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Theory of spin waves in magnetic interfaces, superlattices and disordered layer structures

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Abstract. A general recursion method for calculating the exact local spin-wave Green function in an arbitrary ferromagnetic interface, superlattice and disordered layer structure is developed. The method is applied to magnetic insulator structures described by a nearest-neighbour exchange Hamiltonian. It is shown that the complete response function of an arbitrary layer structure can be generated from a single matrix element of the Green function in the surface plane of a magnetic overlayer. The proposed algorithm for overlayers is very simple, computationally stable and extremely accurate. The method is used to determine the exact exchange stiffness D of a ferromagnetic superlattice and of a disordered layer structure. The range of validity of the exact result for D is discussed in the light of recent experiments on the temperature dependence of the surface magnetisation. The application of the method to ferromagnets with long-range exchange interactions and to metallic layer structures is also discussed.

1. Introduction

Interest in magnetic overlayers, interfaces and superlattices arises since they hold the promise of new device applications with properties such as microwave response subject to design (Grünberg 1985). They also have potential applications in magnetic information technology (see e.g. White 1985). More fundamentally, it is now possible, using atomic-beam deposition, to create novel layer structures with properties quite different from the bulk properties of the constituents (Arrott *et al* 1987, Bader and Moog 1987).

Magnetic layer structures are also interesting theoretically since they are the simplest magnetically inhomogeneous systems for which first-principles calculations are feasible. In fact, the ground-state properties of some metallic layer structures and superlattices have already been calculated within the local spin-density-functional formalism (see e.g. Freeman and Fu 1987).

Apart from the ground state, the most important characteristic of a magnetic layer structure is its dynamic response function. It determines the dispersion of magnetic excitations, spin-wave stiffness of the structure, neutron scattering cross section and also the local density of spin-wave states which is required in the calculation of the local magnetisation.

For an insulating magnetic structure, the response function reduces to the Green function $G = (E - H)^{-1}$ of the exchange Hamiltonian H of the structure. We shall loosely refer to G as the spin-wave Green function. The spin-wave Green function can

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be also defined for a ferromagnetic metal (Mathon 1988a) and it determines completely its response function (Mathon 1983, 1988a).

The spin-wave Green function is, therefore, a quantity of central importance. The purpose of this paper is to describe a general recursion method for calculating the exact local spin-wave Green function in an arbitrary ferromagnetic overlayer, interface, superlattice and even disordered layer structure. The method is a generalisation of an algorithm we have developed for magnetic overlayers (Mathon and Ahmad 1988, Mathon 1988b).

The plan of the paper is as follows. First the recursion method for overlayers is briefly reviewed in § 2. The generalisation of the method to interfaces and superlattices is described in §§ 3 and 4. Finally, exact results for the exchange stiffness of a superlattice and of a disordered layer structure are derived in § 5 and compared with the exact results for a classical disordered ferromagnetic chain (Harris and Kirkpatrick 1977).

For simplicity, the method is explained for insulating layer structures described by a nearest-neighbour exchange Hamiltonian. The atomic planes of the layer structure are assumed to be parallel to the (100) plane. Generalisation to a longer-range exchange is quite straightforward and is described in § 6. Aplication to metallic layer structures is also briefly discussed in § 6.

2. Magnetic overlayers

Consider a magnetic overlayer consisting of N atomic planes labelled by $n = 1, 2, \ldots, N$. The overlayer is located above the (100) surface of a SC ferromagnet occupying the half-space $z < 0$. The exchange Hamiltonian of the system expressed in terms of the Bose spin raising and lowering operators b_n^+, and b_n is

$$H = E_0 + \sum_{n,m} H_{nm} b_n^+ b_m \tag{1}$$

where

$$H_{nm} = -(S_n S_m)^{1/2} J_{nm} \qquad (n \neq m)$$

$$H_{nn} = \sum_{m \neq n} S_m J_{nm}$$

and n and m label lattice sites. We have $J_{n,n+1} = J$ and $S_n = S$ in the substrate, but the exchange integrals between neighbouring atomic planes and within different planes of the overlayer are arbitrary (ferromagnetic). The local spin S_n in any atomic plane of the overlayer is also arbitrary. The spin-wave Green function of the Hamiltonian (1) is defined by

$$G = (E - H)^{-1}. \tag{2}$$

Because of translational symmetry in the (100) plane, we shall calculate G in the mixed representation $G_{nm}(q, E)$, where n and m now label planes parallel to the (100) plane, q is the two-dimensional wavevector from the surface Brillouin zone $-\pi/a < q_x$, $q_y < \pi/a$, and a is the lattice constant (see e.g. Kalkstein and Soven 1971).

