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The elastic behaviour of heavy-fermion compounds within the MFA approach

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Abstract. The temperature dependence of the velocity of sound is calculated for heavy fermions within a mean field approach. The basic parameters of the periodic Anderson model, V and E_0, are taken to be volume dependent. This leads to a volume dependence of the chemical potential, μ, the renormalized f level energy, $\tilde{\epsilon}_f$, the number of f electrons, n_f, and the renormalized hybridization $\tilde{V}$. These effects are all included in the calculation of the temperature dependence of the sound velocity.

1. Introduction

In recent years a lot of interest has been devoted to heavy-fermion systems (HFS). It is known that HFS show not only very interesting anomalies of their electronic properties (Fulde *et al* 1988, Evans *et al* 1989) but also pronounced instabilities in the temperature and magnetic field behaviour of the lattice properties like elastic constants, thermal expansion, and magnetostriction (Thalmeier and Lüthi 1991, Thalmeier and Fulde 1986, Wojciechowski 1986, Gehring and Wojciechowski 1992, Niksch *et al* 1980, Weber *et al* 1987, Lüthi and Yoshizawa 1987, Harigaya and Gehring 1993).

Some systems, namely UPt_3, $CeAl_3$, $CeCu_6$, $CeRu_2Si_2$, show a sharp depression in the longitudinal modes of the elastic constants at low temperatures while the transverse modes pass through a maximum. These observed step anomalies in the longitudinal modes are especially important as they provide a way of constructing the B–T phase diagram by varying both the temperature and the magnetic field (Bruls *et al* 1990). All these results indicate that the coupling of the heavy electrons with the longitudinal phonons plays an important role within the microscopic structure of the heavy-fermion state. Indeed, it has been proposed that this mechanism is responsible for heavy-fermion superconductivity (Razafimandimby *et al* 1984, Gehring and Major 1994). Here, we shall only concern ourselves with the nature of the elastic instabilities. In particular we shall consider the sound velocity for both the rare earth and the uranium HFS.

The coupling of long-wavelength longitudinal phonons to the heavy quasiparticles originates in the extreme volume dependence of the system's effective Kondo temperature T_K or spin fluctuation temperature (Fulde *et al* 1988) which defines a new energy scale for the heavy-fermion systems. Both the hybridization between the f electron and conduction electrons and the effective f electron energy level depend upon T_K. Thus, they are also strongly dependent upon the volume strain associated with the lattice.

One can also consider the effects of distortion in a cubic material including crystalline field splitting and calculate the linear susceptibility with respect to the crystalline field

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splitting. This approach gives a downward dip of the elastic constants (Harigaya and Gehring 1993, 1994) which appears at a temperature of the order of the crystalline field splitting but much larger than the Kondo temperature.

In this paper the resulting electron–phonon coupling is characterized by the Grüneisen parameter. A concept of the Grüneisen parameter coupling in HFS allows us to describe the experimental anomalies of the lattice properties like thermal expansion and magnetostriction constants at temperatures which are very low in comparison with T_K. At higher temperatures, however, theoretical results are at variance with the experiment (Thalmeier and Lüthi 1991).

In order to obtain the sound velocity at both low and high temperatures we propose an approach based on a mean field version of the Anderson model (Coleman 1984). It is known that the mean field approximation (MFA) is sufficient to extrapolate between the low- and high-temperature regimes yielding, for example, enhanced Pauli-like and Curie–Weiss susceptibilities for the low and high temperatures, respectively which is in good qualitative agreement with experiment (Rasul and Desgranges 1986, Evans *et al* 1989, Gehring *et al* 1994).

We want to consider to what extent this approximation can be successful in describing the sound velocity and ultrasonic attenuation at finite temperatures.

We derive the electron–phonon coupling Hamiltonian resulting from a volume dependence of the bare hybridization strength and bare position of the f level. These two volume dependence quantities together with the width of the conduction electron band, the bare hybridization strength and the bare position of the f level are the model parameters. A similar Hamiltonian has been derived and examined by Keller *et al* (1990) at $T = 0$.

All electronic quantities are determined within the MFA for slave bosons and finally the sound velocity is obtained from the RPA like procedure for the phonon self-energy. The quasiparticle–phonon interaction considered within these approaches changes considerably below and above T_K. Below T_K it is the heavy quasiparticles which directly couple to the phonons, through the Grüneisen parameter. However, above T_K the resident f electrons are well localized so that they feel the lattice deformation via the electric field that surrounds them.

We shall show that even for one electronic Grüneisen parameter we obtain the dip of the elastic constant at finite temparature for both 4f and 5f HFS.

