Chapter 4

Numerical Evaluation

4.1 Introduction

The phonon response properties of the strongly correlated electron systems, mainly heavy fermion (HF) systems, are investigated within the Periodic Anderson Model. In which two different mechanisms of the electron-phonon interaction is considered. These are the usual interaction between the phonons and the electrons in the $f$-bands as well as the interaction arising from that of the hybridization term of the PAM. In this dissertation we have investigated the influence of $f$- and conduction electron mixing as well as the $f$ electron alone on the phonon response functions. Therefore our analysis presents how the phonons in these systems get modified due to these interactions through their self-energy and spectral density functions which in turn involve the electron response functions corresponding to the conduction electrons, the $f$-electrons and $f-d$ mixing densities. To understand these effects and peculiar behavior related to phonon anomalies one need to solve equation (3.57) and (3.59). These again involve equation (3.56) which is to be integrated numerically. The exact evaluation of these equations with all wave vector $q$ and temperature $T$ is quite complicated. So for simplification we, we have opted for certain approximations. Those are the evaluation of frequencies and the spectral density functions either for long wavelength limit i.e., $q = 0$ and in the low temperature limit, or for small values of $q$ in the zero temperature limit, or for small values of both $q$ and $T$. Following the standard technique of Zubarev [112] the different correlation functions involved in these equations are evaluated. These evaluated quantities again substituted back in equation (3.9) and (3.10 - 3.13) to get the expression for the phonon Green function $D_{qq}(\omega)$ required for the calculation.
4.1.1 Parameterization

It is well known that the position of the $f$-level and the strength of hybridization play an important role in heavy fermion systems. The behavior of these systems is well understood by investigating the influence of certain parameters on their different physical properties. This is achieved when dividing suitable energy parameter parameterizes the different dimensional quantities. Thus, the different dimensionless parameters that are involved in these calculations are

$$r = f_2(q)/f_1(q); \quad g = N(0)f_1^2(q)/\omega_q; \quad d = E_0/\gamma_0$$

$$b = \gamma_0/2KT; \quad e = \eta/4\gamma_0^2; \quad z = \omega_q/2\gamma_0; \quad \eta/\omega_q^2 = e/z^2$$

$$\delta = \omega/\omega_q; \quad c = \omega/\gamma_0 = 2\delta z; \quad W' = W/\gamma_0$$

$$b' = \gamma_0/2KT_k; \quad b = b'/\tilde{T}; \quad \tilde{T} = T/T_k; \quad U' = U/\gamma_0$$

$$y_F = e_F/\gamma_0; \quad K = q\nu_F/\gamma_0 \quad \text{and} \quad y = e_F/\gamma_0 \quad (4.1)$$

where $r$, the ratio of electron-phonon coupling strength of phonons with electrons in $f$-band to that of phonons with hybridization band; $g$, the effective coupling parameter involving density of states at Fermi level ($E_f$ is assumed to lie at 0 energy level); $d$, the position of $f$-level with respect to Fermi level $E_f$; $b$, the temperature; $e$, the width of phonon mode; $z$, the scaling parameter; $c$, relates the phonon frequency; $W'$, related to width of conduction band which ranges from $-W'/2$ to $+W'/2$; $\omega$, the reduced frequency; $U'$, onsite coulomb repulsion; $y_F$, effective Fermi level; $\nu_F$, the Fermi velocity; $y$, refers to the energy of conduction band which spreads symmetrically above the Fermi level and $T_k$ is the Kondo temperature. Moreover as per the finding of Razafimandimby et al [153] the value of $r$ is kept at less than 1, in heavy fermion systems, so as to make $f_1(q)$ stronger than $f_2(q)$. But in case of other strongly correlated systems like fluoride scheelites $r$ is greater than 1, i.e., $f_2(q)$ is stronger than $f_1(q)$. For simplicity it is assumed that the $f$-level to be half filled so that the average value of $\langle n_f \rangle$ is taken as 1. The value of $g$, the effective coupling parameter is kept low so as to produce the result of weak coupling regime as well as the softening effect in the correct spin fluctuation temperature range pertinent to the heavy fermion systems. Since the
Fermi level is set equal to zero \((E_f = 0)\), the value of \(d\) is negative, if the \(f\)-level lies below the Fermi level and is positive if it is above the Fermi level. The values of these parameters more or less influence and play a dominant role in determining the physical characteristics of heavy fermion systems.

In this chapter we have discussed the detailed numerical evaluation to study the effect of electron-phonon interaction and influence of finite \(U\) i.e. the Coulomb correlation between \(f\)-electrons on phonon excitation spectrum, the spectral density, the elastic constant and the effective mass using some approximations. In section 4.2 the electron-phonon interaction and temperature dependence of elastic constants is discussed. The results presented in this section are in the limit of \(U = 0\) and the numerical calculations has been made for \(q = 0\) and finite temperature. In section 4.3 microscopic theory of electron-phonon coupling mechanism in heavy fermion systems i.e., phonon response functions for the heavy fermion system is calculated for finite wave vector \(q\) and temperature \(T\). In section 4.4 the effect of electron-phonon interaction on effective mass i.e., the increase or decrease of effective mass with the variation of system parameters is studied. To compare the derived results with experiment one need to calculate the spectral density function. The effect of electron-phonon interaction on different model parameters is discussed through the shift and width of spectral density function in section 4.5. In section 4.6 the effect correlation \(U\) on electron-phonon interaction with a finite \(q\) is calculated. We have also made an attempt to study the effect of the correlation on effective mass in section 4.7. The influence of finite \(U\) on phonon self-energy is studied for various model parameters namely, the effective coupling strength \(g\), the position of \(f\)-level \(d\) and the ratio of electron-phonon coupling strengths \(f_1(q)\) and \(f_2(q)\) i.e., \(r\). In the last section 4.8 we have discussed the effect of electron-phonon interaction on spectral density function of fluoride scheelites \(LiYF_4\) and \(LiLnF_4\) with \(Ln = Ho, Er, Tm\) and \(Yb\). These systems are not heavy fermion systems but show a strong electron-phonon interaction. We have used our method to study the effect and found that the results are in agreement with that of experiments.
4.2 Electron-Phonon interaction and the Temperature dependence of elastic constants.

4.2.1 Introduction

The heavy fermion systems not only exhibit very interesting anomalies of their electronic properties but also pronounced instabilities in the temperature and field behavior of the lattice properties, like elastic constant, thermal expansion and magnetostriction. There is an influence of the quasi particle phonon interaction in the heavy fermion systems on the sound velocity. It is shown that [36, 154] for temperatures less than spin fluctuation temperature $T^*$ the change in sound velocity depend strongly on the detailed shape of quasi particle density of states. Measurements of longitudinal and shear elastic constants in polycrystalline $\mathrm{CeAl}_3$ shows that at low temperature a strong softening for longitudinal elastic constant was observed and even stronger softening occurs at very low temperature [155].

Some recent experiments on elastic constants found that systems, particularly $\mathrm{UPt}_3$, $\mathrm{CeAl}_3$ show a sharp depression or a dip in the longitudinal modes of elastic constant at extremely low temperature while transverse modes pass through the maximum [155, 156]. However for some other systems like $\mathrm{CeCu}_6$, $\mathrm{CeRu}_2\mathrm{Si}_2$ the dip or minimum is neither distinct nor present. All these findings show that the coupling of heavy electron with longitudinal phonon play an important role within the microscopic structure of heavy fermion state. To explain the microscopic origin of this difference in the behavior of the elastic constant both at low and high temperature attempts has been made to through electron-phonon coupling mechanisms through different approaches. Wojciechoski et. al. [114] used the concept of Grüneisen parameter coupling to explain the different phonon anomalies associated with elastic constants. In doing so they have considered the volume dependence of the bare hybridization strength and the bare position of the $f$-level in the electron-phonon term. In addition they have also taken in to account the additional term coming from the implicit volume dependence of the renormalized hybridization strength through the number of $4f$ electron per site.

In this section we have tried to explain the temperature dependence of elastic constants by introducing the electron-phonon interaction through a different approach.
We have introduced the electron-phonon interaction in the normal state of the heavy fermion system and have used the Periodic Anderson Model. Two different mechanisms of electron-phonon interaction are considered. The usual interaction between the phonons and the electrons in the $f$ bands as well as that of phonons with the hybridization band are used in the present calculation to calculate the phonon self energy the phonon excitation spectrum and the self-energy. The self-energy gets modified through the different electron response functions corresponding to the conduction electrons, $f$-electrons and $f-d$ mixing densities. The elastic constant that is related to the real part of the self-energy is also affected by these interactions. For simplicity we have performed the numerical analysis in the zero correlation, long wave length and finite temperature limit.

4.2.2 Evaluation of Elastic Constant

Neglecting the Coulomb term in Equation. (3.16 – 3.18) the different response functions can be rearranged to give the following set of equations

$$\Gamma_3(qq',\omega) = \sum_{kk'\sigma\sigma'} \Gamma_3(kqk'q'\sigma\sigma'\omega)$$

$$= \frac{\delta_{\sigma\sigma'} \delta_{q-kq} \delta_{k-k'q'}}{2\pi D} [A\langle c^\dagger_{k-q,\sigma} c_{k-q',\sigma'} \rangle - \langle f^\dagger_{k\sigma} f_{k\sigma} \rangle]$$

$$+ B\langle f^\dagger_{k-q,\sigma} f_{k-q',\sigma'} \rangle - \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle + C_1\langle c^\dagger_{k-q,\sigma} f_{k-q,\sigma} \rangle - \langle f^\dagger_{k\sigma} c_{k\sigma} \rangle$$

$$- D\langle f^\dagger_{k-q,\sigma} c_{k-q,\sigma'} \rangle - \langle c^\dagger_{k\sigma} f_{k\sigma} \rangle$$

$$- E\langle f^\dagger_{k-q,\sigma} f_{k-q,\sigma'} \rangle - \langle c^\dagger_{k\sigma} c_{k\sigma} \rangle - \langle f^\dagger_{k\sigma} f_{k\sigma} \rangle]$$

$$\Gamma_4(qq',\omega) = \frac{\delta_{\sigma\sigma'} \delta_{q-kq} \delta_{k-k'q'}}{2\pi D} [A\langle c^\dagger_{k-q,\sigma} f_{k-q',\sigma'} \rangle - B\langle f^\dagger_{k\sigma} c_{k\sigma} \rangle]$$

$$- D\langle f^\dagger_{k-q,\sigma} f_{k-q,\sigma'} \rangle - \langle f^\dagger_{k\sigma} f_{k\sigma} \rangle$$

$$+ E\langle f^\dagger_{k\sigma} c_{k\sigma} \rangle - \langle c^\dagger_{k-q,\sigma} f_{k-q,\sigma'} \rangle]$$
\[ \Gamma_{\nu}(q',\omega) = \frac{\delta_{\omega \omega}}{2\pi} \delta_{q \nu} \delta_{\nu \nu} \left[ \langle f_{\nu q}^* c_{k-q} \rangle - \langle c_{k-q} f_{\nu q} \rangle \right] \]

\[ + \frac{\delta_{\omega \omega}}{2\pi} \delta_{q \nu} \delta_{\nu \nu} \gamma_0 \left[ A \left( \langle f_{\nu q}^* f_{k-q} \rangle - \langle c_{k-q} c_{k-q} \rangle \right) \right] \]

\[ + B \left( \langle f_{\nu q}^* c_{k-q} \rangle - \langle c_{k-q} c_{k-q} \rangle - C_i \left( \langle c_{k-q} f_{\nu q} \rangle - \langle f_{\nu q} c_{k-q} \rangle \right) \right) \]

\[ + D \left( \langle f_{\nu q}^* c_{k-q} \rangle - \langle c_{k-q} c_{k-q} \rangle \right) \]

\[ - E \left( \langle c_{k-q} c_{k-q} \rangle - \langle f_{\nu q}^* f_{k-q} \rangle \right) \]

where

\[ A = (\omega - \varepsilon_k + E_0) - \gamma_0^2 f(kq) \]

\[ B = (\omega + \varepsilon_{k-q} - E_0) - \gamma_0^2 f(kq) \]

\[ C_i = \gamma_0 ((2E_0 - \varepsilon_k - \varepsilon_{k-q})/\omega - \varepsilon_k - \varepsilon_{k-q}) \]

\[ D = \gamma_0 (2E_0 - \varepsilon_k - \varepsilon_{k-q})/\omega \]

\[ E = \gamma_0^2 f(kq) \]

\[ |D| = (\omega + \varepsilon_{k-q} - E_0) (\omega - \varepsilon_{k-q} + E_0) - \gamma_0^2 f(kq) \times (2\omega + \varepsilon_{k-q} - \varepsilon_k) \]

and

\[ f(kq) = \left( \frac{2\omega - \varepsilon_k + \varepsilon_{k-q}}{\omega (\omega - \varepsilon_k + \varepsilon_{k-q})} \right) \]

The phonon Green function \( D_{qq'}(\omega) \) given earlier through Equation (3.8) and the phonon self-energy \( \chi(qq'\omega) \) are written as

\[ D_{qq'}(\omega) = \delta_{q-q'}(\omega^2/\pi)[\omega^2 - \omega_0^2 - 4\pi\omega \chi(qq'\omega)]^{-1} \]

\[ \chi(q,\omega) = \sum_{kk'q} \delta_{kk'} \delta_{qq} \left[ f_1^2(q) \Gamma_1(\varepsilon_{kk'q} + f_2(q)) \Gamma_2(\varepsilon_{kk'q}) \right. \]

\[ + \Gamma_3(\varepsilon_{kk'q} + f_1^2(q)) \Gamma_4(\varepsilon_{kk'q}) \]

Replacing \( \sum_k = \int d\varepsilon_k N(\varepsilon_k) \) the final form of \( \chi \) can be written as
\[ \chi(q,\omega) = \left\{ f_1(q)N(\varepsilon_f)/\pi \right\} \left[ \Gamma_1(kq\omega) + \left( f_2(q)/f_1(q) \right) \Gamma_4(kq\omega) \right. \]
\[ \left. + \Gamma'_5(kq\omega) + \left( f_5(q)/f_1(q) \right)^2 \Gamma'_6(kq\omega) \right\} d\varepsilon_k \] (4.15)

