

Conditions for the existence of interface spin waves in a biferromagnetic interface

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Abstract. The eigenproblems of interface spin waves of a (100) biferromagnetic interface are solved exactly by use of the interface rescaling approach. Particularly, the necessary and sufficient conditions for the existence of interface spin waves are obtained analytically.

PACS. 75.70.Cn Magnetic properties of interfaces (multilayers, superlattices, heterostructures) – 75.30.Ds Spin waves – 75.10.Jm Quantized spin models

1 Introduction

Many theoretical works concerning the interface spin waves (ISW) in various layered materials with different configurations and compositions have appeared over the past. Yaniv [1] has investigated the ISW of an exchange-coupled biferromagnetic interface and found that there may exist 0, 1 or 2 branches of ISW for a (100) interface formed by two simple-cubic crystals. Ferromagnetic ISW in cubic crystals were also studied by Xu *et al.* [2] and Wang and Lin [3], very interesting results were obtained for different faces of the same crystal or for the same face of different crystals. Mata and Pestana [4] have considered spin waves at the interface between two antiferromagnets and found a variety of possible magnon states. The ISW in a bilayer of two ferromagnetic sublattices were investigated by Che *et al.* [5]. Their results showed that there may exist two branches of ISW. In another work, Hong and Yang [6] discussed the spin waves at the interface between a ferromagnet and an antiferromagnet. In recent years, Puzzkarski and his co-operators [7–16] had studied extensively the conditions for the existence of ISWs in various bilayer systems, which composed of two ferromagnetic sublayers of the same magnetic material, using the method of Brillouin zone (BZ) mapping [17] for the three interface orientations *sc*(110), *fcc*(110), and *bcc*(110). They showed that the emergence of ISWs occurs much more easily on the edges of the BZ than at its center and that antiferromagnetic interface coupling considerably broadens the

regions of interface spin waves existence (towards the BZ center). In addition to these studies performed on the bilayer system, many authors have also investigated the multi-interface magnon states [18–23], and a extensive review can be found in reference [7].

In this paper, we use the interface-rescaling approach (IRA) developed by Puzzkarski [24,25] to study the ISW for the system consisting of two ferromagnets. Recently, this technique has been widely used for a number of systems [7,26–30]. IRA has the major advantage that it allows one to decompose a coupled system into several independent subsystems so as to solve them exactly. We obtain with IRA the exact solutions of ISW in ferromagnetic bilayer systems. Particularly, we also obtain analytically the necessary and sufficient conditions for the existence of ISW in such kind of systems.

2 Formulations

Consider a (100) interface formed between two ferromagnets *A* and *B*, each one of which has a simple-cubic structure and a finite thickness. For the sake of simplicity, we assume the two ferromagnets still have the periodicity in the atomic planes parallel to the interface and the two outer surfaces. In our theoretical study we neglect the anisotropy in the interface, on the surfaces as well as in the volume of the system, so that the only inhomogeneity of the system is assumed to come from the difference between the interface exchange constant J_{AB} and the bulk ones J_A and J_B . The Heisenberg Hamiltonian of the

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system is written as:

$$H = -\frac{1}{2} \sum_{n,m} \sum_{i,j} J(n,i;m,j) \mathbf{S}(n,i) \cdot \mathbf{S}(m,j) \quad (1)$$

where n, m are the indices of the atomic planes, and i, j the sites in the atomic planes n and m , respectively. The interaction constant $J(n,i;m,j)$ is nonzero only when the sites are nearest neighbors and takes the following value:

$$J(n,i;m,j) = \begin{cases} J_A, & \text{for both sites in } A, \\ J_B, & \text{for both sites in } B, \\ J_{AB}, & \text{for one sites in } A \text{ and the other in } B. \end{cases} \quad (2)$$

We also take

$$\begin{aligned} \mathbf{S}(n,i) \cdot \mathbf{S}(n,i) &= S(n)[S(n)+1] \\ &= \begin{cases} S_A(S_A+1), & \text{for sites in } A, \\ S_B(S_B+1), & \text{for sites in } B. \end{cases} \end{aligned} \quad (3)$$

