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# Influence of electron-phonon interaction on effective mass in some intermetallic compounds

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**Abstract** It is well known that for ordinary metals, the electron-phonon interaction increases the quasi particle mass which is in contrast to the recent finding by Fulde *et al* that, for some Heavy Fermion systems, it decreases. To understand the effect of this interaction on effective mass, we have considered here the electron-phonon interaction in the Periodic Anderson Model (PAM) and derived a simple expression for it. This involves various model parameters namely, the position of 4$f$ level, the effective coupling strength $g$ and the electron-phonon coupling strength $r$. The influence of these parameters on the value of effective mass is studied. For simplicity, the numerical calculation is performed in long wavelength limit. It was found that the position of 4$f$ level and electron-phonon coupling strength influence strongly on effective mass

**Keywords** : Heavy Fermion (HF) systems, effective mass, electron-phonon interaction

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## 1. Introduction

The experimental investigations on some intermetallic compounds and alloys of rare earths and actinides, have revealed very interesting physical properties which can be associated with their partially filled shell of $f$ and $d$ electrons. Some of these systems are known to form highly correlated electronic states and exhibit unusual magnetic, thermodynamic, transport properties in their normal state at low temperature. Heavy Fermion (HF), Valence Fluctuation (VF), Kondo lattices are some of the systems which belong to these groups. These are characteristically different from their counterpart in ordinary metals and have attracted considerable interest in recent years [1-4]. In the present paper, we have studied the effect of electron-phonon interaction on effective mass in some Heavy Fermion systems.

It is a well known fact that for ordinary metals, the electron-phonon interaction increases the quasi particle mass. This is in contrast to a recent finding by Fulde *et al* [5] that for some Heavy Fermion systems, it decreases. Moreover, some recent experiments [6] on HF systems suggest that there exists a strong coupling of the elastic degrees of freedom with those of the electronic and magnetic ones. Particularly, the physical properties related to the observed magneto-elastic effect (coupling of phonons to the $f$-electrons), anisotropic Fermi surface, Kondo volume collapse *etc* and the manifestation of the deformation potential (the coupling of phonons to the conduction electrons), have persuaded many to emphasize the role of electron-phonon interaction to explain some of the low temperature behavior. But direct experimental evidence for phonon anomaly through inelastic neutron scattering or Raman scattering experiments are rare in these systems. However, the measurements on elastic constant, ultrasonic attenuation and sound velocity, have provided indirect evidence of strong electron-phonon coupling. To understand the effect of this interaction on effective mass, we have considered electron-phonon coupling mechanisms in the framework of the Periodic Anderson Model (PAM). These are (i) the usual interaction between the phonons with the electrons in the $f$-bands and (ii) the electron-phonon interaction arising from hybridization term of the PAM. The aim in this paper, as stated earlier, is to see the effect of electron-phonon interaction on effective mass through the self energy which relates to the effective mass in the following way :

$$m^*/m = \tilde{m} = 1/\left[1+\partial\Sigma(k,\omega)/\partial\varepsilon_k\right]. \quad (1)$$

For simplicity, we have first explored the properties of the system in the normal state for long wave length limit in the finite

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temperature limit without keeping the $f-f$ Coulomb correlation term.

## 2. Formalism

Rajafimandimby, Fulde, Luthi and few others, who are the pioneer in this field, have successfully estimated the electron-phonon mechanism in these systems. It was shown by Rajafimandimby *et al* [7] that the existence of super conductivity in HF system $CeCu_2Si_2$, is due to the strong electron-phonon interaction in it. It is also established that all anomalous properties exhibited by these systems, can be understood as arising from the strong hybridization of the correlated $f$-electrons with those in the conduction band near the Fermi level. Moreover, it is also established that the strength of phonon coupling to the hybridization of $f$- and conduction band electrons is stronger compared to the coupling of phonons to that of electrons of $f$-band alone.