In the long wavelength limit i.e. for \( q=0 \) the expressions for these response functions are given by

\[ \Gamma_1(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ 2(E_0 - \varepsilon_k) \left\langle \left( c^\dagger_{k\alpha} c_{k\alpha} \right) - \left( f^\dagger_{k\alpha} f_{k\alpha} \right) \right\rangle \right. \]
\[ \left. + \frac{4\gamma_0}{\omega} \left\langle \left( c^\dagger_{k\alpha} f_{k\alpha} \right) - \left( f^\dagger_{k\alpha} c_{k\alpha} \right) \right\rangle \right\} \] (4.16)

\[ \Gamma_4(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ 2(\omega - \varepsilon_k + E_0) \left\langle \left( c^\dagger_{k\alpha} f_{k\alpha} \right) - \left( \omega + \varepsilon_k - E_0 \right) \left( f^\dagger_{k\alpha} c_{k\alpha} \right) \right\rangle \right. \]
\[ \left. - \frac{4\gamma_0}{\omega} \left\langle \left( c^\dagger_{k\alpha} f_{k\alpha} \right) - \left( f^\dagger_{k\alpha} c_{k\alpha} \right) \right\rangle \right\} \] (4.17)

\[ \Gamma_5(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ 2\omega \left\langle \left( c^\dagger_{k\alpha} f_{k\alpha} \right) - \left( f^\dagger_{k\alpha} c_{k\alpha} \right) \right\rangle + \frac{4\gamma_0}{\omega} \left\langle \left( f^\dagger_{k\alpha} c_{k\alpha} \right) - \left( c^\dagger_{k\alpha} f_{k\alpha} \right) \right\rangle \right\} \] (4.18)

\[ \Gamma_6(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ (\omega - \varepsilon_k + E_0) \left\langle \left( f^\dagger_{k\alpha} c_{k\alpha} \right) \right\rangle \right. \]
\[ \left. - \frac{4\gamma_0}{\omega} \left\langle \left( f^\dagger_{k\alpha} c_{k\alpha} \right) \right\rangle \right\} \] (4.19)

Since for \( q = 0 \), \( \left\langle c^\dagger_{k\alpha} f_{k\alpha} \right\rangle = \left\langle f^\dagger_{k\alpha} c_{k\alpha} \right\rangle \) the set of equations (4.16 - 4.19) further simplified and expressed as

\[ \Gamma_1(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ 2\left( E_0 - \varepsilon_k \right) \left\langle \left( c^\dagger_{k\alpha} c_{k\alpha} \right) - \left( f^\dagger_{k\alpha} f_{k\alpha} \right) \right\rangle \right\} \] (4.20)

\[ \Gamma_4(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ 2\left( E_0 - \varepsilon_k \right) \left\langle \left( c^\dagger_{k\alpha} f_{k\alpha} \right) \right\rangle \right\} \] (4.21)

\[ \Gamma_5(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ 2\gamma_0 \left\langle \left( f^\dagger_{k\alpha} f_{k\alpha} \right) \right\rangle \right\} \] (4.22)

\[ \Gamma_6(q=0,\omega) = \sum_{k\alpha} \frac{\delta_{\alpha\alpha} \delta_{\sigma\sigma}}{2\pi |D|} \left[ 2\gamma_0 \left\langle \left( c^\dagger_{k\alpha} c_{k\alpha} \right) \right\rangle \right\} \] (4.23)

where

\[ |D|_{\omega=0} = (\omega + \varepsilon_k - E_0)(\omega - \varepsilon_k + E_0) - 4\gamma_0^2 \] (4.24)
Following the standard technique of Zubarev [200] the different correlation functions involved in these equations are evaluated and these are expressed as

\[
\langle c_{\alpha \sigma}^+ c_{\beta \rho} \rangle = -\gamma_{12}[\gamma_1 (y_2 - E_0) - \gamma_2 (y_1 - E_0)]
\] (4.25)

\[
\langle f_{\alpha \sigma}^+ f_{\beta \rho} \rangle = -\gamma_{12}[\gamma_1 (y_1 - \varepsilon_\kappa) - \gamma_2 (y_2 - \varepsilon_\kappa)]
\] (4.26)

\[
\langle c_{\alpha \sigma}^+ f_{\beta \rho} \rangle = \langle f_{\alpha \sigma}^+ c_{\beta \rho} \rangle = \gamma_{12} \gamma_0 [\gamma_{11} + \gamma_{22}] 
\] (4.27)

where

\[
\gamma_{11} = \frac{1}{e^{\eta/\theta} + 1} 
\] (4.28)

\[
\gamma_{22} = \frac{1}{e^{\eta/\theta} + 1} 
\] (4.29)

\[
\gamma_{12} = -\frac{\delta_\alpha \delta_\beta \delta_\kappa \delta_\rho}{\gamma_1 - \gamma_2} 
\] (4.30)

\[
y_1 = (1/2) \{ (\varepsilon_\kappa + E_0) + \sqrt{(\varepsilon_\kappa - E_0)^2 + 4\gamma_0^2} \}
\] (4.31)

\[
y_2 = (1/2) \{ (\varepsilon_\kappa + E_0) - \sqrt{(\varepsilon_\kappa - E_0)^2 + 4\gamma_0^2} \}
\] (4.32)

and

\[
\frac{1}{e^{\eta/\theta} + 1} - \frac{1}{e^{\eta/\theta} + 1} = (1/2) [\tanh(y_2/2\theta) - \tanh(y_1/2\theta)]
\] (4.33)

Analyzing in the same way to that of Wojciechowski et al [114] and using the usual relation with change of elastic constant to that of the real part of self-energy, one can write the expression \( C / C_0 \) in the long wavelength limit \( \omega = \nu q \). It well known that the change in sound velocity \( \Delta S = S - S_0 \) is related to the real part of \( \chi(q\omega) \) in the following way

\[
\Delta S / S = (4\pi / \omega_0) \text{Re} \chi(q\omega)
\] (4.34)

where \( \omega_0 \) is the bare value of sound velocity and \( S \) is the sound velocity with interaction.

Further the change in longitudinal elastic constant is related to the change in sound velocity as

\[
\Delta C = 2\rho C_0 \Delta S
\] (4.35)
Here $\rho$ is the mass density and $C$ is the bare elastic constant. $\omega$ and $\omega_q$ are related to $S$ and $q$ as

$$\omega = S q \Rightarrow S / S_0^2 = C / C_0$$  \hspace{1cm} (4.36)

$$\omega_q = S_0 q \Rightarrow \omega^2 / \omega_q^2 = S^2 / S_0^2 = 1 + (4\pi / \omega_q) \text{Re} \chi(q\omega)$$  \hspace{1cm} (4.37)

and

$$S = \sqrt{C / \rho}$$  \hspace{1cm} (4.38)

$$\tilde{C} = C / C_0 = 1 + (4\pi / \omega_q) \text{Re} \chi(q\omega)$$  \hspace{1cm} (4.39)

$$S_0 = \sqrt{C_0 / \rho}$$  \hspace{1cm} (4.40)

Here the zero subscript corresponds to the bare values of the elastic constant. Equation (4.39) is valid for all wave vector $q$ and $T$. This can be simplified by taking some usual approximation performing the numerical evaluation for $q=0$ and for small $T$ and the self-energy $\chi(q\omega)$ can be expressed as

$$\chi(0,\omega) = \left[ \sum_{\alpha} \frac{\tilde{L}_{\alpha}(0)}{2\lambda} N(e_F) \left[ (e_k - E_0)^2 + 2\gamma (e_k - E_0) \tilde{L}_{\alpha}(0) + \tilde{L}_{\alpha}(0)^2 \gamma_{\alpha}^2 \right] \right] \left[ (e_k - E_0)^2 + 4\gamma^2 \right]^{1/2}$$

$$\times \left[ \tanh \left( \frac{\omega}{2\gamma} \right) - \tanh \left( \frac{\omega}{2\gamma} \right) \right]$$

(4.41)

It is evident from Equation (4.41) that $\chi(0,\omega)$ is zero for $T = 0$. This is because in this limit both $\tanh(\omega/2\gamma)$ and $\tanh(\omega/2\gamma)$ become equal to 1. Performing the small $T$ expansion of Equation (4.33) we can express

$$\tanh \left( \frac{\omega}{2\gamma} \right) - \tanh \left( \frac{\omega}{2\gamma} \right) = - \left( 4e^{i(k\xi - E_0) / KT} \right) \sinh \sqrt{(e_k - E_0)^2 + 4\gamma^2} / 2KT$$

(4.42)

Performing the integration over the conduction bandwidth $W$ from $-W/2$ to $W/2$ and parameterizing the different quantities in Equations (4.31 - 4.33, 4.42) we can express the reduced value of the elastic constant $\tilde{C}$ as

$$\tilde{C} = 1 - 4g(I_1 + I_2 + I_3)$$

(4.43)

where,

$$I_1 = 2e^{-\beta d} \int dy \sinh \left[ \frac{2bi(1/4)(y - d)^2 + 1}{D_1} \right]$$

(4.44)
Numerical Evaluation

\[ I_2 = 2D_1e^{-\beta d} \int dy e^{-\beta y} \frac{[2b(1/4)(y-d)^2 + 1]^{1/2}}{D_1D_2} \quad (4.45) \]

\[ I_3 = re^{-\beta d} \int dy(y-d)e^{-\beta y} \frac{[2b(1/4)(y-d)^2 + 1]^{1/2}}{D_1D_2} \quad (4.46) \]

and

\[ D_1 = [(1/4)(y-d)^2 + 1]^{1/2} \quad (4.47) \]

\[ D_2 = [(1/4)(y-d)^2 - C^2] + 1 \quad (4.48) \]

\[ D_3 = (1/4)(C^2 + r^2) + 1 \quad (4.49) \]

Equation (4.42) is evaluated numerically for the different parameter \( r, g, d \) and temperature. The physical meaning of these parameters is already explained in section 4.1.1.

4.2.3 Results and Discussion

The different dimensionless parameters involved in the numerical calculation are \( r, g, d, b' \) and \( \tilde{T} \), which are explained earlier. We have evaluated the Equation (4.43) in the static limit. Considering different values of these for which uniform softening of phonons are observed in the experiment sets the initial parameters. The electron-phonon coupling term of the present calculation consists of two parameters \( f_1(0) \) and \( f_2(0) \) which are related to the strength of coupling of phonons to the hybridization between \( f \) and conduction electrons and to the \( f \) electrons respectively. When one compares these parameters with those of Wojciechowski et al [114] defined through their equations (4.6 - 4.12), it is found that \( f_1(0) \) can be thought of arising from a volume dependence of bare hybridization strength \( \gamma_0 \), i.e., \( f_1(0) = \delta \gamma_0 / \delta \eta \) (our \( \gamma_0 \) is same as their \( \nu \)). Similarly \( f_2(0) \) can be thought of arising from a volume dependence of bare position of the \( f \)-level \( (E_0) \) i.e., \( f_2(0) = \delta E_0 / \delta \eta \). Here \( \eta \) being the volume strain and can be related directly to the phonon operators. Thus, these two volume dependent quantities \( (f_1(0), f_2(0)) \) together with conduction electron band \( (W) \), the bare hybridization strength \( (\gamma_0) \) and bare position of \( f \)-level \( (E_0) \) form the model parameters. It is observed that the strength of
Numerical Evaluation

coupling of phonons $f_i(0)$ with the hybridization plays a dominant role and is stronger compared to the strength of coupling of phonons with that of the $f$-band $f_2(0)$ so as to explain the existence of superconductivity in $\text{CeCu}_2\text{Si}_2$. On the basis of this finding the numerical value of the parameter $r$ which is the ratio of coupling parameter is always taken as less than one. Secondly the numerical evaluation of the integrals of equations (4.44 - 4.46) we have assumed the Fermi level to lie in mid way between the lower and the upper limit of the conduction band. Moreover we have set the Fermi level $E_f$ equal to zero. It implies that whenever the $f$-level lies below the Fermi level, the parameter $d$ associated with its position is negative and above $E_f$ is positive. Considering the limitations of these parameters and uniform softening of phonon energy with temperature the other parameters may be set in the process as $\gamma = 0.01$, $g = 0.1$ and $d = -2.0$.

In this section we have shown the variation of $\tilde{C}$ for different values of $r$, $d$, $g$ and temperature $T(=T/T_k)$ through three figures (Fig 4.1- 4.3). In Fig 4.1, we have shown the variation of $\tilde{C}$ with temperature for different values of $r$ i.e., 0.01, 0.1 and 0.5 keeping other parameters $g$ and $d$ fixed at values 0.01 and -2.0 respectively. From the variation of $\tilde{C}$, it is found that as the values of $r$ decrease so also the value of $\tilde{C}$. It implies that stronger the strength phonons with hybridization band than that of $f$-band, the more softening at low temperature.

![Fig. 4.1: Plot of $\tilde{C}(= C/C_0)$ versus temperature $\tilde{T} = T/T_k$ for $r = 0.01$, 0.1 and 0.5 for fixed values of $g = 0.1$ and $d = -2.0$](image)

The Fig. 4.2 is the plot of same quantities for different values of $g$ i.e., 0.1, 0.5 and 1.0 for fixed values of $r = 0.01$ and $d = -2.0$. Here the variation is exactly the opposite to that of Fig. 4.1. From the variation of $\tilde{C}$ it is clearly noticed that as $g$ values increase, the reduced elastic constant $\tilde{C}$ values decrease. This implies that the
Numerical Evaluation

electron-phonon coupling with hybridization produces more softening and is prominent at low temperature.

A similar plot has also been made in Fig 4.3 for different values of $d (= -2.0, -1.5$ and $1.5)$ for the fixed values of $r=0.01$ and $g=0.1$. Here we observed that as the values of $d$ increase from the negative to positive values the degree of softening decreases. For negative values of $d$ the softening is stronger than the positive values. In all these plots it is found that the different parameters which are intimately related to the heavy fermion systems have strong influence at extremely low temperature. Moreover in all cases $C$ approaches gradually to a maximum and ultimately saturates at high temperature.

