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Study of dynamic spin susceptibility in Kondo lattice

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ABSTRACT

The dynamic spin susceptibility $\chi(q,\omega)$, which is related to the inelastic neutron scattering cross-section, gives important information about the low energy excitations of the systems. The spectral density distribution function (SDF) of the neutron scattering is directly proportional to the imaginary part of the $\chi(q,\omega)$. Attempt is made in the present communication to calculate the longitudinal spin susceptibility for heavy fermion systems (HFS) to study resonance peaks at correlation temperature (T_N) and Kondo temperature (T_K). The model Hamiltonian consists of c–f electron exchange term and Heisenberg type inter-site spin–spin correlation in a mean-field approximation, besides the terms containing the conduction electron and f-electron contributions in presence of the hybridization between them in the Hamiltonian. The two particle Green functions are calculated using the equations of motion by method of Zubarev's technique. The microscopic model calculation shows two resonance peaks, one at Kondo excitation energy and another at correlation energy exhibiting the excellent interplay between them for different model parameters.

1. Introduction

The ground state of Kondo atom is a non-magnetic singlet state in case of a single impurity [1], while there is a strong competition between the Kondo effect and the magnetic ordering in the heavy fermion compounds [2]. Thus some Cerium (Ce) Kondo compounds are, at low temperature, either non-magnetic, as in case of single impurity, or magnetically ordered [3,4]. The well-known "Doniach diagram" gives a qualitative description of the competition between the Kondo effect and the magnetic ordering as a function of the exchange integral J_K (with $J_K<0$). Kondo temperature T_K increases experimentally with $|J_K|$, while the real ordering temperature T_N increases initially with increasing $|J_K|$, then passes through a maximum and tends to zero at a critical value. Such behaviour of T_N has been observed experimentally in $CePd_2Al_3$, $CeAl_2$, $CePd_2Si_2$ and $CeRb_2Si_2$ [5]. The description of phase diagram by Doniach to explain the above effects appears to be too simplified for the really observed Kondo temperature T_K. In a paper by Iglesias and coworkers [6,7] have taken the effect of anti-ferromagnetic correlation in the non-magnetic phase. Moreover, the occurrence of short range magnetic correlation has been observed experimentally by neutron diffraction experiment at low temperatures in $CeCu_6$ and $CeRu_2Si_2$ [8,9]. It has been found that incommensurate and anti-ferromagnetic correlations develop at low temperature bellow $T_N \simeq 60-70$ K in $CeRu_2Si_2$ [8,9] or $T_N \simeq 10$ K in $CeCu_6$ [8] which are clearly larger than Kondo temperature $T_K \simeq 14-23$ K in $CeRu_2Si_2$ or $T_K \simeq 5$ K in $CeCu_6$.

The dynamic spin susceptibility $\chi(\omega)$, which is related to the inelastic neutron scattering (INS) cross-section, gives important information about the low energy excitation of the system. In this paper, we apply random phase approximation (RPA) theory [10] to calculate dynamical longitudinal magnetic susceptibility of conduction electron in the Kondo model. The magnetic excitation in heavy fermion systems (HFS) provides valuable information for the nature HF states in Ce and uranium compounds [10]. Aeppli et al. [11] performed neutron scattering measurements on $CeCu_6$ which is a typical HF compound with an exceptionally large specific heat constant at low temperatures [12,13]. The cross-section of the inelastic scattering for $k_BT\langle\langle\hbar\omega$ is proportional to $\mathrm{Im}\,\chi(q,\omega)$, where χ is the dynamical spin susceptibility. Some authors [14–18] have calculated $\chi(q,\omega)$ in Anderson model applying $1/N_f$ method, where N_f is degeneracy of 4f-electrons. In above model, they could explain the Kondo peak but could not explain the f-electron correlation interaction peaks. In their calculation, they assumed f–f Coulomb interaction U to be infinity.

