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G.M. Japiassú, L.J.El-Jaick and X.A. da Silva

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by

G.M. Japiassú
Instituto de Física
Universidade Federal do Rio de Janeiro
Rio de Janeiro, RJ, Brasil

L.J. El-Jaick
Centro Brasileiro de Pesquisas Físicas
Rio de Janeiro, RJ, Brasil

X.A. da Silva
Centro Brasileiro de Pesquisas Físicas
Rio de Janeiro, RJ, Brasil

In this paper we study the self-excitations of coupled localized and itinerant spin systems. We calculate the transverse dynamic susceptibility of the itinerant part, using the method of double-time Green's functions. In the narrow band limit the role of the coupling parameter on the poles and the susceptibility itself is physically interpreted.

1. Introduction

The self-excitations of localized and itinerant spin systems have been extensively studied in the literature[1,2], individual or collective excitations being obtained according to the approximations used.

The possibility of coexistence and mutual influence of itinerant and localized spins has been considered by several authors[3,4,5,7,8]. A possible example where this might occur is the case of $Eu_{1-x}Gd_xB_6$ $(0<x<1)$. These compounds were investigated by Glaunsinger[6] using EPR. EuB_6 is a ferromagnetic semiconductor with a conduction-electron density of about 0.09 eℓ/Eu, and GdB_6 is a metal with one conduction electron per Gd site. Since both Eu^{2+} and Gd^{3+} have identical magnetic moments and Gd^{3+} can be substituted for Eu^{2+} in EuB_6 with only a slight change in lattice parameter, the variation of x in $Eu_{1-x}Gd_xB_6$ provides a series of materials having different conduction-electron, but identical magnetic-ion, concentrations. If one assumes that the effective coupling between Eu in EuB_6 is Bloemberg-Rowland-like, whereas for Gd in GdB_6 it is RKKY-like, it is reasonable to think that for $Eu_{1-x}Gd_xB_6$ $(0<x<1)$ the two mechanisms may coexist.

In this paper we consider a system consisting of conduction electrons and localized spins. The localized spins are coupled, via exchange, to the itinerant electrons. The localized spins interactions are Heisenberg-like and the conduction band is described in the Hartree-Fock (H-F) approximation. Our purpose is to obtain the dynamic susceptibilities of the itinerant spins and the excitation spectra. Using the RPA approximation and the narrow band limit our results are compared with the corresponding localized spin susceptibilities obtained by Wortmann[7,8]. The results are discussed considering the non-interacting systems and the role of the coupling parameter.

The plan of the paper is as follows. In section 2 the model Hamiltonian as well as the quantities of interest are introduced. In section 3, the double-time Green's function (GF) which represent the dynamic susceptibilities are obtained in the RPA approximation. Finally, in the narrow band limit, the excitation spectra and the susceptibilities which now have optical and accoustic branches, are physically interpreted considering the role of the coupling parameter, and the susceptibilities of the non-interacting systems. A comparison with Wortmann's work[8] where the localized dynamic susceptibilities are studied is also made.

2. Formulation of the Problem.

The Hamiltonian of the system is

$$H = H_E + H_L + H_{int} \tag{2.1}$$

H_E describes the conduction electrons

$$H_E = \sum_{i,j,\sigma} T^{\sigma}(ij)\ c^{+}_{i\sigma}\ c_{j\sigma} \tag{2.2}$$

$c^{+}_{i\sigma}(c_{j\sigma})$ stand for Wannier creation (destruction) operator,

$T^{\sigma}(ij)$ is the energy of the conduction band

$$T^{\sigma}(ij) = T(ij) - \frac{1}{2}(\sigma-1)\,\Delta\delta_{ij}$$

where Δ is the shift of the bands. In the H-F approximation $\Delta = I\langle n_{\uparrow} - n_{\downarrow}\rangle$, I is the Coulomb interaction, σ(algebraic symbol) = ±1, and σ(index) = $\uparrow$ or $\downarrow$.
H_L stands for the Heisenberg part

$$H_L = -\sum_{i,j}{}' J(ij)\ \vec{S}_i\cdot\vec{S}_j \tag{2.3}$$

with the spin operators $\vec{S}_i$, and the interaction parameter J(ij), which depends on the lattice sites. We consider only interaction between nearest neighbouring spins, and J(ij) should be isotropic because of lattice symmetry.
H_{int} describes the exchange interaction between the localized and itinerant spins

$$H_{int} = -\frac{g}{2}\sum_i \left\{ S_i^z(n_{i\uparrow}-n_{i\downarrow}) + S_i^+\, c_{i\downarrow}^+ c_{i\uparrow} + S_i^-\, c_{i\uparrow}^+\, c_{i\downarrow} \right\} \tag{2.4}$$

Here g is the coupling parameter and $n_{i\sigma}$ stands for the number operator $c_{i\sigma}^+ c_{i\sigma}$.