From the results presented in this section it is found that the temperature variation of the elastic constant agrees well with that of experimental observations for the compounds CeCu$_6$ and CeRu$_2$Si$_2$ and for some other systems like CeAl$_3$ and UPt$_3$ the variation is poor [114]. The measurements of the elastic constant for the later two systems show a dip at extremely low temperatures. These dips are thought due to the volume dependence of hybridization and $f$-level energy as well as the local screening effect [157]. As it is difficult to carry out these effects in the present approach

Fig. 4.2: Plot of $\tilde{C}(= C / C_0)$ versus temperature $\tilde{T} = T / T^*$ for $g = 0.1, 0.5$ and $1.0$ for fixed values of $r = 0.01$ and $d = -2.0$.

Fig. 4.3: Plot of $\tilde{C}(= C / C_0)$ versus temperature $\tilde{T} = T / T^*$ for $d = -2.0, -1.5$ and $1.5$ for fixed values of $r = 0.01$ and $g = 0.1$. 

102
we have neglected them and fail to explain the dip seen in some systems. However our present calculation give satisfactory agreement for the whole temperature range for some other systems.

4.3 **Microscopic theory of electron-phonon coupling**

**Mechanism in Heavy Fermion systems.**

**4.3.1 Introduction**

There are several observations, which suggest the existence of strong electron-phonon interaction in heavy fermion systems. The most prominent effect of these are the softening of elastic constant, temperature dependence of thermal expansion and the strong softening of phonons below the Kondo temperature. As discussed earlier we considered two different mechanisms of electron-phonon coupling through Periodic Anderson Model [90]. Our aim here is to calculate the influence of \( f \) and conduction electron 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 conduction electrons, \( f \)-electrons and \( f - d \) mixing densities.

**4.3.2 Evaluation for small \( q \) and \( T \) limit**

Since we are interested in the calculation phonon response functions it is necessary to evaluate the phonon Green function [112], which is defined as

\[
D_{qq'}(t-t') = \langle \langle A_q(t); A_{q'}(t') \rangle \rangle 
= -i \delta(t-t') \langle [A_q(t); A_{q'}(t')] \rangle \tag{4.50}
\]

The Fourier transformed Green function \( D_{qq'}(\omega) \) for the system defined by the Hamiltonian Equation (3.1) is evaluated to express the phonon self-energy. The phonon self-energy is defined as

\[
\omega^2 - \omega_q^2 = 4\pi \omega_q \chi_{qq'}(\omega) = 0 \tag{4.51}
\]

where

\[
\chi_{qq'}(\omega) = f_1(-q)f_1(-q')\Gamma_1(qq'\omega) + f_1(-q)f_2(-q')\Gamma_2(qq'\omega) + f_2(-q)f_1(-q')\Gamma_3(qq'\omega) + f_2(-q)f_2(-q')\Gamma_3(qq'\omega) \tag{4.52}
\]
Numerical Evaluation

here Γ's (i=1 to 4) represent the electron response functions.

\[ \Gamma_1(kq,k'q',\omega) = \frac{\delta_{qq'}\delta_{kk'}}{2\pi |D|} \left[ \{(\omega - \varepsilon_k + E_0) - 2\gamma_0^2 F(kq)\} A_0 + \{(\omega + \varepsilon_{k-q} - E_0) - 2\gamma_0^2 F(kq)\} A_1 - \frac{2E_0 - \varepsilon_{k-q} - \varepsilon_k}{\omega - \varepsilon_k + \varepsilon_{k-q}} \right] + \gamma_0 \left[ \frac{2E_0 - \varepsilon_{k-q} - \varepsilon_k}{\omega} \right] A_3 \]

\[ \Gamma_2(kq,k'q',\omega) = \frac{\delta_{qq'}\delta_{kk'}}{2\pi |D|} \left[ \gamma_0 \{(\varepsilon_k + \varepsilon_{k-q} - 2E_0)/\omega \} A_4 + \{(\omega + E_0 - \varepsilon_k) - 2\gamma_0^2 F(kq)\} A_5 + \{(\omega - E_0 + \varepsilon_{k-q}) - 2\gamma_0^2 F(kq)(A_2 - A_3)\} \right] \]

\[ \Gamma_3(kq,k'q',\omega) = \frac{\delta_{qq'}\delta_{kk'}}{2\pi \omega |D|} \left[ \{(\varepsilon_k - E_0 - \omega) A_0 - \gamma_0 \left[ \frac{2\omega + \varepsilon_{k-q} - \varepsilon_k}{\omega + \varepsilon_{k-q} - \varepsilon_k} \right] A_2 + (\omega + \varepsilon_{k-q} - E_0) A_3 \right] \]

\[ \Gamma_4(kq,k'q',\omega) = \frac{\delta_{qq'}\delta_{kk'}}{2\pi \omega |D|} \gamma_0 \left[ \{(\varepsilon_k + \varepsilon_{k-q} - 2E_0)/(2\omega + \varepsilon_{k-q} - \varepsilon_k)\} A_4 - (\omega - \varepsilon_k + E_0) A_5 - (\omega + \varepsilon_{k-q} - E_0) A_6 \right] \]

Where

\[ A_0 = \left\langle c_{k-q,\sigma}^+ c_{k-q,\sigma} \right\rangle - \left\langle f_{k,\sigma}^+ f_{k,\sigma} \right\rangle \]

\[ A_1 = \left\langle f_{k-q,\sigma}^+ f_{k-q,\sigma} \right\rangle - \left\langle c_{k,\sigma}^+ c_{k,\sigma} \right\rangle \]

\[ A_2 = \left\langle c_{k-q,\sigma}^+ f_{k-q,\sigma} \right\rangle - \left\langle f_{k,\sigma}^+ c_{k,\sigma} \right\rangle \]

\[ A_3 = \left\langle f_{k-q,\sigma}^+ c_{k-q,\sigma} \right\rangle - \left\langle c_{k,\sigma}^+ f_{k,\sigma} \right\rangle \]

\[ A_4 = \left\langle f_{k-q,\sigma}^+ f_{k-q,\sigma} \right\rangle - \left\langle c_{k,\sigma}^+ c_{k,\sigma} \right\rangle \]

\[ A_5 = \left\langle f_{k,\sigma}^+ f_{k,\sigma} \right\rangle \]

\[ A_6 = \left\langle c_{k,\sigma}^+ c_{k,\sigma} \right\rangle \]

and

104
Numerical Evaluation

\[ |D| = (\omega + \varepsilon_{k-q} - E_0) \left( \omega - \varepsilon_k + E_0 \right) - \gamma_0^2 F(kq)(2\omega + \varepsilon_{k-q} - \varepsilon_k) \]  
\[ (4.64) \]

\[ F(kq) = \frac{(2\omega + \varepsilon_{k-q} - \varepsilon_k)}{(\omega + \varepsilon_{k-q} - \varepsilon_k)} \]  
\[ (4.65) \]

In view of our interest we have evaluated Equations. (4.51, 4.52) for small \( q \) and \( T \) limit. In doing so we have expanded \( \varepsilon_{k-q} \) and the Fermi function \( m_{k-q} \) up to the order linear in \( q \) as

\[ \varepsilon_{k-q} = \varepsilon_k - q\nu_F \]  
\[ (4.66) \]

\[ m_{k-q} = m_k - q\nu_F \delta(\varepsilon_k - \varepsilon_F) \]  
\[ (4.67) \]

where

\[ \nu_k = \frac{\partial \varepsilon_{k-q}}{\partial k_{q=0}} \]  
\[ (4.68) \]

and

\[ \delta(\varepsilon_k - \varepsilon_F) = \frac{\partial m_{k-q}}{\partial \varepsilon_{k-q}} \]  
\[ (4.69) \]

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

\[ \tanh(y_1/2\theta) - \tanh(y_2/2\theta) = -2 \exp((\varepsilon_k - E_0)/2\theta) \sinh(\sqrt{(\varepsilon_k - E_0)^2 + 4\gamma_0^2})/2\theta \]  
\[ (4.70) \]

where

\[ y_{1,2} = 1/2\{(\varepsilon_k + E_0) \pm \sqrt{(\varepsilon_k - E_0)^2 + 4\gamma_0^2} \} \]  
\[ (4.71) \]

When these are substituted in Equation. (4.51) the renormalized phonon dispersion takes the form

\[ (\omega/\omega_q)^2 = 1 + (4\pi/\omega_q)\chi(\omega, q, T) \]  
\[ (4.72) \]

and

\[ \chi(\omega, q, T) = \chi(\omega, q = 0, T) + \chi(\omega, q, T = 0) + \chi(\omega, q, T) \]  
\[ (4.73) \]

After paramaterizing the different quantities of Equation. (4.73) the Equation. (4.72) can be put in the compact form as defined below

\[ (\omega/\omega_q)^2 = 1 - 4g(I_1 + I_2 + I_3) \]  
\[ (4.74) \]
Numerical Evaluation

where

\[ I_1 = 4A(B + C) \]  \hspace{1cm} (4.75)

\[ I_2 = \int dx F \exp(-bx) \sinh(bD) / DE \]  \hspace{1cm} (4.76)

\[ I_3 = \int dx(J + H) \exp(-bx) \sinh(bD) / E \]  \hspace{1cm} (4.77)

\[ A = 4k(c-yf+d)/\{(yf-d)^2-c^2+4\} \]  \hspace{1cm} (4.78)

\[ B = 2r/\{(yf-d)-1\} \]  \hspace{1cm} (4.79)

\[ C = r^3(c+yf-d)/\{(yf-d)^2(c-yf+d)\} \]  \hspace{1cm} (4.80)

\[ D = \sqrt{(x-d)^2+4} \]  \hspace{1cm} (4.81)

\[ E = \{(x-d)^2+4-c^2\} \]  \hspace{1cm} (4.82)

\[ F = \{(x-d)^2+2r(x-d)+r^2\} \exp(-bd) \]  \hspace{1cm} (4.83)

\[ G = \{(c-x+d)/(x-d+c)\} \]  \hspace{1cm} (4.84)

\[ H = [kG+2rkG(2(x-d)+c)/(x-d)^2] \]  \hspace{1cm} (4.85)

\[ I = [(2r^2k(x-d)(x-d-1)+c(x-d-c))/(x-d)^2(x-d-c)] \]  \hspace{1cm} (4.86)

\[ 4.3.3 \text{ Results and Discussion} \]

The different dimensional parameters those are involved in the numerical calculations are \( r, g \) and \( d \) and they have their usual meaning as described in the beginning of this chapter. The other parameters involved in the calculation are \( yf, x, c \) and \( k \), which represent 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 heavy fermion systems. The results of the calculations are presented in three figures (Fig. 4.4 – 4.6). Figure 4.4 shows the variation of renormalized phonon energy \( \tilde{\omega} \) with \( b \), the inverse of the

Fig.4.4: Plot \( \tilde{\omega}(=\omega / \omega_o) \) verses \( b \) for \( q=0, r=0.01, g=0.01 \) for \( d=-5.0, -2.0 \) and \( 2.0 \).
Numerical Evaluation

temperature for $q=0$ and for different values of $d$(-5.0, -2.0, 0, 2.0). It is found that the degrees of phonon softening decreases as $f$-level move towards the Fermi level. But for positive values of $d$ there is hardly any softening. Figure 4.5 shows the variation of $\omega$ with $q$ for $T=0$ and for same values of $d$. It is found that the softening is poor compared to the variation $\omega$ with that of temperature shown in Figure 4.4. Moreover hardening of phonon is observed when the $d$ value is positive. Finally the Figure 4.6 shows the variation of $\omega$ for finite values of $q$ and $T$. Thus to study the effect the plot is made for $\omega$ versus $q$ for different values of $T$ i.e., for different values of $b (=0, 0.1, 0.2, 0.3)$ with same values of $r$ and $g$ (as taken in Figure 4.4 and 4.5) with $d = -2.0$. It is observed that as the temperature is decreased the softening of phonon becomes faster.

Comparing this plot with the other two plots described earlier it is observed that both $q$ and $T$ have finite contribution to the phonon spectrum. The other two parameters $r$ and $g$ which, also influence phonon softening are discussed latter.
4.4 Influence of Electron-Phonon Interaction on Effective mass in some Intermetallic Compounds.

4.4.1 Introduction

In ordinary metals the electron-phonon interaction increases the quasi particle mass $m^*$. In heavy fermion systems the effect of electron-phonon interaction is quite different. In heavy fermion systems the electron-phonon interaction results in decreasing of quasi particle mass considering the system as a Kondo lattice. When a singlet is formed at low temperature at each rare earth or actinide site between the $f$-electrons and the conduction electrons, the energy gain due to this is $E_0 = -k_B T^*$. Here $T^*$ is the equivalent of the Kondo temperature. It defines a low energy scale. The quasi particle mass $m^*$ is proportional to inverse of $(T^*)^{-1}$ [158].

Due to the electron-phonon interaction the energy gain in singlet formation increases. The hybridization of $f$-electrons with conduction electrons, on which $T^*$ crucially depends, increases when the neighbors move closer to an $f$ site. Electron-phonon interaction and decrease in effective mass increase the energy gain due to the singlet formation. Because the excitations which breaks the singlets are spread over a large energy interval [159]. Some recent experiments on heavy fermion systems suggest that there exist a strong coupling of the elastic degrees of freedom with these at the electronic and magnetic ones. To understand the effect of electron-phonon interaction on effective mass we have considered the electron-phonon coupling mechanism in the framework of PAM. In this section we have tried to observe the effect of electron-phonon interaction on effective mass through self-energy, which is related to the effective mass in the following way

$$
m^* / m = \tilde{m} = 1 / [1 + \frac{1}{v_F} \frac{\partial}{\partial k} \Sigma(k,\omega)]_{k=k_F} \quad (4.87)$$

$$
\text{Numerical Evaluation}
$$
For simplicity we have first explored the properties of the system in the normal state for long wavelength limit in the finite temperature limit without keeping the $f-f$ correlation term. Later we will also discuss the effect of the correlation on effective mass.