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In the present communication, we attempt to study the interplay between the Kondo coupling and short range f–f correlations within the mean-field approximation. Therefore, we investigate the momentum and frequency dependent dynamical spin susceptibility $\chi(q,\omega)$ for HFS. In particular, we compare the formation of the resonant spin excitations (resonance peaks) with the resonance peak in the inelastic neutron scattering experiment. For this purpose, a model Hamiltonian is formulated in Section 2. The mean-field Kondo parameter (λ), magnetic correlation parameter (Γ) and the chemical potential (μ) are calculated by minimizing the total energy of the system as described in Section 3. The calculation of dynamic spin susceptibility $\chi(q,\omega)$ is presented in Section 4. Finally, the results and discussion are presented in Section 5.

2. Formalism

Iglesias and coworkers [6,7] have considered the Kondo-lattice model including nearest neighbour magnetic exchange interaction and studied both the Kondo state and inter-site magnetic correlations using a mean-field approximation. Later Baral et al. [19] have considered the similar model and reported the interplay of Kondo effect and superconductivity in HFS. We consider the following Hamiltonian [6,19] to describe the Kondo lattice with short-range magnetic correlation:

$$\mathscr{H} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + E_0 \sum_{i,\sigma} f^\dagger_{i,\sigma} f_{i,\sigma} - J_H \sum_{i,j} \vec{S}^f_i \cdot \vec{S}^f_j - J_K \sum_i \vec{s}^c_i \cdot \vec{S}^f_i \quad (1)$$

where $c_{k,\sigma}(c^\dagger_{k,\sigma})$ and $f_{i,\sigma}(f^\dagger_{i,\sigma})$ are the annihilation (creation) operators of conduction and f-electrons for wave vector $\vec{k}$ and spin σ at site i, respectively. $\vec{s}^c_i$ and $\vec{S}^f_i$ are the spin operators for conduction and f-electrons. In Eq. (1), the third term describes the Heisenberg interaction between neighbouring f-magnetic moments and under the condition $J_H > 0$ for a ferromagnetic coupling and $J_H < 0$ for an anti-ferromagnetic coupling. The last term is the c–f exchange term for $J_K(<0)$ being the Kondo coupling. We treat the Hamiltonian in Eq. (1) in a "mean-field" approximation to find simultaneously the Kondo effect and the anti-ferromagnetic correlation. The two mean-field parameters are: (i) $\lambda = \langle f^\dagger_{i,\sigma} c_{i,\sigma}\rangle$ which describes the formation of Kondo singlet and (ii) $\Gamma = \langle f^\dagger_{i,\sigma} f_{i,\sigma}\rangle$ accounts for magnetic correlation between neighbouring localized spins. Within the mean-field approximation the Hamiltonian Eq. (1) can be written after Fourier transformation as

$$\mathscr{H} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_{k,\sigma} \varepsilon_f(k) f^\dagger_{k,\sigma} f_{k,\sigma} + V(\lambda) \sum_{k,\sigma} (c^\dagger_{k,\sigma} f_{k,\sigma} + f^\dagger_{k,\sigma} c_{k,\sigma}) - 2J_K\lambda^2 - ZJ_H\Gamma^2 \quad (2)$$

where effective f-level $\varepsilon_f(k) = E_0 + B\varepsilon_k$ with $B = 2ZJ_H\Gamma/W$ and effective c–f hybridization $V(\lambda) = J_K\lambda$ and W is the band width of conduction band, with the nearest neighbour sites Z. In Eq. (1), f-band is taken as dispersion-less with constant density of states. Within this mean-field interaction, the magnetic interaction J_H leads to a finite band width for the f-states, while the Kondo interaction J_K produces a hybridization between conduction band of width W and the f-band of effective width $\varepsilon_f(k)$.