In this paper, we only consider the ferromagnetic case with $J(n,i;m,j) > 0$. The ground state of the present system is all spin parallel. We now discuss the excitation of this system at low temperatures. We first apply to H the well-known Holstein–Primakoff transformation and only take quadratic terms, then we have

$$\begin{aligned} H = H_0 + \frac{1}{2} \sum_{n,m} \sum_{i,j} J(n,i;m,j) \{ & S(m) \mathbf{C}^+(n,i) \cdot \mathbf{C}(n,i) \\ + S(n) \mathbf{C}^+(m,j) \cdot \mathbf{C}(m,j) - \sqrt{S(n)S(m)} [& \mathbf{C}^+(n,i) \cdot \mathbf{C}(m,j) \\ + \mathbf{C}(n,i) \cdot \mathbf{C}^+(m,j)] \}, \end{aligned} \quad (4)$$

where H_0 is a constant. Due to the periodicity in the atomic planes parallel to the interface, we perform the following Fourier transformation:

$$\begin{aligned} b(m, \mathbf{k}) &= \frac{1}{\sqrt{N_{\parallel}}} \sum_{j \in m} \exp(-i\mathbf{k} \cdot \mathbf{j}) \mathbf{C}(m, j), \\ b^+(m, \mathbf{k}) &= \frac{1}{\sqrt{N_{\parallel}}} \sum_{j \in m} \exp(+i\mathbf{k} \cdot \mathbf{j}) \mathbf{C}^+(m, j), \end{aligned} \quad (5)$$

where N_{\parallel} is the number of sites in the m th atomic planes, \mathbf{k} the wave vector parallel to the interface and the operators b and b^+ satisfy the following commutating relations:

$$\begin{aligned} [b(n, \mathbf{k}), b^+(m, \mathbf{k}')] &= \delta_{nm} \delta_{\mathbf{k}\mathbf{k}'}, \\ [b(n, \mathbf{k}), b(m, \mathbf{k}')] &= [b^+(n, \mathbf{k}), b^+(m, \mathbf{k}')] = 0. \end{aligned} \quad (6)$$

We can then obtain from equations (4) and (5) the following expression:

$$\begin{aligned} H = H_0 + \sum_k \sum_n \{ & [J(n, n)S(n) + J(n, n+1)S(n+1) \\ + J(n, n-1)S(n-1)] & b^+(n, \mathbf{k}) \cdot b(n, \mathbf{k}) \\ - J(n, n+1) \sqrt{S(n)S(n+1)} & b^+(n, \mathbf{k}) \cdot b(n+1, \mathbf{k}) \\ - J(n, n-1) \sqrt{S(n)S(n-1)} & b^+(n, \mathbf{k}) \cdot b(n-1, \mathbf{k}) \} \end{aligned} \quad (7)$$

where

$$\begin{aligned} J(n, n) &= 2[2 - \cos k_x - \cos k_y] J(n, i; n, i \pm 1) \\ &\equiv 2\gamma J_n, \\ J(n, n \pm 1) &= J(n, i; n \pm 1, i) = J(n \pm 1, n). \end{aligned} \quad (8)$$

Here we have chosen the three lattice constants as unit lengths and the parameter γ varies from zero to four. In order to diagonalize the Hamiltonian (7), we introduce the following further transformation:

$$\begin{aligned} a(p, \mathbf{k}) &= \sum_n f^*(n, p) b(n, \mathbf{k}), \\ a^+(p, \mathbf{k}) &= \sum_n f(n, p) b^+(n, \mathbf{k}), \end{aligned} \quad (9)$$

where $f(n, p)$ is an orthonormalized wave function to be determined by

$$\begin{aligned} E_{pk} f(n, p) &= [J(n, n)S(n) + J(n, n+1)S(n+1) \\ + J(n, n-1)S(n-1)] & f(n, p) \\ - J(n, n+1) \sqrt{S(n)S(n+1)} & f(n+1, p) \\ - J(n, n-1) \sqrt{S(n)S(n-1)} & f(n-1, p). \end{aligned} \quad (10)$$

With the above transformations, the Hamiltonian (7) is finally diagonalized

$$H = H_0 + \sum_{p, \mathbf{k}} E_{pk} a^+(p, \mathbf{k}) \cdot a(p, \mathbf{k}), \quad (11)$$

where $E_{pk} \geq 0$ is the excitation energy of the spin waves in the system at low temperatures and can be obtained from the eigenvalues of the solutions of equation (10). We shall study it by the IRA [24, 25] as follows.