### 4.4.2 Evaluation

Effective mass is related to the original mass $m$ as

$$\frac{1}{m^*} = \frac{1}{m} + \frac{1}{\hbar v_F k_F} \frac{\partial \Sigma}{\partial k_{\parallel k_F}}$$

which ultimately can be put in the form

$$\frac{m^*}{m} = \frac{1}{\mu + \frac{\partial \Sigma(k, \omega, q)}{\partial \varepsilon_k}}$$

The conduction electron Green Function $G(k, \omega)$ is calculated as

$$G_{\omega \omega'}(t-t') = \langle \{ c_{\omega}(t); c_{\omega'}^\dagger(t') \} \rangle$$

The equation of motion for $G_{\omega \omega'}(t-t')$ we have

$$i \frac{d}{dt} G_{\omega \omega'}(t-t') = \theta(t-t') \{ [c_{\omega}(t), H] \} + \left\{ i \frac{d}{dt} c_{\omega}(t); c_{\omega'}^\dagger(t') \right\}$$

When the time derivative for different electron operators given in Equations\,(3.75 - 3.78) are substituted in Equation\,(4.91) additional higher order Green functions are generated, the Fourier transformed of which can be defined as

$$\Gamma_1(k, \omega, q) = \langle \{ f_{\omega-q, \alpha} A_{\alpha}; c_{\omega}^\dagger \} \rangle$$

$$\Gamma_2(k, q, \omega) = \langle \{ c_{\omega-q, \alpha} A_{\alpha}; c_{\omega}^\dagger \} \rangle$$

$$\Gamma_3(k, q, q) = \langle \{ f_{\omega-q, \alpha} B_{\alpha}; c_{\omega}^\dagger \} \rangle$$

$$\Gamma_4(k, \omega, \omega) = \langle \{ c_{\omega-q, \alpha} B_{\alpha}; c_{\omega}^\dagger \} \rangle$$

Writing the equation of motion for each we get the following set of equations

$$[\omega - \varepsilon_k - \{ \gamma_q \frac{\omega}{\hbar} / (\omega - E_\alpha) \}] G(k, \omega) = (1/2\pi) \sum_q f_q(q) \Gamma_1$$

$$(\omega - E_\alpha) \Gamma_1 = \gamma_q \Gamma_2 + \omega_q \Gamma_3 + N_q \{ f_q(-q) + \frac{\delta(q-q)}{\delta(q-q)} \} G(k, \omega)$$
Numerical Evaluation

\[
(\omega - \varepsilon_{k-q}) \Gamma_2 = \frac{\left\langle \phi_{k-q} \right\rangle}{2\pi} + \gamma_0 \Gamma_1 + \omega \gamma_0 \Gamma_4 + f_1(-q) N_q G_{1}(k, \omega) \tag{4.99}
\]

\[
(\omega - E_0) \Gamma_3 = \gamma_0 \Gamma_4 + \omega \gamma_0 \Gamma_1 + \{2 f_2(-q)(1 - n_{k-q}^f) - 2 f_1(-q) \varphi_{k-q} \sigma f_2(-q) M_q \} G_1
\]
\[+ f_1(-q) (2(1 - n_{k-q}^f) + M_q) G_{1}(k, \omega) \tag{4.100}
\]

\[
(\omega - \varepsilon_{k-q}) \Gamma_4 = \frac{\left\langle \phi_{k-q} \right\rangle}{2\pi} + \gamma_0 \Gamma_3 + \omega \gamma_0 \Gamma_2 - 2 f_2(-q) \rho_{k-q} \sigma G(k, \omega)
\]
\[+ (2 f_1(-q)(1 - n_{k-q}^f) - 2 f_2(-q) \rho_{k-q} \sigma + M_q f_1(-q)) G_1 \tag{4.101}
\]

where

\[
N_q = \gamma_q + \gamma_{-q} + 1 = 2 \gamma_q + 1 \tag{4.102}
\]

\[
\gamma_0 = \frac{1}{e^{\hbar \omega/kT} - 1} \tag{4.103}
\]

\[
\varphi_{k-q,\sigma} = \left\langle \gamma_q - \gamma_{-q} - 1 \right\rangle \tag{4.104}
\]

\[
\varphi'_{k-q,\sigma} = \left\langle f^1_{k-q,\sigma} c_{k-q,\sigma} \right\rangle \tag{4.105}
\]

\[
n_{k-q,\sigma}^f = \left\langle f^f_{k-q,\sigma} c_{k-q,\sigma} \right\rangle \tag{4.106}
\]

\[
n_{k-q,\sigma}^c = \left\langle c^c_{k-q,\sigma} c_{k-q,\sigma} \right\rangle \tag{4.107}
\]

\[
\gamma_q = b_q b_q \tag{4.108}
\]

From the above Green Functions the conduction electron Green functions can be calculated as

\[
G(k, \omega) = \frac{1}{2\pi} \left[ \frac{1 + \sum_{1}(kq\omega) \left\langle A_0 \right\rangle + \sum_{2}(kq\omega) \left\langle B_0 \right\rangle}{\omega - \varepsilon_k - (\gamma_q / (\omega - E_0)) - \sum_{3}(kq\omega)} \right] \tag{4.109}
\]

where

\[
\sum_{1}(kq\omega) = \sum_{q} f_1(q) \gamma_0 (1 + \frac{\omega^2}{|D_3|} \frac{1}{|D_3|}) \tag{4.110}
\]

\[
\sum_{2}(kq\omega) = \sum_{q} f_1(q) \left\{ \frac{(2\omega - \varepsilon_{k-q} - E_0) \gamma_0 \omega_k}{|D_3|} \right\} \tag{4.111}
\]

\[
\sum_{3}(k, \omega, q = 0) = \sum_{q} \left[ \frac{f_1^2(0)}{|D_3|} \left[ \omega - \varepsilon_k \omega_q^0 (1 - n_{k,\sigma}^f)ight.ight.
\]
\[- (2f_1 \varphi_{k,q} (\omega - E_0)) \left( \omega - \varepsilon_k \right)^2 \omega_{k,\sigma} - 2(2\omega - \varepsilon_k - E_0) \gamma_0 \omega_k \varphi_k
\]
\[+ \gamma (\omega - \varepsilon_k)^2 \gamma_0 \omega_0 (\omega - E_0) (1 - \omega_{k,\sigma}^f) + \gamma (\omega - \varepsilon_k)^2 \gamma_0 N_0 \right] \tag{4.112}
\]

110
The electron self-energy is written as

$$\Sigma(k, q, \omega) = \omega - G^{-1}(k, \omega)$$

$$= \omega - 2\pi \left\{ \frac{\omega - \varepsilon_k - \left( \gamma_0^2/(\omega - E_0) \right) - \sum_j (kqo_j)}{1 + \sum_j (kqo_j) \langle A_j \rangle + \sum_j (kqo_j) \langle B_j \rangle} \right\}$$

with special condition $q=0$, $T \neq 0$. Keeping terms up to $\gamma_0^2, \omega_0^2$ and $\gamma_0\omega_0$ the effective mass is calculated as

$$m^* = \frac{1}{m + \left[ \frac{\delta}{\delta \omega} \Sigma(k, q, \omega) \right]_{q=0}}$$

Keeping the term linear in $\gamma_0, \omega_0$ and putting $|D_3| = |D_3|$ we get

$$\sum_k (k, \omega, q = 0) = \sum \frac{f_1^2(0)}{|D_2||D_3|} \left[ \omega_0(\omega - \varepsilon_k)^2(1 - 2n_{k,x}^0) + (\omega - E_0)(\omega - \varepsilon_k)^2 N_0 \right]$$

$$+ \gamma(\omega - \varepsilon_k)^2 \gamma_0 N_0$$

$$\approx \frac{3f_1^2(0)}{|D_3|^2} \left[ \omega_0(\omega - \varepsilon_k)^2(1 - 2n_{k,x}^0) + (\omega - E_0 + \gamma_0 N_0) \right]$$

$$\approx \frac{3g}{|D_3|^2} \left[ \omega_0^2(\omega - \varepsilon_k)^2(1 - 2n_{k,x}^0) + \omega_0(\omega - \varepsilon_k)^2(\omega - E_0 + \gamma_0 N_0) \right]$$

$$\sum_{-k} (-k, \omega, q = 0) = \sum \frac{f_1(0)\gamma_0}{|D_2||D_3|} (|D_3| + \omega_0^2) = \frac{3f_1(0)\gamma_0}{|D_3|}$$

$$\sum_{-k} (-k, \omega, q = 0) = \sum \frac{f_1(0)(2\omega - \varepsilon_k - E_0')\gamma_0 \omega_0}{|D_2||D_3|} = 0$$

where

$$|D_3| = (\omega - \varepsilon_{k+q})(\omega - E_0) - \gamma_0^2$$

$$|D_2| = \{\omega - \varepsilon_{k+q} - \left( \frac{\omega - \varepsilon_k}{|\beta|} \right) \} (\omega - E_0 - \left( \frac{\omega - \varepsilon_k}{|\beta|} \right)) - \gamma_0^2 (1 + \frac{\omega^2}{|\beta|^2})$$

$$1 + \sum \langle A_0 \rangle + \sum \langle B_0 \rangle = 1 + \sum \langle A_0 \rangle$$

$$\sum (k, \omega, q = 0) = \omega - 2\pi \left\{ \frac{\omega - \varepsilon_k - \gamma_0^2}{1 + \sum \langle A_0 \rangle} \right\}$$
Numerical Evaluation

\[
\frac{\partial \Sigma}{\partial \varepsilon_k} = -2\pi \left[ \frac{\partial}{\partial \varepsilon_k} \left( \frac{\omega - \varepsilon_k - \frac{\gamma_k^2}{(\omega - \varepsilon_k)^2} - \Sigma_3}{1 + \Sigma_1 \langle A \rangle} \right) \right]
\]

\[
= -2\pi \left[ \frac{-1 - \frac{\delta \omega_0}{\delta \varepsilon_k} \omega - \varepsilon_k - \frac{\gamma_k^2}{(\omega - \varepsilon_k)^2} - \Sigma_3 \frac{\partial \Sigma_1}{\partial \varepsilon_k} \langle A \rangle}{1 + \Sigma_1 \langle A \rangle} \right]
\]

\[
(4.122)
\]

Let

\[
a = \frac{1 + \frac{\delta \omega_0}{\delta \varepsilon_k}}{1 + \Sigma_1 \langle A \rangle}
\]

\[
b = \frac{\omega - \varepsilon_k - \frac{\gamma_k^2}{(\omega - \varepsilon_k)^2} - \Sigma_3}{1 + \Sigma_1 \langle A \rangle} \frac{\partial \Sigma_1}{\partial \varepsilon_k} \langle A \rangle
\]

\[
\Rightarrow \frac{\partial \Sigma}{\partial \varepsilon_k} = 2\pi (a + b)
\]

\[
(4.123)
\]

\[
C = \frac{\partial}{\partial \varepsilon_k} \left( \Sigma_1 \langle A \rangle \right) = \frac{\partial}{\partial \varepsilon_k} \left[ 3\sqrt{g} \gamma \omega_0 \frac{(\omega - \varepsilon_k)(\omega - E_0) - \gamma_0^2}{|D_3|^3} \right]
\]

\[
= 3\sqrt{g} A \frac{(\omega - \varepsilon_k)(\omega - E_0) - \gamma_0^2}{|D_3|^3} \frac{\partial}{\partial \varepsilon_k} [(\omega - \varepsilon_k)(\omega - E_0) - \gamma_0^2]
\]

\[
(4.126)
\]

\[
= 3\sqrt{g} \gamma \omega_0 \frac{(\omega - E_0)}{A}
\]

\[
(4.127)
\]

\[
\frac{\partial \Sigma_3}{\partial \varepsilon_k} (k, \omega, q = 0) = \frac{\partial}{\partial \varepsilon_k} \left[ 3g (\omega - \varepsilon_k)^2 \left( \omega_0^2 (1 - 2n'_{\omega}) + \omega_0 (\omega - E_0 + \gamma_0) N_0 \right) \right]
\]

\[
= 3g \left[ \frac{\{2(\omega - \varepsilon_k)\} \{\omega - \varepsilon_k\}(\omega - E_0) - \gamma_0^2 + 2(\omega - \varepsilon_k)^2(\omega - E_0)}{|D_3|^3} \right]
\]

\[
\times \left[ \omega_0^2 (1 - 2n'_{\omega}) + \omega_0 (\omega - E_0 + \gamma_0) N_0 \right] \frac{2\omega_0^2 (\omega - \varepsilon_k)^2}{|D_3|^3} \frac{\partial n'_{\omega}}{\partial \varepsilon_k}
\]

\[
= 3g \left[ \frac{-2\omega_0^2 (\omega - \varepsilon_k)^2}{|D_3|^3} \frac{\partial n'_{\omega}}{\partial \varepsilon_k} \right]
\]

\[
(4.127)
\]

neglecting $\gamma_0^2 \omega_0^3$ term. And

\[
n'_{\omega} = \frac{1}{4\Delta} \left[ (\varepsilon_k + E_0 + \Delta) \tanh(y_2 / 2kT) + (\varepsilon_k - E_0 - \Delta) \tanh(y_1 / 2kT) \right]
\]

\[
y_1 = \frac{\varepsilon_k + E_0 + \Delta}{2}
\]

\[
y_2 = \frac{\varepsilon_k - E_0 - \Delta}{2}
\]

\[
(4.128)
\]

\[
(4.129)
\]
Numerical Evaluation

\[ y_2 = \frac{\varepsilon_k + E_0 - \Delta}{2} \quad (4.130) \]

\[
\frac{\partial y_1}{\partial \varepsilon_k} = \frac{1}{2} \left[ 1 + \frac{2\varepsilon_k - E_0}{2\sqrt{(\varepsilon_k - E_0)^2 + 4\gamma_0^2}} \right] = \left[ \frac{\varepsilon_k - E_0 + \Delta}{2\Delta} \right] \quad (4.131)
\]

\[
\frac{\partial y_2}{\partial \varepsilon_k} = \frac{1}{2} \left[ 1 - \frac{2\varepsilon_k - E_0}{2\sqrt{(\varepsilon_k - E_0)^2 + 4\gamma_0^2}} \right] = \left[ \frac{-\varepsilon_k + E_0 + \Delta}{2\Delta} \right] \quad (4.132)
\]

\[
\frac{\partial \Delta}{\partial \varepsilon_k} = \frac{1}{2} \left[ \frac{2(\varepsilon_k - E_0)}{\Delta} \right] = \frac{\varepsilon_k - E_0}{\Delta} \quad (4.133)
\]

