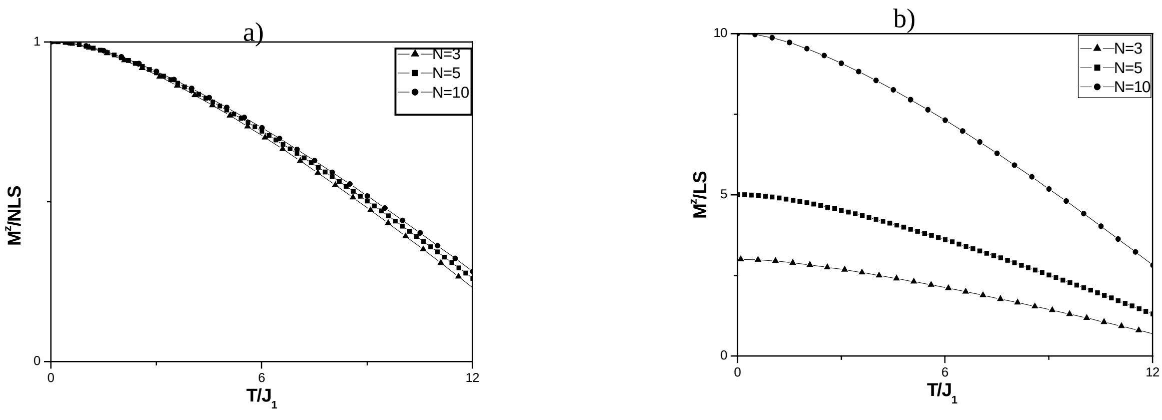

Fig.2: Thermal variation of the magnetization: a) magnetization per spin. b) global magnetization.

The anisotropy and the magnetic field are absent, and for lowest frequency mode, the logarithmic factor diverges. This fact confirms the anisotropy important role as deduced above from the gap analysis. Figure (2-a), shows that each super-lattice site produces the same average contribution to the total magnetization, while the total magnetization increases when N increases (fig. 2-b).

Moreover, the NNN exchange interaction effect on the magnetization is deduced from expression (8) and is displayed in figure 3. So, comparing the presence (fig. 4-a) and absence (fig. 4-b) of this interaction, we see that the NNN exchange interaction increases the transition temperature, thus reinforcing the ferromagnetic order.

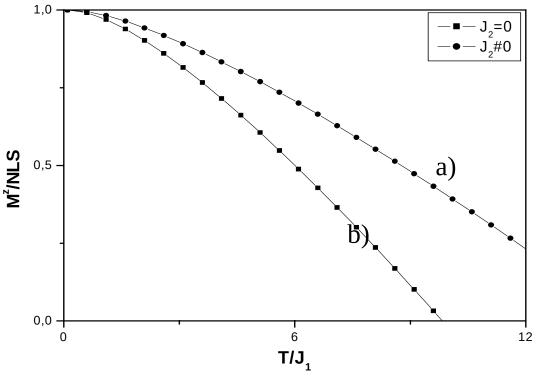

Fig.3: Thermal variation of the magnetization. The parameters are the same as fig. 1

On the other hand, to analyse the dipolar interactions and surface anisotropy effects, we start again from the resolution of (4) with $\alpha \neq 0$ and $D \neq 0$. The spectral theorem [17] allows us to calculate the spin wave average number and the magnetization expression (8). Therefore,

$$< a^+_{k_{//},l}, a_{k_{//},l} >= -2\int \frac{\mathrm{Im} << a^+_{k_{//},l}, a_{k_{//},l} >>}{e^{\beta E_l(k)}-1}. \quad (15)$$

The Green's functions $G_{ll}=<<a^+_{k,l},a_{k,l}>>$ are expressed here according to the passage matrix elements and its inverse (P and P^{-1}, respectively) which diagonalise the Hamiltonian:

$$< a^+_{k,l}, a_{k,l} >= \sum_{n=1}^{N}\left[\frac{P_{\ln}P^{-1}_{nl}-P_{\ln'}P^{-1}_{n'l}}{e^{\beta E_l(k)}-1}-P_{\ln'}P^{-1}_{n'l}\right]$$

with $n'=N+n$,

$$\frac{M^z}{NLS}=1-\frac{1}{S}\frac{1}{N}\frac{v}{(2\pi)^2}\sum_{l=1}^{N}\sum_{n=1}^{N}\int_{BZ}\left[\frac{P_{\ln}P^{-1}_{nl}-P_{\ln'}P^{-1}_{n'l}}{e^{\beta E_l(k)}-1}-P_{\ln'}P^{-1}_{n'l}\right]dk_x dk_z \quad (16)$$

The exact analytical solution of (4) is more complex than in the simple case with α=D=0. We thus performed a numerical solution. The results are reported in figure 5, where we display the magnetization thermal variation ratio compared to the obtained one when the dipolar interaction and the surface anisotropy have the same weight (α=D) in the magnetic order stability. It comes out that for temperatures lower than a "threshold temperature" $T_s(N)$, these two parameters don't have an effect (see fig. 5).

We will qualify this situation as a "standard" state where these two effects contribute with the same weight *(α =D)* to the super-lattice magnetic properties. However the decreasing of $T_s(N)$ with N increasing suggests the presence of effects increasingly significant when the super-lattice becomes wide. For the temperature higher than $T_s(N)$, an asymmetry of their influence is also recorded. The anisotropy effect would be greater in the evolution of the magnetic state of the super-lattice.

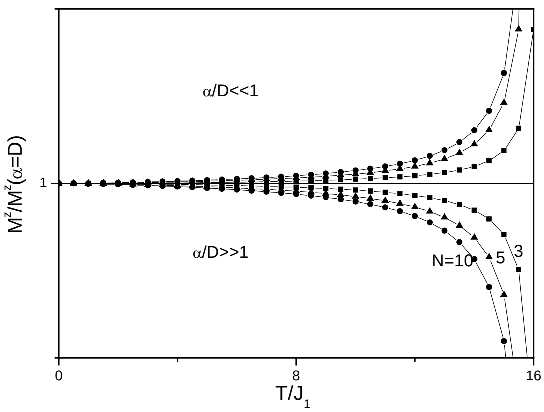

Fig. 5: Thermal evolution of the dipolar interaction and surface anisotropy effects on the magnetization.

Its impact is indeed perceived more rapidly than in the dipolar interaction case, when T increases. Furthermore, a competitive character between these two effects is clearly highlighted in this temperature zone. When *α/D>>1*, the magnetization decreases, while if the dipolar interaction is dominant (α/D<<1), the magnetization increases compared with the "standard" case *(α =D)*. Indeed, dipolar interaction tends to align magnetic moments in the film plane, and consequently to reinforce the magnetization in the plane. The surface anisotropy,

however, tends to align moments perpendicularly to the plane, and as a result to decrease the magnetization.

IV- CONCLUSION

In this work, we have studied the elementary magnetic excitations of a super-lattice having bcc structure by using the linear spin-wave theory. The excitation spectrum calculated shows the existence of N planar modes coupled for all wavevector **k** value in the film plane of the super-lattice to N planes. The obvious dependence of a gap on the surface anisotropy shows the role played by this anisotropy in the existence of a magnetic order. A competition between surface anisotropy and dipolar interaction effects on the stability of this long-range magnetic order is also shown for the temperatures higher than a threshold temperature $T_s(N)$ which decreases with the increasing layers number N.

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