Let N_A and N_B denote the numbers of atomic planes of the two ferromagnets A and B , respectively. We assume the atomic planes $n = -1, -2, \dots, -N_A$ are occupied by A spins, whereas the atomic planes $n = 0, 1, 2, \dots, N_B - 1$ are occupied by B spins. In this way, the interface is formed between the planes $n = 0$ and $n = -1$ and the interface spins interact *via* the interface coupling J_{AB} . On the other hand, the two surfaces are the planes at $n = -N_A$ and $n = N_B - 1$.

After applying the IRA to equation (10), we have the following two subsets of eigenequations:

$$\begin{aligned} E f_A(-N_A) &= J_A S_A [(2\gamma + 1)f_A(-N_A) - f_A(-N_A + 1)], \\ E f_A(n) &= J_A S_A [(2\gamma + 2)f_A(n) - f_A(n + 1) \\ &\quad - f_A(n - 1)], \quad -N_A + 1 \leq n \leq -2, \\ E f_A(-1) &= J_A S_A [(2\gamma + 2 - \mu_A)f_A(-1) - f_A(-2)] \end{aligned} \quad (12a)$$

and

$$\begin{aligned} E f_B(0) &= J_B S_B [(2\gamma + 2 - \mu_B)f_B(0) - f_B(1)], \\ E f_B(n) &= J_B S_B [(2\gamma + 2)f_B(n) - f_B(n + 1) \\ &\quad - f_B(n - 1)], \quad 1 \leq n \leq N_B - 2, \\ E f_B(N_B - 1) &= J_B S_B [(2\gamma + 1)f_B(N_B - 1) \\ &\quad - f_B(N_B - 2)], \end{aligned} \quad (12b)$$

where we have omitted the indices p , k of E_{pk} and p of $f(n, p)$, and set

$$f(n) = \begin{cases} f_A(n), & \text{for } n \leq -1 \\ f_B(n), & \text{for } n \geq 0. \end{cases} \quad (13)$$

The parameters μ_A and μ_B in equations (12a) and (12b) are given by

$$\begin{aligned} \mu_A &= 1 + \frac{J_{AB} S_B}{J_A S_A} (\alpha^{-1} R^{-1} - 1), \\ \mu_B &= 1 + \frac{J_{AB} S_A}{J_B S_B} (\alpha R - 1), \end{aligned} \quad (14)$$

where

$$\alpha = \sqrt{S_A/S_B}, \quad (15)$$

and R is the interface-rescaling coefficient that is defined as [24, 25]

$$f_A(-1) = R f_B(0). \quad (16)$$

It is obvious that equations (12a) and (12b) are two formally independent subsets and become much easier to be solved exactly. The general solutions of them have the following form:

$$\begin{aligned} f_A(n) &= CD [\exp(-ink_A) - \theta_A \exp(ink_A)], \\ \theta_A &= \exp [i2(N_A + 1)k_A], \quad -N_A \leq n \leq -1, \end{aligned} \quad (17a)$$

and

$$\begin{aligned} f_B(n) &= C [\exp(-ink_B) - \theta_B \exp(ink_B)] \\ \theta_B &= \exp [i2N_B k_B], \quad 0 \leq n \leq N_B - 1, \end{aligned} \quad (17b)$$

where k_A and k_B are the wave vectors of the spin waves in A and B perpendicular to the interface; C is the

normalization coefficient and D a constant with respect to n . Inserting equations (17a) and (17b) into (12a), (12b) and (16), we obtain

$$D = R \exp(ik_A) \times [1 - \exp(i2N_A k_A)] / [1 - \exp(i2N_B k_B)], \quad (18)$$

and

$$\begin{aligned} \mu_A &= \sin [(N_A + 1)k_A] / \sin(N_A k_A), \\ \mu_B &= \sin [(N_B + 1)k_B] / \sin(N_B k_B). \end{aligned} \quad (19)$$