Differentiating \( n'_n \) with respect to \( \varepsilon_k \) and using the Equations (4.131 - 4.133) we get

\[
\frac{\partial n'_n}{\partial \varepsilon_k} = -\frac{1}{4\Delta^3} \left\{ (\varepsilon_k - E_0) / \Delta \right\}^2 [(-\varepsilon_k + E_0 + \Delta) \tanh(y_2 / 2kT) + (\varepsilon_k - E_0 + \Delta) \tanh(y_1 / 2kT)] + \frac{1}{4\pi} \left[ -\tanh(y_2 / 2kT) + \tanh(y_1 / 2kT) \right] + \frac{1}{4\Delta} [(-\varepsilon_k + E_0 + \Delta) \{ \sec^2 h(y_2 / 2kT) \} \{ (-\varepsilon_k + E_0 + \Delta) / 2\Delta.2kT \} + (\varepsilon_k - E_0 + \Delta) \{ (\varepsilon_k - E_0 + \Delta) / 2\Delta.2kT \} \{ \sec^2 h(y_1 / 2kT) \}]
\]

Neglecting \( \gamma^2 \omega_0^2 \) term, we get

\[
\frac{\partial n'_n}{\partial \varepsilon_k} = \frac{1}{4\Delta^3} \left\{ (\varepsilon_k - E_0) / \Delta \right\}^2 [(-\varepsilon_k + E_0 + \Delta) \{ \tanh(y_2 / 2kT) + \tanh(y_1 / 2kT) \} + (\varepsilon_k - E_0 + \Delta) / 4kT \{ \sec^2 h(y_2 / 2kT) \} \{ \sec^2 h(y_1 / 2kT) \}] \quad (4.135)
\]

Using the value of \( (\partial n'_n / \partial \varepsilon_k) \) in the expression for \( (\partial \Sigma / \partial \varepsilon_k) \) we obtain

\[
\frac{\partial \Sigma_{13}}{\partial \varepsilon_k} = 3g \left[ \frac{2\omega_0^2 (\omega - \xi_k)^2 \partial n'_n}{|D_k|^2 \partial \varepsilon_k} \right] = 3g \frac{\omega_0^2 (\omega - \xi_k)^2}{2|D_k|^2 \Delta^2} \left\{ (\varepsilon_k - E_0) \{ \tanh(y_2 / 2kT) + \tanh(y_1 / 2kT) \} + (\varepsilon_k - E_0 + \Delta) / 4kT \{ \sec^2 h(y_2 / 2kT) \} \{ \sec^2 h(y_1 / 2kT) \} \right\} \quad (4.136)
\]

\[
\frac{\partial \Sigma(k, \omega, q = 0)}{\partial \varepsilon_k} = 2\pi \left[ \frac{1 + \frac{\varepsilon_k}{\varepsilon_0}}{1 + \sum \langle A_0 \rangle + (1 + \sum \langle A_0 \rangle) \frac{\partial \Sigma}{\partial \varepsilon_0} \langle A_0 \rangle} \right] \quad (4.137)
\]
Numerical Evaluation

\[
a = \left[ \frac{1 + \frac{\xi_3}{\xi_4}}{1 + \Sigma_i \langle A_i \rangle} \right] = (1 + \frac{\xi_3}{\xi_4})(1 - \Sigma_i \langle A_i \rangle) = 1 + \frac{\xi_3}{\xi_4} - \Sigma_i \langle A_i \rangle
\]

(4.138)

\[
b = \frac{(\omega - \varepsilon_k - \frac{\xi_1^2}{\omega - \varepsilon_k} - \Sigma_j) \frac{\partial \Sigma_i \langle A_i \rangle}{\partial \varepsilon_k}}{(1 + \Sigma_i \langle A_i \rangle)^2}
\]

(4.139)

Substituting the values of \(a\) and \(b\) from Equations (4.138 - 4.139) in Equation (4.137) we get

\[
\frac{\partial \Sigma(k, \omega, q = 0)}{\partial \varepsilon_k} = 2\pi [a + b]
\]

(4.140)

where

\[
F(k, \omega, q = 0) = \left[ \frac{\xi_3}{\xi_4} - \Sigma_i \langle A_i \rangle + (\omega - \varepsilon_k - \frac{\xi_1^2}{\omega - \varepsilon_k} - \Sigma_j) \frac{\partial \Sigma_i \langle A_i \rangle}{\partial \varepsilon_k} \right]
\]

(4.141)

Let

\[
a_i = \left[ \frac{\partial \Sigma_1}{\partial \varepsilon_k} - \Sigma_2 \left( \frac{\partial \Sigma_1}{\partial \varepsilon_k} \langle A_i \rangle \right) \right]
\]

(4.142)

\[
\frac{3 f_i^2(0)(\omega - \varepsilon_k)^5}{2 |D \Delta^2} \left[ \omega_0 \left( \varepsilon_k - E_0 \right) \left( \tanh(\frac{\nu}{2\Delta}) + \tanh(\frac{\nu}{2\Delta}) \right) \right]
\]

and

114
Numerical Evaluation

\[ b_i = \left( -\Sigma_i \langle A_0 \rangle + \frac{|D_1|}{\omega - E_0} \frac{\partial \Sigma_i}{\partial e_i} \langle A_0 \rangle \right) \]

\[ = -\frac{3 f_i (0) y_0 \langle A_0 \rangle}{|D_1|} + \frac{3 f_i (0) y_0 \langle A_0 \rangle}{|D_1|} = 0 \]  

(4.143)

So,

\[ F(k, \omega, q = 0) = a_i + b_i = a_i \]  

(4.144)

Then the effective mass takes a very simple form as

\[ \tilde{m} = \frac{1}{[1 + 2\pi \{1 + F(k, \omega, q = 0)\}]} \]  

(4.145)

where

\[ F(k, \omega, q = 0) = A(P - Q - R - S) \]  

(4.146)

and

\[ A = 3 f_i (0)^2 (\omega - \varepsilon_f)^2 / 2D^2 \Delta^2 \]  

(4.147)

\[ P = \omega_0 \left( \varepsilon_f - E_0 \right) \left( \tanh \left( y_1 / 2kT \right) + \tanh \left( y_2 / 2kT \right) \right) \]  

(4.148)

\[ Q = \left( \frac{\omega_0}{4kT} \right) \left( E_0 - \varepsilon_f + \Delta \right)^2 \left( \sec h \left( y_2 / 2kT \right) \right)^2 \]  

(4.149)

\[ R = \left( \frac{\omega_0}{4kT} \right) \left( \varepsilon_f - E_0 + \Delta \right)^2 \left( \sec h \left( y_1 / 2kT \right) \right)^2 \]  

(4.150)

\[ S = B C \]  

(4.151)

\[ B = 6 f_i (0) y_0 \left( \omega - E_0 \right) \langle a_0 \rangle \Delta^2 / D^2 \]  

(4.152)

\[ C = \left( 1 - 2N_{\alpha}^0 \right) a_0 \left( \omega - E_0 + \gamma y_0 \right) \]  

(4.153)

\[ D = \left( \omega - \varepsilon_f \right) \left( \omega - E_0 \right) - \gamma^2 = \left( \omega - y_1 \right) \left( \omega - y_2 \right) \]  

(4.154)

\[ \Delta = \left[ \left( \varepsilon_f - E_0 \right)^2 + 4y_0^2 \right]^{1/2} \]  

(4.155)

\[ N_{\alpha}^0 = \left( 1 / 4\Delta \right) \left( E_0 - \varepsilon_f + \Delta \right) \left( \tanh y_2 / 2kT \right) + \left( \varepsilon_f - E_0 + \Delta \right) \left( \tanh y_1 / 2kT \right) \]  

(4.156)

\[ N_0 = 2 / \left[ \exp \left( \omega_0 / 2kT \right) - 1 \right] + 1 \]  

(4.157)

\[ \langle a_0 \rangle = \left( b_0 + b^*_0 \right)_{\alpha = 0} \]  

(4.158)

\[ y_1 = \left( \varepsilon_f + E_0 + \Delta \right) / 2 \]  

(4.159)

\[ y_2 = \left( \varepsilon_f + E_0 - \Delta \right) / 2 \]  

(4.159)
4.4.3 Results and Discussion

The different dimensionless parameters those are involved in these calculations are the ratio of the two electron-phonon interaction strength $r$ and the effective coupling constant $g$. All the energies in the system are measured with respect to the strength of the hybridization ($\gamma_0$), the single dominant parameter, where $d$ the position of the f-level. The inverse of the temperature is given by $b = \gamma_0 / 2kT$, the Fermi energy $x_f = \varepsilon_f / \gamma_0$ and the normalized phonon frequency $x_m = \omega / \omega_0$ 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 $D_i = D / \gamma_0^2$.

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. Considering the physically allowed values of these parameters at random sets the initial parameters, so as to give uniform softening as evident from the experiment.

The results of the numerical calculations are presented in two figures (Fig 4.7 - 4.8) showing the variation of effective mass $\tilde{m}$ with the effective coupling strength ‘$g$’.

![Fig. 4.7: Plot of $m^*/m$ verses $g$ for $r=0.1$, $b=0.2$ and $d=-2$](image)

![Fig. 4.8: Plot of $m^*/m$ verses $g$ for $r=0.1$, $b=0.2$ and $d=-1$](image)

116
keeping the other parameters constant. In the Figure (4.7) the variation of $\tilde{m}$ is made with 'g' keeping 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 the other figure (4.8) the same plot is made for a different value of $d (\approx -1)$ 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.[*]. The effective mass is also affected by other parameters, which can be studied similarly. In section 4.7 the effect of correlation on the effective mass is discussed.

4.5 Electron Phonon interaction and Phonon Response in Heavy Fermion systems.

4.5.1 Introduction

The results of some recent experiments on heavy fermion systems suggest that there exist a strong coupling of elastic degrees of freedom with those of the electronic
and magnetic ones. Though direct experimental evidence for phonon anomaly through inelastic neutron scattering or Raman scattering experiments are rare in these systems, but the measurements on elastic constant, ultrasonic attenuation and sound velocity have provided some evidence of strong electron-phonon coupling. Some Uranium based heavy fermion systems show phonon anomalies due to anharmonic interaction with the zone boundary phonons and exhibit soft mode behavior [160]. Here we have investigated the phonon response property of heavy fermion systems to explain the observed phonon anomalies. To understand the microscopic origin of these anomalies we have considered the same two mechanisms of electron-phonon interaction in the framework of Periodic Anderson Model (PAM) as discussed earlier. The influence of Coulomb correlation $U$ on the phonon excitation spectrum and the spectral density function are also studied.

4.5.2 Evaluation of Electron Response Function

With the help of the electronic part of the Hamiltonian given in equation (3.2) the equation of motion of different electronic operators are calculated. After carrying out these calculations and retaining the terms linear in correlation the exact form of the response functions are expressed as

\[
\Gamma_i(kq,k'q',\omega) = \\
(\delta_{oo} \delta_{-qq} \delta_{\epsilon_{k',q} - \epsilon_k} / 2\pi |D|)[\{(\omega - \epsilon_k + E_0) - 2\gamma^2 F(kq)\} A_0 \\
+ \{(\omega + \epsilon_{-k' - q} - E_0) - 2\gamma^2 F(kq)\} A_1 - \gamma_0 \{(2E_0 - \epsilon_{k' - q} - \epsilon_k)/(\omega - \epsilon_k + \epsilon_{k' - q})\} A_2 \\
+ \gamma_0 \{(2E_0 - \epsilon_{k' - q} - \epsilon_k) / \omega\} A_3 + (U / 2) \langle n_{k' - \sigma} \rangle (A_0 - A_1)]
\]

\[
\Gamma_2(kq,k'q',\omega) = \\
(\delta_{oo} \delta_{-qq} \delta_{\epsilon_{k',-q} - \epsilon_k} / 2\pi |D|)[\gamma_0 \{(\epsilon_k + \epsilon_{k' - q} - 2E_0) / \omega\} A_4 \\
+ \{(\omega + E_0 - \epsilon_k) - 2\gamma^2 F(kq)\} A_5 \\
+ \{(\omega - E_0 + \epsilon_{k' - q}) - 2\gamma^2 F(kq)\} (A_2 - A_3) + (U / 2) \langle n_{k' - \sigma} \rangle [2A_5 - A_2 - (\gamma_0 / \omega) A_4]
\]

\[
\Gamma_3(kq,k'q',\omega) = \\
(\delta_{oo} \delta_{-qq} \delta_{\epsilon_{k',-q} - \epsilon_k} / 2\pi \omega)[\{(1 + (\gamma_0 / |D|))(\gamma_0 / \omega)(\omega + \epsilon_{k' - q} - \epsilon_k)\} A_3 \\
+ (\epsilon_k - E_0 - \omega) A_0 - \gamma_0 \{(2\omega + \epsilon_{k' - q} - \epsilon_k)/(\omega + \epsilon_{k' - q} - \epsilon_k)\} A_2 \\
+ (\omega + \epsilon_{k' - q} - E_0) A_1 - (U / 2) \langle n_{k' - \sigma} \rangle (A_0 - A_1)]
\]

(4.160) (4.161) (4.162)
Numerical Evaluation

\[
\Gamma_4(k_q, k'_q, \omega) =
(\delta_{\omega \omega} \delta_{-\omega \omega} \delta_{k'-k} \mid 2\pi \omega \mid D \mid \gamma_0 \{(\gamma_0 \omega)(2\omega + \varepsilon_{k'-q} - \varepsilon_k)\} A_4
-(\omega - \varepsilon_k + E_o)A_3 - (\omega + \varepsilon_{k-q} - E_o)A_6 - (U/2)(n'_{\omega_o})A_2
\]  
(4.163)

