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Spin waves at an interface between ferromagnetic and antiferromagnetic materials

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Abstract. The interface spin waves at the (001) interface between a ferromagnet and an antiferromagnet, both with body-centred crystal structures, were investigated in the context of the Heisenberg model. The transfer matrix technique was employed to derive the Green functions at the interface layers. Interface spin waves which are localized in the neighbourhood of the interface were found to exist. The spectrum of these bound states was calculated for a number of different sets of parameters. The possible extensions of the present work were discussed.

1. Introduction

The investigation of magnetic excitations or spin waves at the interface between magnetic materials has received extensive attentions [1–15] in the past decade. Interface spin waves (ISW) were found in many different configurations and compositions of materials. Camley and Maradudin [1] have considered the ISW at an interface between two ferromagnetic materials in the dipole–dipole interaction dominant regime, i.e. the magnetostatic waves. Interesting properties, such as the non-reciprocality of the propagation of ISW, etc were found. In another work, Yaniv [4] investigated the ISW of an exchange-coupled biferromagnetic interface and predicted that either 0, 1 or 2 branches of ISW may exist for an (100) interface formed by two simple cubic crystals with the same lattice constant. An extension to the same kind of study by Xu *et al* [5] and Wang and Lin [6] revealed that the ISW are sensitively dependent on the geometric structures of the two materials forming the interface. In addition to these studies performed on the interface between two ferromagnetic materials, Mata and Pestana [7] have examined the magnetic properties of an interface between two antiferromagnets. Most recently, Che *et al* [8] studied the ISW in a bilayer of two sublattice ferrimagnets and found that two branches of ISW may exist.

The investigation of ISW on other kinds of compositions has also been carried out in the past few years. Hinchey and Mills [9] have considered a multi-interface magnon state in a hypothetical ferromagnetic/antiferromagnetic superlattice. Novel properties, such as spin reconstructions, etc were found.

In this paper, we concentrate on the ISW at an interface between materials with different spin structures, i.e. the interface formed by a ferromagnet and an antiferromagnet. To our knowledge, there is no investigation on such a problem in the current literature. The couplings between spins in the two materials and across the interface are taken to be of exchange type. The study of dipole–dipole dominated spin waves in such a structure can be carried out easily following the procedures in [1]. We will use the transfer matrix technique [12–14] to study the energy spectrum of ISW. We can see from the formalism below that in comparison with other Green function methods [8], transfer matrix techniques are more powerful and more clear in physical meaning in dealing with layered structures. Specifically, we will assume that the crystal structures of the two materials are body-centred tetragonal lattices with the same lattice constant and we will consider the (001) surface between them.

2. Formalism and results

We now consider the interface between two semi-infinite Heisenberg magnets, one is ferromagnetic and the other is antiferromagnetic. The system is schematically shown in figure 1. The structure of the antiferromagnet can be divided into two sublattices which are themselves simply cubic. The (001) surface of the body-centred tetragonal antiferromagnet has spins from only one of the sublattices. We denote the atomic layers by integers $n = 0, \pm 1, \pm 2, \ldots$, with the interfaces being $n = 0$ and $n = 1$, respectively.

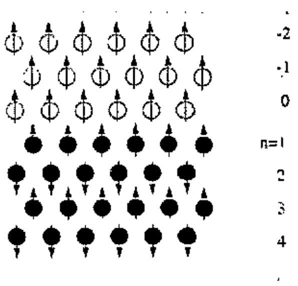

Figure 1. Schematic diagram of the system considered in this paper. The open circles are the spins of the ferromagnetic material. The black and shaded circles are the spins of the up and down sublattices of the antiferromagnet, respectively. The interfaces are denoted by $n = 1$ and $n = 0$. The coupling constant across the interface is assumed to be ferromagnetic, thus the spins are lined up across the interface.

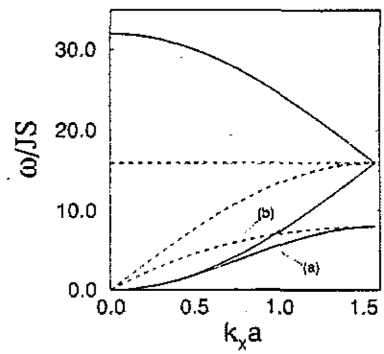

Figure 2. The surface states spectra of the (001) surfaces of a ferromagnet and an antiferromagnet. We have taken $J_1 = J_2 = J$, $S_1 = S_2 = S$ and $k = (k_x, 0)$. The area between the solid curves is the bulk states region for the ferromagnet, that between the dashed curves is the bulk states region for the antiferromagnet. Curves (a) and (b) are the spectra of the surface states of the ferromagnet and antiferromagnet, respectively.