2. Hamiltonian

Our starting point is the Anderson lattice Hamiltonian in the second quantized representation:

$$H = \sum_{km} \varepsilon_k c^{\dagger}_{km} c_{km} + \sum_{im} E_0(i) f^{\dagger}_{im} f_{im} + \sum_{lm} V_m(i)(f^{\dagger}_{im} c_{im} + \text{HC}) + \sum_{im\ (\neq m')} U n_{im} n_{im'} \qquad (1)$$

where i is the site label. The N-fold degeneracy of both bands is labelled by m. Here, ε_k is the conduction band dispersion relation, E_0 is the bare f level energy; V is the bare hybridization term, which is usually assumed to be independent of k and m. We assume the same degeneracy for both c and f electrons to avoid a complicated form of the hybridization matrix elements (Hewson 1993). In our approach the hybridization matrix reduces to one parameter only. This makes it possible to calculate the sound velocity, as well as all other thermodynamic quantities (Evans *et al* 1989) taking the minimum number of initial parameters. It is worth mentioning that this simplified model possesses a $1/N$ expansion analogous to that in the single impurity problem (Millis and Lee 1987).

Moreover, we neglect the volume dependence of the conduction electron energy (for instance, it can be incorporated into the bare elastic constant), and therefore the degeneracy

of the conduction electrons is not a crucial factor in determining the sound velocity.

The large local Coulomb repulsion parameterized by U can be eliminated by introducing the slave boson technique (Coleman 1984). The mean field approximation for the slave boson operators gives the following effective Hamiltonian:

$$H_0 = \sum_{km} \varepsilon_k c^\dagger_{km} c_{km} + \sum_{im} \tilde{\varepsilon}_f(i) f^\dagger_{im} f_{im} + \sum_{im} r(i) V(i) (f^\dagger_{im} c_{im} + \text{HC}) + \text{constant} \tag{2}$$

where $\tilde{\varepsilon}_f$ and r are the renormalized 4f level and the mean value of the boson field operator ($r = \sqrt{1 - n_f}$). The mean field approximation leads to the following three coupled integral equations for n_f, $\tilde{\varepsilon}_f$ and the chemical potential μ (Evans *et al* 1989):

$$n_f = N\rho_0 \int_{-W}^{(N-1)W} \left[A_+(k) f(E_-(k) - \mu) + A_-(k) f(E_+(k) - \mu) \right] \mathrm{d}\varepsilon_k \tag{3}$$

$$\varepsilon_f = E_0 + N\rho_0 V^2 \int_{-W}^{(N-1)W} \frac{f(E_-(k) - \mu) - f(E_+(k) - \mu)}{E_+(k) - E_-(k)} \mathrm{d}\varepsilon_k \tag{4}$$

$$\begin{aligned} n_f + n_c = {} & N\rho_0 \int_{-W}^{(N-1)W} (f(E_-(k) - \mu) + f(E_+(k) - \mu)) \, \mathrm{d}\varepsilon_k \\ & + sN\rho_0 \int_{-W}^{(N-1)W} f(\varepsilon_k - \mu) \, \mathrm{d}\varepsilon_k \end{aligned} \tag{5}$$

$$E_\mp = \tfrac{1}{2} \left(\varepsilon_k + \varepsilon_f \mp \sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4\tilde{V}^2} \right) \tag{6}$$

$$A_\mp = \frac{1}{2} \left(1 \mp \frac{\varepsilon_k - \varepsilon_f}{\sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4\tilde{V}^2}} \right) \tag{7}$$

where E_0 is the bare f electron energy, $f(x)$ is the Fermi function, W is the conduction electron band width, ρ_0 ($= 1/NW$) is the conduction electron density of states, $V^2 = \langle V_k^2 \rangle_{\text{Fermisurface}}$ is the bare hybridization and $\tilde{V}^2 = (1 - n_f)V^2$ is the effective hybridization. $E_\mp$ are the dispersion relations of the upper (+) and lower (−) quasiparticle energy bands.

In the following we want to derive the quasiparticle–phonon interaction Hamiltonian which results from the volume dependence of the bare parameters E_0 and V. We expand therefore as

$$\begin{aligned} \tilde{\varepsilon}_f(\eta(v_i)) &= \tilde{\varepsilon}_f + \frac{\partial \tilde{\varepsilon}_f}{\partial \eta(v_i)} \eta(v_i) \\ \tilde{V}(\eta(v_i)) &= \tilde{V}(i) + \frac{\partial \tilde{V}(i)}{\partial \eta(v_i)} \eta(v_i). \end{aligned} \tag{8}$$

The volume strain $\eta(v)$ can be expressed in terms of phonon creation and annihilation operators:

$$\eta(v_i) = \sum_q \frac{|q|}{\sqrt{2N_0 M \omega_q}} (b_q + b^\dagger_{-q}) \exp(\mathrm{i} q \cdot R_i) \tag{9}$$

where M, N_0, ω_q and R_i are the ion mass, the number of sites, the phonon dispersion and the ion position, respectively.