Here, following Fulde *et al* [1], we have considered two different electron-phonon coupling mechanisms in the framework of the Periodic Anderson Model (PAM) [8]. For proper description of the phonon anomalies in the HF systems, the model Hamiltonian takes the form

$$H = H_0 + H_{e-p} + H_p \tag{2}$$

which consists of three terms, (i) the electronic Hamiltonian $H_0$, (ii) the Hamiltonian for the phonons $H_p$, (iii) the electron-phonon interaction term $H_{e-p}$. The electronic Hamiltonian $H_0$ correspond to the PAM and is given by

$$H_0 = \sum_{k\sigma} \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} + E_0 \sum_{k\sigma} f^{+}_{k\sigma} f_{k\sigma} + \gamma_0 \sum_{k\sigma} \left( f^{+}_{k\sigma} C_{k\sigma} \quad C^{+}_{k\sigma} f_{k\sigma} \right), \tag{3a}$$

where $C^{+}_{k\sigma}(C_{k\sigma})$ and $f^{+}_{k\sigma}(f_{k\sigma})$ are the creation (annihilation) operators for conduction and $f$-electrons with momentum $k$ and spin $\sigma$ respectively, $\varepsilon_k$ is the energy of the electron in the conduction band, $E_0$ is the position of the $f$-level and $\gamma_0$ representing the strength of the hybridization between the $f$-electrons and the conduction electrons.

Considering the importance of the Lanthanide contraction in these systems, the phonons are assumed to interact predominantly with the $f$-electrons. While the interaction of the phonons with the conduction electrons is neglected, Fulde has argued that their interaction with the hybridization term can contribute substantially to the phonon anomalies. Thus the electron-phonon interaction Hamiltonian is given by

$$H_{e-p} = \sum_{kq\sigma} \Big[ f_1(q) \left( f^{+}_{k+q,\sigma} C_{k,\sigma} + C^{+}_{k+q,\sigma} f_{k,\sigma} \right) + f_2(q) f^{+}_{k+q,\sigma} f_{k,\sigma} \Big] \Big[ b_q + b^{+}_{-q} \Big], \tag{3b}$$

where $f_1(q)$ and $f_2(q)$ are the coupling constants, the former being the interaction arising between phonons with the hybridization term and the later corresponding to the strength of interaction with the $f$-electrons. Finally, the Hamiltonian for the phonon is given by

$$H_p = \sum \omega_q b^{+}_q b_q , \tag{3c}$$

$b^{+}_q (b_q)$ being the creation (annihilation) operator for the phonons with wave vector $\omega_q$.

Since we are interested in the calculation of phonon response functions, it is necessary to evaluate the phonon Green function [9] defined as

$$D_{qq'}(t-t') = \langle\langle A_q(t);\, A_{q'}(t') \rangle\rangle$$

$$= i\nu(t-t') \left\langle \left[ A_q(t);\, A_{q'}(t') \right]_- \right\rangle, \tag{4}$$

where

$$A_q = b_q + b^{+}_{-q} \quad \text{and} \quad B_q = b_q - b^{+}_{-q} \tag{5}$$

are respectively the $q$-th Fourier component of the displacement and momentum of the ions.

The phonon green function [eq.(4)] can be calculated by writing its equation of motion using the Hamiltonian of eq. (1) which when Fourier transformed, $D_{qq'}(\omega)$ can be expressed in the form

$$D_{qq'}(\omega) = \delta_{-qq'} \left( \omega_q / \pi \right) \left[ \omega^2 - \omega_q^2 - \sum (q,\omega) \right]^{-1}, \tag{6}$$

where $\sum (q,\omega) = 4\pi\omega_q \chi_{qq'}(\omega)$. (7)

The fourier transform of the response functions entering in the self energy, is given by

$$\chi_{qq'}(\omega) = f_1(-q) f_1(-q') \Gamma_1(qq'\omega) + f_1(-q) f_2(-q') \Gamma_2(qq'\omega) + f_2(-q) f_1(-q') \Gamma_3(qq'\omega) + f_2(-q) f_2(-q') \Gamma_4(qq'\omega), \tag{8}$$

where the $\Gamma_i's (i = 1\text{-}4)$ represent the electron response functions. These electron response functions are higher order Green functions of the electron operators and are evaluated from the equations of motion of these Green functions using only the electronic Hamiltonian as given by eq. (2) without the phonon and the electron-phonon interaction term *i.e.*

$$H_0 = \sum_{k\sigma} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma} + E_0 \sum_{k\sigma} f^{+}_{k\sigma} f_{i} + \gamma_0 \sum_{k\sigma} \left( f^{+}_{k\sigma} c_{k\sigma} + c^{+}_{k\sigma} f_{k\sigma} \right). \tag{9}$$