The constants involved in the Equations (4.160 - 4.163) are defined in the Equations (4.57 - 4.65) discussed earlier. Following the standard technique of Zubarev [112], the different correlation functions involved in these systems are evaluated. The expressions of these are given by

\[
\langle c_{\omega}^\dagger c_{\omega} \rangle = -y_{12} \left[ y_{11} (y_1 - \bar{E}_o) - y_{22} (y_2 - \bar{E}_o) \right]
\]  
(4.164)

\[
\langle f_{\omega}^\dagger f_{\omega} \rangle = -y_{12} \left[ y_{11} (y_1 - \varepsilon_k) - y_{22} (y_2 - \varepsilon_k) \right]
\]  
(4.165)

\[
\langle c_{\omega}^\dagger f_{\omega} \rangle = \langle f_{\omega}^\dagger c_{\omega} \rangle = y_{12} y_o \left[ y_{11} + y_{22} \right]
\]  
(4.166)

\[
\langle c_{k-q,\sigma}^\dagger c_{k-q,\sigma} \rangle = -z_{12} [z_{11}(z_1 - E_o) - z_{22}(z_2 - E_o)]
\]  
(4.167)

\[
\langle f_{k-q,\sigma}^\dagger f_{k-q,\sigma} \rangle = -z_{12} [z_{11}(z_1 - \varepsilon_k) - z_{22}(z_2 - \varepsilon_k)]
\]  
(4.168)

\[
\langle c_{k-q,\sigma}^\dagger f_{k-q,\sigma} \rangle = \langle f_{k-q,\sigma}^\dagger c_{k-q,\sigma} \rangle = z_{12} y_o [z_{11} + z_{22}]
\]  
(4.169)

Where

\[
y_{11} = 1/(e^{\psi_1/\tau} + 1); \quad y_{22} = 1/(e^{\psi_2/\tau} + 1); \quad y_{12} = -\delta_{4k,4\omega_o} / (y_1 - y_2)
\]  
(4.170)

\[
z_{11} = 1/(e^{\psi_1/\tau} + 1); \quad z_{22} = 1/(e^{\psi_2/\tau} + 1); \quad z_{12} = \delta_{4k,4\omega_o} / (z_1 - z_2)
\]  
(4.171)

\[
y_1 = (1/2)(\psi_k + \bar{E}_o) + (1/2)(\psi_k - \bar{E}_o)^2 + 4\gamma_o^2
\]  
(4.172)

\[
y_2 = (1/2)(\psi_k + \bar{E}_o) - (1/2)(\psi_k - \bar{E}_o)^2 + 4\gamma_o^2
\]  
(4.173)

And

\[
\bar{E}_o = E_o + (U/2)(n'_{\omega_o})
\]  
(4.174)

\(z_1\) and \(z_2\) have the same form as \(y_1\) and \(y_2\) with \(\varepsilon_k\) replaced by \(\varepsilon_{k-q}\).

The values of time correlation function given in Equations (4.164 - 4.169) are substituted in Equations (4.57 - 4.65) to get the final form of different Green functions, which involve different parameters related to these systems. These evaluated quantities are further substituted to get the final expression for the phonon Green function \(D_{qq'}(\omega)\) sought for the calculation. The phonon Green function \(D_{qq'}(\omega)\) is related to different
Numerical Evaluation

electron response functions \( \chi(q,\omega) \). The phonon excitation spectrum depend on different model parameters through the electron-response functions which in turn gives its effect in the spectral density function. Therefore, in order to compare the derived results with experiment or to see the effect of the electron-phonon interaction on different model parameters through the shift and the width of the phonon peaks, we need to know the spectral density function, which is defined through equation

\[
S(0,\omega) = -2 \text{Im} \, D_{qq'}(\omega + i\eta)|_{q=0} \quad (4.175)
\]

The phonon excitation spectrum is determined from the solutions of the equation

\[
\omega^2 - \omega_q^2 - 4\pi\omega_q \chi(q,\omega) = 0 \quad (4.176)
\]

The roots of this equation will show up peaks in the spectral density function. Replacing \( \sum_k = \int d\varepsilon_k N(\varepsilon_k) \) the final form of \( \chi \) can be written as

\[
\chi(q,\omega) = \left\{ f_1^2(q)N(\varepsilon_F)/\pi \right\} \left[ \Gamma_1(k,q,\omega) + \{ f_2(q)/f_1(q) \} \{ \Gamma_2(k,q,\omega) + \Gamma_3(k,q,\omega) \} + \{ f_2(q)/f_1(q) \}^2 \Gamma_4(k,q,\omega) \right] d\varepsilon_k \quad (4.177)
\]

This on substitution into Equations (4.175) and (4.176), the correct form of the dispersion relation and the spectral density function are expressed as

\[
(\omega/\omega_q)^2 = 1 + (4\pi/\omega_q)\chi(q,\omega) \quad (4.178)
\]

and

\[
S(q,\omega) = \frac{2(\eta/\omega_q^2) - (4\pi/\omega_q) \text{Im} \chi(q,\omega)}{(\eta/\omega_q)^2} \left( (\omega/\omega_q)^2 - 1 - (4\pi/\omega_q) \text{Re} \chi(q,\omega) \right)^2 + (\eta/\omega_q^2) \left( (\omega/\omega_q)^2 - 1 - (4\pi/\omega_q) \text{Re} \chi(q,\omega) \right)^2 \quad (4.179)
\]

The equation (4.178) and (4.179) are the two final equations, which are to be evaluated numerically. These two equations are exact and valid for all wave vector \( q \) and temperature \( T \). The solutions of these equations for finite \( q \) and \( T \) are quite complicated. Therefore, to avoid this, the numerical calculation are performed for \( q=0 \) i.e. in the long wavelength limit. This approximation is valid and useful to explain far-infrared measurements on some heavy fermion systems reported recently [161, 162]. Carrying out these limitations the different response functions defined in Equations (4.57 - 4.65) reduces to the following forms.

\[
A_1 = -A_0; A_2 = A_3 = A_4 = 0 \quad (4.180)
\]
Numerical Evaluation

where

\[
y_{11} = z_{11} = \frac{1}{(e^{\psi/\theta} + 1)}
\]

\[
y_{22} = z_{22} = \frac{1}{(e^{\psi/\theta} + 1)}
\]

\[
y_{12} = z_{12} = -\delta_{ak} \delta_{\alpha\alpha} / (y_1 - y_2)
\]

\[
y_1 = z_1 = \frac{1}{2} \left[ \frac{\sigma_k^2}{\epsilon_k + E_0} \right] + \frac{1}{2} \left[ \frac{\sigma_k^2}{\epsilon_k + E_0} \right] + 4y^2
\]

\[
y_2 = z_2 = \frac{1}{2} \left[ \frac{\sigma_k^2}{\epsilon_k + E_0} \right] - \frac{1}{2} \left[ \frac{\sigma_k^2}{\epsilon_k + E_0} \right] + 4y^2
\]

\[
\langle c_{\alpha\alpha} f_{\alpha\alpha} \rangle = \langle f_{\alpha\alpha} c_{\alpha\alpha} \rangle = y_{12} y_0 \left[ y_{11} + y_{22} \right]
\]

\[
\langle c_{\alpha\alpha} c_{\alpha\alpha} \rangle = -y_{12} \left[ y_{11} (y_1 - E_0) - y_{22} (y_2 - E_0) \right]
\]

\[
\langle f_{\alpha\alpha} f_{\alpha\alpha} \rangle = -y_{12} \left[ y_{11} (y_1 - \epsilon_k) - y_{22} (y_2 - \epsilon_k) \right]
\]

\[
\bar{E}_0 = E_0 + (U / 2) \left(n'_{\epsilon,\epsilon} \right)
\]

On substituting these values into Equations (3.2) and (4.160- 4.163) we can write the different response functions for \( q = 0 \) as

\[
\Gamma_1(q = 0, \omega) = \sum_{k,k'} \Gamma_1(k,k',\omega)
\]

\[
= (\delta_{\alpha\alpha} \delta_{kk'} / 2\pi) \left| D \right|^{q=0} \left[ 2(E_0 - \epsilon_k) \langle c_{\alpha\alpha} c_{\alpha'\alpha'} \rangle - \langle f_{\alpha\alpha} f_{\alpha'\alpha'} \rangle \right]
\]

\[
+ 2(U/2) \left(n'_{\epsilon,\epsilon} \right) \left( c_{\alpha\alpha} c_{\alpha'\alpha'} \right) - \langle f_{\alpha\alpha} f_{\alpha'\alpha'} \rangle
\]

\[
\Gamma_2(q = 0, \omega) = (\delta_{\alpha\alpha} \delta_{kk'} / 2\pi) \left| D \right|^{q=0} \left[ 2(E_0 - \epsilon_k) + (U/2) \left(n'_{\epsilon,\epsilon} \right) \right] \left( c_{\alpha\alpha} f_{\alpha'\alpha'} \right)
\]

\[
\Gamma_3(q = 0, \omega) = (\delta_{\alpha\alpha} \delta_{kk'} / 2\pi \omega) \left| D \right|^{q=0} \left( \langle f_{\alpha\alpha} c_{\alpha'\alpha'} \rangle \right) - \langle c_{\alpha\alpha} c_{\alpha'\alpha'} \rangle
\]

\[
\Gamma_4(q = 0, \omega) = (\delta_{\alpha\alpha} \delta_{kk'} / 2\pi \omega) \left| D \right|^{q=0} \left( \langle f_{\alpha\alpha} c_{\alpha'\alpha'} \rangle \right) - \langle c_{\alpha\alpha} c_{\alpha'\alpha'} \rangle
\]

where

\[
\left| D \right|^{q=0} = (\omega + \epsilon_k - E_0)(\omega - \epsilon_k + E_0) - 4y^2 + 2(U/2) \left(n'_{\epsilon,\epsilon} \right) \left( \epsilon_k - E_0 \right)
\]

The values of these time correlation function are substituted in Equations (4.57 – 4.65) to get the final form of different Green functions, which involve different parameters related to these systems. These evaluated quantities are again substituted back
to get the final expression for the phonon Green function \( D_{\text{eq}}(\omega) \) sought for the calculation. The phonon excitation spectrum is determined from the pole of this Green function, which is given by solution of the equation
\[
\omega^2 - \omega_0^2 - 4\pi \omega_0 \chi(q = 0, \omega) = 0 
\] (4.193)

where
\[
\chi(q = 0, \omega) = \left\{ f_1^2(0)N(e_F) / \pi \right\} \left[ (e_k - E_0)^2 + 2\gamma_0 (e_k - E_0) \{ f_2(0) / f_1(0) \} \right]
+ \{ f_2^2(0) / f_1^2(0) \} \gamma_0 \frac{4\pi}{\{ |D_1| \} \{ y_1 - y_2 \}} \left\{ \tanh(y_2 / 2\theta) - \tanh(y_1 / 2\theta) \right\} \right\} dE_k 
\] (4.194)

and
\[
\left( 1 / \left( e^{h_2 / 2\theta} + 1 \right) \right) \left( 1 / \left( e^{h_1 / 2\theta} + 1 \right) \right) = \left( 1 / 2 \right) \left\{ \tanh(y_2 / 2\theta) - \tanh(y_1 / 2\theta) \right\} 
\] (4.195)

It is evident from Equation (4.194) that \( \chi(q = 0, \omega) \) is zero for \( T = 0 \). This is because, in this limit both \( \tanh(y_1 / 2\theta) \) and \( \tanh(y_2 / 2\theta) \) becomes equal to 1. However, on performing a low temperature expansion, Equation (4.195) can be expressed as
\[
\tanh(y_2 / 2\theta) - \tanh(y_1 / 2\theta) = -4e^{-h_2 / 2kT} \sinh \sqrt{\frac{(e_k - E_0)^2 + 4\gamma_0^2}{2kT}} 
\] (4.196)

The energy integration is taken over the conduction bandwidth \( W \) from \(-W/2\) to \( W/2\), in numerical calculation of phonon energy. In the static limit \( \epsilon = \omega / \gamma_0 = 0 \), the phonon self energy can be expressed as
\[
\chi(q = 0, \omega) = -4 \left( f_1^2(0)N(0) / \pi \right) \int \left\{ (I_1 + I_2 + I_3) \right\} \left( e^{-h k / 2kT} \right) \left[ \sinh \sqrt{\frac{(e_k - E_0)^2 + 4\gamma_0^2}{2kT}} \right] dE_k 
\] (4.197)

Where
\[
I_1 + I_2 + I_3 = (e_k - E_0)^2 + 2\gamma_0 (e_k - E_0) + (f_2(0) / f_1(0)) + (f_2^2(0) / f_1^2(0)) \gamma_0 \frac{4\pi}{|D_1| \{ y_1 - y_2 \}} 
\] (4.198)

and \( |D_1| \) is the value of \( |D| \) in the static limit \( \epsilon = 0 \) i.e.
\[
|D_1| = (e_k - E_0)(e_k + E_0) - 4\gamma_0^2 + (U / 2) \left\{ n_{k-a} \right\} (e_k - E_0) 
\] (4.199)

Moreover, the renormalized phonon frequencies in the static long wavelength limit can be expressed as
\[
(\omega / \omega_0)^2 = 1 + (4\pi / \omega_0) \chi(q = 0, \omega = 0) 
\] (4.200)
Numerical Evaluation

The phonon frequencies thus calculated will acquire temperature dependence through Equation (4.197) besides depending on the various parameters such as the electron-phonon coupling constants and the intra-atomic Coulomb repulsion. Similarly the expression of the spectral density function calculated in this limit becomes

\[
S(q = 0, \omega) = 2 \left[ \frac{(\eta / \omega_0^2) - (4\pi / \omega_0) \text{Im} \chi(q = 0, \omega)}{(\pi \omega_0)} \right]^{\frac{1}{2}} \left[ \left( \frac{\omega}{\omega_0} \right)^2 - 1 - \frac{4\pi}{\omega_0} \text{Re} \chi(q = 0, \omega) \right] \left[ \left( \frac{\eta}{\omega_0} \right)^2 - 4\pi \text{Im} \chi(q = 0, \omega) \right]^{-1/2}
\]

(4.201)

4.5.3 Results and Discussion

It is well known that the positions of f-level relative to the Fermi level and the strength of hybridization plays an important role in heavy fermion systems. To understand in detail the behavior of phonons in these systems, it is necessary to investigate the influence of different system parameters on phonon response functions. The 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 dimensionless coupling constant \( g = N(0) f_1^2(0) / \omega_0, N(0) \) being the density of states at the Fermi level. All the energies in the system are measured with respect to the strength of hybridization \( \gamma_0 \) which is the single dominant parameter, e.g., the position of the f-level is given by \( d = E_0 / \gamma_0 \), the onsite Coulomb repulsion \( U' = U / \gamma_0 \), the band width \( W' = W / \gamma_0 \) and the inverse of the temperature by \( b = \gamma_0 / 2K \). Similarly the variable band energies are denoted by \( \nu = \varepsilon_k / \gamma_0 \), the width of the phonon mode as \( \epsilon = \eta / \gamma_0^2 \) and the renormalized phonon frequency \( c = \omega / \gamma_0 \) is expressed as the product of reduced frequency \( \tilde{\omega}(= \omega / \omega_0) \), and the scaling parameter \( z = \omega_0 / \gamma_0, \omega_0 \) being the frequency of bare phonon. For simplicity, it is assumed that the f-level is half filled so that the average value of \( \langle n_f \rangle \) is taken to be one. The Fermi level is set equal to zero \( (E_F = 0) \) so that the value of \( d \) is negative, if the f-level lies below the Fermi level, and is positive if it is
above the Fermi level. The initial values of these parameters are considered at random in such a way that these are physically acceptable and relevant to heavy fermion systems. To realize this the value of \( r \) is always kept less than one so as to make \( f_1(0) \) more stronger than \( f_2(0) \) in consistent with the findings of Razafimandimby et al [153] and the value of \( g \), the effective coupling parameter, is kept low so as to reproduce the result of weak coupling regions as well as the softening effect in the correct spin fluctuation temperature range pertinent to heavy fermion systems. This is explained in detail where the figure for \( g \) variation is discussed.

