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Dynamic spin susceptibility in f-electron Systems in the ferromagnetic state

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Abstract: In order to make a theoretical study of dynamic spin susceptibility due to strong spin fluctuations of f-electrons, in low temperature ferromagnetic state, in lanthanide or actinide compounds, called as f-electron systems, and their anomalous physical properties, we use Zubarev's technique and the periodic Anderson model (PAM) with f-electron Coulomb correlation energy in a mean-field approximation in ferromagnetic limit. The f-electron occupancies for spin up and spin down and the magnetization are calculated numerically and self-consistently, from f-electron Green's function. The difference for up spin and down spin f-electron occupancy, gives rise to ferromagnetism in the system. We calculate temperature dependent susceptibility and by varying the different model parameters such as the position of f-level, Coulomb interaction energy and strength of hybridization between conduction and f-electrons of the system, we study the variation of temperature dependent susceptibility. It is found in the ferromagnetic limit of the coulomb interaction, the susceptibility is enhanced up to Curie temperature (T_c) throughout the temperature and with increase of Coulomb correlation energy, the Curie temperature is enhanced.
Keywords: f-electron systems, Ferromagnetism, Susceptibility
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1. INTRODUCTION

Compounds consisting of lanthanides or actinides with partly filled 4f or 5f orbitals are called f-electron systems. These systems, at low temperature, have large electronic specific heat coefficient and magnetic susceptibility γ corresponding to their enhancement of electronic mass. The low temperature large Sommerfeld coefficient and ordered magnetic moment suggest both itinerant and localized f-electron behaviour [1,2]. The characteristic of both itinerant and localized f-electrons is revealed from neutron scattering experiments on f-electron systems like U_2Zn_{17} [3]. The itinerancy of f-electrons due to hybridization of f-electrons with the conduction electrons and Coulomb interaction between localized f-electrons readjust f-level position with respect to the Fermi level. For f-level, nearer to Fermi level, the systems exhibit mixed valent behavior and away from Fermi level, the systems show heavy fermion behavior. The 4f electrons of lanthanides are highly localized hybridizing weakly with the conduction electrons, whereas the 5f electrons of actinides hybridize strongly with the conduction electrons due to spatially extended dispersive f bands [4- 6]. At high temperatures, the f-electrons remain localized and weakly interact with the conduction electrons.

In low temperature regime, below characteristic temperature T^*, the f-electron spins remain strongly fluctuating, leading to different low temperature magnetic orderings and anomalous physical properties. The magnetism of these systems depends on the degree of localization of f-electrons and their spin fluctuations. The difference between f-electron occupancies for up spin and down spin gives rise to ferromagnetism. At low temperature, below 10K, the specific heat coefficient γ of $CeFePo$ increases logarithmically to the value 700 $mJ/molK^2$ and levels off down to 1K. This compound has strong f-electron correlations and FM fluctuations below 0.4K. Above 0.4K, there is no evidence for magnetic ordering[7]. In $YbNi_4P_2$ magnetically ordered f-electron system, ferromagnetism sets in at Curie temperature T_c= 0.17K in the heavy fermion state. It has a huge Sommerfeld coefficient 2000 $mJ/molK^2$ well below the T_c [8]. The f-electron system $CeAgSb_2$ undergoes ferromagnetic transition below the Curie temperature $T_c = 9.6K$. Neutron diffraction [9] confirms the ferromagnetic ground state of $CeAgSb_2$. Sm-based skutterudite compounds such as $SmFe_4P_{12}$ and $SmOs_4Sb_{12}$ exhibit heavy fermion behaviour and ferromagnetism. Below 2.6K$SmOs_4Sb_{12}$ has electronic specific heat coefficient $\gamma \simeq 820mJ/molK^2$ in heavy fermion ferromagnetic state[10-13]. In heavy fermion state, for the systems $UCo_2Zn_{20}$and URh_2Zn_{20}, the magnetic susceptibility χ(T) acquire maximum value at 7K and 9K respectively. Around this temperature i.e. below 10K, the Sommerfeld coefficient γ = 450 $mJ/molK^2$for $UCo_2Zn_{20}$and γ = 300$mJ/molK^2$ for URh_2Zn_{20}[14]. The magnetic susceptibility χ(T) of URu_2Zn_{20} increases monotonically as the temperature decreases, to the value $\chi \simeq 11.1 \times 10^{-3}\, emu/mol$ at temperature 2K. At 2K, the susceptibility of UCo_2Zn_{20} is about $37.2 \times 10^{-3}\, emu/mol$, which is 3.3 times larger than for the Ru case. C/T for URu_2Zn_{20} has the magnitude γ = 190 $mJ/molK^2$at 2K. The uranium based heavy fermion compound UIr_2Zn_{20} undergoes ferromagnetic state at 2.1 K with a large electronic specific heat coefficient 450 $mJ/molK^2$[15]. Rout et.al. have earlier studied dynamic spin susceptibility in Kondo lattice [16]. Recently, they have studied velocity of sound and ultrasonic attenuation in f-electron systems both in paramagnetic and ferromagnetic states [17-20].