We shall show in §§ 3 and 4 that the complete response function of an arbitrary layer structure can be generated from a single matrix element $G_{NN}(q, E)$ of the Green function in the surface plane $n = N$ of an overlayer. In principle, this key matrix element could be calculated by one of the traditional recursion methods for the Green function (see

e.g. Haydock 1982, Lopez Sancho *et al* 1985 and references therein). However, a serious disadvantage of all these methods is that they are iterative and give only an approximate G_{NN}. In the applications described in §§ 3–5, an exact rather than approximate Green function is required. We have, therefore, developed a new version of the recursion method which gives the exact surface Green function for an arbitrary overlayer (Mathon and Ahmad 1988, Mathon 1988b).

To calculate G_{NN}, we first assume that the overlayer is physically removed from the substrate. The matrix element of the exact spin-wave Green function $G^0_{00}(q, E)$ in the now exposed surface plane of the substrate ($n = 0$) is assumed to be known (we shall show in § 4 how to determine $G^0_{00}(q, E)$ self-consistently). As a next step, we reinstate the first atomic plane of the overlayer $n = 1$ and give a prescription for calculating the matrix element G^1_{11} of the Green function in the new surface plane $n = 1$ in terms of the old G^0_{00}. The superscript '1' indicates that G^1 refers to the substrate covered with one 'adlayer'. Once G^1_{11} is known, the second layer $n = 2$ is reinstated and G^2_{22} is expressed in terms of G^1_{11}. This procedure is repeated until the whole overlayer is 'rebuilt'. After N recursion steps, we end up with the exact G^N_{NN} in terms of G^0_{00}.

The general recursion step from a layer n to the layer $n + 1$ is given by (Mathon and Ahmad 1988, Mathon 1988b)

$$(G^{n+1}_{n+1,n+1})^{-1} = \omega + W_{n+1,n+1} - W^2_{n,n+1} G^n_{nn}(1 - W_{nn} G^n_{nn})^{-1} \tag{3}$$

where

$$\begin{aligned} &W_{nn} = J_{n,n+1} S_{n+1} \\ &W_{n,n+1} = -J_{n,n+1}(S_n S_{n+1})^{1/2} \\ &W_{n+1,n+1} = 2SJ - S_n J_{n,n+1} + [1 - (S_{n+1}/S)(J_{n+1,n+1}/J)](E - \omega - 2SJ) \\ &\omega = E - 6SJ - 2SJ[\cos(q_x a) + \cos(q_y a)]. \end{aligned} \tag{4}$$

Here $J_{n,n+1}$ is the exchange integral between layers n and $n + 1$, and J_{nn} is the exchange integral and S_n the local spin in the layer n.

Equations (3) and (4) provide a very simple and efficient computational algorithm for calculating the exact surface Green function of an arbitrary overlayer. The results obtained by this method for specific magnetic overlayers have already been discussed (Mathon and Ahmad 1988, Mathon 1988b). The method as it stands is applicable only to overlayers but it can be easily generalised to interfaces and superlattices.

3. Magnetic interfaces

Consider an interface of N atomic planes separating two magnetically homogeneous semi-infinite ferromagnets (figure 1). The exchange integrals between neighbouring atomic planes and within atomic planes of the interface and the local spin S_n in the interface are again arbitrary.