The quantities of interest are the dynamic susceptibilities of the itinerant spins. The transverse susceptibilities are the Fourier transform of the double-time Green's functions (GF)[2] $\langle\langle A;B\rangle\rangle$ with $A = s_k^+$, $B = s_{-k}^-$ or S_{-k}^- , where

$$S_k^{\pm} = \frac{1}{\sqrt{N}}\sum_i e^{ikR_i}\ S_i^{\pm} \tag{2.5a}$$

$$s_k^+ = \frac{1}{\sqrt{N}} \sum_q c_{q\uparrow}^+ c_{k+q\downarrow} \quad , \quad s_k^- = \frac{1}{\sqrt{N}} \sum_q c_{q\downarrow}^+ c_{k+q\uparrow} \tag{2.5b}$$

$$c_{k\sigma}^+ = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} c_{i\sigma}^+ \quad , \quad c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{-ikR_i} c_{i\sigma} . \tag{2.5c}$$

These susceptibilities must satisfy the equation of motion(9)

$$\omega <<A;B>> = \frac{1}{2\Pi} <[A,B]_{\pm}> + <<[A,H]_-; B>>. \tag{2.6}$$

In the following section we study the equations of motion of the susceptibilities $<<s_k^+ ; s_{-k}^->>$ and $<<s_k^+ ; s_{-k}^->>$.

3. Equations of motion, approximations and dynamic magnetic responses.

In the computation of the susceptibilities the following results will be used

$$\begin{aligned} \left[c_{i\uparrow}^+ c_{j\downarrow}, H\right]_- = & \sum_m \left\{ T(mj)\, c_{i\uparrow}^+ c_{m\downarrow} - T(im)\, c_{m\uparrow}^+ c_{j\downarrow} \right\} \\ & + \frac{g}{2} \left\{ (S_i^z + S_j^z)\, c_{i\uparrow}^+ c_{j\downarrow} \right. \\ & \qquad \left. - S_j^+ c_{i\uparrow}^+ c_{j\uparrow} + S_i^+ c_{i\downarrow}^+ c_{j\downarrow} \right\} \\ & + \Delta\, c_{i\uparrow}^+ c_{j\downarrow} \quad , \end{aligned} \tag{3.1}$$

$$\left[S_i^+, H\right]_- = 2 \sum_\ell J(i\ell)(S_\ell^z S_i^+ - S_\ell^+ S_i^z) + \frac{g}{2} S_i^+ (n_{i\uparrow} - n_{i\downarrow})$$

$$- g\, S_i^z c_{i\uparrow}^+ c_{i\downarrow}. \tag{3.2}$$

In order to obtain the GF $<<s_k^+ ; s_{-k}^->>$ we begin studying the GF $<<c_{i\uparrow}^+ c_{j\downarrow}; c_{\ell\downarrow}^+ c_{m\uparrow}>>$. These two GF are related by (2.5).

From (3.1) and (2.6) we obtain

$$\left\{ \omega - \Delta \right\} <<c_{i\uparrow}^+ c_{j\downarrow}; c_{\ell\downarrow}^+ c_{m\uparrow}>> =$$

$$= \frac{1}{2\Pi} \left\{ <c_{i\uparrow}^+ c_{m\uparrow}> \delta_{j\ell} - <c_{\ell\downarrow}^+ c_{j\downarrow}> \delta_{im} \right\}$$

$$+ \sum_p \left\{ T(pj) <<c_{i\uparrow}^+ c_{p\downarrow}; c_{\ell\downarrow}^+ c_{m\uparrow}>> \right.$$

$$\left. - T(ip) <<c_{p\uparrow}^+ c_{j\downarrow} ; c_{\ell\downarrow}^+ c_{m\uparrow}>> \right\}$$

$$+ \frac{g}{2} <<(S_i^z + S_j^z)\, c_{i\uparrow}^+ c_{j\downarrow} ; c_{\ell\downarrow}^+ c_{m\uparrow}>>$$

$$- \frac{g}{2} \left\{ <<S_j^+ c_{i\uparrow}^+ c_{j\uparrow}; c_{\ell\downarrow}^+ c_{m\uparrow}>> \right.$$

$$\left. - <<S_i^+ c_{i\downarrow}^+ c_{j\downarrow}; c_{\ell\downarrow}^+ c_{m\uparrow}>> \right\}. \tag{3.3}$$

