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Effect of next-nearest-neighbour interactions on spin waves in magnetic superlattices

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Abstract. Results are presented for 3D magnetic superlattices consisting of alternating films of cubic Heisenberg ferromagnets. Taking into account the next-nearest-neighbour (NNN) interactions, an explicit equation for the spin-wave dispersion relation is obtained by means of a transfer matrix method. Numerical results are presented for FCC ferromagnetic films with different values of the exchange constant ratio $\eta = J(\mathrm{NNN})/J(\mathrm{NN})$. If $\eta \neq 0$, for every frequency ω, there are two pairs of allowed values of wavenumbers k and in some frequency range both can be real if $\eta \geqslant 1$. For the superlattice, a comparison with the dispersion relation obtained considering only NN interaction is made and the main physical features are discussed.

1. Introduction

The recent development of exceptionally good quality magnetic superlattices has made possible the study of the intriguing properties of these artificial periodic layered structures, in which the thicknesses of the constituent films can be as thin as a few atomic layers (Parkin *et al* 1990). It is known that when the layer thicknesses are very small, the spectrum of the elementary excitations may possess unique physical properties which are distinct from those of the individual layers. These differences may be accounted for by the fact that the excitations of neighbouring layers are coupled via the interfilm exchange interaction, both in the magnetostatic (Camley *et al* 1983, Camley and Cottam 1987 and Almeida and Mills 1988) and exchange regimes (Albuquerque *et al* 1986). The specific regime is determined by the wavenumber K of the excitation.

The magnetostatic limit has already been proved to be particularly important for long-wavelength modes on the surface of a semi-infinite specimen, as well as in a thin film, and has been extensively investigated; for a review see Cottam and Tilley (1989) and references therein. On the other hand, for wavelengths comparable with the interatomic spacing a, the exchange interaction between adjacent spins is the main physical parameter and must determine the general behaviour of the magnetic excitations. Moreover, in this wavelength regime, it is necessary to use a microscopic theory to study these modes which are usually called spin waves.

In this paper we present a detailed study of 3D magnetic superlattices composed of alternating cubic Heisenberg films. The dispersion relations for spin waves will be obtained taking into account the exchange interaction between not only nearest

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neighbours (NN) but also next-nearest neighbours (NNN). It must be said that, beyond academic curiosity, the rapid development of deposition techniques has allowed preparation of very thin films and their possible applications in practical devices, such as delay lines and filters (Camley 1987), require a more realistic model to describe them.

The discussion presented here follows similar work recently presented by Hadizad *et al* (1991a, b) where the authors study lattice dynamics for 1D superlattices including NNN as well as NN interactions.

The plan of this paper is as follows: in section 2 we present the equation for the dispersion relation of bulk spin waves which provides the wavevectors for each medium. An equation for the spin-wave dispersion relation in a magnetic superlattice composed of two cubic Heisenberg ferromagnetic films is obtained in section 3. Numerical results are presented for the case when both constituent films have their spins localized in FCC lattices. A comparison with the dispersion relation obtained taking into account only NN interaction is also made in this section. Finally, in section 4, the main results are briefly summarized.

2. Bulk modes

To study spin waves in magnetic superlattices (MSL), taking into account the exchange interaction between nearest and next-nearest neighbours, we consider a MSL as shown in figure 1. This artificial layered structure is described by the Hamiltonian

$$\mathcal{H} = -\sum_i \sum_{\delta_1} K(i, i+\delta_1) \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\delta_1} - \sum_i \sum_{\delta_2} K(i, i+\delta_2) \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\delta_2} \tag{2.1}$$

where $K(i, i+\delta_1)$ denotes the exchange force between NN, which is equal to J_{1A} (J_{1B}) if both spins belong to the layer A (B), or I_1 if they are in different layers; $K(i, i+\delta_2)$ is the equivalent parameter for NNN and can assume the values J_{2A}, J_{2B} and I_2 for layer A, B or interlayer exchange, respectively.