Let us assume that we require the local Green function G_{nn} in the nth layer of the interface. To obtain G_{nn}, we first pass an imaginary cleavage plane between the layers n and $n + 1$, separating the whole structure into two independent semi-infinite systems (i.e. there are no exchange bonds between the right- and left-hand halves). We can then define a Green function G^{cl} for the cleaved system by

$$G^{\mathrm{cl}}_{nm} = \begin{cases} G^{\mathrm{L}}_{nm} & n, m \in \mathrm{L} \\ 0 & n \in \mathrm{L},\ m \in \mathrm{R} \text{ (or vice versa)} \\ G^{\mathrm{R}}_{nm} & n, m \in \mathrm{R} \end{cases} \tag{5}$$

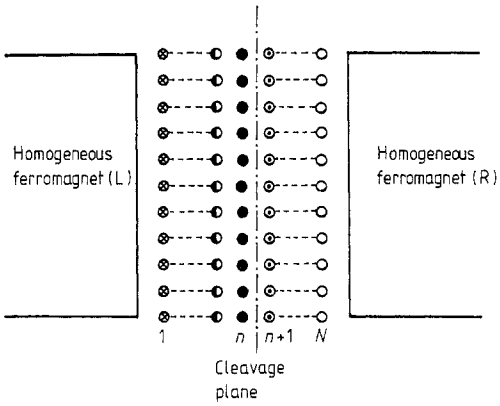

Figure 1. Cleaved interface of N atomic planes separating two homogeneous ferromagnets. Different types of circle denote atomic planes with different magnetic properties.

where G^{L} and G^{R} are the Green functions for the left- and right-hand halves of the cleaved interface. Since each half is just a magnetic overlayer on a homogeneous substrate, the matrix elements G^{cl}_{nn} and $G^{cl}_{n+1,n+1}$ can be calculated by the recursion method for overlayers described in § 2.

To determine the exact G_{nn} in the interface we need only to switch on the exchange $J_{n,n+1}$ between the layers n and $n+1$, and reconnect the two halves using the Dyson equation

$$G^{n+1} = G^{n} + G^{n}WG^{n+1}.$$

When the two halves are being reconnected, both the diagonal elements G^{cl}_{nn} and $G^{cl}_{n+1,n+1}$ are perturbed. Since we consider nearest-neighbour exchange only, the perturbation to the diagonal elements is equivalent to the perturbation caused by the deposition of a single atomic layer (the surface layer of the other half of the cleaved structure), i.e. is again described by the matrix W defined in equation (4). It is, therefore, useful first to 'prepare' two auxilliary Green functions, G^{D}_{nn} and $G^{D}_{n+1,n+1}$, which include this diagonal perturbation. They are given by

$$\begin{aligned} G^{D}_{nn} &= G^{L}_{nn}\,(1 - W_{nn}G^{L}_{nn})^{-1} \\ G^{D}_{n+1,n+1} &= G^{R}_{n+1,n+1}(1 - W_{n+1,n+1}G^{R}_{n+1,n+1})^{-1} \end{aligned} \tag{6}$$

where W_{nn} and $W_{n+1,n+1}$ are given by equation (4). When these two auxilliary Green functions are finally reconnected, only the off-diagonal element $W_{n,n+1}$ defined by equation (4) needs to be considered in the Dyson equation. It is easy to show that the required G_{nn} is given by

$$G_{nn} = G^{D}_{nn}(1 - G^{D}_{nn}W^{2}_{n,n+1}G^{D}_{n+1,n+1})^{-1}. \tag{7}$$

By passing the cleavage plane between any two atomic planes of the interface, we can determine from equations (3)–(7) all the diagonal elements G_{nn}, $n = 1, 2, \ldots, N$, of the exact interface Green function.

For example, to compute by this method the local density of spin-wave states (DOS) in every layer of the interface, all G^{L}_{nn} and G^{R}_{nn} for $n = 1, 2, \ldots, N$ are required. Since these are just the intermediate Green functions used in the recursion equation (3), one only needs to calculate G^{L}_{NN} and G^{R}_{11} once and store all the intermediate matrix elements in the computer memory. The computational effort needed to evaluate the local DOS in every layer of the interface is, therefore, equivalent to the effort required to calculate by the method of § 2 the surface density of states for two overlayers (left and right), i.e. minimal.