The derivatives $\partial\tilde{\varepsilon}_f/\partial\eta(v)$ and $\partial\tilde{V}/\partial\eta(v)$ may be written in terms of $\partial E_0/\partial\eta(v) = \gamma_1$ and $\partial V/\partial\eta(v) = \gamma_2$ as

$$\frac{\partial\tilde{\varepsilon}_f}{\partial\eta(v_i)} = \gamma_1\frac{\partial\tilde{\varepsilon}_f}{\partial E_0} + \gamma_2\frac{\partial\tilde{\varepsilon}_f}{\partial V}$$
$$\frac{\partial\tilde{V}}{\partial\eta(v_i)} = \gamma_1\frac{\partial\tilde{V}}{\partial E_0} + \gamma_2\frac{\partial\tilde{V}}{\partial V}. \tag{10}$$

From the MFA equations we can see that $\tilde{\varepsilon}_f$, $\tilde{V}$ and n_f depend on E_0 and V. Thus we obtain

$$\frac{\partial\tilde{V}}{\partial\eta(v_i)} = \gamma_2\sqrt{1-n_f} - \frac{V}{2\sqrt{1-n_f}}\left[\gamma_1\frac{\partial n_f}{\partial E_0} + \gamma_2\frac{\partial n_f}{\partial V}\right]. \tag{11}$$

The numerical plots of the derivatives of equation (10) are shown in figures 1 and 2.

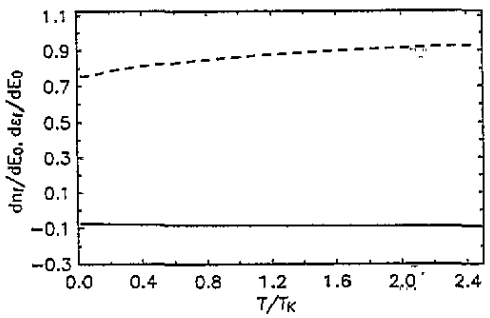

Figure 1. The temperature dependence of $\partial n_f/\partial E_0$ (solid line) and $\partial\varepsilon_f/\partial E_0$ (dashed line) for $E_0 = -0.5$ eV, $V = 1.0$ eV, $W = 10$ eV and $N = 6$.

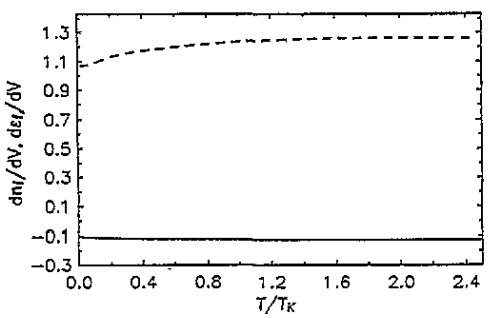

Figure 2. The temperature dependence of $\partial n_f/\partial V$ (solid line) and $\partial\varepsilon_f/\partial V$ (dashed line) The input parameters are the same as those in figure 1.

The electron–phonon interaction is then obtained by substituting equations (8)–(11) into the slave boson Hamiltonian. This contains two separate components: an expression containing the total electronic energy of the system, given by the original Hamiltonian (2), and an electron–phonon term (for clarity we neglect the volume dependence of the conduction electron energy)

$$H_{\text{qp-ph}} = \sum_{kqm} X_q\left\{\frac{\partial\tilde{\varepsilon}_f}{\partial\eta(v_i)}f^\dagger_{k+qm}f_{km} + \frac{\partial\tilde{V}}{\partial\eta(v_i)}(c^\dagger_{k+qm}f_{km} + f^\dagger_{k+qm}c_{km})(b_q + b^\dagger_{-q})\right\} \tag{12}$$

where

$$X_q = \frac{|q|}{\sqrt{2N_0M\omega_q}}.$$

The total Hamiltonian is then given by the sum of these terms and an expression for the free phonon energy of the system,

$$H_{\text{ph}} = \sum_q \omega_q b^\dagger_q b_q \tag{13}$$

where ω_q is simply the phonon energy. Thus, the total Hamiltonian

$$H_T = H_0 + H_{\text{ph}} + H_{\text{qp-ph}}. \tag{14}$$

We now perform a Bogoliubov transformation which leads to a new Hamiltonian given in terms of two quasiparticle bands, and the phonon coupling between them. The lower- (α) and upper- (β) band quasiparticles are given by the usual expressions,

$$\alpha^{\dagger}_{km} = x_k f^{\dagger}_{km} + y_k c^{\dagger}_{km} \tag{15}$$

$$\beta^{\dagger}_{km} = -y_k f^{\dagger}_{km} + x_k c^{\dagger}_{km}. \tag{16}$$

The coefficients $x_k$and y_k can be found by simple algebra,

$$x_k = -\frac{1}{\sqrt{2}}\left(1 + \frac{(\varepsilon_k - \tilde{\varepsilon}_f)}{\sqrt{(\varepsilon_k - \tilde{\varepsilon}_f)^2 + 4\tilde{V}^2}}\right)^{1/2} \tag{17}$$

$$y_k = -\frac{1}{\sqrt{2}}\left(1 - \frac{(\varepsilon_k - \tilde{\varepsilon}_f)}{\sqrt{(\varepsilon_k - \tilde{\varepsilon}_f)^2 + 4\tilde{V}^2}}\right)^{1/2}. \tag{18}$$

Upon substitution, these expressions diagonalize the Hamiltonian (2) into quasiparticle energy bands:

$$H_{qp} = \sum_k E^{\alpha}_{km}\alpha^{\dagger}_{km}\alpha_{km} + \sum_k E^{\beta}_{km}\beta^{\dagger}_{km}\beta_{km} \tag{19}$$

where E^{α}_{km} and E^{β}_{km} are the lower- and upper-heavy-fermion-band energies given by equation (6).