The long wavelength limit of the self-energy is evaluated and when the derivative of the same with respect to $\varepsilon_k$ is substituted, the effective mass takes a very simple form as

$$\tilde{m} = 1/\left[1 + 2\pi(1 + F(k,\omega,q = 0))\right], \tag{10}$$

where

$$F(k,\omega,q=0) = A(P - Q - R - S) \tag{11}$$

and

$$A = 3f_1(0)^2\,(\omega - \varepsilon_f)^2 / 2D^2\Delta^2, \tag{12a}$$

$$P = \omega_0(\varepsilon_f - E_0)(\tanh(y_1/2kT) + \tanh(y_2/2kT)), \tag{12b}$$

$$Q = (\omega_0/4kT)(E_0 - \varepsilon_f + \Delta)^2(\mathrm{sec}\,h(y_2/2kT))^2, \tag{12c}$$

$$R = (\omega_0/4kT)(\varepsilon_f - E_0 + \Delta)^2(\mathrm{sec}\,h(y_1/2kT))^2, \tag{12d}$$

$$S = BC, \tag{12e}$$

$$B = 6f_1(0)\gamma_0(\omega - E_0)\langle a_0\rangle\,\Delta^2/D^2, \tag{12f}$$

$$C = \left(1 - 2N^f_{k\sigma}\right)\omega_0 + (\omega - E_0 + r\gamma_0)N_0, \tag{12g}$$

$$D = \left(\omega - \varepsilon_f\right)(\omega - E_0) - \gamma_0^2 = (\omega - y_1)(\omega - y_2), \tag{12h}$$

$$\Delta = \left[\left(\varepsilon_f - E_0\right)^2 + 4\gamma_0^2\right]^{1/2}, \tag{12i}$$

$$N^f_{k\sigma} = (1/4\Delta)\left[\left(E_0 - \varepsilon_f + \Delta\right)(\tanh y_2/2kT) + \left(\varepsilon_f - E_0 + \Delta\right)(\tanh y_1/2kT)\right], \tag{12j}$$

$$N_0 = 2/\left[\exp(\omega_0/2kT) - 1\right] + 1, \tag{12k}$$

$$\langle a_0\rangle = \left\langle b_q + b^+_{-q}\right\rangle_{q=0}, \tag{12l}$$

$$y_1 = \left(\varepsilon_f + E_0 + \Delta\right)/2, \tag{12m}$$

$$y_2 = \left(\varepsilon_f + E_0 - \Delta\right)/2. \tag{12n}$$

Most of the notations used here are same as that of our two earlier papers [10,11].

## 3. Results and discussion

The different dimensionless parameters that are involved in these calculations are the ratio of the two electron-phonon interaction strengths $r = f_2(0)/f_1(0)$; the effective coupling constant $g = N(0)f_1^2(0)/\omega_0$, where $N(0)$ being the density of states at the Fermi level. All the energies in the system are measured with respect to the strength of the hybridization $(\gamma_0)$, the single dominant parameter, where the position of the $f$-level is given by $d = E_0/\gamma_0$, the inverse of the temperature given by $b = \gamma_0/2kT$, the fermi energy $x_f = \varepsilon_f/\gamma_0$. The normalized phonon frequency $\omega = \omega/\omega_0$ is measured with respect to the frequency $(\omega_0)$ of the bare phonon. The other dimensionless parameters, which are required for scaling different energy quantities are $\delta = \Delta/\gamma_0$, $z = \omega_0/\gamma_0$, $c = \omega/\gamma_0$ and $D_1 = D/\gamma_0^2$. However, the most prominent parameters that influence the phonons are $d$, $g$ and $r$. To appreciate the behavior of these parameters in these systems, we have investigated their influence on renormalized phonon energy, which again influence the effective mass. The initial parameters are set by considering the physically allowed values of these parameters at random, so as to give uniform softening as evident from the experiment.

