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N.B.Perkins, N.M.Plakida

SPIN DYNAMICS IN THE GENERALIZED
FERROMAGNETIC KONDO MODEL
FOR MANGANITES

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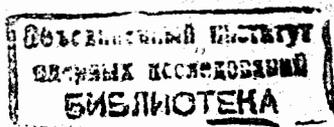
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1 Introduction

Manganites of the perovskite structure of the form $R_{1-x}B_xMnO_3$ (where R are trivalent rare-earth and B are divalent alkaline ions, respectively) and related compounds that present the phenomenon of "colossal" magnetoresistance (CMR) have recently attracted much attention both from the basic point of view and due to their potential application [1], [2]. The large magnetoresistance occurs close to the metal-insulator and the paramagnetic-ferromagnetic transitions where the interplay of transport, magnetic and structural properties is of the great importance (see [3]). The key elements of the manganese oxides are Mn ions. In the parent compound $LaMnO_3$ the electronic configuration of Mn^{+3} is $(t_{2g}^3e_g)$. In this configuration due to a strong intra-orbital Hund's coupling t_{2g}^3 electrons go into tightly bound d_{xy} , d_{yz} , d_{zx} core states and make up an electrically inert core Heisenberg spins S of magnitude $3/2$. The t_{2g}^3 configuration is very stable and remains localized over the entire range of doping.

In the undoped case, with one e_g electron per Mn ion, two e_g orbitals, $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ types, are splitted due to the Jahn-Teller effect. At low temperature e_g electrons occupy $d_{3z^2-r^2}$ and $d_{3y^2-r^2}$ ordered alternately in ab plane with their spins aligned to the core spin by interorbital Hund's coupling. Due to the Goodenough-Kanamori rules [4] it results in the A-type antiferromagnet (AFM) ground state (AFM vector $Q=(0, 0, 0.5)$) with spin $S = 2$ for $LaMnO_3$. Upon doping with holes by substituting La with Sr or any other divalent ions system becomes ferromagnetic (FM) and conducting. The hopping between two Mn sites is maximal when the core spins are parallel and minimum when they are antiparallel. That results in effective ferromagnetic exchange between the nearest neighbor core spins and thus leads to the FM metallic ground state of doped compounds. This behavior is qualitatively well described within the framework of the double exchange (DE) mechanism (see [5],[6],[7]). At higher hole concentration, $x \geq 0.5$, a charge ordering for holes is observed, and at $x = 1$ an insulating G-type AFM state (with $Q = (0.5, 0.5, 0.5)$) takes place for $CaMnO_3$ compound. Therefore to describe the experimentally obtained phase diagram (see, for example, [8]) one should take into account both the Heisenberg type of AFM exchange between the core t_{2g} electrons and the strong Hund coupling between t_{2g} and e_g electrons (see, e.g. [9, 10]). These competing interactions could be responsible for a coexistence of AFM and FM states observed recently in neutron scattering experiments in $(La_{0.25}Pr_{0.75})_{0.7}Ca_{0.3}MnO_3$ [11] and in the bilayer manganite $La_{1.2}Sr_{1.8}Mn_2O_7$ [12]. Also a crossover from an ideal isotropic FM spin-wave behaviour at low temperature to a diffusive spin propagation observed in $La_{0.7}Ca_{0.3}MnO_3$ [13] could be explained if one takes into account both the localized t_{2g} spin ($S = 3/2$) and the itinerant e_g spin ($\sigma = 1/2$) subsystems.

In the present paper we study the spin dynamics in manganites within the generalized ferromagnetic Kondo model (FKM) allowing for the AFM exchange interaction between t_{2g} spins. Unlike to the DE model (see, [14]), where $J_H/t \rightarrow \infty$ is considered and the system is treated as perfectly spin polarized with $S = 2$, in our work both the fluctuation of the localized and itinerant spins are taking into account. However, we ignore in the present calculations a possible orbital ordering



which is very important in explaining different types of AFM ordering in the insulating phases [10, 15] but plays less essential role in the FM state considered here. To take into account strong Coulomb interaction between e_g electrons which excludes the double occupancy of e_g electrons for a lattice site we employ the Hubbard operator technique. The spectrum of spin waves in the FM state is calculated by employing equations of motion for the matrix Green function (GF) for the localized and itinerant spins. In the next Section the model and general formalism for the GF are presented. The spin-wave spectrum in a generalized mean field approximation (MFA) is calculated in Sec. 3 and self-energy corrections and spin-wave damping are evaluated in Sec. 4.

2 The model

We consider an effective Hamiltonian of the generalized FM Kondo model which can be written in the following form [9]:

$$H = - \sum_{i,j,\sigma} t_{ij} X_i^{\sigma 0} X_j^{0\sigma} - \frac{J_H}{2S} \sum_i \mathbf{S}_i \cdot \boldsymbol{\sigma}_i + \frac{1}{2} \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (1)$$

The first term of Eq. (1) describes an electron hopping between Mn-ions where $X_i^{\sigma 0}$ is the creation operator of an electron with spin σ in one of the e_g orbitals. Here we neglect orbital degeneracy of e_g electrons and introduce orbital independent hopping parameter t_{ij} with $t_{ij} = t$ for the nearest neighbors. The second term describes the ferromagnetic Hund coupling ($J_H > 0$) between e_g and t_{2g} spins where \mathbf{S}_i refers to the localized Mn core spin $S = 3/2$. The third term describes the antiferromagnetic coupling of localized spins between the nearest neighbor sites. In real materials the coupling of core spins is not the same in different directions and should be described in the matrix form, but for simplicity we are analyzing the isotropic case ($J_{ij} = J$). We exclude the doubly occupied e_g state from the effective Hamiltonian by using the Hubbard operator representation because the electron-electron interaction has the largest energy scale (intra-atomic Coulomb interaction in the e_g orbitals) and can be estimated as 7–8 eV while $J_H \sim 1$ eV. Due to large Hund energy we neglect superexchange interaction between e_g electrons of the order of t^2/U [10]. The conduction bandwidth is smaller than the Hund coupling energy and from density-functional studies can be estimated as $t \simeq 0.15$ eV [16].