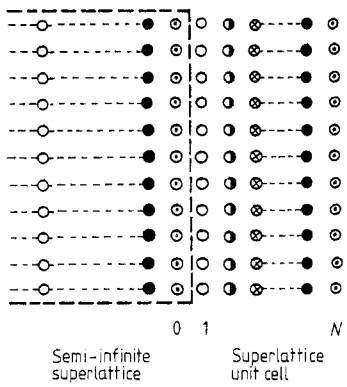

Figure 2. Semi-infinite superlattice with one additional unit cell of N atomic planes deposited on its surface. Different types of circle denote atomic planes with different magnetic properties.

4. Magnetic superlattices

Consider a magnetic superlattice with a unit cell of N atomic planes in the direction perpendicular to the (100) plane. The exchange integrals J_{nn} and $J_{n,n+1}$ and the local spin S_n in any atomic plane of the superlattice satisfy the periodic conditions

$$J_{n+N,n+N} = J_{nn} \qquad J_{n+N,n+1+N} = J_{n,n+1} \qquad S_{n+N} = S_n$$

but are otherwise arbitrary.

The calculation of the local Green function in any atomic plane of the superlattice is essentially a combination of the methods described in §§ 2 and 3. We again pass a cleavage plane between any two atomic planes of the superlattice. Without loss of generality, we label these planes by $n = 0$ and $n = 1$. Let us assume for a moment that the two surface matrix elements G^{L}_{00} and G^{R}_{11} of the Green function for the cleaved superlattice are known. The exact Green function G_{00} of the original (uncleaved) superlattice is then expressed in terms of G^{L}_{00} and G^{R}_{11} via equations (6) and (7). The general superlattice problem, therefore, reduces to the calculation of the surface Green function for a semi-infinite superlattice.

We shall assume that a semi-infinite superlattice occupies the half-space $z < 0$ and its surface plane is at $n = 0$ (see figure 2). The first step in the calculation of the surface Green function G^0_{00} is to deposit on the semi-infinite superlattice, one by one, all the atomic planes from a superlattice unit cell. This additional unit cell forms an overlayer of N atomic planes above the old surface at $n = 0$. The Green function G^N_{NN} in the new surface at $n = N$ can, therefore, be again expressed from equations (3) and (4) in terms of G^0_{00} using the recursion method for overlayers. The fact that the 'substrate' on which the overlayer is deposited is not a homogeneous ferromagnet is immaterial since only the surface matrix element G^0_{00} is required in our recursion method.

The periodicity of the superlattice implies that the surface at $n = N$ is identical with the surface at $n = 0$ and, therefore, the following self-consistency condition must be satisfied:

$$G^N_{NN}[G^0_{00}(q, E)] = G^0_{00}(q, E) \tag{8}$$

where the bracket [. . .] indicates that G^N_{NN} is a functional of G^0_{00}. The explicit form of the functional $G^N_{NN}[G^0_{00}(q, E)]$ is determined recursively by equations (3) and (4). Equation (8) combined with equations (3) and (4) provides, therefore, a simple computational algorithm for calculating G^0_{00}. Since G is a complex function, equation (8) is equivalent to a system of two coupled non-linear equations for Re G^0_{00} and Im G^0_{00} which

can be solved numerically for any fixed values of q and E.

As a simple illustration, we shall use equation (8) to determine the exact surface Green function G^0_{00} for a homogeneous semi-infinite ferromagnet (as promised in § 2).

A semi-infinite homogeneous ferromagnet is a trivial special case of a semi-infinite superlattice with $N = 1$. Using $J_{10} = J_{11} = J$ and $S_1 = S$ in equation (4), it is easy to see that $W_{00} = W_{11} = -W_{10} = SJ$. We need only one recursion step (3), which means that equation (8) reduces to a simple quadratic equation for G^0_{00}:

$$(G^0_{00})^{-1} = \omega + SJ - (SJ)^2 G^0_{00}(1 - SJG^0_{00})^{-1}. \tag{9}$$

Its solution is the well known result for the surface spin-wave Green function of a semi-infinite ferromagnet with (100) surface (see e.g. Mathon and Ahmad 1988)

$$G^0_{00}(q, E) = (2SJ)^{-1}[1 + (\omega - 2SJ)^{1/2}(\omega + 2SJ)^{-1/2}] \tag{10}$$

(of the two roots of equation (9), the root which has the correct analytic properties at $E \to \pm\infty$ is chosen).