3. Expressions for magnetic correlation Γ and Kondo singlet λ

In order to diagonalize the mean-field Hamiltonian in Eq. (2) and to calculate Kondo singlet parameter λ and correlation parameter Γ, we define two Green functions for the conduction electrons as

$$G_1(k,\omega) = \langle\langle c_{k,\sigma}; c^\dagger_{k,\sigma}\rangle\rangle_\omega \quad (3)$$

$$G_2(k,\omega) = \langle\langle f_{k,\sigma}; c^\dagger_{k,\sigma}\rangle\rangle_\omega \quad (4)$$

These Green functions are calculated by equations of motion by Zubarev's technique [20] and expressed as closed form as

$$G_1(k,\omega) = \frac{(\omega - \varepsilon_f(k))}{2\pi|D(\omega)|} \quad (5)$$

$$G_2(k,\omega) = \frac{V(\lambda)}{2\pi|D(\omega)|} \quad (6)$$

where

$$|D(\omega)| = (\omega - \varepsilon_k)(\omega - \varepsilon_f(k)) - V^2(\lambda) \quad (7)$$

Equating $|D(\omega)| = 0$, the two quasi-particle bands are found to be

$$\omega_{1,2}(k) = \tfrac{1}{2}[\varepsilon_k - \mu + \varepsilon_f(k) \pm \sqrt{(\varepsilon_k - \mu - \varepsilon_f(k))^2 + 4V^2(\lambda)}] \quad (8)$$

The position of f-level E_0 and chemical potential μ are determined self-consistently in order to satisfy the following conditions:

$$\sum_{k,\sigma} \langle f^\dagger_{k,\sigma} f_{k,\sigma}\rangle = 1 \quad (9)$$

$$\sum_{k,\sigma} \langle c^\dagger_{k,\sigma} c_{k,\sigma}\rangle = 1 \quad (10)$$

Thus within this mean-field approach, we deal with two quasi-particle bands of energies $\omega_\alpha(k)$ for $\alpha = 1,2$ given in Eq. (8) and, by using the two conditions in Eqs. (9) and (10), the total energy of system is given by

$$E = 2\sum_{k,\alpha} \omega_\alpha(k) f(\beta\omega_\alpha(k)) - ZJ_H\Gamma^2 - 2J_K\lambda^2 \quad (11)$$

where $f(\beta\omega_\alpha)$ describes the Fermi–Dirac distribution function. The temperature dependent mean-field parameters $\lambda(T)$ and $\Gamma(T)$ are determined by minimizing the total energy E. The minimization of the total energy for $\lambda(T)$ (i.e., $\partial E/\partial\lambda = 0$) gives

$$1 = \sum_k \frac{J_K}{P(k)}[K(\beta\omega_1(k)) - K(\beta\omega_2(k))] \quad (12)$$

The minimization of the total energy for $\Gamma(T)$ (i.e., $\partial E/\partial\Gamma = 0$) gives

$$1 = \frac{1}{\Gamma}\sum_k \frac{\varepsilon_k}{WP(k)}[(\omega_1(k) - B\varepsilon_k - E_0)K(\beta\omega_2(k)) - (\omega_2(k) - B\varepsilon_k - E_0)K(\beta\omega_1(k))] \quad (13)$$

We know that the chemical potential $\mu(T)$ is the free energy of conduction electrons per particle. The minimization of total energy w.r.t. chemical potential $\mu(T)$ at finite temperature, (i.e., $\partial E/\partial\mu = 0$) we get the temperature dependent of chemical potential μ

$$0 = \sum_k \frac{1}{P(k)}[(\omega_2(k) - B\varepsilon_k - E_0)K(\beta\omega_2(k)) - (\omega_1(k) - B\varepsilon_k - E_0)K(\beta\omega_1(k))] \quad (14)$$

where the functions $K(\beta\omega_\alpha(k))$ for $\alpha = 1,2$ are given by

$$K(\beta\omega_\alpha(k)) = \frac{1 + (1 - \beta\omega_\alpha(k))\exp(\beta\omega_\alpha(k))}{[\exp(\beta\omega_\alpha(k)) + 1]^2} \quad (15)$$

and

$$P(k) = \sqrt{(\varepsilon_k - \mu - \varepsilon_f(k))^2 + 4V^2(\lambda)} \quad (16)$$

Then, the temperature dependence of $\Gamma(T)$, $\lambda(T)$ and $\mu(T)$ can be calculated self-consistently along with conditions in Eqs. (9) and (10). When λ equals to zero, the correlation function $(s^c_i \cdot S^f_j)$