ENERGY RENORMALISATION AND DAMPING OF SURFACE SPIN WAVES IN HEISENBERG FERROMAGNETS

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Résumé - En utilisant la théorie de fonctions de Green, nous étudions l'effet d'une surface sur les interactions magnon-magnon dans un corps ferromagnétique de Heisenberg. On en déduit l'énergie renormalisée et l'amortissement d'ondes de spin de surface.

Abstract - A Green function theory is employed to study the effect of a surface on magnon-magnon interactions in a Heisenberg ferromagnet. Results are deduced for the renormalised energy and damping of the surface spin waves.

It is well known that under certain conditions localised surface spin waves are predicted to exist in Heisenberg ferromagnets. The properties of these modes, and their influence on thermodynamic behaviour, spin wave resonance, light scattering, etc., have been summarised in various review articles, e.g. /1-3/. Since spin waves are not exact eigenstates of the Heisenberg Hamiltonian, interaction effects will occur resulting in an energy renormalisation and damping of the modes. In infinite ferromagnets the treatment of interactions between bulk spin waves has been put on a rigorous basis by Dyson /4/. However, the presence of a surface will give rise to much richer and more complicated schemes of spin wave interactions, since scattering processes may take place involving surface spin waves as well as bulk spin waves (which in any case have modified properties close to the surface).

In this paper we employ a Green function formalism to study spin wave interactions in semi-infinite Heisenberg ferromagnets at low temperatures $T \ll T_c$. Specifically we deduce expressions for the energy renormalisation and damping of surface spin waves due to their interactions either with bulk spin waves or with surface spin waves. Previous related work has, for example, included a calculation of the surface spin wave damping in a simple cubic Heisenberg ferromagnet with a (001) surface for the special case of nearest-neighbour exchange and zero surface anisotropy /5/. In the present analysis we consider the energy renormalisation as well as the damping, and we examine effects of next-nearest-neighbour exchange, modified exchange near the surface, surface anisotropy and applied magnetic field. Only a brief outline is given here; details will be published elsewhere.

We consider a semi-infinite ferromagnet occupying the half-space $z \leqslant 0$ and described by the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J(i,j)\underline{S}_i\cdot\underline{S}_j - g\mu_B\sum_i\left[H+D(i)\right]S_i^z \qquad (1)$$

where $\underline{S}_i$ is a spin operator, $J(i,j)$ is an exchange interaction, and the summations are over all magnetic sites. The quantities H and $D(i)$ denote respectively an applied magnetic field and a surface anisotropy field perpendicular to the surface; we assume $D(i)$ to be zero except in the surface layer ($z = 0$) where it has the value D. We consider here a simple cubic lattice with (001) crystallographic orientation of the surface; more generally we have also derived results for b.c.c. and f.c.c. ferromagnets and for (011) surfaces. For the exchange terms we restrict attention

to two simple models:
Model 1: Exchange $J(i,j)$ couples nearest neighbours only, having the value J_S if both spins are in the surface layer and the bulk value J_1 otherwise.
Model 2: All exchange interactions are the same as in the bulk specimen, with $J(i,j)$ equal to J_1 between nearest neighbours, J_2 between next-nearest neighbours and zero otherwise.

Using the Holstein-Primakoff representation the Hamiltonian (1) may be transformed to boson operators, keeping terms up to fourth order. As is well known this type of approach can lead to inconsistencies for small values of the spin S, but these difficulties are avoided if 1/S is formally treated as a small parameter and calculations are carried out consistently to each power in 1/S (see /6/). The linear spin wave part of the Hamiltonian can then be diagonalised by a further transformation to normal mode operators, and $\mathcal{H}$ takes the form

$$\mathcal{H} = \sum_{\underline{q},\mu} E(\underline{q}\mu)\, a^+(\underline{q}\mu)\, a(\underline{q}\mu) + \mathcal{H}_{int} \tag{2}$$