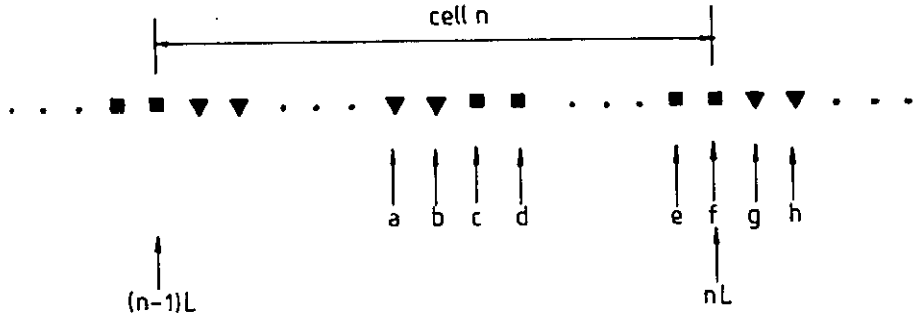

Figure 1. Notation for superlattice calculations.

By using the random phase approximation, i.e. considering $(S_i^z)_\alpha$ equal to the thermal expectation value of the z-component of $(\boldsymbol{S})_\alpha$ the equation of motion for

$S_i^+ = S_i^x + iS_i^y$ can be written as:

$$i\hbar\frac{\partial S_i^+}{\partial t} = 2\langle S_\alpha^z\rangle\Big(\sum_{\delta_1}(J_{1\alpha}S_i^+ - K(i,i+\delta_1)S_{i+\delta_1}^+) + \sum_{\delta_2}(J_{2\alpha}S_i^+ - K(i,i+\delta_2)S_{i+\delta_2}^+)\Big). \tag{2.2}$$

For an infinite specimen A or B (either n_A or $n_B \to \infty$) there are only bulk spin waves. The dispersion relation curves for these modes are obtained from the infinite series of equations represented by (2.2). Solutions for these equations can be found by the *ansatz*

$$(S_i^+)_\alpha = \exp[i(\boldsymbol{k}_\alpha \cdot \boldsymbol{r} - \omega t)]. \tag{2.3}$$

The substitution of (2.3) in (2.2) gives

$$\hbar\omega = 2S_\alpha\,[J_{1\alpha}(z_1 - \gamma_{1k}^\alpha) + J_{2\alpha}(z_2 - \gamma_{2k}^\alpha)] \tag{2.4}$$

where $S_\alpha = \langle S_\alpha^z\rangle$, z_1 and z_2 are the number of the NN and NNN sites respectively and γ_{1k}^α and γ_{2k}^α are given by

$$\gamma_{1k}^\alpha = \sum_{NN}\exp(i\boldsymbol{k}_\alpha \cdot \delta_1) \qquad \alpha = A \text{ or } B \tag{2.5a}$$

$$\gamma_{2k}^\alpha = \sum_{NNN}\exp(i\boldsymbol{k} \cdot \delta_2) \qquad \alpha = A \text{ or } B. \tag{2.5b}$$

If we assume the spins to be localized in a simple cubic structure ($z_1 = 6$ and $z_2 = 12$) γ_{ik}^α are given by

$$\gamma_{1k}^\alpha = 2(\cos q_\alpha^x a + \cos q_\alpha^y a + \cos q_\alpha^z a) \tag{2.6a}$$

$$\gamma_{2k}^\alpha = 4(\cos q_\alpha^x a \cos q_\alpha^y a + \cos q_\alpha^x a \cos q_\alpha^z a + \cos q_\alpha^y a \cos q_\alpha^z a) \tag{2.6b}$$

with a denoting the length of the unit cell of the specimen.

It should be noted that for modes propagating parallel to the z-axis ($q_\alpha^x = q_\alpha^y = 0$, and $q_\alpha^z = q_\alpha$), $\gamma_{1k}^\alpha = 2(2 + \cos q_\alpha a)$ and $\gamma_{2k}^\alpha = 4(1 + 2\cos q_\alpha a)$. Therefore, the dispersion relation for these modes can be written as

$$\Omega_\alpha/(1 + 4\eta_\alpha) = 1 - \cos q_\alpha a \tag{2.7}$$

where we have defined the characteristic parameters $\Omega_\alpha = \hbar\omega/4S_\alpha J_{1\alpha}$ and $\eta_\alpha = J_{2\alpha}/J_{1\alpha}$. As can be seen in (2.7), for a simple cubic lattice, the effect of the NNN interaction on the spin waves propagating along the z-axis is only the introduction of a scale factor in the energy. As a consequence, the dispersion curves have no qualitative difference from that obtained considering only nearest neighbours.

