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A Heisenberg model of a two-component magnetic superlattice

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Abstract. We study an (m, n) superlattice consisting of two alternating magnetic materials (components) of m and n atomic layers, respectively. The superlattice is modelled by a simple cubic lattice of spins coupled via nearest-neighbour exchange (Heisenberg model). Using recurrence relations, the dispersion equations of surface and bulk spin waves are derived for both finite and semi-infinite systems. The numerical results of the (1, 1), (3, 1) and (3, 2) cases are shown graphically. For a range of the surface exchange J_s, the maximum number of surface modes, equal to $m + n$, is obtained.

1. Introduction

Superlattices of excellent quality can nowadays be synthesized, following the advances in sputtering [1, 2] and epitaxial [3–5] techniques. The superlattice may possess new physical properties which are very different from those of their component materials [6]. We can design the superlattices that we need with the aid of theoretical studies. These factors have aroused great interest in superlattice materials in recent years.

As regards spin excitations, there have been many theoretical studies of the spin wave dispersion in the long-wavelength or magnetostatic limit [7–11]. In the short-wavelength limit, where the exchange coupling is dominant, comparatively fewer studies have been done. Several different techniques have been developed for the exchange-dominated spin waves, including the Green function method [12], the interface rescaling technique [13] and the transfer matrix formalism [14–16].

In this paper, we study a semi-infinite and a finite stack of two different ferromagnetic films by the method of recurrence relations. This method was first developed for electron Tamm state problems [17] and has been used for magnetostatic modes [11]. The superlattice is modelled by a simple cubic lattice of spins coupled via nearest-neighbour exchange (Heisenberg model). We obtain the dispersions for both semi-infinite and finite structures with one surface layer modification. We also find that the maximum number of surface modes in a semi-infinite superlattice is equal to the atomic layer number $m + n$ of a superlattice unit. We also obtain the range of J_s when there are $m + n$ surface modes, and when all the surface modes disappear.

Some of our results are equivalent to those obtained for finite and infinite systems by Barnas [15, 16] in the transfer matrix formalism. In our calculation, the recurrence relations are used and solved for each of the atomic layers in one component, as well as from one superlattice unit to another. In [15, 16], only the eigenvalue value results for the superlattice unit matrix are solved. Hence our results are more general for arbitrary and large m and n. In earlier work also, there has been no discussion of how the number of surface modes changes with the surface exchange J_s.

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2. Recurrence relations for (m, n) superlattices in the Heisenberg model

We consider here the following Heisenberg Hamiltonian:

$$H = -\sum_{(i,j)} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - g\mu_B B_0 \sum_i S_i^z \tag{1}$$

where J_{ij} represents the exchange couplings between the spins $\boldsymbol{S}_i$ and $\boldsymbol{S}_j$ of the nearest neighbours. $\boldsymbol{B}_0$ is an applied magnetic field in the superlattice z direction (see figure 1).

From this Hamiltonian, we can obtain the coupled equations [14–16] for S_l (spin operator for the lth layer):

$$[(\omega - g\mu_B B_0)/s - J_{l,l+1} - J_{l,l-1} - 4J_{l,l}\Lambda]S_l + J_{l,l-1}S_{l-1} + J_{l,l+1}S_{l+1} = 0 \tag{2}$$

where $\Lambda = 1 - \frac{1}{2}[\cos(q_x a_0) + \cos(q_y a_0)]$, a_0 is the lattice constant for the simple cubic structure, q_x and q_y are the components of the spin wave vector in the x and y directions, ω is the angular frequency and s is the spin constant.

The (m, n) superlattice that we consider is formed from two different ferromagnetic layered structures stacked alternately: material A with m layers and material B with n layers. Each material A or B is characterized by its exchange interaction J_a or J_b and spin constant s_a or s_b. The constant describing the exchange interaction between interface atoms is J. The elementary unit cell is indicated by $k = 1, 2\ldots$ (see figure 1).