Here $\underline{q} = (q_x, q_y)$ is a wavevector parallel to the surface, and μ labels the normal modes of the semi-infinite system which consist of a quasi-continuum of bulk spin waves with wavevectors $\underline{Q} = (\underline{q}, q_z)$ and a discrete surface spin wave branch characterised by wavevector $\underline{q}$. As expected, the eigenvalues $E(\underline{q}\mu)$ have the usual form (e.g. see /1/) for the energies $E_B(\underline{Q})$ and $E_S(\underline{q})$ of bulk and surface spin waves respectively in a linear approximation. The surface mode dispersion relation is

$$E_S(\underline{q}) = g\mu_B H + S\left[u(0) - u(\underline{q})\right] + 2Sv(0) + Sv(\underline{q})\left[\Delta(\underline{q}) + \Delta^{-1}(\underline{q})\right] \tag{3}$$

with

$$\begin{array}{lll} u(\underline{q}) = 4J_1\gamma(\underline{q}) & v(\underline{q}) = J_1 & \text{(Model 1)} \\ u(\underline{q}) = 4J_1\gamma(\underline{q}) + 4J_2\cos(q_x a)\cos(q_y a) & v(\underline{q}) = J_1 + 4J_2\gamma(\underline{q}) & \text{(Model 2)} \end{array} \tag{4}$$

$$\Delta(\underline{q}) = \begin{cases} d - \left[1 + 4(1 - J_S/J_1)(1 - \gamma(\underline{q}))\right] & \text{(Model 1)} \\ (d-1)(J_1 + 4J_2)/(J_1 + 4J_2\gamma(\underline{q})) & \text{(Model 2)} \end{cases} \tag{5}$$

where $\gamma(\underline{q}) = \left[\cos(q_x a) + \cos(q_y a)\right]/2$, $d = g\mu_B D/Sv(0)$, and a is the lattice constant. The existence conditions for surface spin waves are $\Delta(\underline{q}) < -1$ for an acoustic mode and $\Delta(\underline{q}) > 1$ for an optic mode respectively, and these restrict the values of the parameters.

The term $\mathcal{H}_{int}$ in (2), which describes the leading effect of magnon-magnon interactions in the semi-infinite ferromagnet, is quartic in the operators $a^+(\underline{q}\mu)$ and $a(\underline{q}\mu)$. Here we discuss the resulting energy renormalisation and damping of the surface spin waves. The calculations can be conveniently performed by evaluating Green functions $\langle\langle a(\underline{q}\mu); a^+(\underline{q}'\mu')\rangle\rangle$ within a diagrammatic perturbation expansion in $\mathcal{H}_{int}$, and then analysing the complex energy poles of these Green functions.

I - ENERGY RENORMALISATION

To first order of perturbation there is a shift ΔE in the spin wave energies. For the surface modes we write $\Delta E_S = \Delta E_{SS} + \Delta E_{SB}$, where ΔE_{SS} and ΔE_{SB} are the contributions due to interactions with surface modes and bulk modes respectively. We find

$$\begin{aligned} \Delta E_{SS}(\underline{q}) &= \frac{1}{N_\perp} \sum_{\underline{k}} W_{SS}(\underline{q},\underline{k})\, n\left[E_S(\underline{k})\right] \\ \Delta E_{SB}(\underline{q}) &= \frac{1}{N_\perp N_\parallel} \sum_{\underline{K}} W_{SB}(\underline{q},\underline{K})\, n\left[E_B(\underline{K})\right] \end{aligned} \tag{6}$$

where $\underline{k}$ is a two-dimensional wavevector parallel to the surface, $\underline{K} = (\underline{k}, k_z)$ is a three-dimensional wavevector, and $n(E) = 1/\left[\exp(E/k_B T) - 1\right]$. $N_\parallel$ and $N_\perp$ denote respectively the number of atomic layers parallel to the surface and the number of magnetic sites in each layer (both numbers macroscopically large). The interaction vertices W_{SS} and W_{SB} in the case of Model 1 are