On the other hand, for an FCC lattice we have $z_1 = 12$, $z_2 = 6$ and the sums are given by

$$\gamma_{1k}^{\alpha} = 4(\cos q_{\alpha}^{x} a/2 \cos q_{\alpha}^{y} a/2 + \cos q_{\alpha}^{x} a/2 \cos q_{\alpha}^{z} a/2 + \cos q_{\alpha}^{y} a/2 \cos q_{\alpha}^{z} a/2) \quad (2.8a)$$

$$\gamma_{2k}^{\alpha} = 2(\cos q_{\alpha}^{x} a + \cos q_{\alpha}^{y} a + \cos q_{\alpha}^{z} a). \quad (2.8b)$$

Therefore, for propagation along the z-axis, the bulk dispersion relation curves are obtained from:

$$\eta_{\alpha} \cos^2 k_{\alpha} a + 2 \cos k_{\alpha} a - (2 + \eta_{\alpha} - \Omega_{\alpha}/2) = 0 \quad (2.9)$$

with $k_{\alpha} = q_{\alpha}/2$.

Equation (2.9) has two solutions for k_{α}, say k_1^{α} and k_z^{α}. In the low-frequency region, i.e. $\Omega_{\alpha} \leqslant 2(1+\eta_{\alpha})^2/\eta_{\alpha}$, at least one of these values is real. Moreover, from (2.9) it can be seen that there is a critical value for $\eta_{\alpha}(\eta_{\alpha}^{c} = 1.0)$ above which there is a frequency interval where both values of k_{α} are real. The frequency region is determined by $8 \leqslant \Omega_{\alpha} \leqslant 2(1 + \eta_{\alpha})^2/\eta_{\alpha}$. It should be noted that the critical value for η_{α} obtained here corresponds to the case where the NNN and NN forces are equal and is much bigger than critical value 0.25 found for the equivalent parameter by Hadizad *et al* in 1D lattice dynamics. In figure 2 we show the spectra of these spin waves for $\eta_{\alpha} = 0.5$ (figure 2(a)) and 1.5 (figure 2(b)). In the first case one root, k_1^{α} say, has a similar form to that found for NN exchange for frequencies below $\Omega_{\alpha} = 8$. In this interval k_2^{α} has the form $\pi/a + iy$. For $8 < \Omega_{\alpha} < 9$ both roots have the form $\pi/a + iy$. In the high-frequency region $\Omega_{\alpha} > 9$ both roots are in the complex plane and of the general form $x + iy$. In figure 2(b) it is seen that the effect of a larger NNN exchange is to produce a frequency interval above $\Omega = 8$ in which both k_1^{α} and k_2^{α} are real. These forms are very similar to those found by Hadizad *et al* (1991a) for the monatomic 1D lattice.

3. Superlattice

We consider a magnetic superlattice as depicted schematically in figure 1. Each point of this diagram corresponds to one atomic plane. Therefore, for spins localized in a simple cubic lattice, a unit cell of the lattice is represented by two points, while for an FCC structure, the unit cell is represented by three points. As can be seen in figure 1, a spin that is not at the interface or in the next-neighbour atomic plane has the same equation of motion as a spin in the corresponding bulk medium. Thus the spin-wave amplitude must be given, within each film, by a linear combination of the positive and negative solution $\pm k_1^{\alpha}$ and $\pm k_2^{\alpha}$ of the dispersion relation (2.9), namely

$$S_i^{+} = A_n e^{ik_1^{A}(z - z_{nA})} + B_n e^{-ik_1^{A}(z - z_{nA})} + C_n e^{ik_2^{A}(z - z_{nA})} + D_n e^{-ik_2^{A}(z - z_{nA})} \quad (3.1a)$$

in film A of cell n, and

$$S_i^{+} = E_n e^{ik_1^{B}(z - z_{nB})} + F_n e^{-ik_1^{B}(z - z_{nB})} + G_n e^{ik_2^{B}(z - z_{nB})} + H_n e^{-ik_2^{B}(z - z_{nB})} \quad (3.1b)$$