In each material, the interaction between the spins is taken to be of Heisenberg type. The Hamiltonian can be expressed as

$$H = \sum_{(ij)} J_{ij} S_i \cdot S_j \tag{1}$$

where $\langle ij \rangle$ means that only the nearest-neighbour interaction between spins is considered. J_{ij} is the exchange integral between spins at sites i and j, and in this paper it takes the form

$$J_{ij} = \begin{cases} J_1 > 0, & \text{for antiferromagnetic material} \\ J_2 < 0, & \text{for ferromagnetic material} \\ J_I < 0, & \text{for ferromagnetic interface coupling} \\ J_I > 0, & \text{for antiferromagnetic interface coupling.} \end{cases} \qquad (2)$$

Here we only consider the case where the exchange integral across the interface is different from the bulk, though more complicated situations may be easily included in the present work. The spins in the two materials are represented by S_1 and S_2, respectively. For simplicity, we assume the interface coupling constant to be ferromagnetic. The situation for antiferromagnetic coupling can be extended straightforwardly.

Following the usual procedures [11], we define the following relevant double-time Green functions:

$$\begin{aligned} G^{aa}(t,t') &= \langle\langle S_a^{\dagger}(t); S_{a'}^{-}(t')\rangle\rangle \\ G^{ba}(t,t') &= \langle\langle S_b^{\dagger}(t); S_{a'}^{-}(t')\rangle\rangle \\ G^{cc}(t,t') &= \langle\langle S_c^{\dagger}(t); S_{c'}^{-}(t')\rangle\rangle \\ G^{ca}(t,t') &= \langle\langle S_c^{\dagger}(t); S_{a'}^{-}(t')\rangle\rangle \end{aligned} \qquad (3)$$

where the superscripts a and b refer to the up and down sublattices of the antiferromagnetic material respectively, and c is the index for the ferromagnetic material.

After carrying out the Fourier transformation for the Green functions in time and space coordinates, we can write down the equations of motion for the Green functions in k–ω space:

$$(\omega - U_1 + 8J_I S_2) g_{11}^{aa} - U_1 \gamma(k) g_{21}^{ba} + 8J_I S_1 \gamma(k) g_{01}^{ca} = 2S_1 \qquad (4)$$

$$(\omega + U_2 + 8J_I S_1) g_{01}^{ca} - U_2 \gamma(k) g_{-11}^{ca} - 8J_I S_2 \gamma(k) g_{11}^{aa} = 0 \qquad (5)$$

$$(\omega + 2U_1) g_{2m,n}^{ba} + U_1 \gamma(k) g_{2m-1,n}^{aa} + U_1 \gamma(k) g_{2m+1,n}^{aa} = 0 \quad (m \geqslant 1) \qquad (6)$$

$$(\omega - 2U_1) g_{2m+1,n}^{aa} - U_1 \gamma(k) g_{2m,n}^{ba} - U_1 \gamma(k) g_{2m+2,n}^{ba} = 0 \; (m \geqslant 1, n \neq 2m+1) \qquad (7)$$

$$(\omega + 2U_2) g_{m,n}^{cc} - U_2 \gamma(k) g_{m-1,n}^{cc} - U_2 \gamma(k) g_{m+1,n}^{cc} = 0 \quad (m \leqslant -1, n \neq m) \qquad (8)$$

$$(\omega + U_2 + 8J_I S_1) g_{00}^{cc} - U_2 \gamma(k) g_{-10}^{cc} - 8J_I S_2 \gamma(k) g_{10}^{ac} = 2S_2 \qquad (9)$$

where $\gamma(k) = \cos(\frac{1}{2}k_x a)\cos(\frac{1}{2}k_y a)$, k is a two-dimensional vector parallel to the interface and a is the lattice distance. $U_i = 8J_i S_i$, i=1 or 2. $g_{m,n}^{ij}$ is the corresponding component of the Fourier transformations of the Green function defined by equation (3). These equations can be solved by introducing the following transfer functions [12–14] between different atomic layers:

$$\alpha_1(\omega) = g_{2m+1,n}^{aa} / g_{2m,n}^{ba} \qquad \alpha_2(\omega) = g_{2m,n}^{ba} / g_{2m-1,n}^{aa} \qquad (m \geqslant 1) \qquad (10)$$

$$\beta(\omega) = g_{m,n}^{cc} / g_{m-1,n}^{cc} \qquad (m \leqslant -1) \qquad (11)$$

where $\alpha_1(\omega)$ and $\alpha_2(\omega)$ represent the propagation of spin waves between the two sublattice layers of the antiferromagnetic material and $\beta(\omega)$ represents the propagation within the ferromagnetic material.

