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Localized magnetic excitations of coupled impurities in a Heisenberg ferromagnet: Optical defect modes

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ABSTRACT

A Green's function method is used to obtain the spectrum of excitations of two neighboring impurities in a semi-infinite ferromagnet. The equations of motion for Green's functions are determined in the framework of the Heisenberg model. The energies of non-resonant localized modes are calculated as a function of the interaction parameters for the exchange coupling between impurity–spin pairs, host–spin pairs, and impurity–host neighbors, as well as the effective field parameter at the impurity sites. With two impurities the system is less symmetric and has more localized modes when compared with a single impurity case.

1. Introduction

The effect of impurities on the spectrum of elementary excitations of solids is well known from experimental and theoretical studies [1–7]. In some bulk magnetic materials, light scattering experiments have demonstrated that the presence of a low concentration of random impurities can modify their spectrum of the elementary excitations [8–11]. From the experimental viewpoint the investigations of the properties of excitations like surface and impurity modes [12–14] have included the use of Raman scattering and inelastic neutron scattering to elucidate the dynamics of these modes. In particular, light scattering studies have shown that the Heisenberg model can give a good theoretical description of real magnetic materials such as EuO and EuS. Theoretical studies based on Green's function technique have been developed by several authors in the context of the Ising [15–19] and the Heisenberg model [20–23]. These developed models allowed the identification of *defect modes* outside the bulk band of spin waves (SW) and of *resonance modes* within the spin wave band.

Previous results for the Ising model [15] and the Heisenberg model [20] in magnetic media with one impurity showed that the presence of impurities creates localized impurity modes. These modes depend on the position of the impurities within the material, as well as on the strength of the exchange coupling between the magnetic impurity sites, impurity host sites and the effective field parameter at the impurity sites. In the present paper, we extend the above-mentioned theory by considering the effect of two nearest neighbor coupled magnetic impurities at arbitrary distances from the surface of a semi-infinite Heisenberg ferromagnet. We consider localized impurities embedded in the magnetic medium in two adjacent magnetic layers aligned along the z-axis (perpendicularly to the surface). The presence of two impurities breaks the translational symmetry along the direction perpendicular to the surface in two adjacent layers of the material. This system has a symmetry lower than the one with a single impurity. The numerical results are obtained adapting Green's function technique for two impurities in the Heisenberg model context.

In Section 2 we present a model and Green-function formalism for the system. The energies of the impurity modes are deduced in Section 3 and numerical results are then given in Section 4.

2. Model and Green's function formalism

The system under study is a semi-infinite ferromagnet with a (0 0 1) surface and a simple cubic structure (lattice constant a). Two nearest neighbors localized impurities spins are placed in the medium at distance $(n-1)a$ from the surface (where integer $n \geq 1$). The Heisenberg Hamiltonian used to describe the system can be written as

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J_{i,j}\mathbf{S}_i \cdot \mathbf{S}_j - \sum_i h_i S_i^z, \quad (1)$$

where $\mathbf{S}_i$ is the spin operator at site i, having spin quantum number S everywhere except at the impurities sites (labeled by

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$o(o')$) where the spin quantum number is denoted by S'. The first term in the right-hand side of Eq. (1) contains the contribution due to the exchange interaction. Throughout this letter we assume that the summation runs over nearest neighbor sites. The second term on the right-hand side of Eq. (1) refers to the effect of the external magnetic field applied to the system in the z direction (where this field is h for the host sites in the bulk and h_S for the host sites at the surface). For convenience, we shall rewrite the Hamiltonian as $\mathcal{H}=\mathcal{H}_0+\mathcal{H}_I$, where $\mathcal{H}_0$ is the Hamiltonian of a pure host ferromagnet, whereas $\mathcal{H}_I$ corresponds to the perturbation caused by impurities:

$$\mathcal{H}_I=\mathcal{H}_{o,d}+\mathcal{H}_{o',d'}+\mathcal{H}_{o,o'}. \tag{2}$$

Here the $\mathcal{H}_{o,d}$ and $\mathcal{H}_{o',d'}$ are the terms for coupling between an impurity at a given site labeled o (o') and its neighboring host sites d (d'):

$$\mathcal{H}_{o,d}=-(J_o-J)\sum_d \mathbf{S}_o\cdot\mathbf{S}_d-(h_o-h)S_o^z, \tag{3}$$

$$\mathcal{H}_{o',d'}=-(J_{o'}-J)\sum_{d'} \mathbf{S}_{o'}\cdot\mathbf{S}_{d'}-(h_{o'}-h)S_{o'}^z, \tag{4}$$

where the d (d') index labels the nearest neighbors host sites. The exchange constant assumes the values $J_o=J'$ ($J_{o'}=J'$) for the interaction between an impurity and a host site inside the medium, and $J_o=J'_S$ ($J_{o'}=J'_S$) when both sites are at the surface. For the pure material the exchange is J_S between neighbors in the surface and J otherwise. Likewise, the term $\mathcal{H}_{o,o'}$ in Eq. (2) comes from the coupling between two impurities:

$$\mathcal{H}_{o,o'}=-(J_I-J)\mathbf{S}_o\cdot\mathbf{S}_{o'}, \tag{5}$$

where J_I is the interaction between two neighboring impurities. The Zeeman contribution in Eqs. (3) and (4) describes the effect of the magnetic field h_o ($h_{o'}$) at the impurity, which can assume the values h'_S at the surface of the medium and h' otherwise.