The HO's in Eq. (1) are defined as $X_i^{\alpha\beta} = |i, \alpha\rangle\langle i, \beta|$ for three possible states at the lattice site i : $|i, \alpha\rangle = |i, 0\rangle$, $|i, \sigma\rangle$ for an empty site and for a singly occupied site with spin $\sigma = (\uparrow, \downarrow) = (+, -)$. The completeness relation for the HO's reads as

$$X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} = 1. \quad (2)$$

For itinerant electrons the spin and density operators in Eq. (1) are expressed by HO's as

$$\sigma_i^{\uparrow} = X_i^{\uparrow\uparrow}, \quad \sigma_i^{\downarrow} = X_i^{\downarrow\downarrow}, \quad \sigma_i^z = \frac{1}{2}(X_i^{\uparrow\uparrow} - X_i^{\downarrow\downarrow}), \quad n_i = X_i^{\uparrow\uparrow} + X_i^{\downarrow\downarrow}. \quad (3)$$

The HO's obey the following commutation relations

$$[X_i^{\alpha\beta}, X_j^{\gamma\delta}]_{\pm} = \delta_{ij} (\delta_{\beta\gamma} X_i^{\alpha\delta} \pm \delta_{\delta\alpha} X_i^{\gamma\beta}). \quad (4)$$

In Eq.(4) the upper sign stands for the case when both HO's are Fermi-like ones (as, e. g., $X_i^{\sigma\sigma}$). The spin and density operators (3) are Bose-like and for them the lower sign in Eq.(4) should be taken.

It is assumed that the core spin operators S_i^{α} obey the standard commutation relations, e.g.,

$$[S_i^+, S_j^-] = 2\delta_{ij} S_j^z. \quad (5)$$

To treat the fluctuations of localized and itinerant spins at the same level of approximation we introduce the dynamic spin susceptibility (DSS) of the system in the matrix form

$$\chi(q, \omega) = \begin{pmatrix} \chi_{11} & \chi_{12} \\ \chi_{21} & \chi_{22} \end{pmatrix} = \langle\langle A_q | A_q^{\dagger} \rangle\rangle_{\omega}, \quad (6)$$

where

$$A_q = \begin{pmatrix} \sigma_q^+ \\ S_q^+ \end{pmatrix}, \quad A_q^{\dagger} = \begin{pmatrix} \sigma_q^- \\ S_q^- \end{pmatrix}.$$

Here

$$\langle\langle A_q | A_q^{\dagger} \rangle\rangle_{\omega} = -i \int_0^{\infty} dt e^{-i\omega t} \frac{1}{N} \sum_{q'} e^{-iq(t-m)} \langle\langle A_l(t), A_m^{\dagger} \rangle\rangle \quad (7)$$

denotes the Fourier transformed two-time retarded commutator Green function (GF) [18, 19]. The diagonal elements $\chi_{11}(q, \omega)$ and $\chi_{22}(q, \omega)$ stands for the itinerant and core spin GF, respectively, while the nondiagonal elements $\chi_{12}(q, \omega)$ and $\chi_{21}(q, \omega)$ define the cross-correlations between the two spin subsystems. The GF (6) obeys the following equation of motion

$$\omega \langle\langle A_q | A_q^{\dagger} \rangle\rangle_{\omega} = \langle\langle A_q, A_q^{\dagger} \rangle\rangle + \langle\langle \imath \dot{A}_q | A_q^{\dagger} \rangle\rangle_{\omega}, \quad (8)$$

$$\omega \langle\langle \imath \dot{A}_q | A_q^{\dagger} \rangle\rangle_{\omega} = \langle\langle \imath \dot{A}_q, A_q^{\dagger} \rangle\rangle + \langle\langle \imath \dot{A}_q | -\imath \dot{A}_q^{\dagger} \rangle\rangle_{\omega}.$$

These equations (8) could be easily combined in a more convenient form of the equation of motion [19]:

$$\omega \langle\langle A_q | A_q^{\dagger} \rangle\rangle_{\omega} = \langle\langle A_q, A_q^{\dagger} \rangle\rangle + \left(\langle\langle \imath \dot{A}_q, A_q^{\dagger} \rangle\rangle + \langle\langle \imath \dot{A}_q | -\imath \dot{A}_q^{\dagger} \rangle\rangle_{\omega}^{irr} \right) \cdot \frac{1}{\langle\langle A_q, A_q^{\dagger} \rangle\rangle} \cdot \langle\langle A_q | A_q^{\dagger} \rangle\rangle_{\omega}, \quad (9)$$

where the current is defined as $\imath \dot{A} = \imath dA/dt = [A, H]$ and in the matrix form can be given by the following expression:

$$\imath \dot{A}_q = \begin{pmatrix} \imath \dot{\sigma}_q^+ \\ \imath \dot{S}_q^+ \end{pmatrix}, \quad (10)$$

and

$$\langle\langle \imath \dot{A}_q | -\imath \dot{A}_q^{\dagger} \rangle\rangle_{\omega}^{irr} = \langle\langle \imath \dot{A}_q | -\imath \dot{A}_q^{\dagger} \rangle\rangle_{\omega}$$

$$- \langle \langle \dot{A}_q | A_q^+ \rangle \rangle_\omega \langle \langle A_q | A_q^+ \rangle \rangle_\omega^{-1} \langle \langle A_q | -\dot{A}_q^+ \rangle \rangle_\omega \quad (11)$$

is the irreducible part of the higher order GF.