Making use of equations (6), (7) and (8), we can show that these transfer functions satisfy the following equations

$$(\omega - 2U_1)\alpha_1(\omega) = U_1\gamma(k) + U_1\gamma(k)\alpha_1(\omega)\alpha_2(\omega) \tag{12}$$

$$(\omega + 2U_1)\alpha_2(\omega) = -U_1\gamma(k) - U_1\gamma(k)\alpha_1(\omega)\alpha_2(\omega) \tag{13}$$

$$(\omega + 2U_2)\beta(\omega) = U_2\gamma(k) + U_2\gamma(k)\beta(\omega)^2 \tag{14}$$

which can be solved directly, i.e.

$$\alpha_1(\omega) = -[(\omega + 2U_1)/(\omega - 2U_1)]\alpha_2(\omega) \tag{15}$$

$$\alpha_2(\omega) = \frac{\omega^2 - 4U_1^2 \pm \{(\omega^2 - 4U_1^2)(\omega^2 - 4U_1^2[1 - \gamma(k)^2)]\}^{1/2}}{2U_1\gamma(k)(\omega + 2U_1)} \tag{16}$$

$$\beta(\omega) = \{2|U_2| - \omega \pm [(\omega - 2|U_2|)^2 - 4U_2^2\gamma(k)^2]^{1/2}\}/(2|U|_2\gamma(k)). \tag{17}$$

The energy band of the bulk spin waves can be obtained when the square root expressions in the transfer functions are negative. Thus from $\alpha_1(\omega)$ or $\alpha_2(\omega)$ we can reproduce the band edges of the antiferromagnet, i.e.

$$2U_1(1 - \gamma(k)^2)^{1/2} \leqslant \omega \leqslant 2U_1 \tag{18}$$

and from $\beta(\omega)$ we know the energy band for a bulk ferromagnet

$$2|U|_2(1 - |\gamma(k)|) \leqslant \omega \leqslant 2|U|_2(1 + |\gamma(k)|). \tag{19}$$

These expressions are exactly the same as those given in the standard textbook [15].

In order to study the ISW, we must know the diagonal Green function at the interface. From equations (4) and (5), we obtain

$$g_{11}^{aa} = 2S_1/(\omega - U_1 + 8J_I S_2 - U_1\gamma(k)\alpha_2(\omega) + 8J_I S_1\gamma(k)T(\omega)) \tag{20}$$

where $T(\omega)$ describes the propagation of spin waves across the interface and $g_{01}^{ca} = T(\omega)g_{11}^{aa}$. Explicitly, $T(\omega)$ can be expressed in terms of J_I and $\beta(\omega)$, i.e.

$$T(\omega) = 8J_I S_2\gamma(k)/(\omega - |U_2| + 8J_I S_1 + |U_2|\gamma(k)\beta(\omega)) \tag{21}$$

where we have used $g_{-11}^{ca} = \beta(\omega)g_{01}^{ca}$, which can be easily derived from equation (8) by setting $m = -1$ and using the definition of $\beta(\omega)$.

Before we start to discuss the ISW, let us look at an intermediate problem: the spin waves when the interface system is decoupled, i.e. the surface system of a antiferromagnet and a ferromagnet. The Green functions in this case may be easily obtained by letting $J_I = 0$ in the above equations. Without any difficulty, we get

$$g_{11}^{aa} = 2S_1/(\omega - U_1 - U_1\gamma(k)\alpha_2(\omega)) \tag{22}$$

$$g_{00}^{cc} = 2S_2/(\omega - |U_2| + |U_2|\gamma(k)\beta(\omega)). \tag{23}$$

In terms of these diagonal elements, the density of states (DOS) of the spin waves for the two surfaces can be written as

$$D^{ii}(\omega) = -\frac{1}{N\pi}\sum_k \operatorname{Im} g^{ii}(\omega) \tag{24}$$

where N is the number of spins in an atomic plane.

In real calculations, there is always the problem of choosing the correct sign in the expressions for the transfer functions. In order to be meaningful, we have chosen the branch for the square roots such that $D^{ii}(\omega) \geqslant 0$ and have found that this is equivalent to the criteria that $|\alpha_1(\omega)\alpha_2(\omega)|^2 \leqslant 1$ and $|\beta(\omega)|^2 \leqslant 1$, which guarantees the convergence of the Green function in each layer.