5. Exact results for the exchange stiffness of layer structures

An interesting application of the method described in §§ 2–4 is to calculate the exact exchange stiffness constant D of a layer structure. It is also a very stringent test of the proposed algorithm since D calculated by this method can be compared with the exact results for a classical disordered chain (Harris and Kirkpatrick 1977).

The exchange stiffness constant D is defined as the coefficient in the dispersion law $E = Dq^2$ of a spin wave with a small wavevector q. We shall first discuss the exchange stiffness of a magnetic overlayer since we showed in §§ 3 and 4 that the spin-wave problem for interfaces and superlattices can always be reduced to an equivalent problem for an overlayer.

An overlayer of a finite thickness on a semi-infinite substrate clearly cannot have any effect on D since D is a global property of the whole infinite system. The coefficient D is, therefore, not a good measure of the local exchange stiffness for an overlayer. The correct quantity to look at is the local density of spin-wave states $\rho_n(E)$ at the bottom of the spin-wave band. It is given by

$$\rho_n(E) = (\pi N_s)^{-1} \sum_q \operatorname{Im} G_{nn}(q, E) \tag{11}$$

where G_{nn} is the local Green function in the nth atomic plane and N_s is the number of atoms in the surface plane. The local density of states reflects the local spin-wave amplitude and, therefore, the local exchange stiffness. For a homogeneous bulk ferromagnet the spin-wave energy at the bottom of the band is $E = Dq^2$ and the global density of states is related to D by the well known formula (Kittel 1971)

$$\rho^{\text{bulk}}(E) = (2\pi)^{-2} D^{-3/2} E^{1/2} \tag{12}$$

where $D = 2SJa^2$ for a nearest-neighbour SC ferromagnet. It follows that, to determine the local exchange stiffness of a magnetically inhomogeneous sytem, it is sufficient to examine the initial energy dependence of the local $\rho_n(E)$.

All our further discussion is based on an exact result for the surface density of states of an arbitrary magnetic overlayer proved by Mathon and Ahmad (1988). It states that the initial $\rho_N(E)$ in the surface plane N of an overlayer of arbitrary (finite) thickness is independent of the exchange in the overlayer and is given by

$$\rho_N(E) = 2(S_N/S)\rho^{\text{bulk}}(E) + O(E^{3/2}). \tag{13}$$

Here, S_N is the surface spin and $\rho^{\text{bulk}}(E)$ is the bulk density of states in the substrate given by equation (12). The result (13) is obtained from equations (3) and (11) in the lowest order in E. It shows that not only the global D but even the local exchange stiffness of an overlayer is determined completely by the substrate, i.e. quite independent of the exchange interactions in the overlayer. It is easy to see using the results of § 3 that the same conclusion holds also for any interface of finite thickness.

The situation for a superlattice is quite different from that for an overlayer since there is no infinite substrate. The exchange stiffness D of a superlattice must, therefore, be determined by the exchange interactions (and spin) in the superlattice unit cell. It can be calculated exactly from equation (13) and the self-consistency condition (8) of § 4.

It follows from § 4 that it is sufficient to determine D for a semi-infinite superlattice. The case of exchange interactions which vary in the direction perpendicular to the surface is most important experimentally (Mauri *et al* 1988, Siegmann and Bagus 1988). To illustrate our method, we shall, therefore, calculate D for a superlattice with $S_1 = S_2 = \ldots = S_N = S$ and $J_{11} = J_{22} = \ldots = J_{NN} = J$ but with arbitrary (ferromagnetic) $J_{n,n+1}$ between the layers $n = 0, 1, \ldots, N-1$.