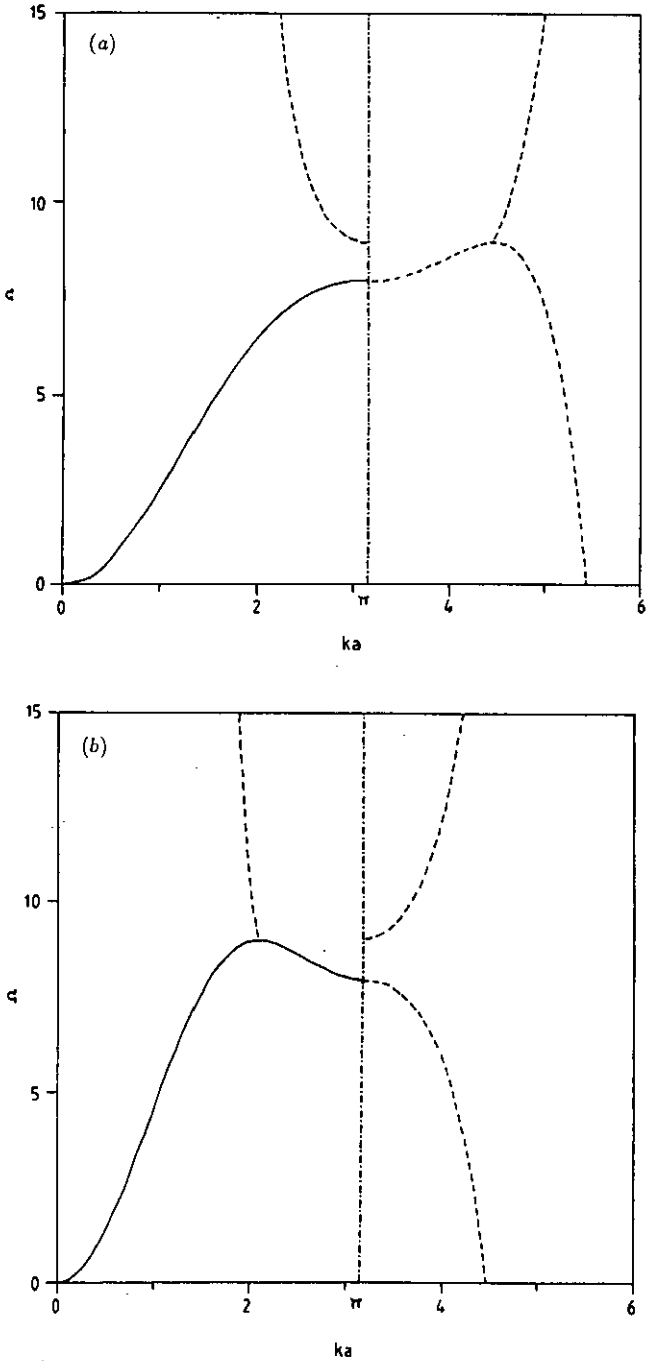

Figure 2. Solutions of bulk dispersion equation (2.9) for spin waves in an FCC lattice represented as $\Omega = \hbar\omega/(4S_A J_{1\alpha})$ versus ka for (*a*) $\eta_\alpha = J_{2\alpha}/J_{1\alpha} = 0.5$ (*b*) $\eta_\alpha = 1.5$. The convention for ka of the form $\pi + iy$ is that these values are represented as broken curves with y as the abscissa measured from π. Roots of the form $x + iy$ are represented as broken curves with x (measured from zero) below π and y as the abscissa measured from π.

in film B of the same cell. Here, z_{nA} and z_{nB} are the position of the first A and B atomic layer in the nth cell of the superlattice and are given by

$$z_{nA} = (n-1)Na + a \tag{3.2a}$$

$$z_{nB} = (n-1)Na + (n_A + 1)a \tag{3.2b}$$

where $Na = (n_A + n_B)a = L$, is the length of the unit cell at the superlattice.