$$W_{SS}(\underline{q},\underline{k}) = -J_1\{[\Delta^2(\underline{q})-1][\Delta^2(\underline{k})-1]/[\Delta^2(\underline{q})\Delta^2(\underline{k})-1]\}$$
$$\times\{\alpha(\underline{q},\underline{k})[1-\sigma(1-\Delta^{-2}(\underline{q})\Delta^{-2}(\underline{k}))]+[1+\Delta^{-1}(\underline{q})][1+\Delta^{-1}(\underline{k})][\Delta^{-1}(\underline{q})+\Delta^{-1}(\underline{k})]\} \tag{7}$$

$$\begin{aligned} W_{SB}(\underline{q},\underline{K}) = -J_1\{ & \alpha(\underline{q},\underline{k})[1-2\sigma(1-\Delta^{-2}(\underline{q}))\sin^2(\theta/2)] \\ & + 2[1+\Delta^{-1}(\underline{q})]^2\sin^2(k_z/2) + [\![[1-\Delta^{-2}(\underline{q})]/[1-2\Delta^{-2}(\underline{q})\cos(2k_z)+\Delta^{-4}(\underline{q})]]\!] \\ & \times [\![[\alpha(\underline{q},\underline{k})+\Delta^{-1}(\underline{q})(1+\Delta^{-1}(\underline{q}))][\Delta^{-2}(\underline{q})\cos(\theta-2k_z)-\cos\theta] \\ & + [1+\Delta^{-1}(\underline{q})]^2[\cos(\theta+k_z)-\Delta^{-2}(\underline{q})\cos(\theta-k_z)]+[1+\Delta^{-1}(\underline{q})][\Delta^{-2}(\underline{q})\cos\theta-\cos(\theta+2k_z)]]\!]\} \end{aligned} \tag{8}$$

where $\sigma = (1-J_S/J_1)$ and $\alpha(\underline{q},\underline{k}) = 4[1+\gamma(\underline{q}-\underline{k})-\gamma(\underline{q})-\gamma(\underline{k})]$. The phase angle θ depends on the reflection properties at the surface of a bulk spin wave with wavevector $\underline{K}$ and is defined by

$$\exp(i\theta) = [\Delta(\underline{k})+\exp(ik_za)]/[\Delta(\underline{k})+\exp(-ik_za)] \tag{9}$$

The quantities W_{SS} and W_{SB} play an analogous role to the Dyson interaction vertex /4/ in the renormalisation of bulk spin waves in an infinite ferromagnet. However, they are very much more complicated due to the lowering of symmetry produced by the surface; they incorporate the statistical weighting of the various modes near the surface.

Because of the Bose factors the summations in (6) are dominated by the behaviour at small $\underline{k}$ and $\underline{K}$, where W_{SS} and W_{SB} simplify. If the wavevector summations are replaced by integrals, they can be evaluated analytically in various limiting cases. The replacement is straightforward for the components of $\underline{k}$ since there is translational invariance parallel to the surface, whilst the correct procedure for replacing the summation over k_z by an integration has been given by Mills /7/. As an example we discuss some results for long wavelenths ($a^2q^2 << 1$) and for zero surface anisotropy ($d = 0$). If $0 < \sigma < 1$ there is a surface branch in the unrenormalised spin wave spectrum occurring just below the continuum of bulk modes. The lower edge of the continuum has energy $E_B(\underline{q},0) \approx g\mu_BH+Sv(0)a^2q^2+O(q^4)$ and the surface mode with energy $E_S(\underline{q})$ is split off below this by an amount $\approx\sigma^2a^4q^4$. In general this close proximity can produce a subtle interplay between effects due to the surface modes and those due to surface perturbation of the bulk modes, e.g. as found in calculations of surface thermodynamic properties /7,8/. On defining $\tau = k_BT/Sv(0)$ and $h = g\mu_BH/Sv(0)$, we obtain the following leading order contributions, assuming $a^2q^2 << \tau << 1$:

$$\Delta E_{SS}(\underline{q}) \approx -(J_1/8\pi)(1-8\sigma^2)\sigma a^4q^4\tau^2F(2,h/\tau) \tag{10}$$

$$\Delta E_{SB}(\underline{q}) \approx -(J_1/32\pi^{3/2})a^2q^2\tau^{5/2}F(5/2,h/\tau)+O(\sigma^2q^4\tau^{3/2}) \tag{11}$$