We can also get the excitation energy

$$\begin{aligned} E &= 2J_A S_A [\gamma + 1 - \cos(k_A)] \\ &= 2J_B S_B [\gamma + 1 - \cos(k_B)]. \end{aligned} \quad (20)$$

Here we can see the k_A and k_B are not independent of each other. On the other hand, we can obtain by canceling R from equation (14) the other constrained equation of k_A and k_B .

$$\left[1 + \frac{J_A S_A}{J_{AB} S_B} (\mu_A - 1) \right] \left[1 + \frac{J_B S_B}{J_{AB} S_A} (\mu_B - 1) \right] = 1, \quad (21)$$

where μ_A and μ_B are given by equations (19).

Up to now, we have solved exactly the eigenequations (12a) and (12b). The eigenvalues of the excitation energy of the spin waves can be derived from equations (20) and (21) when the material parameters of the system are given.

3 Conditions for the existence of ISW

Now we turn to discuss in detail the structure of the magnetic excitations of the system, with particular emphasis on the conditions for the existence of the ISW.

To facilitate our further discussion, we shall use the concept of ‘subbands’ of the two ferromagnets introduced in reference [1]. These subbands span the energy range over which the corresponding bulk spin-wave energies vary with a fixed γ . That is to say, these subbands are described by the union of the bulk spin-wave spectra $E(k_A)$ and $E(k_B)$, equation (20), in which γ equals a constant. The relative relation of the γ subbands of the two bulk ferromagnets depends on the value of the parameter $\beta = J_B S_B / J_A S_A$. Without any loss of generality, we assume in this paper $J_A S_A \geq J_B S_B$, then we have

$$0 < \beta \leq 1. \quad (22)$$

As shown in Figures 1a and 1b, there are two possibilities of the γ subbands: without ($\beta \geq 2/3$) and with ($\beta < 2/3$) an energy gap between the bulk subbands (see Fig. 1).

The eigenfunctions associated with the spin waves in the composite ferromagnets may, in general, show three different types of behavior. In the first case (k_A and k_B are both real) the spin waves can propagate in both ferromagnets and the corresponding eigenfunctions are extended over both constituents. The energy of the spin waves, for this case, lies inside the γ subbands of both ferromagnets.