Using the RPA approximation

$$<<S_i^z c_{i\uparrow}^+ c_{j\downarrow}; c_{\ell\downarrow}^+ c_{m\uparrow}>> \rightarrow <S^z><<c_{i\uparrow}^+ c_{j\downarrow}; c_{\ell\downarrow}^+ c_{m\uparrow}>> \tag{3.4a}$$

$$<<S_j^+ c_{i\uparrow}^+ c_{j\uparrow};\ c_{\ell\downarrow}^+ c_{m\uparrow}>> \rightarrow <c_{i\uparrow}^+ c_{j\uparrow}><<S_j^+;\ c_{\ell\downarrow}^+ c_{m\uparrow}>> \quad (3.4b)$$

$$<<S_i^+ c_{i\downarrow}^+ c_{j\downarrow};\ c_{\ell\downarrow}^+ c_{m\uparrow}>> \rightarrow <c_{i\downarrow}^+ c_{j\downarrow}> <<S_i^+;c_{\ell\downarrow}^+ c_{m\uparrow}>> \quad (3.4c)$$

Combining (3.4) with (3.3)

$$\left\{ \omega - \Delta - g<S^z> \right\} <<c_{i\uparrow}^+ c_{j\downarrow};\ c_{\ell\downarrow}^+ c_{m\uparrow}>> =$$

$$= \frac{1}{2\Pi} \left\{ <c_{i\uparrow}^+ c_{m\uparrow}>\delta_{j\ell} - <c_{\ell\downarrow}^+ c_{j\downarrow}>\delta_{im} \right\}$$

$$+ \sum_p \left\{ T(pj)\ <<c_{i\uparrow}^+ c_{p\downarrow};\ c_{\ell\downarrow}^+ c_{m\uparrow}>> \right.$$

$$\left. -T(ip)<<c_{p\uparrow}^+;\ c_{j\downarrow};\ c_{\ell\downarrow}^+\ c_{m\uparrow}>> \right\}$$

$$- \frac{g}{2}\ <c_{i\uparrow}^+ c_{j\uparrow}><<S_j^+;c_{\ell\downarrow}^+\ c_{m\uparrow}>>$$

$$- <c_{i\downarrow}^+ c_{j\downarrow}><<S_i^+;c_{\ell\downarrow}^+ c_{m\uparrow}>> \quad (3.5)$$

where $<S_i^z> = <S^z>$ due to translation symmetry.

For the new GF $<<S_i^+ ; c_{n\downarrow}^+ c_{m\uparrow}>>$ which appear in (3.5), using (3.2) and (2.6), we have

$$\left\{ \omega -2\ S^z>J(0) - \frac{g}{2}\ <n_\uparrow - n_\downarrow> \right\} <<S_i^+;c_{n\downarrow}^+ c_{m\uparrow}>> =$$

$$= - <S^z> \sum_{i,\ell} J(i\ell)<<S_\ell^+;c_{n\downarrow}^+ c_{m\uparrow}>>$$

$$- g<S^z><<c_{i\uparrow}^+ c_{i\downarrow};c_{n\downarrow}^+ c_{m\uparrow}>> \quad (3.6)$$

Solving for (3.5) and (3.6), via a Fourier transform, we obtain

$$\left\{ \omega - 2\langle S^z\rangle [J(0)-J(k)] - \frac{g}{2}\langle n_\uparrow - n_\downarrow\rangle - \frac{g^2}{2}\langle S^z\rangle \chi(k,\omega)\right\} \langle\langle s_k^+ ; s_{-k}^-\rangle\rangle =$$

$$= \frac{1}{2\pi}\chi(k,\omega)\left\{\omega - 2\langle S^z\rangle [J(0)-J(k)] - \frac{g}{2}\langle n_\uparrow - n_\downarrow\rangle\right\} \qquad (3.7)$$

where J(k), ε(k), and χ(k,ω) are defined by

$$J(ij) = \frac{1}{N}\sum_k J(k)\, e^{-ik(R_i-R_j)} \qquad (3.8a)$$

$$T(ij) = \frac{1}{N}\sum_k \varepsilon(k)\, e^{-ik(R_i-R_j)} \qquad (3.8b)$$

$$\chi(k,\omega) = \frac{1}{N}\sum_q \frac{\langle n_{q\uparrow}\rangle - \langle n_{k+q\downarrow}\rangle}{\{\omega - \Delta - g\langle S^z\rangle - \varepsilon_{k+q} + \varepsilon_q\}} \qquad (3.8c)$$

For g=0, $\langle\langle s_k^+ ; s_{-k}^-\rangle\rangle = \frac{1}{2\pi}\chi(k,\omega)$ is the well known transverse susceptibility for the pure itinerant system. In Eq. (3.7), $\langle n_\uparrow - n_\downarrow\rangle/2$ is the polarization of the conduction electrons and $2\langle S^z\rangle [J(0) - J(k)]$ is the energy of magnons in a Heisenberg ferromagnet.