We can rewrite (9) in the Dyson form

$$\chi_q(\omega) = [\omega \hat{\tau}_0 - \tilde{\Omega}_q - \tilde{\Pi}(q, \omega)]^{-1} \cdot I, \quad (12)$$

where $\hat{\tau}_0$ is the unity matrix and

$$I = \langle \langle A_q, A_q^+ \rangle \rangle = \begin{pmatrix} \langle \langle \sigma_q^+, \sigma_q^- \rangle \rangle & \langle \langle \sigma_q^+, S_q^- \rangle \rangle \\ \langle \langle S_q^+, \sigma_q^- \rangle \rangle & \langle \langle S_q^+, S_q^- \rangle \rangle \end{pmatrix} = \begin{pmatrix} 2\langle \sigma^z \rangle & 0 \\ 0 & 2\langle S^z \rangle \end{pmatrix} \quad (13)$$

where $\langle \sigma^z \rangle = \langle \sigma_i^z \rangle$ and $\langle S^z \rangle = \langle S_i^z \rangle$.

The matrix $\tilde{\Omega}_q = \Omega_q I^{-1}$ describes the mean field (MF) energy spectrum and $\tilde{\Pi}(q, \omega) = \Pi(q, \omega) I^{-1}$ is the self-energy matrix. They are given by

$$\Omega_q = \langle \langle \dot{A}_q, A_q^+ \rangle \rangle = \begin{pmatrix} \langle \langle \dot{\sigma}_q^+, \sigma_q^- \rangle \rangle & \langle \langle \dot{\sigma}_q^+, S_q^- \rangle \rangle \\ \langle \langle \dot{S}_q^+, \sigma_q^- \rangle \rangle & \langle \langle \dot{S}_q^+, S_q^- \rangle \rangle \end{pmatrix}, \quad (14)$$

$$\Pi(q, \omega) = \langle \langle \dot{A}_q | -\dot{A}_q^+ \rangle \rangle^{irr} = \begin{pmatrix} \langle \langle \dot{\sigma}_q^+ | \dot{\sigma}_q^- \rangle \rangle^{irr} & \langle \langle \dot{\sigma}_q^+ | \dot{S}_q^- \rangle \rangle^{irr} \\ \langle \langle \dot{S}_q^+ | \dot{\sigma}_q^- \rangle \rangle^{irr} & \langle \langle \dot{S}_q^+ | \dot{S}_q^- \rangle \rangle^{irr} \end{pmatrix}, \quad (15)$$

with

$$\dot{\sigma}_i^+ = \sum_j t_{ij} (X_i^{\uparrow 0} X_j^{0\downarrow} - X_i^{\downarrow 0} X_j^{0\uparrow}) - \frac{J_H}{2S} (S_i^+ \sigma_i^z - S_i^z \sigma_i^+), \quad (16)$$

$$\dot{S}_i^+ = -\frac{J_H}{2S} (S_i^z \sigma_i^+ - S_i^+ \sigma_i^z) - \sum_j J_{ij} (S_i^z S_j^+ - S_i^+ S_j^z). \quad (17)$$

3 Mean field approximation

Let us now examine the spectrum and DSS in mean field approximation (MFA). The spin-wave dispersion is determined by the following equation

$$\det(\omega \hat{\tau}_0 - \tilde{\Omega}_q) = 0. \quad (18)$$

From (14) we obtain for the matrix elements of $\tilde{\Omega}_q$

$$\tilde{\Omega}_q = \begin{pmatrix} [d + a(1 - \gamma_q)]/2\langle \sigma^z \rangle & -d/2\langle S^z \rangle \\ -d/2\langle \sigma^z \rangle & [d - b(1 - \gamma_q)]/2\langle S^z \rangle \end{pmatrix}, \quad (19)$$

where we are using the following notation:

$$d = \frac{J_H}{2S} (2\langle \sigma_i^z S_i^z \rangle + \langle \sigma_i^+ S_i^- \rangle), \quad (20)$$

$$a = zt(n_1^\uparrow + n_1^\downarrow), \quad b = zJN_1, \quad (21)$$

with $t_q = zt\gamma_q$, $\gamma_q = (2/z)(\cos q_x + \cos q_y + \cos q_z)$, where $z = 6$ for the simple three-dimensional cubic lattice with the nearest-neighbor hopping t . In (21) the nearest neighbor particle-hole and spin correlation functions are defined as follows

$$n_1^\sigma = \frac{1}{N} \sum_k \gamma_k n_k^\sigma, \quad n_k^\sigma = \langle X_k^{\sigma 0} X_k^{0\sigma} \rangle \\ N_1 = \frac{1}{N} \sum_k \gamma_k N_k, \quad N_k = 2\langle S_k^z S_{-k}^z \rangle + \langle S_k^+ S_k^- \rangle. \quad (22)$$