In the present communication, in order to study the longitudinal dynamic spin susceptibility in f-electron systems, we have considered the periodic Anderson model [21] with the repulsive Coulomb interaction between f-electrons considered within mean-field approximation leading to ferromagnetism in the system. The spin up and spin down f-electron occupation numbers and the f-electron magnetization are calculated from f-electron Green's function numerically and self-consistently by using Zubarev's technique. Then the low temperature dependent dynamic spin susceptibility is computed numerically. The susceptibility exhibits high value in heavy fermion state of the system where the position of the f electron level is away from the Fermi level with the lower strength of hybridization between f and conduction electrons. The formalism for the model Hamiltonian is given in section 2 and calculation of longitudinal spin susceptibility in section 3. The results and discussion is described in section 4. The conclusion is given in section 5.

2. Formalism

The f-electron System is described by the periodic Anderson model by the Hamiltonian which is written as

$$H_0 = \sum_{k,\sigma}(\varepsilon_k - \mu - \sigma B_c)\, c^{\dagger}_{k\sigma}c_{k\sigma} + \sum_{k,\sigma}(\varepsilon_f - \sigma B_f)\, f^{\dagger}_{k\sigma}f_{k\sigma} + V\sum_{k,\sigma}\left(f^{\dagger}{}_{k,\sigma}c_{k,\sigma} + c^{\dagger}{}_{k,\sigma}f_{k,\sigma}\right) + U\sum_{k,\sigma} n^f_{i\uparrow}n^f_{i\downarrow} \quad \textbf{(1)}$$

The 1st and 2nd terms describe the bands of conduction and f-electrons with $c^{\dagger}_{k\sigma}(c_{k\sigma})$ and $f^{\dagger}_{k\sigma}(f_{k\sigma})$ as their creation (annihilation) operators. ε_k and ε_f are the conduction and f-electron energies, μ is bare electron chemical potential. B_c and B_f are the magnetic fields applied to conduction and f-electrons. The third term describes the hybridization of conduction and f-electrons with V is strength of hybridization. The fourth term describes Coulomb interaction between f-electrons of opposite spins with U as the Coulomb interaction energy.

Using mean-field approximation and taking Fourier transformation, the Coulomb term can be written as $U\sum_{k,\sigma} < n^f_{-\sigma} > n^f_{k\sigma}$ and the Hamiltonian in eqn.(1) is rewritten as

$$H_0 = \sum_{k,\sigma}\varepsilon_{k\sigma}c^{\dagger}{}_{k,\sigma}c_{k,\sigma} + \sum_{k,\sigma}E_{0\sigma}f^{\dagger}{}_{k,\sigma}f_{k,\sigma} + V\sum_{k,\sigma}\left(f^{\dagger}{}_{k,\sigma}c_{k,\sigma} + c^{\dagger}{}_{k,\sigma}f_{k,\sigma}\right) \quad (2)$$

3. Calculation of Susceptibility

The longitudinal magnetic spin susceptibility of f- electron system is defined as

$$\chi^{zz}(q,\omega) = \ll m_z(q,t);\ m_z(-q',t') \gg_{\omega} \quad (3)$$

Where the z-component of magnetization $m_z(q,t)$ is given by

$$m_z(q,t) = \mu_B\sum_{k,q}(c^{\dagger}_{k+q\uparrow}c_{k\uparrow} - c^{\dagger}_{k+q\downarrow}c_{k\downarrow}) = \mu_B\sum_{k,q,\sigma}\sigma(c^{\dagger}_{k+q\sigma}c_{k\sigma}) \quad (4)$$

and $m_z(-q',t') = \mu_B\sum_{k',q'}(c^{\dagger}_{k'-q'\uparrow}c_{k'\uparrow} - c^{\dagger}_{k'-q'\downarrow}c_{k'\downarrow}) =$

$$\mu_B\sum_{k',q',\sigma'}\sigma'(c^{\dagger}_{k'-q'\sigma'}c_{k'\sigma'}) \quad (5)$$

where μ_B is the Bohr magnetron

The Spin susceptibility $\chi^{zz}(q,\omega)$ which is a two particle Green's function, can be written in the form

$$\chi^{zz}(q,\omega) = \mu_B^2\sum_{k,q,\sigma}\sum_{k',q',\sigma'}\sigma\sigma'\Gamma_1(k,q,\sigma,k',q',\sigma',\omega) \quad (6)$$

with $\Gamma_1(k,q,\sigma,k',q',\sigma',\omega) = \ll (c^{\dagger}_{k+q\sigma}c_{k\sigma};\ c^{\dagger}_{k'-q'\sigma'}c_{k'\sigma'} \gg_{\omega} = \ll \alpha_1;\ \beta \gg_{\omega}$ (7)