Using the Holstein–Primakoff transformation, the spin operators are expressed in terms of boson operators a_l and $a_l^\dagger$. At low enough temperatures ($k_BT\ll JS$), the linearized spin wave approximation can be used to give

$$\begin{aligned} S_l^+&=(2S-a_l^\dagger a_l)^{1/2}a_l\simeq(2S)^{1/2}a_l,\\ S_l^-&=a_l^\dagger(2S-a_l^\dagger a_l)^{1/2}\simeq(2S)^{1/2}a_l^\dagger,\\ S_l^z&=S-a_l^\dagger a_l. \end{aligned} \tag{6}$$

Substituting Eq. (6) into Eqs. (1)–(5), we obtain the linearized Hamiltonian as $\mathcal{H}=\mathcal{H}_0+\mathcal{H}_I$, where

$$\mathcal{H}_0=\sum_i\left(S\sum_j J_{i,j}+h\right)a_i^\dagger a_i-S\sum_{i,j}J_{i,j}a_i^\dagger a_j \tag{7}$$

and the terms of $\mathcal{H}_I$ are given by

$$\mathcal{H}_{o,d}=-JS\sum_d[\gamma(a_o a_d^\dagger+a_o^\dagger a_d)-\varepsilon a_o^\dagger a_o-\rho a_d^\dagger a_d]-\beta a_o^\dagger a_o, \tag{8}$$

$$\mathcal{H}_{o',d'}=-JS\sum_{d'}[\gamma(a_{o'}a_{d'}^\dagger+a_{o'}^\dagger a_{d'})-\varepsilon a_{o'}^\dagger a_{o'}-\rho a_{d'}^\dagger a_{d'}]-\beta a_{o'}^\dagger a_{o'}, \tag{9}$$

$$\mathcal{H}_{o,o'}=-JS\gamma_I(a_o a_{o'}^\dagger+a_o^\dagger a_{o'}-a_{o'}^\dagger a_{o'}-a_o^\dagger a_o), \tag{10}$$

where we have defined the following quantities:

$$\begin{aligned} &\gamma=\frac{J'}{J}\sqrt{\frac{S'}{S}}-1,\quad \varepsilon=\frac{J'}{J}-1,\quad \rho=\frac{J'S'}{JS}-1,\\ &\beta=h'-h\quad\text{and}\quad \gamma_I=\frac{J_IS'}{JS}-1. \end{aligned} \tag{11}$$

The index o (o') takes the values 1 (7) for each impurity site. The second summation runs over *five* neighboring host site to either impurity. In the special case of $n=1$, only one of the impurities is in the surface layer, where it has *four* nearest neighboring host in this layer.

In order to obtain the excitation spectra of these systems, we extend the formalism for a single localized impurity presented in Ref. [20]. Thus, we start by defining the retarded Green function $G_{l,m}(t)=\langle\langle a_l(t);a_m^\dagger\rangle\rangle_E$ for the impure system. These functions must satisfy the standard equation of motion [24]

$$E\langle\langle a_l;a_m^\dagger\rangle\rangle_E=\frac{1}{2\pi}\langle[a_l,a_m^\dagger]\rangle+\langle\langle[a_l,\mathcal{H}];a_m^\dagger\rangle\rangle_E. \tag{12}$$

The corresponding unperturbed Green's function can first be obtained by solving Eq. (12) with $\mathcal{H}$ replaced by $\mathcal{H}_0$ and then decoupling the higher-order Green's functions on the right-hand side using the random phase approximation. The solution, which represents the case of a pure semi-infinite ferromagnet (i.e., with translational symmetry parallel to the surface), is well known and is given by [25]

$$\begin{aligned} G_{l,m}^0(E)=&\frac{1}{M}\sum_{\mathbf{q}_\parallel}\exp[i\mathbf{q}_\parallel\cdot(\mathbf{r}_l-\mathbf{r}_m)]\\ &\times\frac{1}{2\pi JS(x-x^{-1})}\left(x^{|n-n'|}-\frac{1+x^{-1}\Delta}{1+x\Delta}x^{n+n'}\right), \end{aligned} \tag{13}$$