By introducing, in each medium, the column vectors $|\Phi_n\rangle$ and $|\Psi_n\rangle$ defined by

$$|\Phi_n\rangle = \begin{bmatrix} A_n \\ B_n \\ C_n \\ D_n \end{bmatrix} \qquad |\Psi_n\rangle = \begin{bmatrix} E_n \\ F_n \\ G_n \\ H_n \end{bmatrix} \tag{3.3}$$

the equation of motion for spins at the atomic layers labelled by a, b, c and d in figure 1 relates the vectors $|\Phi_n\rangle$ and $|\Psi_n\rangle$ through the matrix equation

$$\mathbf{M}(\omega, k_1^A, k_2^A, A, B, 2n_A)|\Phi_n\rangle = \mathbf{N}(\omega, k_1^A, k_2^A, B, A, 1)|\Psi_n\rangle. \tag{3.4}$$

Similarly, the equation of motion for spins at layers labelled by e, f, g and h allows us to write

$$\mathbf{M}(\omega, k_1^B, k_2^B, B, A, 2n_B)|\Psi_n\rangle = \mathbf{N}(\omega, k_1^B, k_2^B, B, A, 1)|\Phi_{n+1}\rangle. \tag{3.5}$$

The explicit forms of the matrices $\mathbf{M}(\omega, k_1, k_2, \alpha, \beta, N)$ and $\mathbf{N}(\omega, k_1, k_2, \alpha, \beta, N)$ are given in the appendix.

Elimination of $|\Psi_n\rangle$ between (3.4) and (3.5) gives

$$|\Phi_{n+1}\rangle = \mathbf{T}|\Phi_n\rangle \tag{3.6}$$

where the transfer matrix $\mathbf{T}$ is defined by

$$\mathbf{T} = \mathbf{N}^{-1}(\omega, k_1^B, k_2^B, B, A, 1)\ \mathbf{M}(\omega, k_1^B, k_2^B, B, A, 2n_B)\ \mathbf{N}^{-1}(\omega, k_1^A, k_2^A, A, B, 1)$$
$$\mathbf{M}(\omega, k_1^A, k_2^A, A, B, 2n_A). \tag{3.7}$$

The matrix $\mathbf{T}$ has its determinant equal to 1 and therefore its eigenvalues, λ_j ($j = 1$ to 4) obey the relation

$$\lambda_1\lambda_2\lambda_3\lambda_4 = 1. \tag{3.8}$$

On the other hand, Bloch's theorem gives

$$|\Phi_{n+1}\rangle = \exp(\mathrm{i}QL)|\Phi_n\rangle \tag{3.9}$$

where Q is the Bloch wavevector (not necessarily real) and L is the size of the unit cell of the superlattice. Furthermore, time-reversal invariance requires that if Q is a root, so is $-Q$. A comparison between (3.9) and (3.6) show us that $\exp(\mathrm{i}QL)$ are the

eigenvalues of **T** and therefore its eigenvalues occur in pairs $(\lambda_1, \lambda_1^{-1})$ and $(\lambda_2, \lambda_2^{-1})$ related to the Bloch wavevector Q_j by

$$Q_j L = \pm i \ln(\lambda_j) \qquad j = 1,2. \tag{3.10}$$

The formalism that has been presented is similar to that used in the 1D lattice dynamics problem (Hadizad *et al* 1991a). As in the case, once **T** is known, the eigenvalues and therefore the Bloch wavevectors can be obtained numerically by standard methods. Some examples of calculated dispersion curves are shown later; it is convenient to start with results for the limiting case of NN forces only. The dispersion relation for spin waves propagating in an infinite medium with only NN interaction is obtained by taking $\eta_\alpha = 0$ in (2.9). In this case there is only one wavevector which is related to the frequency by

$$k_\alpha a = \pm i \ln(1 - \Omega_\alpha/4) \tag{3.11}$$

where the variables are those used earlier. The dispersion relation for a superlattice can be obtained from (3.11) using the approach of Albuquerque *et al* (1986). Typical results of a numerical calculation of the dispersion curve are shown in figure 3; it may be seen as arising from the usual folding of the bulk curve into the mini Brillouin zone.