Here $F(n,h/\tau)$ is the Bose-Einstein integral function (e.g. see /6/), which simplifies to the Riemann zeta function $\zeta(n)$ if $h = 0$. The dominant contribution to ΔE_S in this case is provided by the first term in (11) and comes from interactions with bulk spin waves. It is interesting to note that this leading order contribution to ΔE_S has the same form as the energy correction for a bulk spin wave with small wavevector $(\underline{q},0)$ in an infinite ferromagnet /4,6/. This result seems reasonable in view of the earlier comments concerning the proximity of the surface branch to the lower edge of the bulk continuum. Moreover the condition $a^2q^2 << \tau$ assumed in deriving (10) and (11) implies that the penetration depth ($\sim 1/\sigma aq^2$) of the surface mode is relatively large, e.g. it is larger than the thickness ($\sim a/\tau^{\frac{1}{2}}$) over which the magnetisation is appreciably perturbed by the surface /8/. The results for larger q will be discussed elsewhere.

A different behaviour for ΔE_S is predicted if there is a surface anisotropy field ($d \neq 0$). We take the case of $d < 0$ and $0 < \sigma < 1$, which ensures the existence of an acoustic surface spin wave (provided the applied field is not too small). For anisotropy fields satisfying $\tau << d^2 << 1$ and $a^2q^2 << d^2$ we find that the dominant contribution to $\Delta E_S(\underline{q})$ is approximately proportional to $d^3\tau F(1,E_S(0)/k_BT)$. It comes mainly from interactions with surface spin waves (i.e. from ΔE_{SS}), unlike the previous example with $d = 0$. This difference can be understood as arising partly due to an approximate node in the bulk spin wave amplitudes at the surface in the present case, and partly due to a relative enhancement in the number of thermally excited surface spin waves (since $E_B(0)-E_S(0) \gtrsim d^2Sv(0)$ for $d^2 << 1$).

We have also carried out calculations to include the effect of next-nearest-neighbour exchange interactions according to Model 2. When $d = 0$ we find that many of the results can be expressed in the same form as for Model 1 but with redefined coefficients. For example, if $a^2q^2 << \tau << 1$ with $J_1 > 0$ and $J_2 > 0$ the same q and τ dependences are predicted as in (10) and (11) but the overall coefficients involve J_2 as well as J_1. The differences between the two models are more significant for $d \neq 0$.

II - DAMPING

Contributions to the damping are obtained on renormalising the spin waves to second order of perturbation. The mechanism is the usual low-temperature scattering process involving four spin waves, except that these may now be bulk modes or surface modes. Hence the damping $\Gamma_S(\underline{q})$ of a surface spin wave will be the sum of four contributions denoted by $\Gamma_S(\underline{q};4S)$, $\Gamma_S(\underline{q};3S,1B)$, $\Gamma_S(\underline{q};2S,2B)$ and $\Gamma_S(\underline{q};1S,3B)$, according to how many surface (S) and bulk (B) modes are involved. We have obtained expressions for all four terms, but for simplicity we discuss here just the contribution $\Gamma_S(\underline{q};4S)$ which is given by

$$\Gamma_S(\underline{q};4S) = \frac{\pi}{8N_\perp^2}\sum_{\underline{k},\underline{p}}\Phi_{4S}(\underline{q},\underline{k},\underline{p})\,\delta\left[E_S(\underline{q})+E_S(\underline{k})-E_S(\underline{p})-E_S(\underline{q}+\underline{k}-\underline{p})\right]$$