where the vectors $\mathbf{r}_l$ and $\mathbf{r}_m$ indicate the positions of two given sites l and m, $\mathbf{q}_\parallel\equiv(q_x,q_y)$ is an in-plane wave vector and M is the number of sites in any layer parallel to the surface, and n and n' are the layer numbers for the sites l and m, respectively (with $n=1$ being the surface layer, etc.). The complex quantity x (satisfying the condition $|x|\le 1$) is defined by

$$x+x^{-1}=\frac{h-E}{JS}+2[3-2\gamma(\mathbf{q}_\parallel)], \tag{14}$$

where $\gamma(\mathbf{q}_\parallel)$ is a structure factor that, in the case of a simple cubic lattice, is given by $\gamma(\mathbf{q}_\parallel)=\frac{1}{2}[\cos(q_xa)+\cos(q_ya)]$. The parameter Δ in Eq. (13) contains the information regarding the surface and is given by

$$\Delta=4\left(\frac{J_S}{J}-1\right)[1-\gamma(\mathbf{q}_\parallel)]-1. \tag{15}$$

The Green function for the semi-infinite ferromagnet with impurities can be constructed from Eq. (12) using the full form of the Hamiltonian equation (7). The result can be expressed in the form of a Dyson equation relating the Green function $G_{l,m}(E)$ for the Heisenberg model system containing impurities to the corresponding $G_{l,m}^0(E)$ for the pure system

$$\sum_j\left(1-\sum_n G_{l,n}^0(E)V_{n,j}\right)G_{j,m}(E)=G_{l,m}^0(E). \tag{16}$$

Here, V is an effective potential related to the perturbation produced by the presence of the impurities, given by

$$V_{n,j}=(V_o)_{n,j}+(V_{o'})_{n,j}+(V_{oo'})_{n,j}, \tag{17}$$

where

$$(V_o)_{n,j}=2\pi JS\left[\sum_d(\rho\delta_{n,d}\delta_{d,j}-\gamma\delta_{n,d}\delta_{o,j}-\gamma\delta_{n,o}\delta_{d,j})+\left(5\varepsilon-\frac{\beta}{JS}\right)\delta_{n,o}\delta_{o,j}\right],$$

$$(V_{o'})_{n,j}=2\pi JS\left[\sum_d(\rho\delta_{n,d'}\delta_{d',j}-\gamma\delta_{n,d'}\delta_{o',j}-\gamma\delta_{n,o'}\delta_{d',j})+\left(5\varepsilon-\frac{\beta}{JS}\right)\delta_{n,o'}\delta_{o',j}\right],$$

$$(V_{oo'})_{n,j}=2\pi JS\gamma_I(\delta_{n,o'}\delta_{o,j}+\delta_{n,o}\delta_{o',j}-\delta_{n,o}\delta_{o,j}-\delta_{n,o'}\delta_{o',j}).$$

We note that, in the presence of *localized* impurities, the translational symmetry does not exist in any of the three directions. Consequently, we have to work in terms of real space to solve Eq. (16).

3. Localized impurity modes

In this section we present results for the energy spectrum of modes associated with two impurities aligned along the z-axis (see Fig. 1). In the site representation, we label the impurity site o (o') in the layer n ($n+1$) by index 1 (7), with $d=2,3,4,5,6$ ($d'=8,\ldots,12$) (see Fig. 1). Clearly the neighbor 6 is absent when $n=1$. Dyson's equation (16) can be rewritten in a matrix form

$$[\mathbf{I}-\mathbf{G}^0(E)\mathbf{V}]\mathbf{G}(E)=\mathbf{G}^0(E). \tag{18}$$

The spectrum of localized modes is then found by numerically calculating the frequencies that satisfy the condition

$$\det[\mathbf{I}-\mathbf{G}^0(E)\mathbf{V}]=0, \tag{19}$$

which represents the poles of $\mathbf{G}^0(E)$ for the system containing impurities. Since each impurity spin couples to five host spins (except when $n=1$) as well as to one impurity spin, we have a 12×12 matrix in Eq. (19).