Consider first the self-consistency condition (8) for $\operatorname{Im} G^N_{NN}$. For a semi-infinite superlattice with $S_1 = S_2 = \ldots = S_N = S$, the exact result (13) implies that the initial $\operatorname{Im} G^n_{nn}(q, E)$ in any surface plane $n = 0, 1, \ldots, N-1$ must be a universal function of E and q independent of n. It follows that, as far as the initial behaviour of $\operatorname{Im} G^n_{nn}(q, E)$ is concerned, any semi-infinite superlattice is equivalent to some effective homogeneous semi-infinite ferromagnetic medium. The surface $\operatorname{Im} G^0_{00}$ for a homogeneous semi-infinite ferromagnet is given by equation (10). Setting $\operatorname{Im} G^n_{nn}(q, E) = F(q, E)$, we find from equation (10) that the universal function $F(q, E)$ is given by

$$F(q, E) = \begin{cases} (1/\omega_0)[(\omega_0 - \omega)/(\omega_0 + \omega)]^{1/2} & \omega^2 < \omega_0^2 \\ 0 & \omega^2 > \omega_0^2 \end{cases} \tag{14}$$

where

$$\begin{aligned} \omega &= E - 4SJ - \omega_0 - 2SJ[\cos(q_x a) + \cos(q_y a)] \\ \omega_0 &= 2SJ^{\text{eff}} \end{aligned} \tag{15}$$

and J^{eff} is the exchange integral in a semi-infinite effective medium perpendicular to the surface which is to be determined self-consistently. Because the initial $\operatorname{Im} G^n_{nn}(q, E)$ is the same in every surface layer of a superlattice, the self-consistency condition (8) for $\operatorname{Im} G^N_{NN}$ is a trivial identity which gives no information about J^{eff}. We need to examine $\operatorname{Re} G^N_{NN}$ at the bottom of the spin-wave band.

The perturbation matrix W in equation (4) takes a very simple form for a superlattice with exchange that varies only in the direction perpendicular to the surface:

$$W_{nn} = -W_{n,n+1} = SJ_{n,n+1} \qquad W_{n+1,n+1} = \omega_0 - SJ_{n,n+1}.$$

To simplify the notation, we shall write $\operatorname{Re} G^n_{nn}(q, E) = R_n$ and $SJ_{n,n+1} = J_n$. The general recursion step (3) for R_n then takes the form

$$R_{n+1} = \{(J_n R_n - 1)[J_n - (\omega + \omega_0)(J_n R_n - 1)] + (\omega + \omega_0)[J_n F(q, E)]^2\} D_n \tag{16}$$

where the denominator D_n is given by

$$D_n = \{[(\omega + \omega_0)(1 - J_n R_n) - J_n]^2 + [(\omega + \omega_0) J_n F(q, E)]^2\}^{-1} \tag{17}$$

and ω_0 is defined in equation (15). At the bottom of the spin-wave band $E \simeq 0$, the condition $\omega \simeq -\omega_0$ must be satisfied for non-zero $F(q, E)$ and it follows from equation (14) that $F(q, E)$ can be approximated by

$$F(q, E) \simeq (2/\omega_0)^{1/2}(\omega + \omega_0)^{-1/2}. \tag{18}$$

Because the factor $(\omega + \omega_0)$ multiplying $F(q, E)$ in equations (16) and (17) removes the singularity of $F(q, E)$ at $\omega = -\omega_0$, we can take equation (16) in the limit $E \to 0$, $\omega \to -\omega_0$. The recursion equation (16) assumes a very simple form in this limit, i.e.

$$R_{n+1} = R_n - 1/J_n + 2/\omega_0 \tag{19}$$

and can be easily solved. Imposing now the self-consistency condition (8), i.e. $R_N = R_0$, we finally obtain the following result for J^{eff}:

$$(1/J^{\text{eff}}) = N^{-1} \sum_{n=0}^{N-1} (1/J_{n,n+1}). \tag{20}$$

The exact exchange stiffness of a superlattice is, therefore, equal to the exchange stiffness of an anisotropic homogeneous ferromagnet with an exchange integral parallel to the (100) plane equal to J and with an exchange integral perpendicular to this plane equal to J^{eff}.