The results of the numerical calculations are presented in seven figures (4.9 - 4.15), out of which the figures 4.12 and 4.15 show the effect of Coulomb correlation parameter \( U' \) on phonon frequency shifts. Figures (4.9 - 4.11) show the variation of the renormalized phonon frequency with inverse temperature while figures 4.13 and 4.14 to that of spectral density \( S(0,\omega) \) with inverse temperature for different values of the parameters using the Coulomb correlation \( U'=0 \). In figures (4.9 - 4.11), the variation of the renormalized phonon frequency \( \bar{\omega} = \omega / \omega_0 \) with inverse temperature parameter \( b \) is plotted for different values of the system parameters \( r, g \) and \( d \). Figure 4.9 shows this variation of \( \bar{\omega} \) with \( b \) for different values of \( r \) keeping the other parameter \( g \) and \( d \) fixed at values 0.001 and -3.0 respectively. From the analysis it is observed that there is a reduction in phonon softening, when the value of \( r \) changes from 0.5 to 0.001. Further it is observed that the reduction of \( r \) beyond 0.01, hardly produces any noticeable affect on the phonon energy, which is evident from the coincidence of the two curves for values of \( r=0.01 \) and 0.001. From physical point of view, it can be interpreted that, small value of \( r \) means either large values of \( f_1(0) \) i.e., the strength of interaction of electrons of hybridization band with phonons or small value of \( f_2(0) \) i.e. strength of f-electrons with phonons. From phonon response curve it is clear that \( f_1(0) \) is effective up to certain value and arbitrary increase of \( f_1(0) \) is ineffective. Similarly, small value of \( f_2(0) \) implies that the strength of f-electron-phonon interaction is so weak that phonons are affected or seen in the experiment. Figure 4.10 shows the variation of \( \bar{\omega} \) with \( b \) for different values of \( g \) (the effective coupling parameter) keeping \( r \) and \( d \) fixed at 0.01 and -3.0 respectively. From this figure it is evident that for the value of \( g=0.001 \) the softening of phonon occurs.
Numerical Evaluation

Fig. 4.9: Plot of $\omega$ verses $b$ for $r = 0.5, 0.1, 0.01, 0.001$ for fixed values of $g=0.001$, $d=-3.0$ and $U' = 0$

Fig. 4.10: Plot of $\omega$ verses $b$ for $g = 0.1, 0.01, 0.001$ and 0.0001 for fixed values of $r=0.01$ and $d=-3.0$ and $U' = 0$
Fig. 4.11: Plot of $\phi$ verses $b$ for $d=-5.0, -4.0, -3.0$ and $-2.0$ for fixed values of $r=0.01$, $g=0.001$ and $U'=0$.

Fig. 4.12: Plot of $\phi$ verses $b$ for $U'=0, 2.0, 4.0$ and $6.0$ for fixed values of $r=0.01$, $g=0.001$ and $d=-3.0$. 
Numerical Evaluation

Fig. 4.13: Plot of spectral density function $S(0, \omega)$ verses $\tilde{\omega} (= \omega / \omega_0)$ for $b = 0.5, 0.55, 0.6$ and $0.65$ for fixed values of $r=0.01, g=0.001, d=-3.0, z=0.01$ and $e=0.1$.

Fig 4.14: Plot of $S(0, \omega)$ versus $\tilde{\omega} (= \omega / \omega_0)$ for $r=0.01, g=0.001, b=0.6$ and $d=-4.0, -3.0, -2.0$.
between temperature parameter range \( b = 0.5 \) to \( 0.9 \), which give the value of hybridization strength between \( 5K \) to \( 9K \). This value is very close to the spin fluctuation temperature of heavy fermion systems, which is about \( 10K \). Again it is found that, if \( g \) values are decreased from \( 0.1 \) to \( 0.0001 \), the degree of softening of the phonon frequency also decreases. Small value of \( g \) means small value of \( \frac{1}{2} (0) \) which implies that the coupling between phonons and hybridization of \( f \) and conduction electrons is weak and the strength is not sufficient to affect phonons. This is also in confirmation with the variation of \( r \) in figure-4.9. Figure-4.11 shows a similar plot with different values of \( d \) (i.e. the position of \( f \)-level) while the other two-parameter \( r \) and \( g \) is kept fixed at \( 0.01 \) and \( 0.001 \) respectively. It is seen that as the value of \( d \) changes from \(-5.0 \) to \(-2.0 \), the phonon softening is small. This implies that as the \( f \)-level moves closer to the Fermi level the degree of phonon softening decreases and covers a wider range of temperature. In all these plots increase of the parameter \( b \) implies the decrease in temperature as \( b \) is an inverse function of temperature. Moreover the change of \( g \) either to high or low values the temperature range of softening also becomes either too low or large to interpret these results of heavy fermion systems.
Numerical Evaluation

In figure 4.12, we have shown the effect of correlation $U'$ on the phonon softening. To visualize this effect, we have studied the variation of phonon energy with temperature considering the same initial values of the parameter $r$, $g$ and $d$ for different values of $U'$ including $U'=0$. On comparison of the different plots it is found that, as the values of $U'$ increases the softening decreases. From the figure it is observed that for $d=-3.0$ and $b=0.6$ the value of $\bar{\omega}$ rises continuously with the values 0.87, 0.94, 0.96 and 0.97 when $U'$ values changed from 0 to 2, 4 and 6 respectively. This increase in correlation leads to hardening of phonons.

Figure 4.13 and 4.14 show the behavior of spectral density function $S(0,\bar{\omega})$ as a function of $\bar{\omega}$ for different values of system parameters and temperature keeping $U'=0$. Figure 4.13 is the plot for different temperature, i.e. $b$, for the fixed values of $r$, $g$ and $d$. The spectral density for different values of the position of the $f$-level, i.e. $d$, for fixed values of $r$, $g$ and $b$ is given in Figure 4.14. If we give a close look to the figure 4.13, it is observed that the spectral density gives three peaks. One of them is prominent with large strength and the other peaks are weak with less strength. For $d=-3$ and for different values of temperature i.e., $b = 0.5, 0.55, 0.6$ and 0.65, the spectral density function shifts smoothly from higher value 0.92 to lower values 0.90, 0.87 and 0.82 respectively. On comparing these values with the renormalized phonon energy plots (Figure 4.11) it is seen that the values of $\bar{\omega}$ for $d=-3$ exactly coincides with the above mentioned values.

The other weak peaks are also phonon peaks, which shift towards higher frequency from 1.11 to 1.21 and also from 1.52 to 1.54 with change of strength. Since the numerical calculation are made in the static limit, i.e., $\omega = 0$, we do not have the scope to compare the behavior of other peaks of the spectral density curve in the similar way. However, these can be explained when the numerical evaluations are performed in the dynamic limit. Secondly in addition to shift the width of the peaks also changes as one goes from one temperature to other indicating the effect of electron-phonon interaction. If we analyze the peaks appeared near $\bar{\omega}=1.11$ to 1.21, it is observed that the width of the peaks gradually increases with decreasing intensity. This is an indication of strong electron-phonon interaction due to which the phonon widens so much that the intensity is suppressed. It is also interesting to note that, the numerical analysis of the present work is
done for $q=0$. Therefore, we expect the $q=0$ phonons are to be affected by electron-phonon interaction, which is found to be correct as explained above.

Figure 4.14 is the plot of spectral density function for different values of the position of $f$-level. Here also it is seen that the phonon peak values shift as the value of $d$ is changed from $d=-4.0$ to $d=-2.0$. The first peak is prominent and it shifts from 0.6 to 0.87 and 0.96 as the $d$ value is changed from −4.0 to −3.0 and −2.0 respectively. The other peaks are weak and distorted. These weak peaks also shift as we from higher value of $d$ to lower values. The distortion of the weak peaks seen in the curve may be attributed to the existence of other interactions in addition to the electron-phonon interactions.

Finally, we have analyzed the effect of correlation on spectral density function in Figure 4.15 keeping the position of $f$-level and temperature i.e. the parameters $d$ and $b$ fixed at $-3.0$ and $0.6$ respectively. From the analysis of this curve it is observed that as $U'$ is changed from 0 to 2.0, 4.0 and 6.0 three different peaks appeared in each case. Out of the three peaks appeared for each strength one is quite prominent and the other two peaks are weak. The position of one weak peak hardly shifts and the other weak peak has a large width, which invariably changes with strength. From the analysis it is evident that, the first peak, prominent one, is phononic in nature and the last weak peak is electronic one. The middle weak peak of large width indicates the effect of electron-phonon interaction and gives a mixed character. It is also observed that with the increase in correlation the phonon hardens, which is in agreement with the predictions of Hirsch [163] and Min et al [164].

4.6 Effect of correlation on electron-phonon Interaction in some Heavy Fermion systems: A finite $q$ Calculation.

4.6.1 Introduction

The electron-phonon interaction in heavy fermion systems manifests itself in numerous ways. The works of Miyake et al [165], Hirsch [163] and a more recent study of Min et al [164] have concluded through their calculations that the coulomb correlation results in the hardening of phonon and enhancement of the strength of electron-phonon coupling constant. In this section we have discussed the influence of 4$f$ and conduction electron mixing and $f$ electron alone on phonon self-energies. Therefore to account for
Numerical Evaluation

these effects, the present calculation analyzes to see how phonons in these systems get modified through the phonon self-energy and the spectral density function which involves response functions corresponding to the conduction electrons, the $f$ electrons, and the $f$ - $d$ mixing densities. The phonon self-energy and the spectral density function are evaluated in the small $q$ limit. This is more appropriate because the general expression for the phonon self-energy and spectral density function are obtained for finite $q$.

4.6.2 Evaluation (small $q$ analysis)

In view of our interest we have evaluated

$$D_{qq}(\omega) = \delta_{qq} \left( \frac{\omega}{\pi} \right)^2 \omega^2 - \omega_0^2 - 4\pi \omega_0 K(q, \omega)$$

and

$$S(q, \omega) = -2 \text{ Im } D_{qq}(\omega + i\eta)$$

for the small $q$ limit. In doing so, we expand $\epsilon_{k,q}$ and the Fermi function $m_{k,q}$ up to the order linear in $q$ as

$$\epsilon_{k,q} = \epsilon_k - qv_f$$

$$m_{k,q} = m_k - qv_f \delta(\epsilon_k - \epsilon_f)$$

where

$$\nu_k = \frac{\epsilon_k}{\nu_k} \text{ and } \delta(\epsilon_k - \epsilon_f) = \frac{\delta m_{k,q}}{\delta m_{k,q}}$$

This when substituted in Equations. (4.202, 4.182, 4.183 and 4.187) yield the phonon energy and the spectral density function as

$$\omega/\omega_0 = \left[ 1 - \frac{Gk(c - y_f + \tilde{d})}{\nu_k} \right] \left[ (y_f - \tilde{d})^2 - \nu_k^2 \right]^{1/2}$$

and

$$S(q, \omega) = \frac{z^4 ep((\tilde{\omega} z - y_f + \tilde{d})^2 + [ez^2 p((\tilde{\omega} z - y_f + \tilde{d})^2]$$

where

$$p = \frac{Gk(\tilde{\omega} z - y_f + \tilde{d})}{\nu_k} \left[ (y_f - \tilde{d})^2 - \nu_k^2 z^2 + \nu_k^2 \nu_k^2 + 1 \right]$$

and

$$\tilde{d} = d + (U/2) \langle n_{\epsilon_0} \rangle$$
The other parameters are same as defined in earlier sections.

4.6.3 Results and Discussion

The different dimensionless parameters involved in the calculations are $r = f_1(q)/f_2(q)$, the ratio of coupling strength of phonons with electrons in the $f$-band and hybridization band, $g$, the effective coupling parameter and $d$, the position of $f$-level. The values of these parameters more or less influence and have a dominant role in determining the physical characteristics of HF systems. In the present calculation the numerical analysis is made for $E_F = 0$ and in the static limit, i.e., $\omega = 0$. The value of $r$ is always taken as less than one considering that the coupling strength of the phonon with hybridization term is stronger than that of phonon with $f$-band electrons. Considering different values for which the softening occurs as observed experimentally has set initial parameters. Here we present only two plots (Figure 4.16 and 4.17). The Figure 4.16 is related to the variation of phonon energy with $k$ with $U' = 0$ and the other i.e., Figure 4.17 with finite $U'$ to show the influence of correlation.