From equations (22) and (23), we know that the bulk spin wave has energy when the $\alpha(\omega)$s and $\beta(\omega)$ have imaginary values, while the surface spin waves occur when the denominator in $g(\omega)$s are zeroes. It can be shown that both the surface systems have surface states which are localized in the surface region and have energy below the corresponding bulk spectrum. We show in figure 2 the surface spin wave spectra [16] together with the bulk ones.

When the two semi-infinite systems are brought together, the ISW are determined by equation (20). It is easy to see that the energy region of the ISW is a combination of the bulk modes of the two semi-infinite materials, which occurs when the transfer functions $\alpha(\omega)$s or $\beta(\omega)$ have imaginary parts. The states in this energy region may propagate throughout the whole crystal if their energy falls into the region where the energy of the two bulk systems overlaps. However, if the energy lies in the bulk energy region of one material but outside that of the other, then the ISW can only propagate without decaying in the former material but is damped exponentially when in the latter, and vice versa.

Besides the ISW mentioned above, there are interface states which are mainly localized in the interface region and decay when propagating into the internal parts of the two materials. It can be shown that these bound states have energy which lies outside both the bulk spectra region of the two materials and their energy is determined by the poles of the Green function, i.e.

$$\omega - U_1 + 8J_I S_2 - U_1\gamma(k)\alpha_2(\omega) + 8J_I S_1\gamma(k)T(\omega) = 0. \qquad (25)$$

Generally, it is hard to determine an analytic solution for this equation. We have studied it numerically and have found that if $|J_I|$ is sufficiently small, the ISW approaches the surface states of the decoupled system. But when $|J_I|$ gets bigger, there exists one interface state which is above the bulk modes of the two materials. The increase of the coupling constant raises the energy of interface modes. The results are schematically shown in figures 3 and 4.

The diagonal Green functions on the other layers in the neighbourhood of the interface can also be obtained in the same way illustrated above. To do this, the equations of motion for the new diagonal Green functions must be solved. The results involve new transfer functions which describe the propagation of spin waves from the interface to the interior of the two materials. When the ISW occurs, the modes of these transfer functions are less than one, demonstrating a characteristic decay for the ISW [17].

In conclusion, the interface structure between ferromagnetic and antiferromagnetic materials usually supports only one branch of interface spin waves when the interface coupling is strong. This spin wave branch is of optical characteristic, meaning that the spin fluctuations are suppressed at the surfaces of the two materials due to the introduction of the interface. In the case of small interface coupling, two branches of interface spin waves appear, which stem from those of the individual surface systems of the two materials.

A simple extension of the present work is to include the differences between the coupling constants near the interface and the bulk ones. We may extend the present work to the study of ISW at an interface formed by materials with different crystal structures as well as different spin structures, e.g. the interface between a two-sublattice ferrimagnet and a ferromagnet or a system in which the (001) surface

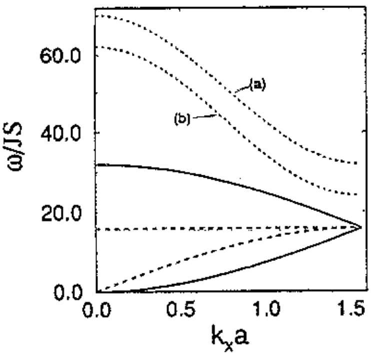

Figure 3. The spectrum of the ISW with $J_1 = J_2 = J$, $S_1 = S_2 = S$ and $\boldsymbol{k} = (k_x, 0)$. Curve (a) was obtained when the interface coupling $|J_I| = 3J$ and curve (b) when $|J_I| = 2J$. Notice that the increase in the strength of the coupling constant results in higher energy interface states. The bulk spectra of the two materials are also presented for comparison, see figure 2.

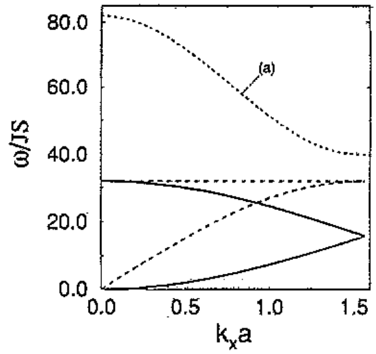

Figure 4. The spectrum of the ISW, curve (a), with parameters $J_1 = J_2 = J$, $S_1 = 2S_2 = 2S$ and $|J_I| = 2J$. As in figure 3, the bulk spin wave spectra are also displayed.

of the antiferromagnet considered in this paper matches with the (100) surface of a ferromagnet with simple cubic structure, etc. The effect of anisotropies can be taken into account by setting the interplane coupling constant to be different from the intraplane ones in the current framework. The inclusion of an external applied magnetic field and the effect of pinning on the interface layers is the subject of our next work [18].

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