On substituting Eq. (17) in the above equation, the determinant can be factorized as in the corresponding calculations for an impurity in an infinite ferromagnet [4],

$$\det[\mathbf{I}-\mathbf{G}^0(E)\mathbf{V}]=D^2_{A_o}(E)D_{B_o}(E)\times D^2_{A_{o'}}(E)D_{B_{o'}}D_C(E) \tag{20}$$

with

$$D_{A_o}(E)=\rho_N[G^0_{2,3}-G^0_{1,1}]+1/2\pi JS \tag{21}$$

$$D_{A_{o'}}(E)=\rho_N[G^0_{8,9}-G^0_{7,7}]+1/2\pi JS \tag{22}$$

$$D_{B_o}(E)=\rho[2G^0_{2,4}-G^0_{1,1}-G^0_{2,3}]+1/2\pi JS \tag{23}$$

$$D_{B_{o'}}(E)=\rho[2G^0_{8,10}-G^0_{7,7}-G^0_{8,9}]+1/2\pi JS \tag{24}$$

$$D_C(E)=\det\mathbf{D}, \tag{25}$$

where for convenience we have omitted the E labeling in the Green functions G^0. The elements of the 6×6 matrix $\mathbf{D}$ are given by

$$D_{1,1}=1/2\pi JS-G^0_{1,1}\varepsilon_N+(4G^0_{1,2}+G^0_{1,6})\gamma_N+G^0_{1,7}\gamma_I,$$

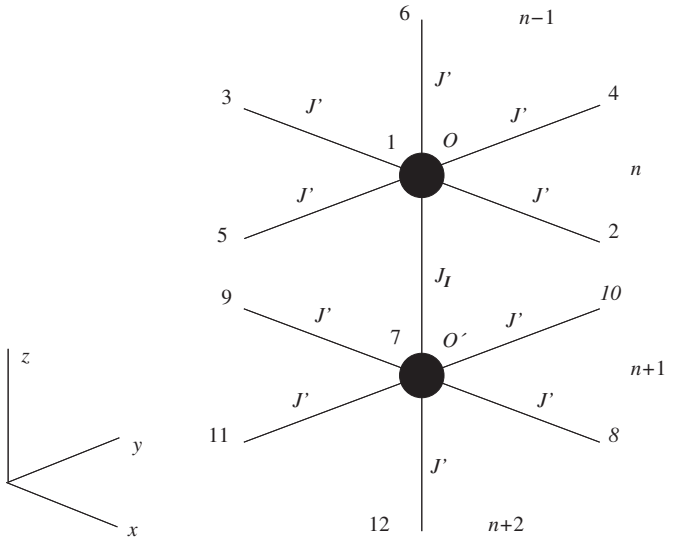

Fig. 1. Interaction scheme for two coupled impurities in a Heisenberg ferromagnet. The spins in each impurity (black circles) are exchange coupled with each other and with their nearest neighbor spins in the host medium. All spins are assumed to be aligned along the z axis.

$$D_{2,1}=-G^0_{1,2}\varepsilon_N+(G^0_{1,1}+G^0_{2,3}+2G^0_{2,4}+G^0_{2,6})\gamma_N+G^0_{2,7}\gamma_I,$$

$$D_{3,1}=-G^0_{1,6}\varepsilon_N+(4G^0_{2,6}+G^0_{6,6})\gamma_N+G^0_{6,7}\gamma_I,$$

$$D_{4,1}=-G^0_{1,7}\varepsilon_N+(4G^0_{2,7}+G^0_{6,7})\gamma_N+G^0_{7,7}\gamma_I,$$

$$D_{5,1}=-G^0_{1,8}\varepsilon_N+G^0_{2,8}\gamma_N+G^0_{7,8}\gamma_I,$$

$$D_{6,1}=-G^0_{1,12}\varepsilon_N+G^0_{7,12}\gamma_I,$$

$$D_{1,2}=4(G^0_{1,1}\gamma_N-G^0_{1,2}\rho_N),$$

$$D_{2,2}=1/2\pi JS+4G^0_{1,2}\gamma_N-(G^0_{1,1}+G^0_{2,3}+2G^0_{2,4})\rho_N,$$

$$D_{3,2}=4(G^0_{1,6}\gamma_N-G^0_{2,6}\rho_N),$$

$$D_{4,2}=4(G^0_{1,7}\gamma_N-G^0_{2,7}\rho_N),$$

$$D_{5,2}=4G^0_{1,8}\gamma_N-G^0_{2,8}\rho_N,$$

$$D_{6,2}=4G^0_{1,12}\gamma_N,$$

$$D_{1,3}=G^0_{1,1}\gamma_N-G^0_{1,6}\rho_N,$$

$$D_{2,3}=G^0_{1,2}\gamma_N-G^0_{2,6}\rho_N,$$

$$D_{3,3}=1/2\pi JS+G^0_{1,6}\gamma_N-G^0_{6,6}\rho_N,$$

$$D_{4,3}=G^0_{1,7}\gamma_N-G^0_{6,7}\rho,$$

$$D_{5,3}=G^0_{1,8}\gamma_N,$$

$$D_{6,3}=G^0_{1,12}\gamma_N,$$

$$D_{1,4}=G^0_{1,1}\gamma_I-G^0_{1,7}\overline{\varepsilon}+(4G^0_{1,8}+G^0_{1,12})\gamma,$$