The equation (18) has two solutions describing two branches of spin wave excitations:

$$E_q^{1(2)} = \frac{1}{2} \left[\tilde{\Omega}_q^{11} + \tilde{\Omega}_q^{22} \mp \sqrt{(\tilde{\Omega}_q^{11} - \tilde{\Omega}_q^{22})^2 + 4\tilde{\Omega}_q^{12}\tilde{\Omega}_q^{21}} \right]. \quad (23)$$

For the model calculation we can expand this equation at $q \rightarrow 0$ and for the finite value of d we obtain

$$E_q^{(1)} \simeq D_1 q^2, \\ E_q^{(2)} \simeq \Delta + D_2 q^2, \quad (24)$$

where $E_q^{(1)}$ corresponds to the gapless (acoustic) spin-wave excitation with the stiffness D_1 given by

$$D_1 = \frac{a - b}{12(\langle S^z \rangle + \langle \sigma^z \rangle)}, \quad (25)$$

and $E_q^{(2)}$ describes the optic mode of the spin fluctuations with the gap Δ and the effective stiffness D_2 determined by the following expressions:

$$\Delta = d \frac{\langle S^z \rangle + \langle \sigma^z \rangle}{2\langle S^z \rangle \langle \sigma^z \rangle}, \\ D_2 = \frac{a\langle S^z \rangle^2 - b\langle \sigma^z \rangle^2}{12\langle S^z \rangle \langle \sigma^z \rangle (\langle S^z \rangle + \langle \sigma^z \rangle)}. \quad (26)$$

The ferromagnetic acoustic spin-wave becomes unstable when the stiffness $D_1 \rightarrow 0$ or $a - b = 0$ in Eq. (25). It may happen for small concentration of itinerant electrons, $n \leq n_c \simeq 2SJ/t \simeq 0.3$. The self-energy corrections considered below (see Eq. (47)) even increase the critical value n_c .

The spectrum of spin fluctuations in MFA are given by the spectral functions

$$B_{\alpha\beta}^{MF}(q, \omega) = -\frac{1}{\pi} \text{Im} \chi_{\alpha\beta}^{MF}(q, \omega + i\epsilon) \quad (27)$$

for the spin susceptibility

$$B_{11}^{MF}(q, \omega) = 2\langle \sigma^z \rangle \left(\frac{\tilde{\Omega}_q^{22} - E_q^{(1)}}{E_q^{(2)} - E_q^{(1)}} \delta(\omega - E_q^{(1)}) + \frac{E_q^{(2)} - \tilde{\Omega}_q^{22}}{E_q^{(2)} - E_q^{(1)}} \delta(\omega - E_q^{(2)}) \right), \quad (28)$$

$$B_{22}^{MF}(q, \omega) = 2(S^z) \left(\frac{\tilde{\Omega}_q^{11} - E_q^{(1)}}{E_q^{(2)} - E_q^{(1)}} \delta(\omega - E_q^{(1)}) + \frac{E_q^{(2)} - \tilde{\Omega}_q^{11}}{E_q^{(2)} - E_q^{(1)}} \delta(\omega - E_q^{(2)}) \right), \quad (29)$$

$$B_{12}^{MF}(q, \omega) = B_{21}^{MF}(q, \omega) = \frac{d}{E_q^{(2)} - E_q^{(1)}} (\delta(\omega - E_q^{(1)}) - \delta(\omega - E_q^{(2)})). \quad (30)$$

The spectral functions (28) - (30) obey the following sum rules:

$$\int_{-\infty}^{+\infty} d\omega B_{\alpha\beta}^{MF}(q, \omega) = I_{\alpha\beta},$$

$$\int_{-\infty}^{+\infty} \omega d\omega B_{\alpha\beta}^{MF}(q, \omega) = \Omega_q^{\alpha\beta} = \langle [i\dot{A}_q, A_q^+] \rangle_{\alpha\beta}, \quad (31)$$

where the matrices $I_{\alpha\beta}$ and $\Omega_q^{\alpha\beta}$ are given by the Eqs.(13), (14).

4 Self-energy corrections

The next step is to consider the self-energy corrections to the MF spectrum. Taking into account the self-energy corrections the equation for the spectrum transforms into the following form:

$$\det (\omega\hat{\tau}_0 - \tilde{\Omega}_q - \tilde{\Pi}(q, \omega)) = 0. \quad (32)$$

First we compute the self-energy matrix elements by using mode-coupling approximation in terms of the dressed particle-hole and spin fluctuations (see, e. g., Götze et al., [17]). This scheme is essentially equivalent to the self-consistent Born approximation in which the vertex corrections are neglected. The proposed scheme is defined by the following decoupling of the time-dependent correlation functions:

$$\langle X_m^{-0}(t) X_i^{0+}(t) X_j^{+0} X_l^{0-} \rangle \simeq \langle X_m^{-0}(t) X_l^{0-} \rangle \langle X_i^{0+}(t) X_j^{+0} \rangle, \quad (33)$$

$$\langle \sigma_i^z(t) S_m^-(t) \sigma_j^z S_l^+ \rangle \simeq \langle \sigma_i^z(t) \sigma_j^z \rangle \langle S_m^-(t) S_l^+ \rangle, \quad (34)$$

$$\langle S_i^z(t) S_m^-(t) S_j^z S_l^+ \rangle \simeq \langle S_i^z(t) S_j^z \rangle \langle S_m^-(t) S_l^+ \rangle. \quad (35)$$

The self-energy matrix elements are obtained by using the above defined decoupling scheme (33) and (35) with the spectral representation for the GF. The diagonal elements involve two contributions:

$$\Pi_{11(22)}(q, \omega) = \Pi_{11(22)}^{(1)}(q, \omega) + \Pi_{11(22)}^{(2)}(q, \omega). \quad (36)$$

The first one describes fluctuations of the internal degrees of freedom of the given spin subsystem. While the second one stems from the Hund's term and describes the coupling between itinerant and core spins.