The Figure 4.16 show the variation of phonon self energy with wave vector $k$ with $U' = 0$ for different values of effective coupling parameter $g$. It is found that the
phonon uniformly softens as the value of $g$ is increased. For very small value of $g$ there is hardly any softening. This is obvious because $g$ is proportional to $f_1(q)$ which is the coupling strength of phonons and hybridization band. Since $f_1(q)$ is stronger than $f_2(q)$ in heavy fermion systems, for small $g$ the effect of phonon softening becomes ineffective. Figure-4.17 show the influence of coulomb correlation $U'$ on phonon self energy with wave vector for a fixed value of $g=0.1$. Here it is observed that as $U'$ is increased the phonon softening decreases or hardens. So in this analysis it is found that the increase in correlation leads to hardening of phonons which, is also in agreement with the predictions of Hirsch [163] and Min et al [164].

4.7 Variation of quasi particle mass due to correlation and electron-phonon interaction in heavy fermion systems.

Over the last thirty years the Periodic Anderson Model (PAM) has emerged as one of the most successful models for explaining many of the properties of the strongly correlated systems. It is believed that, the intra-atomic Coulomb interaction between the $f$-electrons plays a dominant role for explaining the properties of the heavy fermion systems. The strong correlation between the $f$-electrons imposes rather strong local restrictions on the electronic occupancy to be either zero or one at each site. Taking into account the effect of finite bandwidth [166], it has been established that the electron phonon-coupling constant becomes dominant for nearly filled band in the strongly correlated limit. Different conventional approximations were used to deduce the transition temperature, thermal expansion coefficient, magneto-elastic constant, Gruneisen parameter, superconductivity and other physical properties. In this section we consider the electron-phonon interaction and $f$-$f$ correlation $U$ in Periodic Anderson Model (PAM) to see their effect on the quasi particle mass in some heavy fermion systems. Therefore to account for these effects we have considered the phonon coupling mechanism in two ways i.e., the usual interaction between the phonons in the $f$-band and that of electrons of hybridization band and see their influence on phonon self-energy. The phonon self-energy is related to the effective mass as in Equation (4.90) and it involves
Numerical Evaluation

different response functions corresponding to conduction electrons, \(f\)-electrons and \(f-d\) mixing densities. In doing so we have explored the normal properties of the system including the Coulomb correlation in the Hamiltonian as given in Equation (3.2). For simplicity of the calculation the phonon self-energy is calculated in the long wavelength and static limit. The 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 and is defined by Equations (4.145 – 4.159) with \(E_0\) replaced by \(\tilde{E}_0\). The term \(\tilde{E}_0\) is defined as

\[
\tilde{E}_0 = E_0 + \left(U/2\right) \left\langle n'_{\sigma} \right\rangle
\]  

The different dimensionless parameters those are involved in these calculations are the same as described earlier. All the energies of the system are measured with respect to the strength of hybridization \(\gamma_0\), the single dominant parameter. The value of \(r\) is taken as less than one as it is assumed that in heavy fermion systems the coupling strength of phonons with hybridization term is stronger than that of phonons with \(f\)-electrons. 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. Considering the physically allowed values of these parameters at random sets the initial parameters, so as to give uniform softening as evident from the experiment. We have studied the influence of different parameters on effective mass i.e., \(r\), \(g\) and \(d\) with \(U' = 0\) and \(U' \neq 0\). In doing so we present here three figures (Figures 4.18 – 4.20). Out of which the Figure (4.20) shows the effect of Coulomb correlation on

Fig. 4.18: Variation of \(\tilde{m} - r\) for different \(d\)
Numerical Evaluation

Effective mass. In the Figure (4.18) we have shown the variation of effective mass with $r$ for different values of position of $f$-level i.e., $d$ keeping other parameters fixed. Here it is observed that the effective mass remain fixed for different values of $r$. Whereas the Figure (4.19) corresponds to the variation of effective mass with $g$ for different values of $d$ keeping $U' = 0$ and other parameters fixed as in figure one. In this case it is observed that effective mass increases with $g$ for different values of $d$. For larger $d$ values i.e., when $f$-level lies deep in to the core the effective mass increases very sharply compared to closer position. Moreover one interesting fact is that the effective mass decreases as well as increases depending on the

Fig. 4.19: Variation of $\tilde{m} - g$ for different $d$ and $U' = 0$.

Fig. 4.20: Variation $\tilde{m}/m - g$ for $d = 2$ and $U' = 0, 2.0, 4.0$ and $6.0$. 

135
value of \( g \) and \( d \). For example when \( d = -2.0 \) the effective mass is less than one for \( g = 0 \) to 0.29 but increases rapidly and is more than one for the values \( g \) beyond 0.29. In Figure (4.20) we have analyzed the effect of correlation on variation of effective mass with \( g \) for a fixed \( d (= -2.0) \) value and keeping other parameters fixed as in Figures (4.18 – 4.19). As the value of \( U^e \) is changed from 0 to 2.0, 4.0 and 6.0 the sharpness in change of effective mass gradually increases for higher \( U^e \) values.

4.8 PHONONS IN SOME FLUORIDE SCHEELITES

4.8.1 Introduction

LiReF\(_4\) are the series of iso-structural ternary fluoride compounds, which are formed as the mixed system of ReF\(_3\) – LiF, where Re belong to the group of element from Europium (z=63) to Lutetium (z=71). These compounds crystallize in the CaWU\(_4\) (scheelites) structure with two molecules per primitive cell [167, 168] and are generally refereed as fluoride scheelites. These systems are subject of interest in recent years mainly because these are optically transparent and have applications in Laser and other quantum electronic devices. LiYF is the most used flouride laser host crystal generally doped with trivalent Rare earth and more recently with Uranium [169, 170].

On consideration with the structural aspect of both Oxo and fluoride scheelites it is expected that, there are distinct changes in charges, electronegativities and masses when in the lattice of fluorides Ca\(^{2+}\) is replaced by Re\(^{3+}\), W\(^{6+}\) by Li\(^+\) and O\(^{2-}\) by F\(^-\). Moreover due to close packing of scheelites all quantum electronic and magnetic properties of the materials are get influenced by lattice dynamics. Therefore, knowledge of lattice dynamics of LiReF\(_4\) will be useful in connection with their applications in laser optics.

It can be shown that there are thirty six (36) phonon modes with \( q=0 \), which are redistributed among the irreducible representation of \( C_{4h} \) as

\[
\Gamma^{vb} = 3Ag + 5Bg + 5Eg + 5Au + 3Bu + 5Eu
\]

(4.211)

Out of these all u modes are infrared active except one Au and an Eu mode and all g modes are Ramanactive. However, some experiments [167, 170] concerning Raman scattering and infrared spectroscopy in some flouride scheelite systems have reported two
important facts. Those are (i) frequencies of several modes are thought to be missing, which are neither identified nor observed and (ii) softening of some phonon modes. To overcome this deficiency and for a confirmation of earlier results Salaun et al [171, 172] conducted infrared measurements on some of LiYF$_4$ and LiLnF$_4$ compounds with $Ln =$ Ho, Er, Tm and Yb and Raman spectra for $Ln =$ Tm, Hb and Yb. Through group theoretical analysis they could able to give data related to effective changes, the frequency dependence of the optical parameters and atomic movements under some of the vibrational mode. Moreover they could able to explain low-lying $Ag$ modes not predicted earlier. In addition their performance of measurement at different temperatures show clear evidence of phonon softening in specific modes of certain systems. Their measurements from room temperature to 40$^\circ$K revealed the fact that the line width decrease and the frequencies slightly increase except for few specific $B_g$, $E_g$ symmetric modes of LiTmF$_4$ compound. The decrease of this few specific modes, which is unusual, is attributed to the electron-phonon coupling.

To account the phonon softening and missing phonon lines in the Raman spectra we have proposed a strong electron-phonon coupling in these systems. In order to explain this we have considered the Heavy Fermion model, where the electron-phonon interaction is incorporated in the Periodic Anderson Model (PAM) without the Coulomb repulsion term. Fluoride scheelites being an insulator the $f$-electron plays an important role. So, to work out our model for this system we have considered the interaction of $f$-electrons with phonons are stronger than that of phonons either with conduction electrons or with electrons in hybridization band. In order to compare our result with experiments it is necessary know the phonon spectral density function. Double time Green’s function technique [112] is used to calculate this function.

We calculate the phonon response function to see how the phonon get modified through the response functions of the conduction electrons, $f$-electrons and $f-d$ mixing densities. The spectral density function is calculated. It involves various model parameters namely, the position of $f$-level, the effective coupling strength and the electron-phonon coupling strength. Keeping the former two parameters fixed, the softening behavior of phonons with temperature for different strength of electron-phonon coupling is studied. It is observed that even in the static limit the present work provides
large number of phonon peaks of various strengths. There might be some missed phonon lines, which may be interpreted as, due to strong electron-phonon interaction the intensity is sufficiently lowered and not observed in the experiment.

4.8.2 Evaluation

We know that the phonon excitation spectrum is determined through the solution of the denominator of the Green Function. This Green function involves the phonon self-energy, which again influenced by the different response functions corresponding to $f$-electrons, conduction electrons and their mixing. In this analysis we will show that for $f_2(q) > f_1(q)$, i.e. $r$ is greater than one, the phonon excitation spectrum give similar behavior as experimentally observed. That is large number of peaks are observed. However, for $f_1(q) > f_2(q)$ some of the phonon peaks disappear. The phonon excitation spectrum depend on different model parameters through the electron-response functions which in turn gives its effect in the spectral density function. Therefore, in order to compare the derived results with experiment or to see the effect of the electron-phonon interaction on different model parameters through the shift and the width of the phonon peaks, we need to know the spectral density function, which is defined through equation

$$S(q,\omega) = -2 \text{Im} D_{qq}(\omega + i\eta)|_{\eta=0}$$  \hspace{1cm} (4.212)

The phonon excitation spectrum is determined from the solutions of the equation

$$\omega^2 - \omega_q^2 - 4\pi\omega_q \chi(q,\omega) = 0$$  \hspace{1cm} (4.213)

The roots of this equation will show up peaks in the spectral density function. Replacing $\sum_k = \int d\epsilon_k N(\epsilon_k)$ the final form of $\chi$ can be written as

$$\chi(\omega,q) = \{f_1^2(q)N(\epsilon_q)/\pi\} \left[ \Gamma_1(k,q,\omega) + \{f_2(q)/f_1(q)\} \{\Gamma_2(k,q,\omega) + \Gamma_3(k,q,\omega)\} \{\Gamma_4(k,q,\omega)\} \right]$$

Using Equations (4.213) and (4.214) the correct form of the dispersion relation and the spectral density function are expressed as

$$\left(\omega/\omega_q\right)^2 = 1 + (4\pi/\omega_q)\chi(q,\omega)$$  \hspace{1cm} (4.215)

and
Numerical Evaluation

\[ S(q, \omega) = 2(\frac{\eta}{\omega^2} - (4\pi / \omega_q) \Im \chi_{qq}) / (\pi \omega_q) \left[ \left( \frac{\omega}{\omega_q} \right)^2 - 1 - (4\pi / \omega_q) \Re \chi_{qq} \right]^2 \]

The equation (4.215) and (4.216) are the two final equations, which are to be evaluated numerically. These two equations are exact and valid for all wave vector \( q \) and temperature \( T \). The solutions of these equations for finite \( q \) and \( T \) are quite complicated. Therefore, to avoid this, the numerical calculation are performed for \( q=0 \) i.e. in the long wavelength limit for small temperature in the static limit i.e. \( \omega=0 \).

4.8.3 Results and Discussion

These parameters discussed earlier like \( r, d \) and \( g \) play a dominant role on the phonon spectrum. The other parameters are the strength of hybridization \( \gamma_0 \), the bandwidth \( W' \) and the inverse of temperature \( b \). For convenience the Fermi level is not equal to zero and the value of \( d \) is kept negative, as these are Rare-earth compounds, whose \( f \)-level lie deep to the core. The value of \( r \) is always kept more than one so as to make \( f_2(q) \) stronger than \( f_1(q) \). The properties of phonon can be studied with these different parameters. However we present here only two of the important plots (Figure 4.21 and 4.22) with two different values of \( d \) at different temperatures keeping other parameters \( g \) (=0.01), \( r \) (=2.0), \( z \) (=0.01) and \( y \) (=4.0) fixed. Figure-4.21 is the plot of spectral density function \( S(q,0) \) versus \( \omega \) for \( d=-3.0 \), which show large number of peaks within the range between \( \tilde{\omega}=0.62 \) to \( \tilde{\omega}=1.20 \) for different temperatures i.e., \( b=0.05, 0.15 \) and \( 0.25 \). From temperature variation at this value of \( d \), some peaks are identified as phonon peaks as they shift and change in width. The other peaks are of electronic in nature, which remain constant through out the variation of temperature. Out of these about four and five peaks appeared at \( \tilde{\omega}<1 \) and about three peaks appeared at \( \tilde{\omega}>1 \). On comparison our result with that of Salaun et al [171, 172] it is found that there are about eight phonon modes out of

\[ \begin{align*}
\text{Fig. 4.21: Plot of } & S(q,0) \text{ versus } \omega / \omega_0 \text{ for} \\
r=2.0, \ g=0.01, \ z=0.01, \ y=4.0 \text{ and } d=-3.0 \text{ for} \\
\text{different temperatures } & b=0.05, 0.15, 0.25.
\end{align*} \]
which four lies below and four above the value of \( \omega_{r0} \), which gives an agreement with our finding.

Figure-4.22 is the plot between similar quantities for different value \( d \) value i.e., \( d=-2.0 \), it interesting to point out that number of phonon modes appeared above \( \omega_{r0} \) have reduced to one. This implies that for this value of \( d \) some modes above \( \omega_{r0} \) either suppressed or disappeared. This means depending on the position of f-level and the strength of electron-phonon interaction the magnitude of some of the phonon peaks are reduced so much, as appeared in the experiment. Moreover these phonon modes shift as the temperature is varied. On comparison our result with experimental findings it is concluded that our result show the existence of large number of phonon peaks even in the static limit and softening which is in agreement with experimental results.