$$D_{2,4}=G^0_{1,2}\gamma_I-G^0_{2,7}\overline{\varepsilon}+G^0_{2,8}\gamma,$$

$$D_{3,4}=G^0_{1,6}\gamma_I-G^0_{6,7}\overline{\varepsilon},$$

$$D_{4,4}=1/2\pi JS+G^0_{1,7}\gamma_I-G^0_{7,7}\overline{\varepsilon}+(G^0_{7,8}+G^0_{7,12})\gamma,$$

$$D_{5,4}=G^0_{1,8}\gamma_I-G^0_{7,8}\overline{\varepsilon}+(G^0_{7,7}+G^0_{8,9}+2G^0_{8,10}+G^0_{8,12})\gamma,$$

$$D_{6,4}=G^0_{1,12}\gamma_I-G^0_{7,12}\overline{\varepsilon}+(4G^0_{8,12}+G^0_{12,12})\gamma,$$

$$D_{1,5}=4(G^0_{1,7}\gamma-G^0_{1,8}\rho),$$

$$D_{2,5}=4G^0_{2,7}\gamma-G^0_{2,8}\rho,$$

$$D_{3,5}=4G^0_{6,7}\gamma,$$

$$D_{4,5}=4(G^0_{7,7}\gamma-G^0_{7,8}\rho),$$

$$D_{5,5}=1/2\pi JS+G^0_{7,8}\gamma-(G^0_{7,7}+G^0_{8,9}+G^0_{8,10})\rho,$$

$$D_{6,5}=4(G^0_{7,12}\gamma-G^0_{8,12}\rho),$$

$$D_{1,6}=G^0_{1,7}\gamma-G^0_{1,12}\rho,$$

$$D_{2,6}=G^0_{2,7}\gamma,$$

$$D_{3,6}=G^0_{6,7}\gamma,$$

$$D_{4,6}=G^0_{7,7}\gamma-G^0_{7,12}\rho,$$

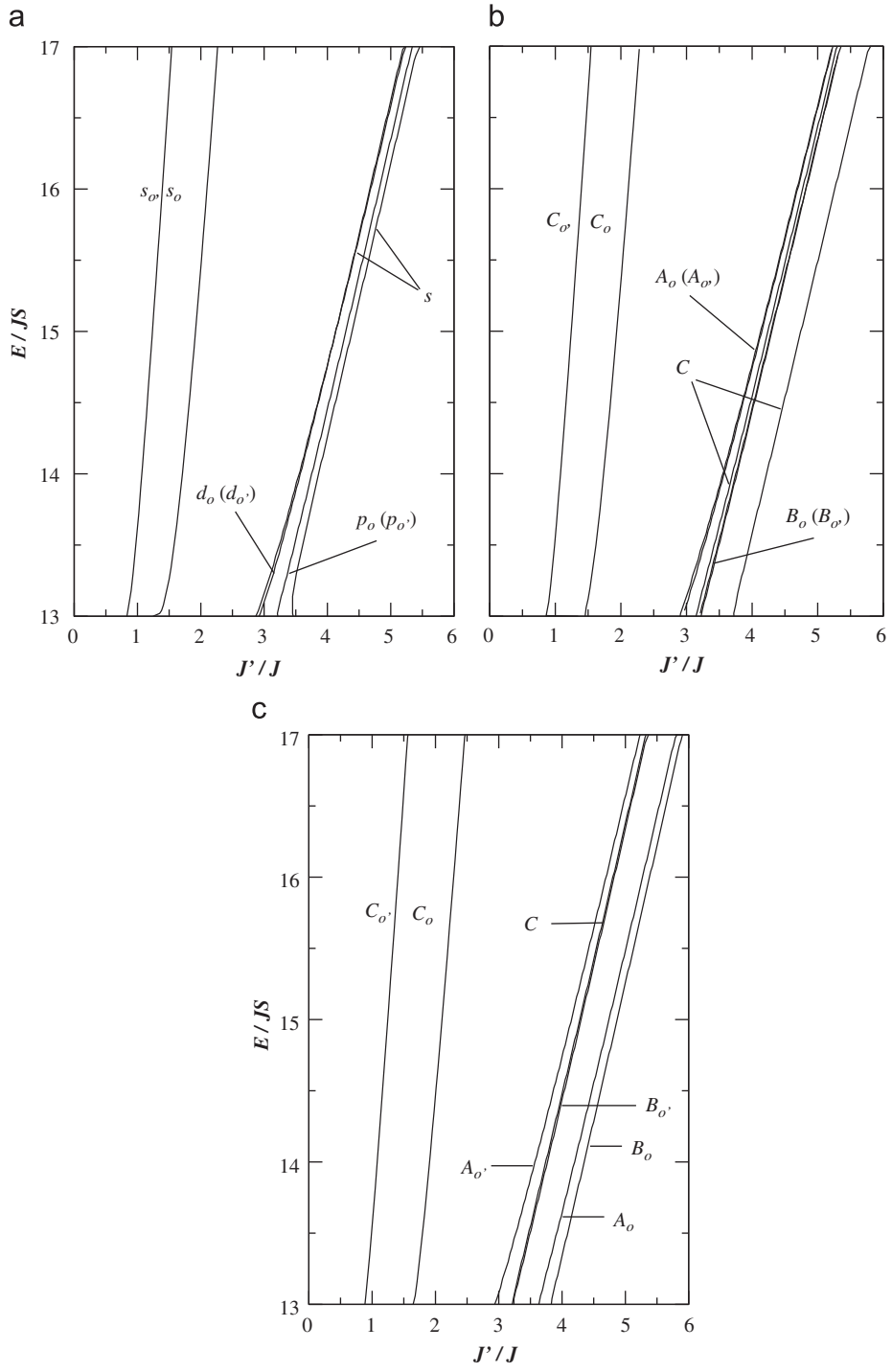

Fig. 2. Localized spin wave spectra of two magnetic impurities in a semi-infinite ferromagnet: (a) impurities located in the bulk (upper impurity in layer $n=10$), (b) upper impurity o in the second layer ($n=2$, see Fig. 1) and (c) upper impurity o located at the surface ($n=1$). The results are plotted as function of J'/J. Parameters are given in the text.