For the itinerant spins the first term in Eq. (36) is due to decay of spin fluctuations into particle-hole pair excitations and reads as

$$\Pi_{11}^{(1)}(q, \omega) = \frac{1}{N} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\omega' d\omega_1 \frac{n(\omega_1 - \omega') - n(\omega_1)}{\omega - \omega' + i\epsilon}$$

$$\times \sum_{k, \sigma} t_{kq}^2 A^\sigma(k - q, \omega_1 - \omega') A^\sigma(k, \omega_1) \quad (37)$$

where $t_{kq} = zt(\gamma_k - \gamma_{k-q})$, $n(\omega) = (e^{\beta\omega} + 1)^{-1}$, and $A^\sigma(k, \omega)$ is the single-electron spectral function. By using the MF approximation for that, Eq. (A.7), we can integrate over the frequencies in Eq. (37) and obtain the following estimation:

$$\Pi_{11}^{(1)}(q, \omega) = \frac{1}{N} \sum_{k, \sigma} t_{kq}^2 (1 - n^\sigma) (1 - n^\sigma) \frac{n(\epsilon_{k-q}^\sigma) - n(\epsilon_k^\sigma)}{\omega + \epsilon_{k-q}^\sigma - \epsilon_k^\sigma + i\epsilon}. \quad (38)$$

It has the standard form for a one-loop particle-hole contribution to the self-energy (see, e.g. [20]).

The second terms in Eq.(36) are the same for both subsystem and coincide with the nondiagonal elements of the self-energy matrix due to the Hund coupling

$$\Pi_{11(22)}^{(2)}(q, \omega) = -\Pi_{12(21)}(q, \omega) = \Pi_H(q, \omega) \quad (39)$$

with

$$\Pi_H(q, \omega) = \left(\frac{J_H}{2S} \right)^2 \frac{1}{N\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\omega' d\omega_1 \frac{1 + N(\omega' - \omega_1) + N(\omega_1)}{\omega - \omega' + i\epsilon}$$

$$\times \sum_k [\text{Im}\chi_{22}^z(k, \omega_1) \text{Im}\chi_{11}(k - q, \omega' - \omega_1) + \text{Im}\chi_{22}(k, \omega_1) \text{Im}\chi_{11}^z(k - q, \omega' - \omega_1)] \quad (40)$$

where $N(\omega) = (e^{\beta\omega} - 1)^{-1}$, χ_{11}^z and χ_{22}^z denotes the longitudinal susceptibility of the itinerant and core spins, respectively.

Let us consider now the remaining $\Pi_{22}^{(1)}$ term which describes the fluctuations in the core spin subsystem. This contribution is due to the Heisenberg exchange between the localized spins and is given by

$$\Pi_{22}^{(1)}(q, \omega) = \frac{1}{N\pi^2} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\omega' d\omega_1 \frac{1 + N(\omega' - \omega_1) + N(\omega_1)}{\omega - \omega' + i\epsilon}$$

$$\times \sum_k J_{kq}^2 \text{Im}\chi_{22}^z(k - q, \omega_1) \text{Im}\chi_{22}(k, \omega' - \omega_1), \quad (41)$$

where $J_{kq} = zJ(\gamma_k - \gamma_{k-q})$.

In order to evaluate the longitudinal susceptibility in Eqs. (40), (41) for both subsystems we will use for them the simplest one-loop approximation (see, e.g. [20]). In this approximation the imaginary part of $\chi_{11}^z(q, \omega)$ is given as the convolution of the single-electron GFs

$$-\frac{1}{\pi} \text{Im}\chi_{11}^z(q, \omega) = \frac{1}{4N} \int_{-\infty}^{+\infty} d\omega' [n(\omega' - \omega) - n(\omega')]$$

$$\times \sum_{k, \sigma} A^\sigma(k, \omega') A^\sigma(k - q, \omega' - \omega). \quad (42)$$

The imaginary part of the core spin susceptibility χ_{22}^z can be expressed in the linear spin-wave approximation as

$$-\frac{1}{\pi} \text{Im}\chi_{22}^z(q, \omega) = \frac{1}{\pi^2 4S^2 N} \int_{-\infty}^{+\infty} d\omega' (N(\omega' - \omega) - N(\omega'))$$

$$\sum_k \text{Im}\chi_{22}(k-q, \omega' - \omega) \text{Im}\chi_{22}(k, \omega'), \quad (43)$$

which follows directly from the Holstein-Primakoff representation.