The calculation involves other Green's function the coupled equations of which , are solved using the mean-field Hamiltonian as given in $eqn.(2)$ and Zubarev's Green's function technique. Using electron commutation rules for the quantities associated in the coupled Green's functions and substituting for them in Γ_1 and taking summation over k', q' and spin σ', we get

$$\Gamma_1(k,q,\sigma,\omega) = \frac{|D_{7\sigma}|}{2\pi|D_{0\sigma}|} \quad (8)$$

where

$$\left.\begin{aligned}
&|D_{7\sigma}| = D_{3\sigma}|\left(< n^c_{k+q,\sigma} > \; - \; < n^c_{k,\sigma} >\right) + |D_4\sigma| < \emptyset_{k,\sigma} > - |D_{5\sigma}| < \emptyset_{k+q,\sigma} > \\
&|D_{0\sigma}| = |D_{1\sigma}||D_{2\sigma}| - |D_{6\sigma}|, |D_{1\sigma}| = (\omega + \epsilon_{1\sigma})(\omega + \epsilon_{2\sigma}) - V^2, \\
&|D_{2\sigma}| = (\omega + \epsilon_{2\sigma})(\omega - \epsilon_{3\sigma}) - V^2 \\
&|D_{3\sigma}| = (\omega + \epsilon_{2\sigma})|D_{2\sigma}| - V^2(\omega - \epsilon_{3\sigma}), |D_{4\sigma}| = V|D_{2\sigma}| + V^3 \\
&|D_{5\sigma}| = V\omega(\omega + \varepsilon_{2\sigma}), |D_{6\sigma}| = V^2\{(\omega + \epsilon_{1\sigma})(\omega - \epsilon_{3\sigma}) + \omega(\omega + \epsilon_{2\sigma}) + V^2
\end{aligned}\right\} \quad (9)$$

and $\epsilon_{1\sigma} = \epsilon_{k+q,\sigma} - \epsilon_{k\sigma}$, $\epsilon_{2\sigma} = \epsilon_{k+q,\sigma} - E_{0\sigma}$, $\epsilon_{3\sigma} = \epsilon_{k\sigma} - E_{0\sigma}$ and $E_{0\sigma} = \varepsilon_f + U < n^f_{-\sigma} > -\sigma B_f$,

The c-and f-electron occupancies $< n^c_{k+q,\sigma'} >$, $< n^c_{k,\sigma} >$, $< \emptyset_{k,\sigma} >$ and $< \emptyset_{k+q,\sigma} >$ are calculated from the mean-field Hamiltonian. Rewriting separately all the above equations for up and down spins we write $\chi^{zz}(q,\omega) = \mu_B^2 \sum_{k,}\{\Gamma_1(k,q,\uparrow,\omega) + \Gamma_1(k,q,\downarrow,\omega)\} = \mu_B^2 \sum_{k,}\{\frac{|D_{7\uparrow}|}{2\pi|D_{0\uparrow}|} + \frac{|D_{7\downarrow}|}{2\pi|D_{0\downarrow}|}\}$ (10)

The momentum summation in eqn.(10) is replaced by $\int_{-w/2}^{+w/2} N(0)d\varepsilon k$, where the energy spans over the conduction band width from -W/2 to +W/2. N(0) is the density of state of conduction electrons at the Fermi level ε_f.

The dimensionless parameters are scaled with respect to the Debye energy ω_D. The parameters are $x = \varepsilon_k/\omega_D$, $d = \varepsilon_f/\omega_D$, $u = U/\omega_D$, $v = V/\omega_D$, $u_m = \mu/\omega_D$, t $= k_B T/\omega_D$ $c = \omega/\omega_D$, neutron momentum transfer energy $\tilde{q} = q v_{F\omega_D}/\omega_D$ and the reduced susceptibility $\tilde{\chi}^{zz}(q,\omega) = \chi^{zz}(q,\omega)/\omega_D$. For small neutron momentum transfer energy, $\varepsilon_{k+q} \simeq \varepsilon_k + q v_F$ where, $v_F = \frac{\partial_{k+q}}{\partial k}|q \to 0$ is conduction electron velocity near the Fermi level.