The quasiparticle–phonon interaction term takes on the following form:

$$\begin{aligned} H_{qp-ph} = \sum_{kqm} \Big\{ & [G_1(k,q) + G_2(k,q)]\alpha^{\dagger}_{k+qm}\alpha_{km} + [G'_1(k,q) - G_2(k,q)]\beta^{\dagger}_{k+qm}\beta_{km} \\ & + \sum_{kqm}[G_3(k,q) + G_4(k,q)]\alpha^{\dagger}_{k+qm}\beta_{km} \\ & + [G'_3(k,q) - G_4(k,q)]\beta^{\dagger}_{k+qm}\alpha_{km}\Big\}(b_q + b^{\dagger}_{-q}) \end{aligned} \tag{20}$$

where

$$\begin{aligned} G_1(k,q) &= x_{k+q}x_k\frac{\partial\tilde{\varepsilon}_f}{\partial\eta(v)} \\ G'_1(k,q) &= y_{k+q}y_k\frac{\partial\tilde{\varepsilon}_f}{\partial\eta(v)} \\ G_2(k,q) &= (y_{k+q}x_k + x_{k+q}y_k)\frac{\partial\tilde{V}}{\partial\eta(v)} \\ G_3(k,q) &= -x_{k+q}y_k\frac{\partial\tilde{\varepsilon}_f}{\partial\eta(v)} \\ G'_3(k,q) &= -x_k y_{k+q}\frac{\partial\tilde{\varepsilon}_f}{\partial\eta(v)} \\ G_4(k,q) &= -(y_{k+q}y_k - x_{k+q}x_k)\frac{\partial\tilde{V}}{\partial\eta(v)}. \end{aligned} \tag{21}$$

An extension to a model in which direct f–f hopping and an external magnetic field are included is straightforward. The main effect of this extension is to renormalize the 4f energy: $\epsilon_f \rightarrow \epsilon_f + hm + \beta\epsilon_k$, where $\beta = (1 - n_f)t/W$ and h and t are the magnetic field strength and the bare f–f hopping, respectively.

3. The phonon Green's function

The phonon Green's function is defined as

$$D(q,\omega) = \langle\langle Y_q | Y_{-q} \rangle\rangle \tag{22}$$

where $\langle\langle\ |\ \rangle\rangle$stands for the retarded Green's function and $Y_q = b_q + b^\dagger_{-q}$.

In order to calculate this, we carry out an RPA-like decoupling procedure. We first rewrite the function in the following way:

$$D(q,\omega) = \frac{\omega_q}{\omega}(D_1 - D_2) \tag{23}$$

where

$$D_1 = \langle\langle b_q | b_q^\dagger \rangle\rangle \qquad D_2 = \langle\langle b^\dagger_{-q} | b_{-q} \rangle\rangle. \tag{24}$$

The equation of motion for the retarded phonon Green's function is given by

$$\omega\langle\langle A|B\rangle\rangle = \langle[A, B]\rangle + \langle\langle [A, H_T]|B\rangle\rangle. \tag{25}$$

Using this we find

$$D_1 = \frac{1 + \sum_{km}\left\{[G_1(k,q) + G_2(k,q)]g_1 + [G_1'(k,q) - G_2(k,q)]g_1'\right\}}{\omega - \omega_q} \tag{26}$$

$$D_2 = \frac{1 + \sum_{km}\left\{[G_1(k,q) + G_2(k,q)]g_2 + [G_1'(k,q) - G_2(k,q)]g_2'\right\}}{\omega + \omega_q}. \tag{27}$$

As we are dealing with the phonon energy which is less than the hybridization gap we neglect the interband terms.