To study the spin wave spectrum including self-energy corrections let us consider the static limit for $q \rightarrow 0$. For the self-energy matrix we can write

$$\lim_{q \rightarrow 0} \Pi(q, 0) = \begin{pmatrix} -Aq^2 - d_1 & d_1 \\ d_1 & -Bq^2 - d_1 \end{pmatrix} \quad (44)$$

where

$$A = -\lim_{q \rightarrow 0} \frac{\Pi_{11}^{(2)}(q, 0)}{q^2}, \quad B = -\lim_{q \rightarrow 0} \frac{\Pi_{22}^{(2)}(q, 0)}{q^2}, \quad d_1 = -\Pi^{J_H}(0, 0). \quad (45)$$

Here the coefficient A, B , and d_1 are positive since $\Pi(q, 0) < 0$ in the second order of the perturbation theory. As it follows from Eqs. (44) and (45), the self-energy corrections coming from the Hund's coupling does not renormalize the spin stiffness and gives input only into the gap. Hence the spin-wave spectrum in the longwavelength limit can be written as

$$\begin{aligned} \omega_q^{(1)} &\simeq \tilde{D}_1 q^2 \\ \omega_q^{(2)} &\simeq \tilde{\Delta} + \tilde{D}_2 q^2 \end{aligned} \quad (46)$$

where the renormalized spin stiffness and the gap are given by

$$\begin{aligned} \tilde{D}_1 &= \frac{a - b - A - B}{12\langle S^z \rangle + \langle \sigma^z \rangle} \\ \tilde{D}_2 &= \frac{(a - A)\langle S^z \rangle^2 - (b + B)\langle \sigma^z \rangle^2}{12\langle S^z \rangle \langle \sigma^z \rangle (\langle S^z \rangle + \langle \sigma^z \rangle)} \\ \tilde{\Delta} &= \frac{(d - d_1)(\langle S^z \rangle + \langle \sigma^z \rangle)}{2\langle S^z \rangle \langle \sigma^z \rangle}. \end{aligned} \quad (47)$$

Now we consider the damping for the acoustic spin wave mode given by the imaginary parts of the self-energy matrix. For the damping induced by particle-hole excitations we get from Eq. (38) in the MF approximation for the single-electron GFs:

$$\begin{aligned} \Gamma_{11}^{(1)}(q, \omega) &= -\text{Im}\Pi_{11}^{(1)}(q, \omega + i\varepsilon) \\ &= \frac{\pi}{N} \sum_{k, \sigma} t_{kq}^2 (1 - n^\sigma)(1 - n^{\bar{\sigma}}) [n(\varepsilon_{k-q}^\sigma) - n(\varepsilon_k^{\bar{\sigma}})] \delta(\omega + \varepsilon_{k-q}^\sigma - \varepsilon_k^{\bar{\sigma}}) \end{aligned} \quad (48)$$

The contribution, due to the finite k -independent gap in single-electron spectrum in the ferromagnetic state disappears in the low frequency limit, $\Gamma_{11}^{(1)}(q, \omega) = 0$ for $\omega < h$ (see Eq. (A.14)).

The damping due to the antiferromagnetic exchange interaction given by the imaginary part of the self-energy $\Pi_{22}^{(1)}(q, \omega)$, Eq. (41), gives a small contribution proportional to q^2 in the longwavelength limit and can be disregarded due to small antiferromagnetic exchange interaction J .

The largest contribution to the damping of spin waves is given by the imaginary part of the self-energy due to the Hund coupling, Eq. (40):

$$\begin{aligned} \Gamma_H(q, \omega) &= -\text{Im}\Pi_H(q, \omega + i\varepsilon) = \left(\frac{J_H}{2S}\right)^2 \frac{1}{\pi N} \int_{-\infty}^{+\infty} d\omega_1 (1 + N(\omega - \omega_1) + N(\omega_1)) \\ &\times \sum_k [\text{Im}\chi_{22}(k - q, \omega - \omega_1) \text{Im}\chi_{11}^*(k, \omega_1) + \text{Im}\chi_{11}(k - q, \omega - \omega_1) \text{Im}\chi_{22}^*(k, \omega_1)]. \end{aligned} \quad (49)$$

Here for the imaginary parts of the spin susceptibilities $\chi_{11}(k, \omega)$ and $\chi_{22}(k, \omega)$ we will use their MF values in Eqs. (28), (29) taking into account only the acoustic $E_q^{(1)}$ mode:

$$-\frac{1}{\pi} \text{Im}\chi_{11}^{MF}(q, \omega) \simeq 2\langle \sigma^z \rangle \frac{\tilde{\Omega}_q^{22} - E_q^{(1)}}{E_q^{(2)} - E_q^{(1)}} \delta(\omega - E_q^{(1)}) = \Lambda_q^{11} \delta(\omega - E_q), \quad (50)$$

$$-\frac{1}{\pi} \text{Im}\chi_{22}^{MF}(q, \omega) \simeq 2\langle S^z \rangle \frac{\tilde{\Omega}_q^{11} - E_q^{(1)}}{E_q^{(2)} - E_q^{(1)}} \delta(\omega - E_q^{(1)}) = \Lambda_q^{22} \delta(\omega - E_q). \quad (51)$$

For the longitudinal spin susceptibilities in (49) we will use Eqs. (42), (43).