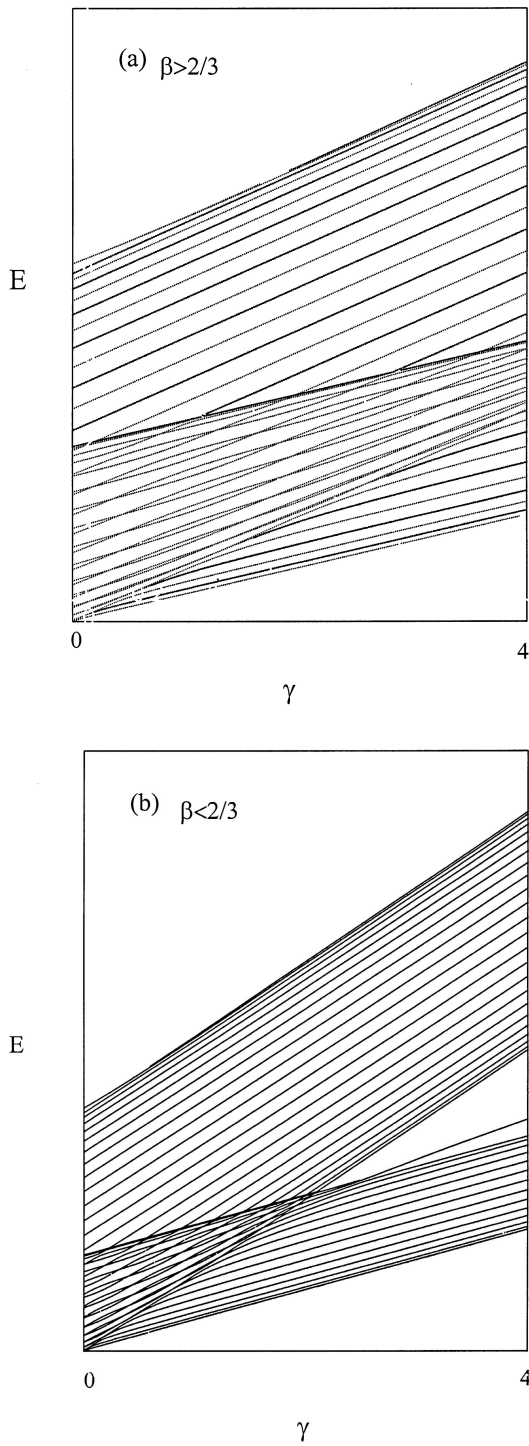


Fig. 1. The γ subbands: (a) without (for $\beta > 2/3$) and (b) with (for $\beta < 2/3$) an energy gap between the bulk subbands.

In the second case (one of k_A and k_B is real, whereas the other is complex) the propagation of the spin waves is only possible in one of the ferromagnets. The eigenfunctions of the spin waves are mostly confined within one of the constituents. Such a kind of behavior occurs for energies that are inside the γ subband of one of the ferromagnets, but outside the corresponding subband of the other.

romagnets, but outside the corresponding subband of the other.

Finally for the third case, with a far interesting behavior, the eigenfunctions of the ISW are localized near the interface and decay exponentially into the interior of each ferromagnets. This property occurs when the wave vectors k_A and k_B are both complex and the corresponding energies of the ISW can only exist either above the two subbands or inside the gap between the γ subbands, when such a gap exists.

It is worthwhile to mention that there does not exist the ISW whose energy can appear below the bulk subbands of the two ferromagnets for any value of the interface exchange coupling $J_{AB} > 0$. As will be shown in the following, the existence of ISW depends on the values of γ and the parameters of the system.

For simplicity, we only consider the limit case of $N_A = N_B \rightarrow \infty$, the system we consider here consists of two semi-infinite ferromagnets [1–3]. We first discuss the ISW whose energies can appear above the bulk subbands of the two ferromagnets. In this case, the wave vector k_A and k_B have the forms

$$k_A = \pi + iq_A \quad \text{and} \quad k_B = \pi + iq_B. \quad (23)$$

The corresponding eigenfunctions of the ISW described by equations (17a) and (17b) become the following expression

$$\begin{aligned} f_A(n) &= (-1)^n C D \exp(nq_A), & (n \leq -1) \\ f_B(n) &= (-1)^n C \exp(-nq_B), & (n \geq 0) \end{aligned} \quad (24)$$

where q_A and q_B are both real and positive numbers, and

$$\begin{aligned} C &= \left\{ R^2 \exp(2q_A) / [\exp(2q_A) - 1] \right. \\ &\quad \left. + \exp(2q_B) / [\exp(2q_B) - 1] \right\}^{-1/2}, \\ D &= -R \exp(q_A). \end{aligned} \quad (25)$$

The parameters μ_A and μ_B in the characteristic equation (21) have the following simple forms

$$\mu_A = -\exp(q_A), \quad \mu_B = -\exp(q_B). \quad (26)$$

To further simplify our discussion about the eigenproblem of the characteristic equations (20) and (21), we introduce the following continuous monotropic transformations

$$\nu_A = \tanh(q_A/2), \quad \nu_B = \tanh(q_B/2). \quad (27)$$

According to our convention, $0 < \nu_A, \nu_B < 1$. Inserting equations (23), (26) into equations (20), and (21) and using the above transformations, we can get

$$\nu_B = \sqrt{\frac{\gamma_c + \beta(\gamma - \gamma_c)(1 - \nu_A^2)}{\gamma_c + \beta\gamma(1 - \nu_A^2)}} \quad (28)$$

and

$$\frac{\nu_A}{J_A S_A^2} + \frac{\nu_B}{J_B S_B^2} = \frac{2}{S_A S_B} \left\{ \frac{1}{J_{AB}^0} - \frac{1}{J_{AB}} \right\}, \quad (29)$$