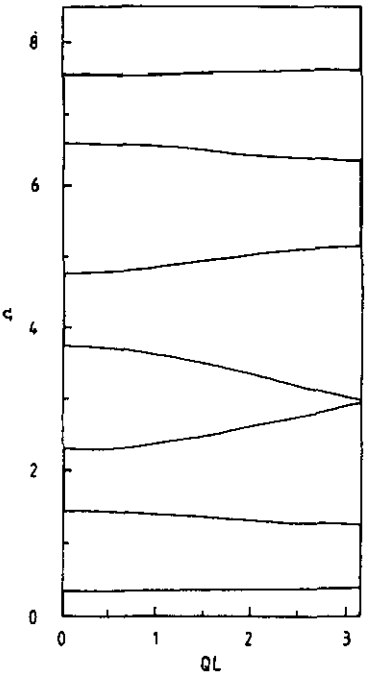

Figure 3. Superlattice dispersion curve for NN interactions only for a superlattice with $n_A = 7$, $n_B = 3$. The graph is presented as $\Omega = \hbar\omega/(4S_A J_{1A})$ versus QL where L is the superlattice period. The other parameters are $S_B = S_A$, $J_{1B} = 1.5J_{1A}$ and $I_1 = 0.5J_{1A}$.

Some dispersion curves to show the effects of inclusion of NNN forces are shown in figure 4. Figure 4(*a*) may be compared with figure 3 to show that the effect of relatively weak NNN forces is to produce some shifting of the dispersion curves in frequency but no qualitative changes. Figure 4(*b*), for stronger NNN forces, shows

somewhat greater changes in the frequency range $\Omega < 8.0$ where there is just one real root in the bulk, figure 2. More importantly, figure 4(*c*) shows a mode-anticrossing region for $\Omega > 8.0$ in the region of two real bulk roots. The form of this is dependent on the monolayer number, as seen in figure 4(*d*). In figures 4(*a*) to (*d*) the interlayer NNN exchange is fairly weak. A striking effect of increasing this parameter is seen by comparing figures 4(*e*) and 4(*c*); the anticrossing becomes so strong as to produce a range of Q in which no propagation occurs.