After integration over ω_1 we get the following result

$$\begin{aligned} \Gamma_H(q, \omega) &= (e^{\omega/T} - 1) \left(\frac{J_H}{2S}\right)^2 \frac{\pi}{4N^2} \sum_{k, k_1, \sigma} \Lambda_{k-q}^{22} (1 - n_\sigma)^2 \\ &\times N(E_{k-q}) n(\varepsilon_{k_1}^\sigma) [1 - n(\varepsilon_{k_1-k}^\sigma)] \delta(\omega - E_{k-q} + \varepsilon_{k_1-k}^\sigma - \varepsilon_{k_1}^\sigma) \\ &+ (e^{\omega/T} - 1) \left(\frac{J_H}{2S}\right)^2 \frac{\pi}{4S^2 N^2} \sum_{k, k_1} \Lambda_{k-q}^{11} \Lambda_{k_1}^{22} \Lambda_{k_1-k}^{22} \\ &\times N(E_{k-q}) N(E_{k_1}) [1 + N(E_{k_1-k})] \delta(\omega - E_{k-q} + E_{k_1-k}^{(1)} - E_{k_1}). \end{aligned} \quad (52)$$

It describes a spin wave damping due to its decay into an electron-hole pair and another spin wave (the first term) and a three spin-wave scattering process (the second term). The latter has a standard form for three magnon scattering (see, (31.2.20) in [21]). At low energy regime ($\omega \rightarrow 0$) and at the longwavelength limit the requirements for conservation of energy and momentum allow only small wave vectors and thus only small energies. Hence we can consider Λ_k^{11} and Λ_k^{22} as k -independent. In the limit $k \rightarrow 0$ we obtain

$$\Lambda_k^{11} \simeq \Lambda_0^{11} = 2\langle \sigma^z \rangle \frac{\langle \sigma^z \rangle}{\langle S^z \rangle + \langle \sigma^z \rangle}, \quad \Lambda_k^{22} \simeq \Lambda_0^{22} = 2\langle S^z \rangle \frac{\langle S^z \rangle}{\langle S^z \rangle + \langle \sigma^z \rangle}. \quad (53)$$

In this approximation from the Eq. (52) follows that at low energies, ($\omega \ll T$), the damping has a linear ω -dependence, $\Gamma^{J_H}(q, \omega) \sim \omega$, and does not depend explicitly on the wave vector q . In the low temperature region, ($\omega \ll T \ll \omega_0$) where ω_0 is the maximal acoustic spin-wave frequency, estimations for $\Gamma_H(q, \omega)/\omega$ show that the first contribution in Eq. (52) is proportional to $(T/\omega_0)(J_H^2/N(\varepsilon_F)v_F k_0)$ where $N(\varepsilon_F)$ is the density of state at the Fermi level and v_F is the Fermi velocity, $k_0 \simeq 2\pi/a$ and a is a lattice constant. The second term gives to the damping the contribution proportional to $(T/\omega_0)(J_H/\omega_0)^2$. To give more accurate estimations for the spin-wave damping numerical studies should be performed which will be considered elsewhere.

5 Conclusions

In the present paper we have calculated dynamical spin susceptibility for the generalized ferromagnetic Kondo model (1) by taking into account explicitly both the strong Hund interaction for the itinerant e_g and localized t_{2g} electrons and AFM interaction between the t_{2g} electrons. We consider the ferromagnetic phase and therefore neglect a possible orbital ordering of the e_g electrons. Strong electron correlations between e_g electrons are treated within the Hubbard operator technique which is important in calculation of the single-electron GF for the itinerant electrons.

We have proved that even in the MFA described by the frequency matrix, Eq. (19), we get the acoustic spin-wave excitations, Eq. (24), due to coupling of the two modes with gaps for itinerant and localized electrons. The gapless mode should appear in the model (1) with rotation symmetry for spin system. A gapless mode in the limit $J_H \rightarrow \infty$, considered in Ref. [14], was obtained only by taking into account self-energy corrections. In our case the self energy corrections calculated in the self-consistent Born approximation, Eqs. (32)-(34), resulted in additional renormalization of the stiffness of the acoustic ferromagnetic spin waves. The imaginary parts of the self-energy gives the damping of spin waves. We have evaluated the most important contribution due to Hund coupling in the second order, Eq. (49), which can be described as a three magnon scattering. The damping of acoustic spin waves is proportional to the frequency for $\omega \ll T$, Eq. (51), and should be small for small wave vectors. To give numerical estimations one should solve self-consistently the system of equations for the matrix spin susceptibility, Eq. (6), and the self-energy functions, Eq. (37). Also the spectrum of single electron excitations, given in the Appendix, should be evaluated to consider the itinerant electron contributions to the spin waves, Eq. (36). These problems will be considered elsewhere.

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Appendix

In this Appendix we evaluate the single-electron Green function defined as

$$G^\sigma(k, \omega) = \langle \langle X_k^{0\sigma} | X_k^{\sigma 0} \rangle \rangle_\omega \quad (A.1)$$

with the corresponding spectral function $A_k^\sigma(\omega) = -(1/\pi) \text{Im} G^\sigma(k, \omega + i\epsilon)$. In the site representation the equation of motion for $G^\sigma(k, \omega)$ reads as

$$\omega \langle \langle X_i^{0\sigma} | X_k^{\sigma 0} \rangle \rangle_\omega = \langle \{ X_i^{0\sigma}, X_j^{\sigma 0} \} \rangle + \langle \langle X_i^{0\sigma} | X_j^{\sigma 0} \rangle \rangle_\omega \quad (A.2)$$

Using the commutation relations, Eq.(4), we obtain

$$X_i^{0\sigma} = [X_i^{0\sigma}, H] = - \sum_{l \neq i} t_{il} [(X_i^{00} + X_i^{\sigma\sigma}) X_l^{0\sigma} + X_i^{\sigma\sigma} X_l^{0\sigma}]$$

$$- \frac{J_H}{4S} [\sigma S_i^z X_i^{0\sigma} + S_i^z X_i^{\sigma\sigma}] \quad (A.3)$$