$$D_{5,6} = G^0_{7,8}\gamma - G^0_{8,12}\rho,$$
$$D_{6,6} = 1/2\pi JS + G^0_{7,12}\gamma - G^0_{12,12}\rho. \quad (26)$$

In Eq. (25), for $n=1$, the constants ρ_N, γ_N must be replaced respectively by ρ_S, γ_S and ε_N by $4\varepsilon_S - \beta/(JS)$, $\varepsilon_N = 5\varepsilon - \beta/(JS)$ when $n \geq 2$, and $\bar{\varepsilon} = 5\varepsilon - \beta/(JS)$. The constants ρ_S, γ_S and ε_S are obtained by replacing J' with J'_S in Eqs. (11).

The localized impurity modes in the semi-infinite ferromagnet may be obtained from Eqs. (21)–(25)) by finding the E values for which $D_{A_o}(E)$, $D_{A_{o'}}(E)$, $D_{B_o}(E)$ or $D_{B_{o'}}(E)$ vanishes.

4. Numerical results

The impurity modes can be classified as resonant modes when the frequencies are found inside the bulk band of the film, and they are called defect modes when they occur outside the bulk band. Because impurity modes inside the bulk bands are more difficult to be experimentally detected, here we considered only the optical defect modes with energies above the upper limit of the bulk band obtained for the film. This limit value of energy is $E/JS = 13$.

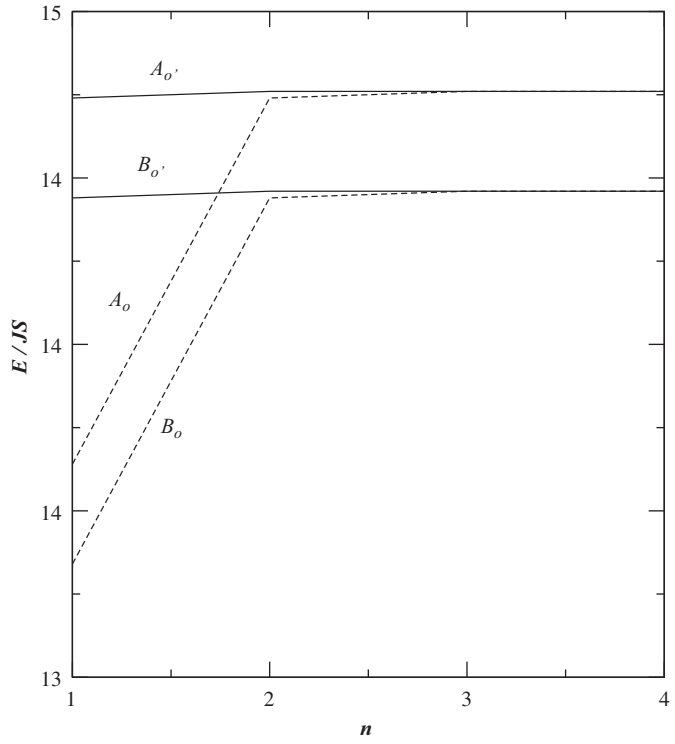

Fig. 3. Localized spin wave modes A and B as a function of the layer index n of the upper impurity o. The parameters are the same as those of Fig. 2.