$$\times\ \{n\left[E_S(\underline{k})\right](1+n\left[E_S(\underline{p})\right]+n\left[E_S(\underline{q}+\underline{k}-\underline{p})\right])-n\left[E_S(\underline{p})\right]n\left[E_S(\underline{q}+\underline{k}-\underline{p})\right]\} \tag{12}$$

where in the case of model 1 we have

$$\Phi_{4S}(\underline{q},\underline{k},\underline{p}) = J_1^2\ \frac{\left[1-\Delta^{-2}(\underline{q})\right]\left[1-\Delta^{-2}(\underline{p})\right]\left[1-\Delta^{-2}(\underline{q}+\underline{k}-\underline{p})\right]\left[1-\Delta^{-2}(\underline{k})\right]}{\left[1-\Delta^{-1}(\underline{q})\Delta^{-1}(\underline{p})\Delta^{-1}(\underline{q}+\underline{k}-\underline{p})\Delta^{-1}(\underline{k})\right]^2}$$

$$\times\ \{4\left[1-\sigma(1-\Delta^{-1}(\underline{q})\Delta^{-1}(\underline{p})\Delta^{-1}(\underline{q}+\underline{k}-\underline{p})\Delta^{-1}(\underline{k}))\right]\left[2\gamma(\underline{p}-\underline{q})+2\gamma(\underline{k}-\underline{p})-\gamma(\underline{q})-\gamma(\underline{p})-\gamma(\underline{k})\right.$$

$$\left.-\gamma(\underline{q}+\underline{k}-\underline{p})\right] + \left[\Delta^{-1}(\underline{q})+\Delta^{-1}(\underline{k})\right]\left[1+2\Delta^{-1}(\underline{p})+2\Delta^{-1}(\underline{q}+\underline{k}-\underline{p})+\Delta^{-1}(\underline{p})\Delta^{-1}(\underline{q}+\underline{k}-\underline{p})\right]$$

$$+\ \left[\Delta^{-1}(\underline{p})+\Delta^{-1}(\underline{q}+\underline{k}-\underline{p})\right]\left[1+\Delta^{-1}(\underline{q})\Delta^{-1}(\underline{k})\right]\}^2 \tag{13}$$

The summations are dominated by the behaviour at small wavevectors, and they may be performed analytically for certain cases. For example, in the absence of surface anisotropy ($d = 0$) and for $\tau << a^2q^2 << 1$ we eventually obtain

$$\Gamma_S(\underline{q};4S) \gtrsim \left[v(0)/32\pi S\right]\sigma^2a^4q^4\tau^3F(3,h/\tau) \tag{14}$$

This agrees with the result obtained previously by Tarasenko and Kharitonov /5/ in the limits of $h << \tau$ and $h >> \tau$. We find the same formal expression holds for

Model 2 provided σ is redefined as $J_2/(J_1+4J_2)$, $(0 < \sigma < 1)$. Our theory also applies when $d \neq 0$. For example, if $d < 0$ such that $\tau \ll d^2 \ll 1$ and $a^2q^2 \ll d^2$ we estimate that $\Gamma_S(\underline{q};4S)$ is proportional to $d^6\tau F(1,E_S(0)/k_BT)$ for Models 1 and 2 provided $k_BT \ll E_S(\underline{q})$.

The other contributions $\Gamma_S(\underline{q};3S,1B)$, $\Gamma_S(\underline{q};2S,2B)$ and $\Gamma_S(\underline{q};1S,3B)$ to the surface spin wave damping are given by much more complicated expressions than (12) and (13), and in general they require numerical evaluation. However, if the surface anisotropy field is sufficiently large ($d^2 \gg \tau$ and $d^2 \gg a^2q^2$) it may be shown that $\Gamma_S(\underline{q};3S,1B)$ and $\Gamma_S(\underline{q};1S,3B)$ are negligibly small. This is essentially because in these processes energy can be conserved only at large wavevectors, and the combination of Bose factors in the summand is then very small.

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