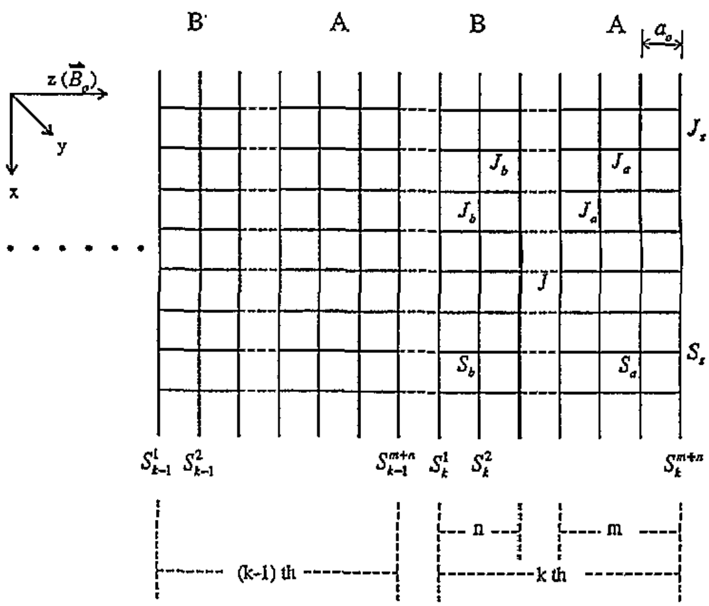

Figure 1. A semi-infinite Heisenberg superlattice model.

The coupled equations (2) for the (m, n) superlattice can be solved by recurrence relation techniques [11, 17] to give

$$\begin{pmatrix} S_k^1 \\ S_k^2 \end{pmatrix} = \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} \begin{pmatrix} S_1^1 \\ S_1^2 \end{pmatrix} = \hat{T} \begin{pmatrix} S_1^1 \\ S_1^2 \end{pmatrix} \tag{3}$$

where

$$\hat{T} = \sin[(k-1)\alpha]\,\hat{N} - \sin[(k-2)\alpha]\,\hat{I}/\sin\alpha. \tag{4}$$

Here S_k^1 and S_k^2 are the spins at the first and second layer, respectively, of the kth unit cell. $\hat{I}$ is the 2×2 unit matrix, and

$$\cos\alpha \equiv b = \tfrac{1}{2}(N_{++} + N_{--}) \qquad \text{for } |b| < 1. \tag{5}$$

For $|b| > 1$, $\cosh\lambda = |b|$, and one replaces $\sin(k\alpha)$ by $\sinh(k\lambda)$ for $b > 1$ and $(-1)^k \sinh(k\lambda)$ for $b < -1$.

$$\hat{N} = \begin{pmatrix} N_{++} & N_{+-} \\ N_{-+} & N_{--} \end{pmatrix} = \begin{pmatrix} B_{++} & B_{+-} \\ B_{-+} & B_{--} \end{pmatrix} \begin{pmatrix} A_{++} & A_{+-} \\ A_{-+} & A_{--} \end{pmatrix} \tag{6}$$

$$\begin{aligned}
A_{++} &= \frac{J_a}{J}\left[\sin[(m-1)\theta_a] - 2f_a\sin[(m-2)\theta_a]\right]/\sin\theta_a \\
A_{+-} &= \frac{J_a}{J}\left[2f_a\sin[(m-1)\theta_a] - \sin[(m-2)\theta_a]\right]/\sin\theta_a \\
A_{-+} &= \left[\left(\frac{J}{J_b} - 4f_a f_b\frac{J_a}{J}\right)\sin[(m-2)\theta_a] + 2f_b\frac{J_a}{J}\sin[(m-3)\theta_a]\right]/\sin\theta_a \\
A_{-+} &= \left[\left(4f_a f_b\frac{J_a}{J} - \frac{J}{J_b}\right)\sin[(m-1)\theta_a] - 2f_b\frac{J_a}{J}\sin[(m-2)\theta_a]\right]/\sin\theta_a
\end{aligned} \tag{7}$$

$$\begin{aligned}
\cos\theta_a &= b_a = -(\omega - g\mu_B B_0 - 2s_a J_a - 4s_a J_a\Lambda)/2s_a J_a \\
f_a &= -(\omega - g\mu_B B_0 - s_a J_a - s_a J - 4s_a J_a\Lambda)/2s_a J_a.
\end{aligned} \tag{8}$$

B_{++}, B_{+-}, B_{-+}, B_{--}, $\cos\theta_b$, b_b and f_b can be obtained by replacing all subscripts a in (7) and (8) by b, b by a and m by n.

The above equations (7) and (8) are also written for $|b_a| < 1$, $|b_b| < 1$. For $|b_a| > 1$, $|b_b| > 1$, the hyperbolic equivalents as in (5) must be used.