The higher-order Green's functions are

$$g_1 = \langle\langle \alpha^\dagger_{k-qm}\alpha_{km} | b_q^\dagger \rangle\rangle \tag{28}$$

$$g_2 = \langle\langle \alpha^\dagger_{k-qm}\alpha_{km} | b_{-q} \rangle\rangle \tag{29}$$

$$g_1' = \langle\langle \beta^\dagger_{k-qm}\beta_{km} | b_q^\dagger \rangle\rangle \tag{30}$$

$$g_2' = \langle\langle \beta^\dagger_{k-qm}\beta_{km} | b_{-q} \rangle\rangle. \tag{31}$$

The equations of motion for these functions in turn lead to

$$g_i = \frac{\sum_{q'}[G_1(k-q',q') - G_2(k-q',q')]\langle\langle \alpha^\dagger_{k-qm}\alpha_{k-q'm}Y_{q'} | b^\pm_{\pm q}\rangle\rangle}{\omega - (E^\alpha_k - E^\alpha_{k-q})} - \frac{\sum_{q'}[G_1(k,q) - G_2(k,q)]\langle\langle \alpha^\dagger_{k+q'-qm}\alpha_{km}Y_{q'} | b^\pm_{\pm q}\rangle\rangle}{\omega - (E^\alpha_k - E^\alpha_{k-q})}. \tag{32}$$

Here $i = 1$ for $b^+$and $i = 2$ for b^- ($b^- \equiv b$). If we replace the lower quasiparticle operators $\alpha^\dagger$ and α with the upper ones, $\beta^\dagger$ andβ, we get a similar expression for g_i'.

To obtain the phonon self-energy we restrict ourselves to second order in the quasiparticle–phonon interaction and perform the following RPA decoupling procedure:

$$\langle\langle \alpha^\dagger_{k-qm}\alpha_{k-q'm}Y_{q'} | b^\pm_{\pm q}\rangle\rangle \approx \delta_{q=q'}\langle\langle b^\mp_{\pm q} | b^\pm_{\pm q}\rangle\rangle\langle\alpha^\dagger_{k-qm}\alpha_{k-qm}\rangle \tag{33}$$

$$\langle\langle \alpha^\dagger_{k+q-q'm}\alpha_{km}Y_{q'} | b^\pm_{\pm q}\rangle\rangle \approx \delta_{q=q'}\langle\langle b^\mp_{\pm q} | b^\pm_{\pm q}\rangle\rangle\langle\alpha^\dagger_{km}\alpha_{km}\rangle \tag{34}$$

where

$$\langle\langle b_q | b_q^\dagger\rangle\rangle = \frac{1}{\omega - \omega_q} \tag{35}$$

$$\langle\langle b^{\dagger}_{-q}|b_{-q}\rangle\rangle = -\frac{1}{\omega+\omega_q}. \tag{36}$$

(Replacing α by β we perform a similar decoupling procedure.)

Thus finally we can express the phonon Green's function in terms of the free phonon Green's function $D_0 = 2\omega_q/(\omega^2-\omega_q^2)$ and the phonon self-energy $\Pi(q,\omega)$,

$$D(q,\omega) = D_0 + D_0\Pi(q,\omega)D_0 \tag{37}$$

where

$$\Pi(q,\omega) = \sum_{qm}[G_1(k,q)+G_2(k,q)]\,[G_1(k-q,q)+G_2(k-q,q)]\,\frac{f^{\alpha}_{k-qm}-f^{\alpha}_{km}}{\omega-(E^{\alpha}_{k}-E^{\alpha}_{k-q})}$$
$$+\sum_{qm}[G_1(k,q)-G_2(k,q)]\,\big[G'_1(k-q,q)-G_2(k-q,q)\big]$$
$$\times\frac{f^{\beta}_{k-qm}-f^{\beta}_{km}}{\omega-(E^{\beta}_{k}-E^{\beta}_{k-q})} \tag{38}$$

where f is the Fermi function and the value of ω is taken to have a small positive imaginary part.

Equating $D(q,\omega)^{-1}$ to zero defines a renormalized phonon energy and yields the following relation:

$$\omega^2-\omega_q^2-2\,\mathrm{Re}\,\Pi(q,\omega)\omega_q = 0. \tag{39}$$

The static approximation to the real part of the phonon self-energy $\mathrm{Re}\,\Pi\ (q,\omega)$ is then applied and the long-wavelength limit taken. We then find

$$\mathrm{Re}\,\Pi(q,\omega) = N\rho_0\int_{-W}^{(N-1)W}\mathrm{d}\varepsilon_k\left\{[G_1(k,q)+G_2(k,q)]^2\frac{\partial f^{\alpha}}{\partial E^{\alpha}_k}\right.$$
$$\left.+[G'_1(k,q)-G_2(k,q)]^2\frac{\partial f^{\beta}}{\partial E^{\beta}_k}\right\}. \tag{40}$$

The change in sound velocity $\Delta s = s - s_0$ is then calculated from the relation

$$\Delta s = \frac{1}{q}\,\mathrm{Re}\,\Pi(q,\omega=0) \tag{41}$$

where s_0 is the bare sound velocity.

We take the degeneracy factor $N = 6$ (the total number of electrons per site $n = 2$) because this is appropriate to describe the $J = \frac{5}{2}$ multiplet in cerium compounds. Then the Fermi level does not move into the hybridization gap at very low temperatures.

