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Microscopic theory of electron-phonon coupling mechanism in heavy fermion systems : a finite q and T calculation

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Abstract : Phonon response function for the heavy fermion (HF) systems for finite wave vector q and temperature T is calculated The electron-phonon interaction in the Periodic Anderson Model (PAM) for the normal state is considered An analytical analysis is carried out for small q and in the limit of low temperature The calculated phonon self-energy is studied for various model parameters of the system The observed behaviour is found to agree well with the general features obtained experimentally for some heavy fermion (HF) systems

Keywords Periodic Anderson model (PAM), Heavy Fermion system, Electron-phonon interaction

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1. Introduction

In recent years, a lot of interest has been developed on heavy fermion (HF) systems. These are the intermetallic compounds with partially filled f-bands of rare earths like Ce, Yb and actinides like U. These form a highly correlated electron system at low temperature and show many interesting anomalies of electronic and lattice properties [1–3].

There are several measurements [2] which suggest the existence of strong electron-phonon interaction in heavy fermion (HF) systems. The most prominent effect of these are the softening of elastic constant, temperature dependence of the thermal expansion, strong softening of phonons below the Kondo temperature. To understand this microscopically, we consider two different mechanisms of electron-phonon couplings through the Periodic Anderson Model (PAM) [4] *i.e.* the usual interaction between the phonons with the electrons in the f-bands as well as the interaction arising from that of the hybridisation band. Our aim in this paper, is to calculate the influence of f and conduction electrons mixing and f-electrons alone on phonon self-energy. Therefore, to account these effects, the present analysis explores how the phonons get modified through the self-energy and the spectral density function which in turn involve response functions corresponding to the conduction electrons, f-electrons and the f-d mixing densities.

2. Formalism

We consider the model system with the Hamiltonian

$$H = H_o + H_p + H_{e-p} \tag{1}$$

which consists of three terms (i) the electronic Hamiltonian H_o, (ii) the Hamiltonian for the phonons H_p and (iii) the electron-phonon interaction term H_{e-p}. The explicit form of these are given by

$$H_o = \sum_{k\sigma} \varepsilon_k C^{\dagger}_{k\sigma} C_{k\sigma} + E_0 \sum_{k\sigma} f^{\dagger}_{k\sigma} f_{k\sigma} + \gamma_0 \sum_{k\sigma} (f^{\dagger}_{k\sigma} C_{k\sigma} + C^{\dagger}_{k\sigma} f_{k\sigma})$$

$$+ U/2 \sum_{i\sigma} n^f_{i\sigma} n^f_{i-\sigma}, \tag{2a}$$

$$H_p = \sum_q \omega_q b^{\dagger}_q b_q, \tag{2b}$$

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

$$+ f_2(q) f^{\dagger}_{k+q,\sigma} f_{k,\sigma} \Big] \left[b_q + b^{\dagger}_{-q} \right]. \tag{2c}$$

The notations used in the above expression are same as described in our earlier paper [5].

Since we are interested in the calculation of phonon response functions, it is necessary to evaluate the phonon Green function [6] defined as

$$D_{qq'}(t-t') = << A_q(t) ; A_{q'}(t') >>$$

$$= -i\vartheta(t-t')\left\langle \left[A_q(t); A_{q'}(t')\right]_- \right\rangle, \quad (3)$$

where $A_q = b_q + b^+_{-q}$ and $B_q = b_q - b^+_q$ (4)

are respectively the q-th Fourier component of the displacement and momentum of the ions. The Fourier transformed Green function $D_{qq'}(\omega)$, were evaluated to express the phonon self-energy which is given by

$$\omega^2 - \omega_q^2 - 4\pi\omega_q \chi_{qq'}(\omega) = 0, \quad (5)$$

where

$$\chi_{qq'}(\omega) = f_1(-q) f_1(-q') \Gamma_1(qq'\omega) + f_1(-q) f_2(-q') \Gamma_2(qq'\omega)$$

$$+ f_2(-q) f_1(-q') \Gamma_3(qq'\omega) + f_2(-q) f_2(-q') \Gamma_4(qq'\omega), \quad (6)$$

where $\Gamma_i's (i = 1 \text{ to } 4)$ 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 Green functions using only the electronic part of the Hamiltonian H_0 given by eq. (2a).