Since equation (20) holds for any N, it can also be applied to a disordered layer structure. A layer structure with a random distribution of exchange in the direction perpendicular to the (100) plane can be modelled by a superlattice with a unit cell so large that $J_{n,n+1}$ within the unit cell can be made random. Equation (20) with $N \to \infty$ and random $J_{n,n+1}$ then gives J^{eff} for a disordered layer structure. This is precisely the result obtained earlier by Harris and Kirkpatrick (1977) for a classical disordered chain.

6. Discussion

Our recursion method for ferromagnetic layer structures can be compared with previous calculations of spin waves in superlattices consisting of two different magnetic materials (van Stapele *et al* 1985, Dobrzynski *et al* 1986, Albuquerque *et al* 1986, Hinchey and Mills 1986) and also with the more general formulations for N-layer superlattices (Masri and Dobrzynski 1988, Barnas 1988).

Our method has several advantages. It is quite general and yet very simple. The complete response function for an arbitrary layer structure is generated from a single matrix element of the response function in the surface plane of a magnetic overlayer. The overlayer calculation itself is based on a very simple and efficient recursion algorithm which has already been tested (Mathon and Ahmad 1988, Mathon 1988b).

The method is computationally very stable and extremely accurate. This means that layer structures consisting of a very large number of different atomic planes $N \simeq$ 50–100 can be easily handled. Our calculation for overlayers of up to 50 atomic layers thick show that the accuracy for $N \simeq 50$ is just as high as for very small N (Mathon 1988b, Eva 1988).

A generalisation of our method to a longer-range exchange is quite straightforward. Consider an overlayer of N atomic planes in which each plane is exchange-coupled to k other planes. When an adlayer is deposited on a semi-infinite substrate, the exchange links coupling the adlayer to the substrate are switched on, one at a time, and with

each new link the Green function is recalculated from equation (3). Computationally, the problem is, therefore, equivalent to an overlayer of kN atomic planes with nearest-neighbour exchange between the planes. The only modification is that the Green function in the overlayer surface plane depends now on k diagonal matrix elements of the substrate Green function. Our tests (Eva 1988) for overlayers in which each layer is coupled to every other layer show that the accuracy for $N = 50$ is just as high as for the nearest-neighbour model.

In § 5 we determined the exact exchange stiffness D of a superlattice and of a disordered layer structure. Exact results for D are available in some special cases of disordered ferromagnets. In particular, Harris and Kirkpatrick (1977) showed that D is directly related to the conductance of a random resistor network. Essentially the same result was obtained recently by Edwards (1988) for a dilute Hubbard model. Using this analogy, our equation (20) for a disordered layer structure is equivalent to the conductance of a random network of resistors connected in parallel. This is precisely the result obtained by Harris and Kirkpatrick (1977) for a classical disordered chain.

Our derivation of the exact D for a layer structure has several interesting features. It shows explicitly that an effective-medium approximation for Im G is exact at the bottom of the spin-wave band but the real part of G must be treated exactly, i.e. multiple scattering from all the layers of a layer structure must be included in Re G.

It is possible, using our recursion method, to determine the range of validity of the exact result for D. The spin-wave energy in a homogeneous ferromagnet is well described by $E = Dq^2$ for E up to about $k_B T_C/3$, where T_C is the Curie temperature. It is universally accepted (see e.g. Edwards and Muniz 1985) that this result holds also for disordered alloys. However, our calculations show that this is certainly not the case for layer structures. It was shown by Mathon and Ahmad (1988) that the initial law $E = Dq^2$ (effective-medium result obtained from equation (13)) breaks down in overlayers for spin-wave energies E as low as $E \simeq 0.01 k_B T_C$. This means that the exact D for a layer structure is virtually not observable. If this result carries through to alloys, all the previous calculations for disordered alloys need to be reconsidered.