3. Surface modes in a semi-infinite superlattice

We next study a semi-infinite system terminated by m A-material layers. All the exchange constants are the same except that the surface layer has the intralayer exchange J_s. To study the possible existence of surface modes for this semi-infinite system (figure 1), we need only replace [11, 17]

$$\pm\frac{\sinh(k-2)\lambda}{\sinh(k-1)\lambda} \text{ by } \pm e^{-\lambda} \qquad \text{and hence } S_{k-1}^p/S_k^p \text{ by } \pm e^{-\lambda}. \tag{9}$$

Applying equations (3) and (9) for the last two unit cells, we get

$$\begin{aligned}
S_{k-1}^{m+n} &= N_{++}S_k^{m+n} + N_{+-}S_k^{m+n-1} = \pm S_k^{m+n}e^{-\lambda} \\
S_{k-1}^{m+n-1} &= N_{-+}S_k^{m+n} + N_{--}S_k^{m+n-1} = \pm S_k^{m+n-1}e^{-\lambda}.
\end{aligned} \tag{10}$$

Using the above equation (10), together with the coupled equations for the surface layer given by

$$\begin{aligned}
S_k^{m+n-1} &= f_s S_k^{m+n} \\
f_s &= -(\omega - g\mu_B B_0 - s_s J_a - 4s_s J_s\Lambda)/s_s J_a
\end{aligned} \tag{11}$$

we get the equations for the surface modes, as follows:

$$f_s N_{+-} + N_{++} \mp \mathrm{e}^{-\lambda} = 0$$
$$\cosh\lambda = \pm\tfrac{1}{2}(N_{++} + N_{--}). \tag{12}$$

Equations (12) are similar to those obtained in [15, 16]. In [15, 16], however, the explicit expressions of $\hat{N}$ for general m, n are not given (equation (6)).

In the special case of $m = n = 1$, and $s_a = s_b = s_s = s$, equations (12) reduce to

$$f'_s f'_b - 1 \mp \mathrm{e}^{-\lambda} = 0$$
$$\cosh\lambda = \pm\left(\tfrac{1}{2} f'_a f'_b - 1\right) \tag{13}$$

where

$$f'_s = -(\omega - g\mu_{\mathrm{B}} B_0 - Js - 4J_s s\Lambda)/sJ$$
$$f'_a = -(\omega - g\mu_{\mathrm{B}} B_0 - 2Js - 4J_a s\Lambda)/sJ \tag{14}$$
$$f'_b = -(\omega - g\mu_{\mathrm{B}} B_0 - 2Js - 4J_b s\Lambda)/sJ.$$

Equation (13) is a quadratic equation in ω. It has at most two solutions. By detailed studies of the equation, we can determine how the number of surface modes changes with J_s algebraically; we find that, under the following conditions, two surface modes appear:

$$\begin{cases} D < 0,\ E > 0 & \text{for } J_a > J_b \\ D > 0,\ E > 0 & \text{for } J_a < J_b \end{cases}$$

where

$$D = 4(J_s - J_a)\Lambda - J$$
$$E = 4(J_s - J_a)(2J_s - J_a - J_b)\Lambda - (4J_s - 3J_a - J_b)J. \tag{15}$$

On the other hand, only one surface mode exists when the following conditions hold:

$$\begin{cases} D < 0,\ E < 0 \text{ or } D > 0,\ E > 0 & \text{for } J_a > J_b \quad (16a) \\ D < 0,\ E > 0 \text{ or } D > 0,\ E < 0 & \text{for } J_a < J_b\,. \quad (16b) \end{cases}$$

An example of the case $J_a > J_b$ is shown in figure 2 for $J_a = 2$, $J_b = 1$, $J = 1.5$ and $\Lambda = 2$. The number of surface spin waves (SSWs) as a function of J_s is shown in figure 2(a). The numerical values are obtained from equations (15) and (16). The results show that all surface modes disappear only in the range $2.19 < J_s < 2.25$.

Figure 2(b) shows the dispersion relation for the maximum case of two surface modes with $J_s = 1.2$. Mode A is an optical wave, and mode B is an acoustic wave. For large Λ, mode A is localized at the surface layer and mode B's peak is at the second atomic layer from the surface (figure 2(c)).