The next step is to define the irreducible part $Z_i^{0\sigma}$ of the current operator $X_i^{0\sigma}$ by

$$X_i^{0\sigma} = \sum_l \epsilon_{il}^\sigma X_l^{0\sigma} + Z_i^{0\sigma}, \quad \langle \{ Z_i^{0\sigma}, X_j^{\sigma 0} \} \rangle = 0 \quad (A.4)$$

The definition gives for the frequency matrix

$$\epsilon_{ij}^\sigma = \langle \{ X_i^{0\sigma}, X_j^{\sigma 0} \} \rangle / (1 - n^\sigma), \quad (A.5)$$

where by using the completeness relation, Eq.(2), we write $\langle \{ X_i^{0\sigma}, X_j^{\sigma 0} \} \rangle = \delta_{i,j} (1 - n^\sigma)$ with $n^\sigma = \langle n_i^\sigma \rangle$. By using equation of motion (A.3) we get

$$\begin{aligned} \langle \{ X_i^{0\sigma}, X_j^{\sigma 0} \} \rangle &= -t_{ij} ((1 - n_i^\sigma)(1 - n_j^\sigma)) - t_{ij} \langle X_i^{\sigma\sigma} X_j^{\sigma\sigma} \rangle \\ &+ \sum_l t_{il} \langle X_l^{\sigma 0} X_i^{0\sigma} \rangle - \frac{J_H}{4S} \sigma \langle S_i^z \rangle (1 - n^\sigma) \delta_{ij} - \frac{J_H}{4S} \langle S_i^z X_i^{\sigma\sigma} \rangle \delta_{ij}. \end{aligned} \quad (A.6)$$

In the present paper we will not include the self-energy correction coming from $Z_i^{0\sigma}$ term (A.4) and treat the single-electron GF within the linear, MF type approximation. That results in the following form of the single-electron GF

$$G^\sigma(k, \omega) = \frac{1 - n^\sigma}{\omega - \epsilon_k^\sigma} \quad (A.7)$$

By introducing the nearest neighbor charge-spin correlation function

$$\begin{aligned} N_{1,\sigma}^{cs} &= \frac{1}{N} \sum_k \gamma_k [\langle X_k^{\sigma\sigma} X_{-k}^{\sigma\sigma} \rangle + \langle X_k^{\sigma\sigma} X_k^{\sigma\sigma} \rangle] \\ &= \langle X_i^{\sigma\sigma} X_{i+a}^{\sigma\sigma} \rangle + \langle X_i^{\sigma\sigma} X_{i+a}^{\sigma\sigma} \rangle \end{aligned} \quad (A.8)$$

we can rewrite the frequency matrix in the form

$$\epsilon_{ij}^\sigma = \epsilon^\sigma \delta_{ij} + \epsilon_{ij}^{\sigma\sigma} \quad (A.9)$$

where

$$\epsilon_{ij}^{\sigma\sigma} = t_{ij} [(1 - 2n^\sigma) + N_{1,\sigma}^{cs}] / (1 - n^\sigma) \quad (A.10)$$

is the one particle spectrum in the linear approximation, and

$$\epsilon^\sigma = - \frac{J_H}{4S} \left[\sigma \langle S^z \rangle + \frac{\langle S_i^z X_i^{\sigma\sigma} \rangle}{1 - n^\sigma} \right] + \frac{z t n_1^\sigma}{1 - n^\sigma}, \quad (A.11)$$

is the spin-dependent energy shift of the spectrum. In the momentum space the spectrum is

$$\epsilon_k^\sigma = \sum_{R_{ij}} e^{-ikR_{ij}} \epsilon_{ij}^\sigma = \epsilon^\sigma - z t_{eff}^\sigma \gamma_k, \quad (A.12)$$

where

$$t_{eff}^\sigma = t [(1 - 2n^\sigma) + N_{1,\sigma}^{cs}] / (1 - n^\sigma), \quad (A.13)$$

is an effective bandwidth that is narrowed and spin dependent due to the spin and charge correlations. In the MFA in the ferromagnetic state we have a spin gap in the single-electron spectrum:

$$\epsilon_k^\sigma - \epsilon_k^\sigma \simeq \sigma (J_H/2S) \langle S^z \rangle = \sigma h. \quad (A.14)$$

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Перкинс Н.Б., Плакида Н.М.

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Спиновая динамика в обобщенной ферромагнитной модели
Кондо для манганитов

Проведено вычисление динамической спиновой восприимчивости в обобщенной модели Кондо, описывающей взаимодействие зонных электронов e_g типа с локализованными электронами, t_{2g} типа, связанными антиферромагнитным обменом. Показано, что спин-волновой спектр системы в ферромагнитной фазе в приближении среднего поля имеет акустическую и оптическую ветви. Рассчитаны собственно-энергетические поправки к спектру и оценено затухание акустических магнонов.

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Perkins N.B., Plakida N.M.

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Spin Dynamics in the Generalized Ferromagnetic Kondo Model
for Manganites

Dynamical spin susceptibility is calculated for the generalized ferromagnetic Kondo model which describes itinerant e_g electrons interacting with localized t_{2g} electrons with antiferromagnetic coupling. The calculations done in the mean field approximation show that the spin-wave spectrum of the system in ferromagnetic state has two branches, acoustic and optic ones. Self-energy corrections to the spectrum are considered and the acoustic spin-wave damping is evaluated.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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