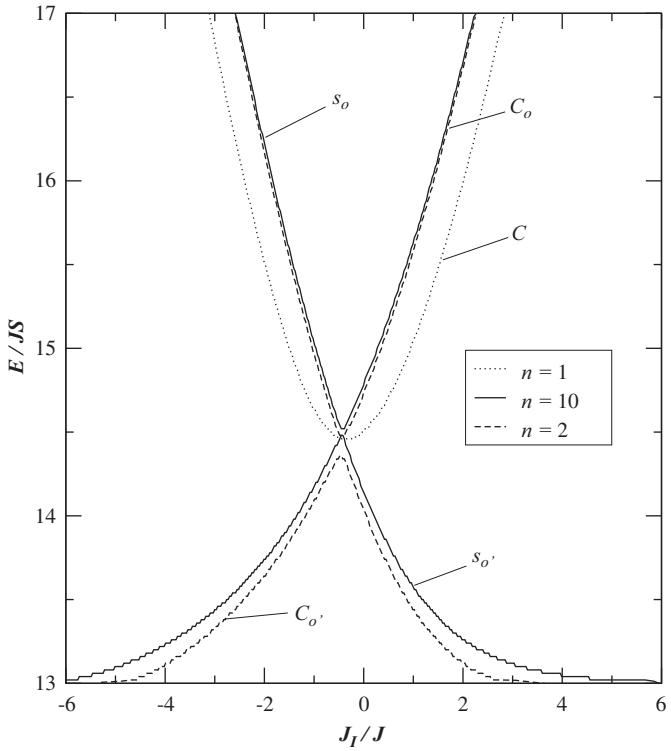

Fig. 4. Localized spin wave energies associated with two magnetic impurities in a semi-infinite ferromagnet: upper impurity o at the surface (dotted line), upper impurity in layer $n=10$ (solid lines), upper impurity o at layer $n=2$ (dashed lines). The results are plotted as function of J_I/J. Parameters are given in the text.

Localized impurity modes spectra may now be obtained as a function of the exchange and effective field parameters related to the impurities like J', J_I and h'. For convenience, in all figures, we take $J_S/J=1$, $J'_S/J'=1$, $h_S/h=1$ and $h'_S/h'=1$.

Figs. 2(a)–(c) show the localized SW energies as a function of the normalized exchange constant J'/J for the coupling between the impurities ($S'=2$) and its neighboring host sites ($S=1$). We have used $J_I/J=2$ and $h'/h=1.5$. For large enough values of n, $n=10$ in Fig. 2(a), each impurity, o and o', and its neighbors have the same symmetry, by that we mean the same kind of neighbor (bulk sites for this case); we find impurity modes which are similar to those occurring in the case of a bulk sample, conventionally labeled as s, p and d, for the case where one considers only one localized impurity [4–6]. Here, this modes are labeled as s_o and $s_{o'}$, p_o and $p_{o'}$ and d_o and $d_{o'}$, associated respectively to impurities o and o' through Eqs. (20)–(25). In this example, the p_o and $p_{o'}$ and d_o and $d_{o'}$ modes appear degenerated. The curves s, p_o ($p_{o'}$) and d_o ($d_{o'}$) correspond to modes that are mainly associated with neighbors of the impurities (like p and d modes at large n).

When the upper impurity o is located at the second layer ($n=2$), Fig. 2(b), the symmetry around the impurities is reduced, since the upper impurity o has a surface site as a neighbor. The symmetry labeling of previous works [4] is no longer applicable, and the modes related to presence of a surface are labeled in the same way as in Ref. [20], however with the addition of an impurity position index. They are labeled as A_o ($A_{o'}$), B_o ($B_{o'}$) (from Eqs. (21) to (24)) and C_o $C_{o'}$ and C (from Eq. (25)), associated respectively to impurities o and o'. The curves C_o and $C_{o'}$ correspond to modes that are mainly localized on the impurities, whereas the curves A_o ($A_{o'}$), B_o ($B_{o'}$) and C correspond to modes that are mainly associated with neighbors of the impurities, as in previous figure. These neighbors do not all have the same symmetry with respect to the surface, and this produces a splitting of the C modes. In this case, the B_o and $B_{o'}$ and A_o and $A_{o'}$ modes still appear with a small degeneracy. This degeneracy is completely lifted when the upper impurity o is located at the surface ($n=1$), as shown in Fig. 2(c). Here, due to absence of a nearest neighbor of the upper impurity o, the symmetry around the impurities is modified and the modes B_o, $B_{o'}$ and A_o and $A_{o'}$ are separated. For this case, only one C mode is found.

In order to verify the dependence of the degeneracy of the A (d) and B (p) modes on the index layer of the upper impurity, we plot in Fig. 3 the localized spin wave modes A and B against n for this impurity, with the same parameters as in Fig. 2. Here, the continuous lines are shown as guides to the eye. We observe that for $n>3$ these modes are completely degenerate. This is expected as can be seen in Fig. 2.