From figure 2(b), we can also see clearly how the surface modes change with J_s. When $J_s < 1.63$, mode B is under the two bulk bands, and mode A is in the gap between two bands. With increasing J_s, the two surface modes move upwards. When $J_s = 1.63$, mode B reaches the bottom of the lower band and disappears first; only mode A is left. When

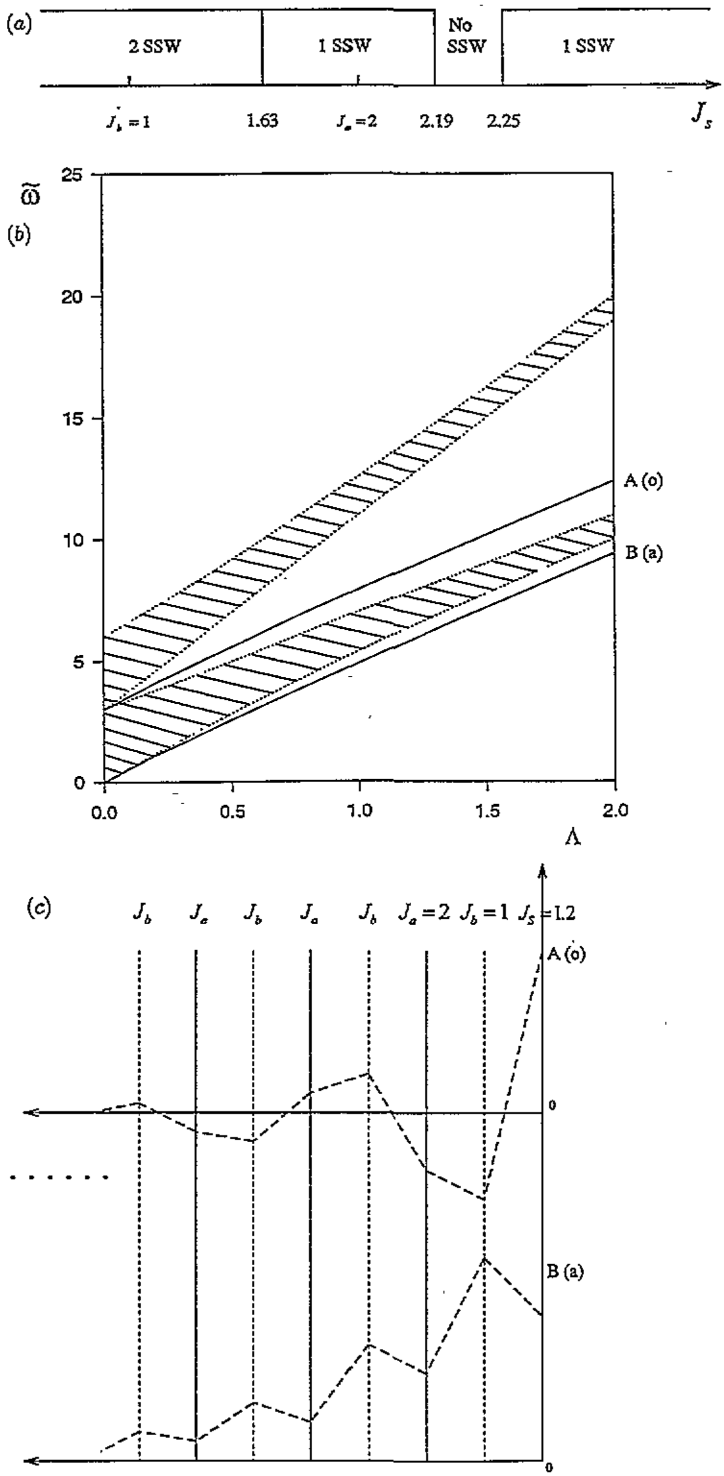

Figure 2. (*a*) Number of surface modes for a (1, 1) superlattice as a function of J_s for $J_a = 2$, $J_b = 1$, $J = 1.5$ and $\Lambda = 2$. (*b*) The two surface modes for $J_s = 1.2$ and $\bar{\omega} = (\omega - g\mu_B B_0)/J_a S_a$; o, optical; a, acoustic. The bulk bands are shown as shaded areas. (*c*) The spin amplitudes for the two surface modes ($\Lambda = 2$).