where

$$J_{AB}^0 = \frac{2S_A S_B J_A J_B}{J_A S_A^2 + J_B S_B^2}. \quad (30)$$

and γ_c is a parameter defined as

$$\gamma_c = 2\beta/(1 - \beta). \quad (31)$$

Substituting equation (28) into equation (29), we immediately obtain a higher-order eigenequation of ν_A , which cannot be solved analytically in general. In order to obtain some useful and essential information on the solutions of equation (29), particularly on the conditions for the existence of solutions, we will proceed by introducing two functions:

$$G_1(\nu_A) = \frac{\nu_A}{J_A S_A^2} + \frac{1}{J_B S_B^2} \sqrt{\frac{\gamma_c + \beta(\gamma - \gamma_c)(1 - \nu_A^2)}{\gamma_c + \beta\gamma(1 - \nu_A^2)}} \quad (32a)$$

and

$$G_2(J_{AB}) = \frac{2}{S_A S_B} \left\{ \frac{1}{J_{AB}^0} - \frac{1}{J_{AB}} \right\}. \quad (32b)$$

Obviously, G_2 is a constant function with respect to ν_A and increases continuously from $-\infty$ to $2/(J_{AB}^0 S_A S_B)$ as J_{AB} varies from 0^+ to $+\infty$. G_1 is a continuous monotropic function of ν_A defined on the closed interval $0 \leq \nu_A \leq 1$. It is easily shown that G_1 is also the monotonically increasing function of ν_A . We, consequently, know that $G_1(\nu_A)$ only at $\nu_A = 0$ and $\nu_A = 1$ has a minimum and a maximum which are given by

$$G_{1\min} = \frac{1}{J_B S_B^2} \sqrt{\frac{\gamma_c + \beta(\gamma - \gamma_c)}{\gamma_c + \beta\gamma}} \quad (33a)$$

and

$$G_{1\max} = \frac{2}{J_{AB}^0 S_A S_B}. \quad (33b)$$

Hence the necessary and sufficient condition for the existence of a nontrivial solution of equation (29) (*i.e.*, $G_1 = G_2$) is

$$G_{1\min} < G_2(J_{AB}) < G_{1\max}. \quad (34)$$

That is to say, the interface coupling constant J_{AB} must obey the requirement:

$$J_{AB} > J_{AB}^{c1} = J_{AB}^0 \left\{ 1 - \frac{\alpha\beta}{1 + \alpha\beta} \sqrt{\frac{\gamma_c + \beta(\gamma - \gamma_c)}{\gamma_c + \beta\gamma}} \right\}^{-1}. \quad (35)$$

Furthermore, it is easy to know from the above discussion that there can only exist one solution of ISW satisfying condition (35).

We now turn to discuss the ISW whose energies can exist inside the energy gap between the bulk subbands of the two ferromagnets. As noted before, the condition for the existence of such a gap is $\beta < 2/3$. For such a case,

$$k_A = iq_A \quad \text{and} \quad k_B = \pi + iq_B \quad (36)$$

and the corresponding wave functions are

$$\begin{aligned} f_A(n) &= CD \exp(nq_A), & (n \leq -1) \\ f_B(n) &= (-1)^n C \exp(nq_B), & (n \geq 0) \end{aligned} \quad (37)$$

where q_A and q_B are both real positive numbers, and C is also given by equation (25), whereas

$$D = R \exp(q_A), \quad \mu_A = -\exp(q_A), \quad \mu_B = -\exp(q_B). \quad (38)$$

The transformations corresponding to equation (27) are changed into the following forms

$$\nu_A = \coth(q_A/2), \quad \nu_B = \tanh(q_B/2). \quad (39)$$

Where $1 < \nu_A < \infty$ and $0 < \nu_B < 1$ for our convention. Using these transformations and inserting equations (36) and (38) into equations (20) and (21), we can obtain two characteristic equations that are similar to equations (28) and (29). One of them is

$$\nu_A = \sqrt{1 + \frac{2(1 - \nu_B^2)}{\gamma(1 - \beta)(1 - \nu_B^2) - 2\beta}}. \quad (40)$$