4. Results and Discussion

The electron occupancy for up spin electrons and for down spin are calculated from the periodic Anderson model H_0 within mean-field approximation given in eqn.1. They are solved numerically and self-consistently for half-filled band situation i.e. $n^c + n^f = 2$. The plots of $n^f_\uparrow$ and $n^f_\downarrow$ vs. temperature t are shown in the inset of Fig.1(a)

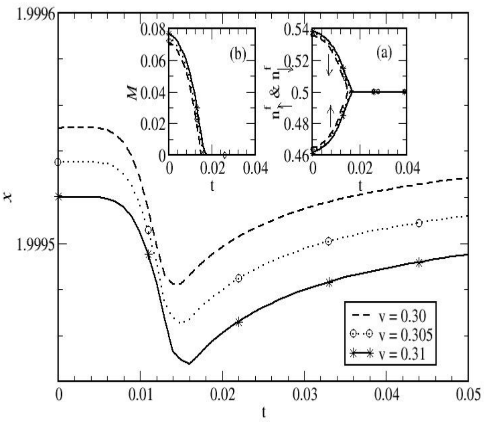

Figure 1. Plot of susceptibility($\boldsymbol{\chi}$) vs. temperature (t) and in the inset (a) plot of f electron occupancies for up spin $\boldsymbol{n_{\uparrow}^{f}}$ and down spin$\boldsymbol{n_{\downarrow}^{f}}$ vs. temperature (t) and in the inset (b) plot of Magnetization vs. temperature (t) for different values of hybridization strength $\boldsymbol{v}$ = 0.305, 0. 31, 0. 315 with fixed values of Coulomb correlations u = 1.34 and f-level energy d = -u/2 = –0.67, frequency $\boldsymbol{c = 2.0x10^{-7}}$, chemical potential p=2.0 and magnetic field b = 0.0

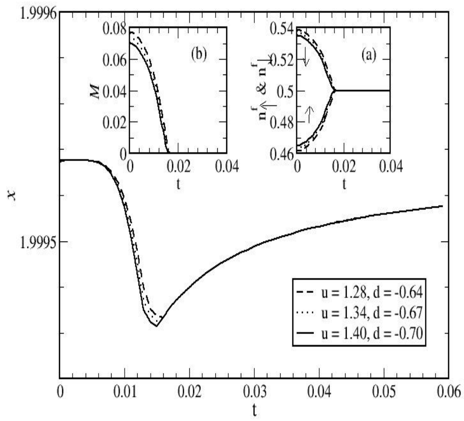

Figure 2. Plot of susceptibility($\boldsymbol{\chi}$) vs. temperature (t) and in the inset (a) plot of f electron occupancies for up spin $\boldsymbol{n_{\uparrow}^{f}}$ and down spin$\boldsymbol{n_{\downarrow}^{f}}$ vs. temperature (t) and in the inset (b) plot of Magnetization vs. temperature (t) for different values of Coulomb correlations $\boldsymbol{u = 1.28, 1.34, 1.4}$, f-level energy $\boldsymbol{d = -u/2}$ with fixed values of hybridization strength $\boldsymbol{v = 0.305}$, frequency $\boldsymbol{2.0x10^{-7}}$, chemical potential p = 2.0 and magnetic field b = 0.0

The electron occupancy for down spin gradually decreases with temperature and attains a half filled condition. Similarly, the electron occupancy for of up spin electrons gradually increases and attains half-filled condition i.e. ($n_{\uparrow}^{f}= n_{\downarrow}^{f}$ = 0.5) at a temperature called Curie temperature below which the system is in ferromagnetic state and above which the system is in paramagnetic phase. The difference ($n_{\downarrow}^{f} - n_{\uparrow}^{f}$) between these occupation numbers gives rise to net magnetization of f-electrons due to Coulomb interaction is shown in inset Fig. 1(b). For a given hybridization strength $v = 0.35$, the susceptibility gradually decreases with increase of temperature and reaches a minimum value at Curie temperature t_c= 0.016, and then gradually increases with increase of temperature. For example, for f-electron systems t_c= 0.016 ($T_c \simeq 0.4K$) for. $CeFePo$ [7] and in $YbNi_4P_2$ ($T_c = 0.17K$) [8]. It is further to note that with decrease of hybridization, the Curie temperature shifts to lower temperatures and susceptibility is enhanced to high values indicating the f-electron system moving from mixed valent state to heavy fermion state.