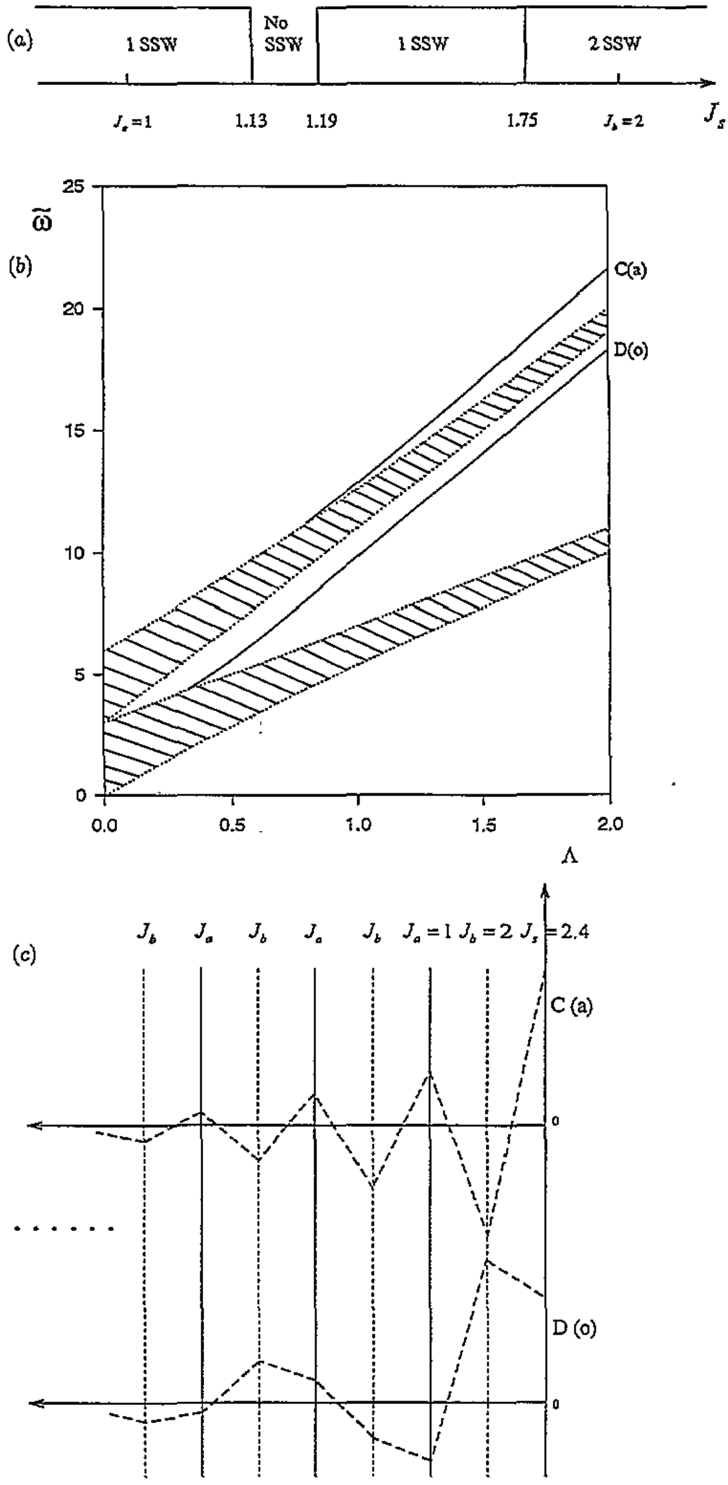

Figure 3. (*a*) Number of surface modes as a function of J_s for $J_a = 1$, $J_b = 2$, $J = 1.5$ and $\Lambda = 2$. (*b*) The two surface modes for $J_s = 2.4$. (*c*) The spin amplitudes for the two surface modes ($\Lambda = 2$).

$J_s = 2.19$, mode A reaches the bottom of the upper band and disappears also. From $J_s = 2.19$, no SSW exists until $J_s = 2.25$, when mode A appears above the upper band.

As an example of the $J_a < J_b$ case, we choose $J_a = 1$, $J_b = 2$, $J = 1.5$, $\Lambda = 2$. The number of SSWs as a function of J_s is shown in figure 3(a). In figure 3(b), we have shown the maximum case of two SSWs with $J_s = 2.4$. Mode C is an acoustic wave, and mode D is an optical wave. For large Λ, mode C is localized at the surface layer, and mode D's peak is at the second atomic layer (figure 3(c)).