Our approach can be applied to any value of N . As we use the square conduction electron density of states, $\rho_0 = 1/NW$ then $N\rho_0V^2$ is independent of N and therefore the effective Kondo temperature T_K will depend on V, W and E_0 only. Of course, there is a general problem of the validity of the Anderson model for heavy-fermion systems for large values of N. The hope is that the extrapolation to large N provides a reasonably good description of the basic physics (Hewson 1993, Millis and Lee 1987). The problem of the degeneracy is also important if we want to consider the spin–orbit and crystal field effects. These effects can be included in our approach in a similar way to that developed by Evans (1992).

The crystal field effects in the case of the elastic anomaly of heavy-fermion systems were considered by Harigaya and Gehring (Harigaya and Gehring 1993) where the shear modulus was obtained from the linear susceptibility with respect to the crystal field splitting.

The formalism was also based on the Anderson model and was independent of the real band structure and degeneracy structure yielding a good description of the low-temperature anomalies for heavy-fermion systems.

The ultrasonic attenuation coefficient (α) can be obtained from the formula

$$\alpha = \frac{1}{s} \operatorname{Im} \Pi(q, w). \tag{42}$$

We can express the longitudinal elastic constant in terms of the change in sound velocity as

$$\Delta c = 2\rho c_0 \Delta s \tag{43}$$

where ρ is the mass density and c_0 is the bare elastic constant. The temperature dependence of the elastic constant is shown in figure 3.

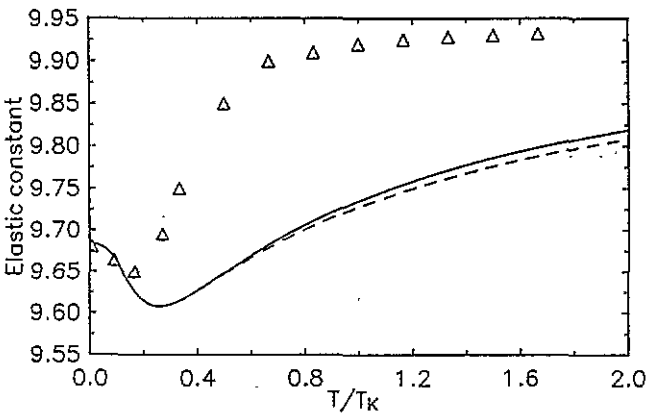

Figure 3. The temperature dependence of the longitudinal elastic constant c (10^{11}erg cm^{-3}) for rare earth systems, $\gamma_2 = 0.015$ eV. The remaining parameters are the same as those in figures 1 and 2. Solid line: the lower-quasiparticle-band contribution. Dashed line: the lower- and upper-quasiparticle-band contributions. Triangles: experimental data of Niksch *et al* (1980) for $CeAl_3$.

In order to compare our quasiparticle–phonon interaction with that obtained by Keller *et al* (1990) for the rare earth systems we need to calculate only the first term of equation (20) i.e. we have to evaluate G_1 and G_2 at $T = 0$. In the mean field approach it is easy to get analytical expressions of all physical quantities in terms of the bare parameters E_0, V, W and the degeneracy factor N.

We obtain the following expressions for G_1 and G_2 (see the appendix) ($q \to 0$):

$$G_1 = \frac{|q|}{\sqrt{2N_0 M\omega_q}} x_k^2 \frac{\partial \tilde{\varepsilon}_f}{\partial V} \gamma_2 \tag{44}$$

$$G_2 = \frac{2|q|}{\sqrt{2N_0 M\omega_q}} x_k y_k \frac{\partial \tilde{V}}{\partial V} \gamma_2 \tag{45}$$

$$\frac{\partial \tilde{\varepsilon}_f}{\partial V} = -\frac{1-n_f}{2-n_f}\left[\frac{2(E_0-\tilde{\varepsilon}_f)}{V} - \frac{1}{N\rho_0}X_V\right] - \frac{1}{N\rho_0}X_V \tag{46}$$

$$\frac{\partial \tilde{V}}{\partial V} = \sqrt{1-n_f}\left[1 - \frac{n_f}{1+K} - \frac{n_f^2(E_0-\tilde{\varepsilon}_f)}{N\rho_0 V^2(1+K)}\right] \tag{47}$$

where

$$X_V = \frac{2n_f^2(1-n_f)(E_0-\tilde{\varepsilon}_f)}{N\rho_0 V^3(1+K)}. \tag{48}$$

These results differ from that obtained by Keller *et al* (1990) because of X_V and K, which come from the hybridization dependence of the chemical potential. This dependence is very important in the lattice case as was shown by Evans *et al* (1989).

Using the mean field results of

$$x_k^2 \cong 1$$
$$x_k y_k \cong \tilde{V}/W$$

neglecting X_V and putting $K = 0$ (see the appendix, (A3) and (A4)) we deduce

$$G_1 + G_2 = -\frac{2|q|(E_0 - \tilde{\varepsilon}_f)W}{\sqrt{2N_0 M\omega_q}\, V^3}\gamma_2[x_k^2 T_K - x_k y_k V\sqrt{1-n_f}]$$
$$\cong -\frac{2|q|(E_0 - \tilde{\varepsilon}_f)W}{\sqrt{2N_0 M\omega_q}\, V^3}\gamma_2\left[T_K - \frac{V^2(1-n_f)}{W}\right] = 0. \tag{49}$$

Therefore Keller's result is only of the order of T_K^2. In our case there in no cancellation of of the two contributions G_1 and G_2 in the leading order in T_K. This result is independent of N in the mean field aproximation.