Fig. 4 shows the localized SW energies as a function of the normalized exchange coupling constant J_I/J for the interaction between the impurities o and o'. The results were obtained for ferromagnetic ($J_I>0$) as well as antiferromagnetic ($J_I<0$) coupling when the coupling between the impurities and its neighboring host sites is $J'/J=1.5$ and the effective external applied magnetic field $h'/h=1.5$. The remaining parameters are the same as in previous figures. The results were obtained for $n=1$ (dotted line), when the upper impurity o is at the surface, $n=10$ (solid lines), when the impurities are at the bulk, and $n=2$ (dashed lines) when the upper impurity o is at the second layer. The figure shows one localized mode when the upper impurity is on the surface. This mode increases when the exchange between the impurities increases. When the upper impurity is in the bulk region ($n=2$ and 10) we see two modes; one increasing and other decreasing with J_I. For $n>1$ we see the two modes crossing. That crossing depends on the parameters used, mainly h' and J'. One would expect the crossing to occur when $J_I=0$. But as we have an external applied field and other parameters. The two modes are degenerated for a different value of J_I.

Next, we analyze the influence of the effective external applied magnetic field on the SW energies for impurity modes. Fig. 5 shows the localized modes as a function of h'/h. The coupling

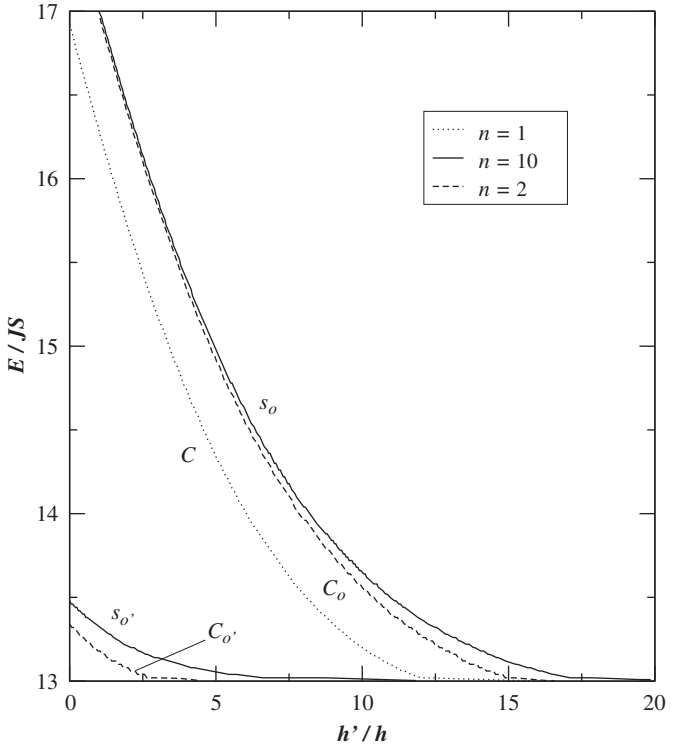

Fig. 5. Localized spin wave energies associated with two magnetic impurities in a semi-infinite ferromagnet: upper impurity o at the surface (dotted line), impurities in the bulk ($n=10$) (solid lines), upper impurity o is at the second layer ($n=2$) (dashed lines). The results are plotted as function of h'/h and the parameters are given in the text.

between the impurities and their neighboring host sites as a well the coupling between the impurities are J'/J and $J_I/J=2.0$. The remaining parameters are the same as in previous graphs. The results were obtained for $n=1$ (dotted line), when the upper impurity o is at the surface, $n=10$ (solid lines), when the impurities are at the bulk, and $n=2$ (dashed lines) when the upper impurity o is at the second layer. The figure shows that all modes decreases in energy when the effective field acting on the impurities increases.

5. Conclusions

In this paper we have investigated the effects of two coupled localized impurities in a simple-cubic Heisenberg ferromagnet. We employed a Green's function method and generalized random phase approximation at low temperatures ($T \ll T_C$). Numerical results were shown for optical non-resonant modes existing above the bulk SW energy bands. The results obtained show the influence of the impurities' position within the film, the strength of the exchange coupling, and the effective field parameter on the excitation spectra of the system. The coupling modifies the spectra when comparing the results for single impurities, especially when the upper impurity is in the layer $n=1$ or $n=2$. If n becomes very large we recover previous results for infinite ferromagnets, for each impurity, as expected. The main result here is that the impurity-related modes behave like the single impurity case, however the number of modes are different, as expected because of the lower symmetry system of the model. As a theoretical perspective for this study, we point the fact that the same formalism used here can be useful to the study of impurities in fermionic systems, such as carbon based materials, since such systems can be accurately described by a microscopic nearest neighbor tight-binding Hamiltonian similar to the Hamiltonian (Eq. (7)) employed here [26].

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