With decrease in J_s, the two surface modes (C and D) move downwards (figure 3(b)). When $J_s = 1.75$, mode C reaches the top of the upper band and disappears. After that only mode D is left. When $J_s = 1.19$, mode D reaches the top of the lower band and disappears. At $J_s = 1.13$, it appears again below the lower band.

For a general case with m layers of material A and n layers of B, the maximum number of surface modes is $m+$ n. These are localized at each of the $m+n$ layers of the surface superlattice unit. However, with larger m and n, the range of J_s in which all $m+n$ surface modes appear at the same time becomes much smaller. The condition can be obtained by solving numerically dispersion equation (12). For a (1, 3) superlattice, there are four surface modes for the following choice of exchange constants: $J_a = 2$, $J_b = 1$, $J = 1.5$ and $J_s = 1.0$. These are shown in figure 4.

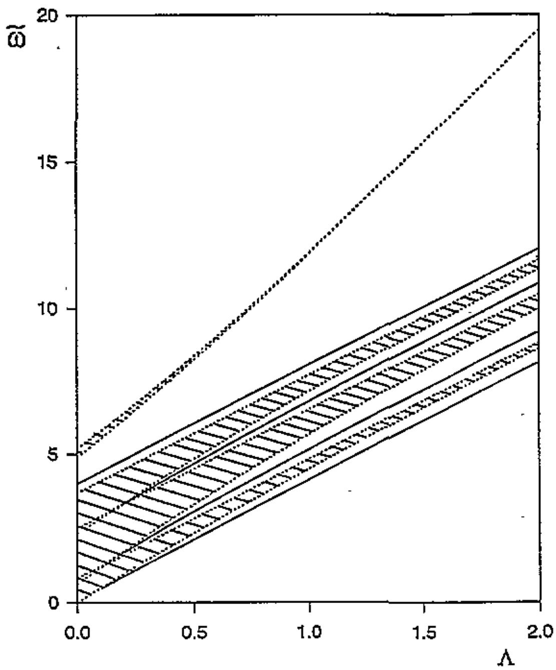

Figure 4. The four surface modes for a (1, 3) superlattice with $J_a = 2$, $J_b = 1$, $J = 1.5$ and $J_s = 1.0$.

4. Surface and bulk modes in a finite superlattice

We next consider a finite superlattice (figure 5), the two ends of which are A layers with the modification J_s to the outermost layers.

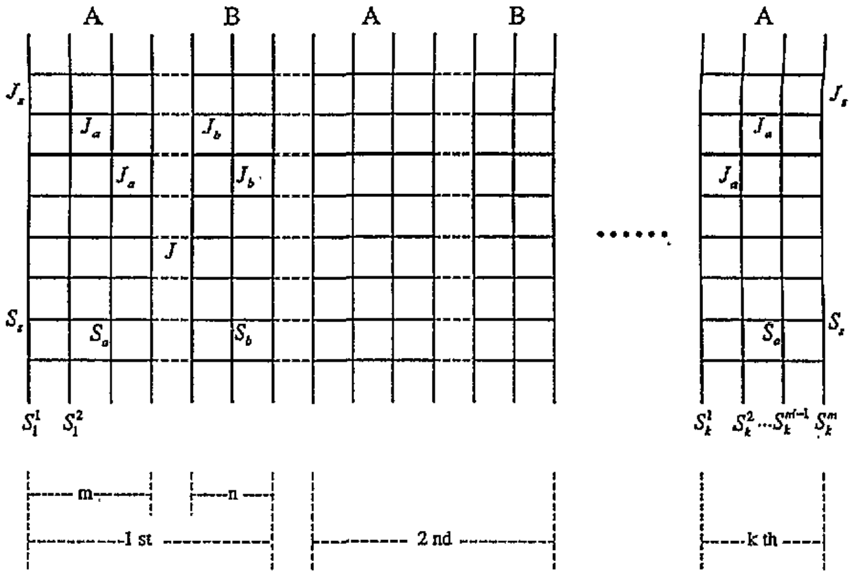

Figure 5. A finite superlattice with $k \times m$ A layers and $(k-1) \times n$ B layers. The outermost A layers have exchange J_s.