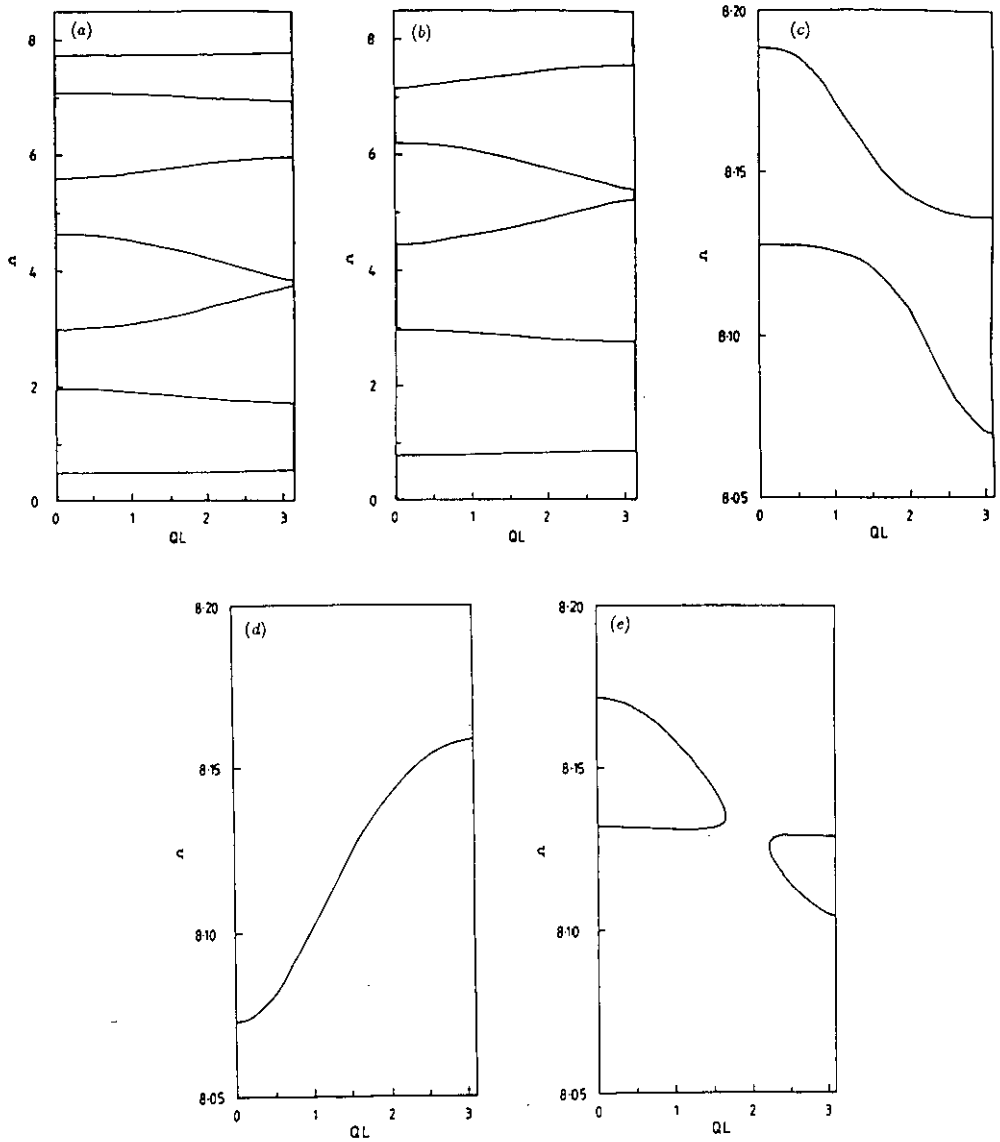

Figure 4. Superlattice dispersion curves with NNN interactions included. The NN parameters are the same as in figure 3. Layer numbers are $n_A = 7$, $n_B = 3$ except for in figure 4(*d*) in which $n_A = 5$, $n_B = 3$. NNN parameters are $J_{2A}/J_{1A} = J_{2B}/J_{1B} = I_2/I_1 = 0.5$ in figure 4(*a*), $J_{2A}/J_{1A} = J_{2B}/J_{1B} = 1.5$, $I_2/I_1 = 0.5$ in figures 4(*b*) to 4(*d*) and $J_{2A}/J_{1A} = J_{2B}/J_{1B} = I_2/I_1 = 1.5$ in figure 4(*e*).

4. Conclusions

The derivation of the bulk mode dispersion equation in section 2 leads to results which are similar to those found in the corresponding lattice dynamical calculation. As in that case, for a sufficiently large value of the NNN exchange constant two real values of the wavenumber are found in a frequency range above the frequency $\Omega = 8$ of the top of the band when only NN forces are included. However the critical value $J_2/J_1 = 1$ for this to appear is much larger than the value of 0.25 found in one-dimensional lattice dynamics.

The main result of this paper is the derivation of the dispersion relation which is given in implicit form in section 3. In view of the large number of parameters, illustration has been restricted to a small number of cases which are intended to bring out points of particular interest. As might be expected from the analogous lattice dynamics, qualitatively new results are found in the range $\Omega > 8$ for strong NNN interactions.

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Appendix

The matrices used in section 3 can be obtained by substituting equations (3.1*a*) and (3.1*b*) in equation (2.2), to obtain an equation of motion for spins localized at positions labelled by a, b, c and d in figure 1. The algebra is straightforward (if laborious) and details are omitted.