We can also use the zero-temperature mean field solutions (Rasul and Harrington 1987) to derive $\partial\tilde{\varepsilon}_f/\partial V$ and $\partial\tilde{V}/\partial V$ for uranium systems. We thus find

$$\frac{\partial\tilde{\varepsilon}_f}{\partial V} = \frac{(n_f-2)(3-n_f)}{n_f + (n_f-2)(3-n_f)}\left[\frac{-2(E_0-\tilde{\varepsilon}_f)}{V} + W\frac{\partial n_f}{\partial V}\right] - W\frac{\partial n_f}{\partial V} \tag{50}$$

and

$$\frac{\partial\tilde{V}}{\partial V} = \frac{1}{2}V(5-2n_f)\sqrt{(n_f-2)(3-n_f)}\left(\frac{2n_f(3-n_f)}{3}\right)\left(\frac{1/V - W(\tilde{\varepsilon}_f - E_0)/V^3}{1-2n_f(3-n_f)W^2/3V^2}\right) \tag{51}$$

where

$$\frac{\partial n_f}{\partial V} = \left(\frac{2n_f(3-n_f)}{3}\right)\left(\frac{1/V - W(\tilde{\varepsilon}_f - E_0)/V^3}{1-2n_f(3-n_f)W^2/3V^2}\right). \tag{52}$$

We can simplify the integral in equation (40) further by employing the linear approximation to the Fermi function (Hong *et al* 1993). This in fact makes the evaluation easier and yet still maintains the essential trends we are concerned with. We then have, combining expressions (40) and (43),

$$\Delta c = 2\rho_0 c_0/q \int_{\mu-\Delta}^{(\mu+\Delta)} d\varepsilon_k\, N(\varepsilon_k)\left\{[G_1(k,q) + G_2(k,q)]^2\right.$$
$$\left. +[G_1'(k,q) - G_2(k,q)]^2\right\}\left(\frac{-1}{2\Delta}\right) \tag{53}$$

where the $-1/2\Delta$ terms come from differentiating the linear Fermi function with respect to temperature and $\Delta = 4T\ln(2)$. $N(\varepsilon)$ is the quasiparticle density of states. The numerical plots for the uranium systems in the linear approximation are shown in figures 4 and 5. A good agreement is found with the experimental findings of Yoshizawa *et al* (1985). As we increase the degeneracy, N, the accuracy of the theoretical plots does seem to improve. This is indeed what we would expect from a mean field theory essentially zeroth order in the expansion parameter $1/N$. Moreover, larger N causes the low-temperature dip to deepen.

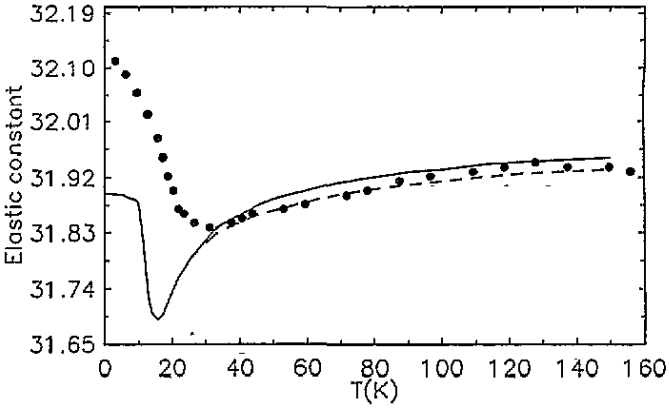

Figure 4. The elastic constant as a function of temperature, with (dashed line) and without (solid line) the upper-quasiparticle-band contribution. The input parameters here were $W = 10$ eV, $V = 1$ eV, $N = 10$ and $E_0 = -0.4$ eV. Circles: experimental data of Yoshizawa *et al* (1985) for UPt_3.

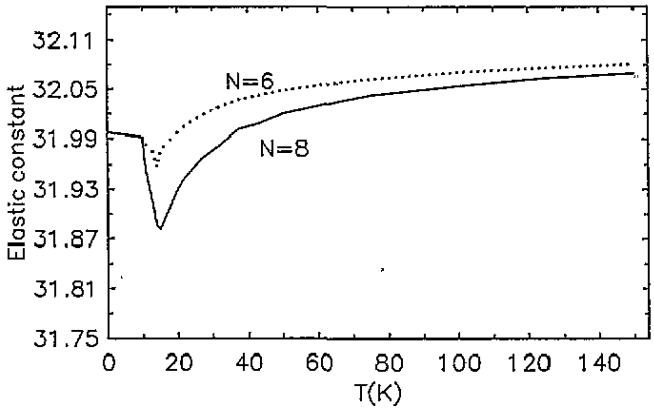

Figure 5. The elastic constant c (10^{11}erg cm^{-3}) as a function of temperature. This was evaluated for different values of degeneracy, N. The input parameters are the same as those in figure 4.