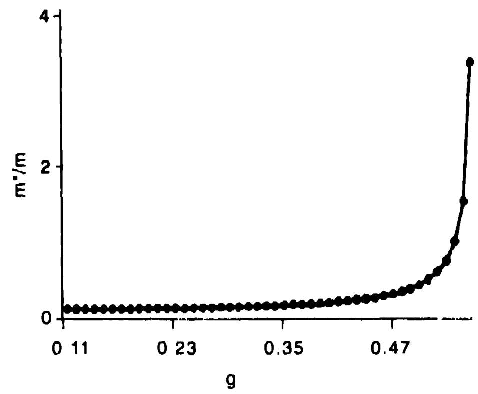


**Figure 1.** Plot of $m^*/m$ *versus* $g$ for $r = 0.1$, $z = 2.5$, $x_m = 0.1$, $a_0 = 0.1$, $x_f = 0$, $b = 0.2$ and $d = -2$

The results of the numerical calculations are presented in two figures showing the variation of effective mass $\tilde{m}$ with the effective coupling strength $g$ keeping the other parameters constant. In Figure 1, the variation of $\tilde{m}$ is made with $g$ keeping

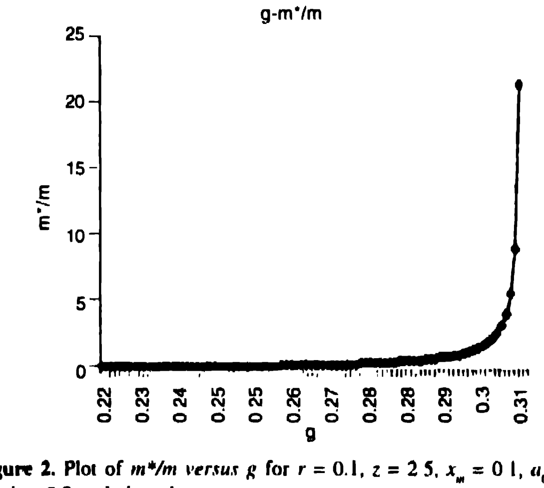


**Figure 2.** Plot of $m^*/m$ *versus* $g$ for $r = 0.1$, $z = 2.5$, $x_m = 0.1$, $a_0 = 0.1$, $x_f = 0$, $b = 0.2$ and $d = -1$.

other parameters at fixed values as $r = 0.1$, $z = 2.5$, $x_m = 0.1$, $a_0 = 0.1$, $x_f = 0$, $b = 0.2$ and $d = -2$. In Figure 2 the same plot is made for a different value of $d$ ( $= -1$ ) where the values of the other parameters have been retained as it appeared in the first case. In both the plots it is observed that, depending on the values of $g$ and $d$, the effective mass increases as well as decreases. In other words, for some range of $g$ values the effective mass is less than one, while for some other range, its value is more than one. Moreover, the range of $g$ value is also very sensitive to the value of the location of the $f$-level. In the first case the range of $g$ values goes from 0 to 0.53 and the corresponding values of the effective mass is less than one. But when the $g$ values crosses this limit *i.e.* 0.53 the effective mass increases rapidly and approaches $\tilde{m} = 4.0$ for $g$ equal to 0.56. If $g$ is further increased the system becomes unstable and the effective mass give unphysical results. Similarly for the second curve, when $d$ changes from $-2$ to $-1$, for the range of $g$ values from 0 to 0.294, the effective mass is less than one. When the value of $g$ is larger than 0.294, the effective mass is more than one and the value of $\tilde{m}$ goes up to $\tilde{m} = 21$ at value of $g = 0.301$.

So from these two figures it is concluded that the range of $g$ values is very sensitive to the location of $f$-level $d$. It is evident that the nearer the $f$-level to the fermi level the larger the value of effective mass ( $\tilde{m}$ ). It is obvious that as $f$-level is close to fermi level the electron density increases Since effective mass is directly proportional to this quantity, the value of effective mass becomes larger. Moreover, the present analysis also explains the decrease of effective mass for some Heavy Fermion systems as predicted by *Fulde et al* [5]. The effective mass is also affected by other parameters, which can be studied similarly. But due to constraint of space we have presented only two cases. The other results will be reported elsewhere.

## 4. Conclusion

The effect of electron-phonon interaction in the Heavy Fermion systems, which directly influence the effective mass, is explained. To understand this mechanism microscopically, the phonon interaction is introduced to both $f$-electrons as well as to the hybridization of conduction and $f$-electrons. The phonon self-energy in normal state is calculated with Coulomb correlation equal to zero. *Zubarev* [9] type Green function is used to evaluate this quantity. The influence of various model parameters is studied, which are presented in two plots. The prediction of decrease in effective mass due to electron-phonon interaction in some Heavy Fermion systems by *Fulde et al* [5] is consistent with our result as presented.

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