These four equations relate the coefficients (A_n, B_n, C_n, D_n) of the layer A with those (E_n, F_n, G_n, H_n) in B in the matrix form shown below:

$$\begin{bmatrix} \xi(\Omega,-k_1^{\mathrm{A}},A) & \xi(\Omega,k_1^{\mathrm{A}},A) & \xi(\Omega,-k_2^{\mathrm{A}},A) & \xi(\Omega,k_2^{\mathrm{A}},A) \\ \eta(\Omega,-k_1^{\mathrm{A}},A) & \eta(\Omega,k_1^{\mathrm{A}},A) & \eta(\Omega,-k_2^{\mathrm{A}},A) & \eta(\Omega,k_2^{\mathrm{A}},A) \\ \Gamma(-k_1^{\mathrm{A}},B) & \Gamma(k_1^{\mathrm{A}},B) & \Gamma(-k_2^{\mathrm{A}},B) & \Gamma(k_2^{\mathrm{A}},B) \\ -2i_{2\mathrm{B}} & -2i_{2\mathrm{B}} & -2i_{2\mathrm{B}} & -2i_{2\mathrm{B}} \end{bmatrix}$$

$$\times \begin{bmatrix} \mathrm{e}^{-k_1^{\mathrm{A}}a\ 2n_{\mathrm{A}}} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{k_1^{\mathrm{A}}a\ 2n_{\mathrm{A}}} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{-k_2^{\mathrm{A}}a\ 2n_{\mathrm{A}}} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{k_2^{\mathrm{A}}a\ 2n_{\mathrm{A}}} \end{bmatrix} \begin{bmatrix} A_n \\ B_n \\ C_n \\ D_n \end{bmatrix}$$

$$= \begin{bmatrix} -2i_{2\mathrm{A}} & -2i_{2\mathrm{A}} & -2i_{2\mathrm{A}} & -2i_{2\mathrm{A}} \\ \Gamma(k_1^{\mathrm{B}},A) & \Gamma(-k_1^{\mathrm{B}},A) & \Gamma(k_2^{\mathrm{B}},A) & \Gamma(-k_2^{\mathrm{B}},A) \\ \eta(\Omega,-k_1^{\mathrm{B}},B) & \eta(\Omega,k_1^{\mathrm{B}},B) & \eta(\Omega,-k_2^{\mathrm{B}},B) & \eta(\Omega,k_2^{\mathrm{B}},B) \\ \xi(\Omega,-k_1^{\mathrm{B}},B) & \xi(\Omega,k_1^{\mathrm{B}},B) & \xi(\Omega,-k_2^{\mathrm{B}},B) & \xi(\Omega,k_2^{\mathrm{B}},B) \end{bmatrix}$$

$$\times \begin{bmatrix} \mathrm{e}^{-k_1^{\mathrm{B}}a} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{k_1^{\mathrm{B}}a} & 0 & 0 \\ 0 & 0 & \mathrm{e}^{-k_2^{\mathrm{B}}a} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{k_2^{\mathrm{B}}a} \end{bmatrix} \begin{bmatrix} E_n \\ F_n \\ G_n \\ H_n \end{bmatrix} \tag{A1}$$

where the functions used above are defined by

$$\xi(\Omega,k,\alpha)=\left(\Omega-4\frac{J_{1\alpha}S_\alpha}{J_{1A}S_A}(1-\cos ka)-\frac{J_{2\alpha}S_\alpha}{2J_{1A}S_A}(2-\exp(i2ka)\right)\exp(ika)$$

$$\eta(\Omega,k,\alpha)=\left(\Omega-2\frac{J_{1\alpha}S_\alpha}{J_{1A}S_A}(2-\exp(ika)-\frac{J_{2\alpha}S_\alpha}{2J_{1A}S_A}(2-\exp(i2ka)\right)$$

$$\Gamma(k,\alpha)=-\tfrac{1}{4}[I_1S_\alpha/J_{1A}S_A+(I_2S_\alpha/J_{1A}S_A)\exp(ika)] \qquad i_{2\alpha}=I_2S_\alpha/J_{1A}S_\alpha.$$

A comparison between the equations (A1) and (3.4) gives the matrices **M** and **N** used in the body of the paper.

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