3. Evaluation

In view of our interest, we have evaluated eqs. (5) and (6) for small-q and T limit. In doing so, we expand ε_{k-q} and the Fermi function m_{k-q} upto the order linear in q as

$$\varepsilon_{k-q} = \varepsilon_k - qv_F, \quad (7a)$$

$$m_{k-q} = m_k - qv_F \delta(\varepsilon_k - \varepsilon_F), \quad (7b)$$

where $v_k = \partial\varepsilon_{k-q} / \partial k|_{q=0}$ and

$$\delta(\varepsilon_k - \varepsilon_F) = \partial m_{k-q} / \partial \varepsilon_{k-q}. \quad (7c)$$

Similarly, the temperature dependent term which appears in the analytical expression is $(\tanh(y_1/2\theta) - \tanh(y_2/2\theta))$ (here $\theta = kT$). This is the term which links the different time correlation functions to their corresponding Green functions. The expansion of this in the limit of small temperature is given by

$$\tanh(y_1/2\theta) - \tanh(y_2/2\theta)$$

$$= -2\exp\left((\varepsilon_k - E_0)/2\theta\right) \sinh\sqrt{(\varepsilon_k - E_0)^2 + 4\gamma_0^2}/2\theta, \quad (8)$$

where $y_{1,2} = 1/2(\varepsilon_k + E_0) \pm 1/2\sqrt{(\varepsilon_k - E_0)^2 + 4\gamma_0^2}$. (9)

When these are substituted in eq. (5), the renormalised phonon dispersion takes the form

$$(\omega/\omega_q)^2 = 1 + (4\pi/\omega_q)\chi(\omega, q, T), \quad (10)$$

where

$$\chi(\omega, q, T) = \chi(\omega, q = 0, T) + \chi(\omega, q, T = 0) + \chi(\omega, q, T). \quad (11)$$

After parametrising the different quantities of eq. (11) in the following way, the eq. (10) can be put in a compact form as given below

$$(\omega/\omega_q)^2 = 1 - 4g(I_1 + I_2 + I_3), \quad (12)$$

where

$$I_1 = 4A(B + C), \quad (13a)$$

$$I_2 = \int dx\, F \exp(-bx) \sinh(bD)/(DE), \quad (13b)$$

$$I_3 = \int dx\, (J + H) \exp(-bx) \sinh(bD)/E, \quad (13c)$$

$$A = 4k(c - yf + d)/((yf - d)^2 - c^2 + 4), \quad (14a)$$

$$B = (2r/(yf - d) - 1), \quad (14b)$$

$$C = r^2(c + yf - d)/((yf - d)^2(c - yf + d), \quad (14c)$$

$$D = ((x - d)^2 + 4)^{0.5}, \quad (14d)$$

$$E = ((x - d)^2 + 4 - c^2), \quad (14e)$$

$$F = ((x - d)^2 + 2r(x - d) + r^2)\exp(-bd), \quad (14f)$$

$$G = (c - x + d)/(x - d + c), \quad (14g)$$

$$H = (kG + 2rkG(2(x - d) + c)/(x - d)^2), \quad (14h)$$

$$I = 2r^2k(x - d)(x - d - 1) + c(x - d - c))$$

$$/((x - d)^2(x - d - c)), \quad (14i)$$

and the different dimensionless parameters are

$$r = f_2(q)/f_1(q),\ g = N(\varepsilon_F)f_1(q)^2/\omega_q,\ d = E_0/\gamma_0,$$

$$yf = \varepsilon_F/\gamma_0,\ c = \omega/\gamma_0,\ k = qv_F/\gamma_0,\ x = \varepsilon_k/\gamma_0. \quad (15)$$

4. Results and discussion

The different dimensional parameters that are involved in the numerical calculations are : $r = f_2(q)/f_1(q)$ the ratio of coupling strength of phonons with electrons in the f-band and the hybridisation band ; g, the effective coupling parameter and d, the position of the f-level. yf, x, c, k relate to the Fermi energy, energy of the conduction band, phonon energy and wave vector respectively. The values of these parameters more or less influence and play a dominant role in determining the physical characteristics of the HF systems. The results of the numerical calculations are presented in three figures. Figure 1 shows the variation of renormalised phonon energy $\tilde{\omega}$ with b (the inverse of temperature) for $q = 0$ and for different values of $d = -5, -2, 0, 2$. It is found that the degree of phonon softening decreases as f-level is moved towards the Fermi level. But for positive values of d there is hardly any softening. Figure 2 shows the variation of $\tilde{\omega}$ with q for $T = 0$ and for the same values of d. It is found that

the softening is poorer compared to the variation $\tilde{\omega}$ with that of temperature shown in Figure 1. Moreover, there is phonon

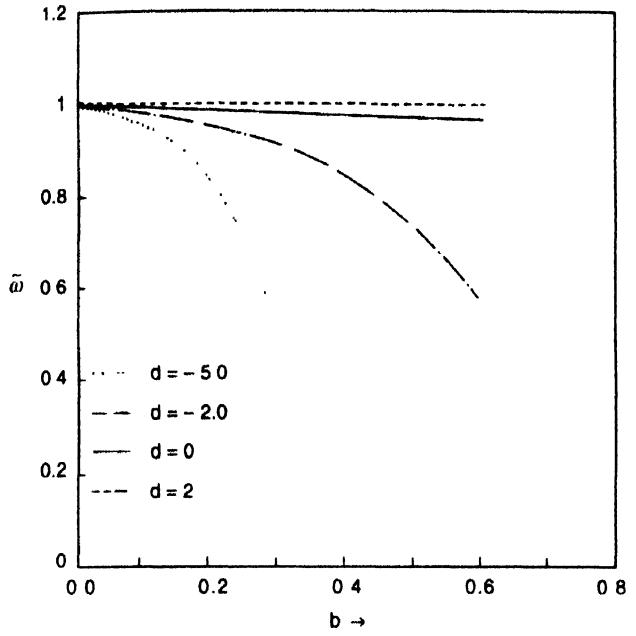

Figure 1. Plot of $\tilde{\omega}(=\omega/\omega_0)$ *versus* Temperature b for $q = 0$, $r = 0.01$, $g = 0.01$ and for different values of $d = -5.0, -2.0, 0$ and 2.0