The other is identical with equations (29) and (30). After performing the discussion similar to that in this section before, we can derive the necessary and sufficient condition for the existence of such ISW, *i.e.*, the interface coupling J_{AB} and the parameter γ must obey the follow equations

$$J_{AB} > J_{AB}^{c2} = J_{AB}^0 \left\{ 1 - \frac{\beta\alpha^2}{1 + \beta\alpha^2} \sqrt{\frac{\gamma + 2}{\gamma - \gamma_c}} \right\}^{-1} \quad (41)$$

and

$$\gamma_c(1 + 2\beta\alpha^2 + \beta\alpha^4)/(1 + 2\beta\alpha^2) < \gamma \leq 4. \quad (42)$$

Obviously, if the interface coupling J_{AB} is large enough and all of the conditions, *i.e.*, equations (35), (41) and (42) are satisfied, there will exist two ISW. One is inside the gap and the other above the subbands of the two ferromagnets. For convenience we have plotted the reduced interface exchange constant $\bar{J}_{AB}^{c1}(\gamma) = J_{AB}^{c1}(\gamma)/J_{AB}^0$ and $\bar{J}_{AB}^{c2}(\gamma) = J_{AB}^{c2}(\gamma)/J_{AB}^0$ as functions of γ in Figure 2.

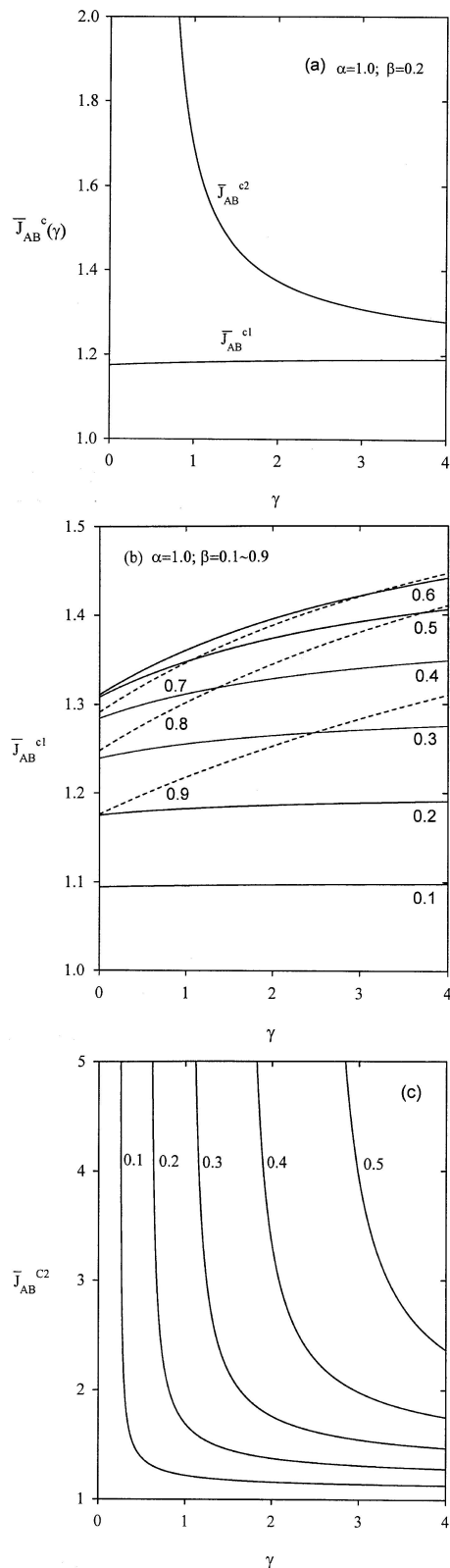


Fig. 2. The conditions for the existence of ISWs: (a) the curves of $\bar{J}_{AB}^{c1}(\gamma)$ and $\bar{J}_{AB}^{c2}(\gamma)$ for $\alpha = 1.0$ and $\beta = 0.2$; (b) the curves of $\bar{J}_{AB}^{c1}(\gamma)$ for $\alpha = 1.0$ and $\beta = 0.1 \sim 0.6$ (solid lines) and $0.7 \sim 0.9$ (dash lines); and (c) the curves of $\bar{J}_{AB}^{c2}(\gamma)$ for $\alpha = 1.0$ and $\beta = 0.1 \sim 0.5$.

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