Fig. 2 shows the temperature variation of susceptibility for different values of Coulomb interaction energy (u) and f -level energy (d) numerically equal to half of Coulomb energy. For a given value of Coulomb energy, the susceptibility gradually decreases with increase of temperature and reaches a minimum value at Curie temperature and then gradually increases with increase of temperature in paramagnetic phase. With the increase of Coulomb energy, the Curie temperature T_c shifts to the lower temperature indicating the system moving from mixed valent sate to heavy fermion state.

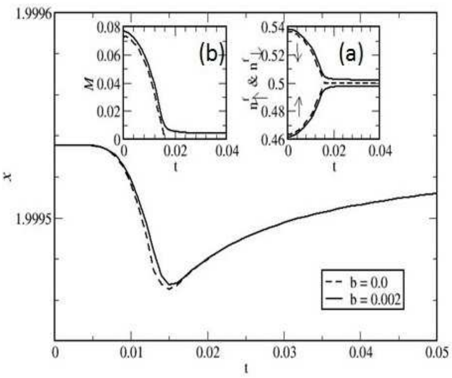

Figure 3. Plot of susceptibility (χ) vs. temperature (t) and in the inset (a) plot of electron occupancies for up spin $n_\uparrow^f$ and down spin $n_\downarrow^f$ vs. temperature (t) and in the inset (b) plot of Magnetization vs. temperature (t) for different values of applied magnetic field b = 0.001, 0.002 with fixed values of Coulomb correlations $u =$ 1.34, f-level energy $d = -0.67$, hybridization strength $v = 0.305$, frequency $2.0x10^{-7}$, chemical potential p = 2.0.

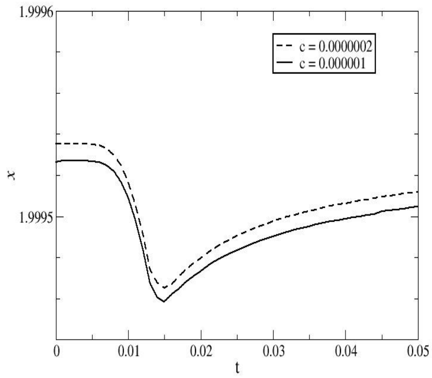

Figure 4. Plot of susceptibility (χ) vs. temperature (t) for different values of applied frequency c = $2.0x10^{-7}$, $1.0x10^{-7}$ with fixed values of Coulomb correlations $u = 1.34$, f-level energy $d = -0.67$, hybridization strength $v =$ 0.305, chemical potential p = 2.0 and magnetic field b = 0.0.

As shown in Fig. 3 a, due to application of magnetic field, the f-electron occupancies for up-spin ($n_\uparrow^f$) and down spin ($n_\downarrow^f$) and show tailing behavior at T_c. With increase of magnetic field, while the down spin occupancy is enhanced the up spin occupancy is suppressed with magnetic field throughout the temperature range. The net difference f electron occupancy gives rise to net magnetic moment and hence ferromagnetism in f electrons as shown in Fig. 3(b). Fig. 3(b) shows the ferromagnetic magnetization gradually decreases with temperature and shows a tail near T_c. Using this temperature dependence of $n_{\uparrow}^{f}$ and $n_{\downarrow}^{f}$ we have plotted temperature dependence of susceptibility in Fig. 3. It is seen that the susceptibility is enhanced with the increase of external magnetic field and the enhancement is larger near T_c. However, the external magnetic field has less effect on susceptibility in paramagnetic phase. Figure 4 shows the effect of external periodic frequency on temperature dependent susceptibility. With increase of applied frequency, the dynamic spin susceptibility is suppressed throughout the temperature range and the Curie temperature shifts to higher temperature.

5. Conclusion

We have considered the periodic Anderson model in order to investigate the temperature anomaly in susceptibility in f-electron systems. The Coulomb repulsive interaction due to f-electrons are considered within Hartree-Fock mean-field approximation for ferromagnetic limits. The f electron occupancies for up spin, down spins and magnetization are computed self-consistently and hence the temperature dependent susceptibility is studied by varying the different model parameters of the system. The up and down spin orientations of f- electrons give rise to ferromagnetism in the system. In the ferromagnetic limit of the coulomb interaction, the susceptibility is enhanced throughout the temperature up to Curie temperature (T_c). The Curie temperature is enhanced with increase of Coulomb correlation energy and decrease of strength of hybridization between f-electrons and conduction electrons indicating the heavy fermion state of the f-electron systems.

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