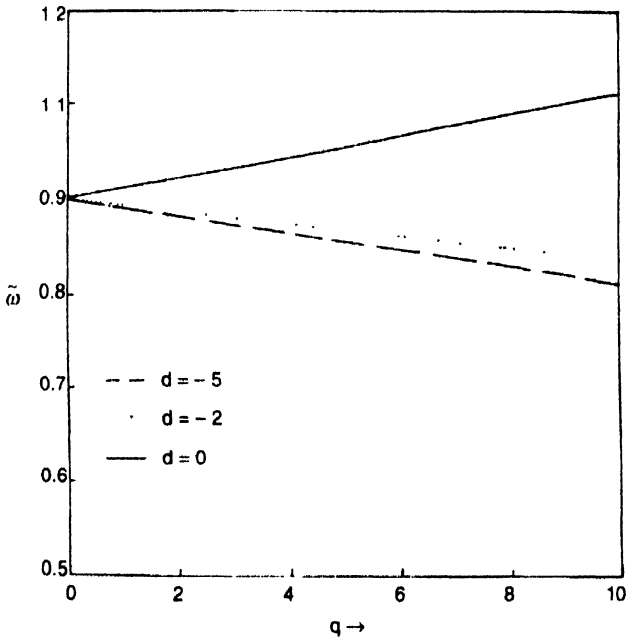

Figure 2. Plot of $\tilde{\omega}(=\omega/\omega_0)$ *versus* q for zero temperature and for different values of $d = -5.0, -2.0, 0$.

hardening when the d value is positive. Finally the Figure 3 shows the variation of $\tilde{\omega}$ for finite values of q and T. Thus to study this effect, the plot is made for $\tilde{\omega}$ *versus* q for different values of T *i.e.* for different b values 0, 0.1, 0.2, 0.3 and for same values of r and g with $d = -2.0$. It is observed that as the temperature is decreased, the phonon softening becomes faster. Moreover, on comparing this plot with the two plots described above, it shows that both q and T have finite contributions to the phonon spectrum. The other two parameters r and g also influence the phonon softening. The study of their influence on phonon softening for different values of these will be published elsewhere.

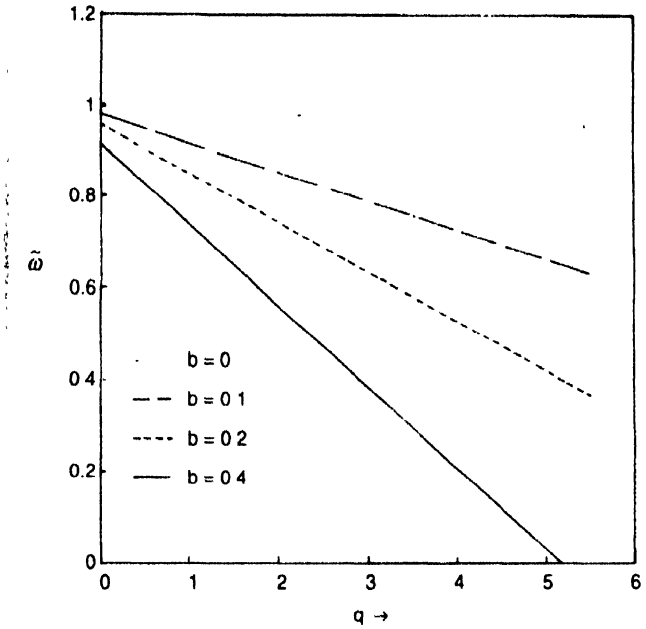

Figure 3. Plot of $\tilde{\omega}(=\omega/\omega_0)$ *versus* q for different values of temperature $b = 0, 0.1, 0.2, 0.3$ with $r = 0.1$, $g = 0.01$, $d = -2.0$

5. Conclusion

An attempt has been made to explain the influence of different system parameters on the electron-phonon interaction in the HF systems. To understand the mechanism microscopically, phonons are assumed to interact with both the f-electron as well as to the hybridisation of conduction of f-electrons. The phonon response functions are evaluated exactly for all wave vectors (q) and temperatures (T). Zubarev type Green functions are used to evaluate these quantities. To achieve simplification, the phonon self-energy is evaluated in the static limit.

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