In the narrow conduction band limit we can put $\varepsilon_q \simeq \varepsilon_{k+q}$, for all k,q in the first Brillouin zone.

This simplifies the term in g^2 of (3.7) and the poles of the GF $\langle\langle s_k^+ ; s_{-k}^-\rangle\rangle$, so that we get as a final result

$$\langle\langle s_k^+ ; s_{-k}^-\rangle\rangle = \frac{\langle s^z\rangle}{\pi}\left\{\frac{D_o(k)}{\omega - \omega_o(k)} + \frac{D_a(k)}{\omega - \omega_a(k)}\right\} \qquad (3.9)$$

where

$$\omega_o(k) = \frac{1}{2}\left[\omega_1(k) + \omega_3\right] + \left\{\frac{1}{4}\left[\omega_1(k) - \omega_3\right]^2 + \omega_2\right\}^{1/2} \tag{3.10a}$$

$$\omega_a(k) = \frac{1}{2}\left[\omega_1(k) + \omega_3\right] - \left\{\frac{1}{4}\left[\omega_1(k) - \omega_3\right]^2 + \omega_2\right\}^{1/2} \tag{3.10b}$$

$$D_o(k) = \left[\omega_o(k) - \omega_1(k)\right]/2\left\{\frac{1}{4}\left[\omega_1(k) - \omega_3\right]^2 + \omega_2\right\}^{1/2} \tag{3.11a}$$

$$D_a(k) = \left[\omega_1(k) - \omega_a(k)\right]/2\left\{\frac{1}{4}\left[\omega_1(k) - \omega_3\right]^2 + \omega_2\right\}^{1/2} \tag{3.11b}$$

$$\omega_1(k) = 2\langle S^z\rangle\left[J(0)-J(k)\right] + \frac{g}{2}\langle n_\uparrow - n_\downarrow\rangle \tag{3.12a}$$

$$\omega_2 = \frac{g^2}{2}\langle S^z\rangle\langle n_\uparrow - n_\downarrow\rangle \tag{3.12b}$$

$$\omega_3 = g\langle S^z\rangle + \Delta \tag{3.12c}$$

$$\langle s^z\rangle = \frac{1}{2}\langle n_\uparrow - n_\downarrow\rangle \tag{3.12d}$$

From (3.11) we have

$$D_o(k) + D_a(k) = 1 \tag{3.13}$$

Equation (3.9) corresponds to equation (10) of reference 8, changing s, $D_o(k)$ and $D_a(k)$ for S, $C_a(k)$ and $C_o(k)$, respectively. Worth noting is the change from optical to acoustic indices ($D_o(k)$ to $C_a(k)$) as we go from the itinerant to the localized susceptibilities.

An analysis of both itinerant and localized dynamic susceptibilities, $\langle\langle s_k^+ ; s_{-k}^-\rangle\rangle$ and $\langle\langle S_k^+ ; S_{-k}^-\rangle\rangle$, and the above mentioned connection suggest how to interpret the coefficients

D's and C's as well as the existence of the optical and acoustic branches in the excitation spectra of the coupled system.

For g=0, in the narrow band limit, $\omega_o(k)$ is a line centered in Δ, and $\omega_a(k)$ reproduces the magnon spectrum of the localized system. For $g \neq 0$, the dynamic susceptibilities of the itinerant part now have features of the localized part. The coefficients $D_o(k)(D_a(k))$and the poles $\omega_o(k)(\omega_a(k))$ reflect, as a function of k, the importance of the itinerant and localized contributions. The same analysis can be made for the localized dynamic susceptibility, changing $D_o(k)(D_a(k))$ for $C_a(k)(C_o(k))$. The poles of the susceptibilities have also optical and acoustic contributions.

To conclude, we also consider the hybrid dynamic susceptibility $\langle\langle S_k^+ ; s_{-k}^- \rangle\rangle$, that can be obtained from (3.6) and (3.7). In the narrow band limit we have

$$\langle\langle s_k^+ ; S_{-k}^- \rangle\rangle = \frac{g}{\pi} \langle S^z \rangle \langle s^z \rangle \, B(k) \left\{ \frac{1}{\omega - \omega_a(k)} - \frac{1}{\omega - \omega_o(k)} \right\} \qquad (3.14)$$

where

$$B(k) = \frac{1}{2\left\{ \frac{1}{4}\left[\omega_1(k) - \omega_3\right]^2 + \omega_2 \right\}^{1/2}} \cdot \qquad (3.15)$$

An analysis of B(k) versus k shows that B(k) has a maximum at a k_o value for which $\omega_o(k)$ and $\omega_a(k)$ are closest to each other (see fig. 1 of ref. 8) and where the system may equally respond in either branch.

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