Using the recurrence relations as in (3), and the coupled equations for the two surface layers as in (11), we can easily obtain the dispersion equations for the $[k \times m, (k-1) \times n]$ finite superlattice:

$$f_s^2 R_{--} + f_s(R_{-+} - R_{+-}) - R_{++} = 0 \tag{17}$$

where

$$\hat{R} \equiv \hat{S}\hat{T} \tag{18}$$

$$\hat{S} = \begin{bmatrix} -\sin[(m-3)\theta_a] & \sin[(m-2)\theta_a] \\ -\sin[(m-2)\theta_a] & \sin[(m-1)\theta_a] \end{bmatrix} \tag{19}$$

and $\hat{T}$ is given by equation (4).

Equations (17)–(19) are equivalent to the results in [16] for finite k. However, in our results, explicit expressions of $\hat{T}$ for general m and n are given by solving the recurrence equations for each component (in equations (4) and (6)).

Equation (17) must be solved numerically. As an example, we have chosen a $(3 \times 3, 2 \times 2)$ superlattice of $m = 3$, $n = 2$ with $J_a = 1$, $J_b = 2$, $J = 1.5$ and $J_s = 1.5$. The dispersion curves are shown in figure 6, together with the five bulk bands. There are 13 spin waves. Spin waves $\{2, 3\}$, $\{5, 6\}$ and $\{8, 9\}$ appear as three pairs of surface modes associated with the three surface A layers. Because of the finite superlattice thickness, there is coupling within each pair, and the pair becomes non-degenerate for small Λ. The highest two modes 12 and 13 are very close, and cannot be resolved on the graph.

The method that we have used in this paper can be generalized to other structures. In the semi-infinite case (figure 1), we can introduce other kinds of surface modification. For example, if we modify more than one layer, we shall need more (and different) equations of the type of equation (11).

Similarly, in studying the finite systems, we have only discussed the case in which there are exactly m additional A layers with the same surface exchange J_s at both ends. If we

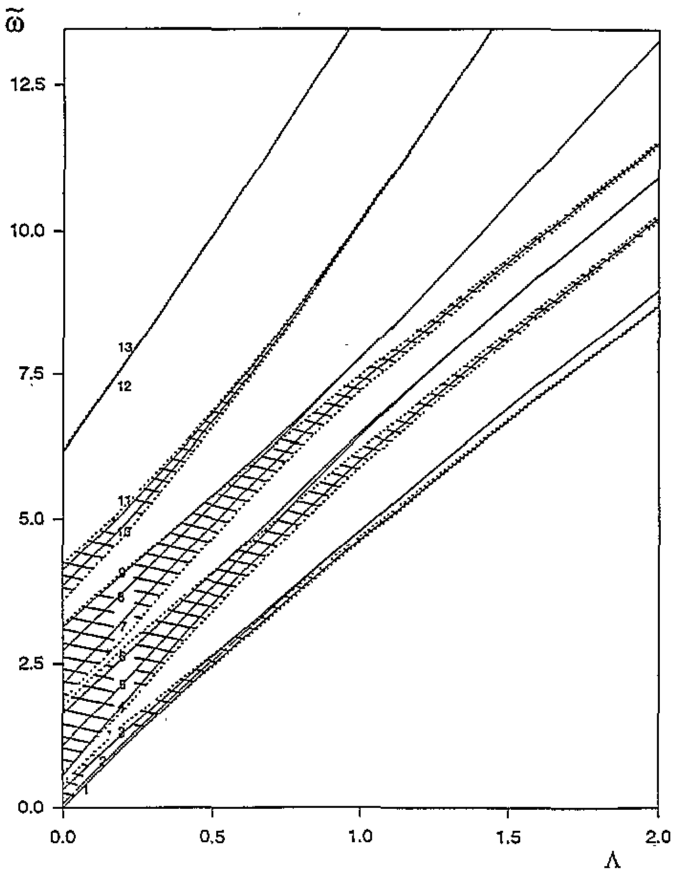

Figure 6. The 13 spin waves for a $(3\times3, 2\times2)$ finite superlattice with $J_a = 1$, $J_b = 2$, $J = 1.5$ and $J_s = 1.5$.

allow the two surface exchange constants to be different, equation (17) will be modified. If we allow other types (or numbers) of additional A layer, the matrix $\hat{S}$ (equations (18) and (19)) will be changed.

We expect more fabrication of superlattices with two types of ferromagnetic material, like that studied in this paper. The different surface and bulk spin waves that we obtain can be observed by Brillouin scattering experiments such as in [18, 19].

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