Since D governs the temperature dependence of the magnetisation, it can be determined experimentally. Measurements of the temperature dependence of the surface magnetisation $M_S(T)$ for $Ni_{40}Fe_{40}B_{20}$ glass (Pierce *et al* 1982) and for Fe (1 1 0) surface (Walker *et al* 1984, Korecki and Gradmann 1985, 1986) show clearly that $M_S(T)$ deviates from the simple Bloch law with the initial exact D (see Mathon and Ahmad (1988) for detailed interpretation). Most recently, this problem was investigated very thoroughly by Mauri *et al* (1988) using the method of spin polarisation of low-energy cascade electrons. They showed quite convincingly that the surface magnetisation is not determined by the initial exact D of the substrate, which is in complete agreement with our theoretical prediction.

Our calculation of the exact D is also applicable to metallic layer structures where contact can be made with the work of Edwards (1988). It was shown by Mathon (1983) that the spin-wave Green function of a metal in the random-phase aproximation is exactly equivalent in the long-wavelength limit to the spin-wave Green function of a Heisenberg ferromagnet with long-range RKKY exchange integrals. Our calculation of D, therefore, carries through, but the method would first have to be extended to long-range exchange as discussed above.

An interesting problem arises for disordered metallic ferromagnets. Since the RKKY exchange integrals are oscillatory, there is always a random admixture of

antiferromagnetic bonds for any disordered ferromagnetic metal. This could lead to Anderson localisation of spin waves, a problem touched upon by Edwards (1988).

Finally, it should be noted that our method is applicable not only to spin waves but also to phonons and electrons in the tight-binding approximation since they are also described by a Hamiltonian of the form (1).

References

Albuquerque E L, Fulco P, Sarmento E F and Tilley D R 1986 *Solid State Commun.* **58** 41–4
Arrott A S, Heinrich B, Purcell S T, Cochran J F and Urquhart K B 1987 *J. Appl. Phys.* **61** 3721–8
Bader S D and Moog E R 1987 *J. Appl. Phys.* **61** 3729–34
Barnas J 1988 *J. Phys. C: Solid State Phys.* **21** 1021–36
Dobrzynski L, Djafari-Rouhani B and Puszkarski H 1986 *Phys. Rev.* B **33** 3251–6
Edwards D M 1988 *Physica* **149** 199–206
Edwards D M and Muniz R B 1985 *J. Phys. F: Met. Phys.* **15** 2339–56
Eva J 1988 *Final Year Project* The City University (unpublished)
Freeman A J and Fu C L 1987 *J. Appl. Phys.* **61** 3356–61
Grünberg P 1985 *J. Appl. Phys.* **57** 3673–7
Harris A B and Kirkpatrick S 1977 *Phys. Rev.* B **16** 542–76
Haydock R 1982 *Solid State Phys.* **35** 215–94 (New York: Academic)
Hinchey L L and Mills D L 1986 *Phys. Rev.* B **33** 3329–43
Kalkstein D and Soven P 1971 *Surf. Sci.* **26** 85–99
Kittel C 1971 *Introduction to Solid State Physics* (New York: Wiley)
Korecki J and Gradmann U 1985 *Phys. Rev. Lett.* **55** 2491–4
—— 1986 *Hyperfine Interact.* **28** 931–4
Lopez Sancho M P, Lopez Sancho J M and Rubio J 1985 *J. Phys. F: Met. Phys.* **15** 851–8
Masri P and Dobrzynski L 1988 *Surf. Sci.* **198** 285–99
Mathon J 1983 *Phys. Rev.* B **27** 1916–8
—— 1988a *Rep. Prog. Phys.* **51** 1–56
—— 1988b *Physica* B **149** 31–36
Mathon J and Ahmad S B 1988 *Phys. Rev.* B **37** 660–3
Mauri D, Scholl D, Siegmann H C and Kay E 1988 *Phys. Rev. Lett.* **61** 758–61
Pierce D T, Celotta R J, Unguris J and Siegmann H C 1982 *Phys. Rev.* B **26** 2566–74
Siegmann H C and Bagus P S 1988 *Phys. Rev.* B **38** submitted
van Stapele R P, Greidanus F J A M and Smits J W 1985 *J. Appl. Phys.* **57** 1282–90
Walker J C, Droste R, Stern G and Tyson J 1984 *J. Appl. Phys.* **55** 2500–2
White R M 1985 *Science* **229** 11