4. Discussion

In this paper we discuss the role of the volume dependence of the bare hybridization and bare 4f energy on the longitudinal sound velocity in heavy-fermion compounds. Recently it has been shown (Evans *et al* 1989) that the MFA solutions not only describe correctly the low-temperature Fermi liquid behaviour but also are sufficient for a discussion of the high-temperature region. Also, the MFA solutions extrapolate smoothly between the two regimes. The latter results from the fact that for the lattice case the Fermi energy decreases with temperature (see the appendix). Hence $n_f \rightarrow 1$ at higher temperature than for an impurity case.

It would seem that the slave boson mean field theory is quite able to incorporate the processes which couple the lattice vibrations with the anomalously heavy electrons. Again we see that the changing chemical potential is a crucial factor within the lattice model: the inclusion of its temperature dependence leads to the negative feedback effect which extends the range of mean field theory well beyond T_K, while the inclusion of its volume

dependence yields a more accurate description of the underlying elastic properties than has been achieved by previous approaches.

The electron–phonon interaction resulting from the volume dependence of the 4f level (E_0) and the bare hybridization strength (V) yields two different parameters, namely γ_1 and γ_2.

Also, we take into account an additional term coming from the implicit volume dependence of the renormalized hybridization strength through the number of 4f electrons per site (n_f). This term is necessary for obtaining the sound velocity in the same form that is yielded when the sound velocity is calculated directly from the free energy (Fulde *et al* 1988). It should also be emphasized that this term is influenced strongly by the bare hybridization dependence on the 4f occupation number (n_f), described by the derivative of n_f with respect to V and cannot be neglected in comparison with $\partial\tilde{\varepsilon}_f/\partial E_0$ and $\partial\tilde{\varepsilon}_f/\partial V$ which are usually very small. The results are shown in figures 1 and 2 where we have plotted $\partial\tilde{\varepsilon}_f/\partial E_0$, $\partial n_f/\partial E_0$ and $\partial\tilde{\varepsilon}_f/\partial V$, $\partial n_f/\partial V$ against temperature divided by T_K (the parameters $W = 10$ eV, $V = 1$ eV and $E_0 = -0.5$ eV give $T_K \approx 38$ K) . In spite of the small values of the derivatives (see figures 1 and 2 they play an important role. At low temperatures they lead to the decreasing of the elastic constant. Thus we obtain a minimum of the elastic constant at finite temperature because the elastic constant increases with the temperature and reaches its bare value at high temperature.

From figures 3, 4 and 5 it is seen that there is a minimum of the elastic constant at about one quarter of the Kondo temperature T_K, defined at $T = 0$ K. This is consistent with the experimental data concerning the elastic constant for $CeAl_3$ (Niksch *et al* 1980, see figure 3) and UPt_3 (Yoshizawa *et al* 1985, see figure 4). However, as it is difficult to fit our results to experimental data for the whole range of temperatures, we can fit our results either at low (see figure 3) or high (see figure 4) temperatures. Changing the input parameters we can fit $CeAl_3$ and UPt_3 data at high and low temperatures, respectively.

The value of this paper is in showing the origin of the dip in the elastic constant. The detailed fitting was disappointing, possibly because we had no underlying anharmonicity data to include in the fit. These calculations show that the minimum appears if, according to the mean field equations, the Fermi energy is allowed to change with temperature.

Since in other heavy-fermion systems such as $CeCu_6$, $CeRu_2Si_2$, the minimum is not so distinct, or even not present, we assume, on the basis of our results, that the diminution or even vanishing of the minimum can be a consequence of the reduction of the negative feedback effect due to the local screening cloud in these materials (Newns and Read 1987). This can mean that the screening effects play a more important role in these componds than they do in $CeAl_3$ or UPt_3 where the dip of the elastic constants is observed. As it is very difficult to include the screening effects within our approach, we have neglected them and therefore we are not able to estimate the role they play in the anomalous behaviour of the temperature dependence of the elastic constant.

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Appendix

In this appendix we calculate G_1 and G_2 terms defined in equation (20) for $\gamma_1 = 0$ and at $T = 0$. For this purpose we only need to evaluate two derivatives $\partial\tilde{\varepsilon}_f/\partial V$ and $\partial\tilde{V}_f/\partial V$.

To obtain a proper quasiparticle–phonon interaction for a lattice case we have to include the hybridization dependence of the chemical potential μ. In the mean field and at $T = 0$ μ can be obtained from the equation

$$n = n_f + N\rho_0(\mu - E_-) \tag{A1}$$

where

$$E_- = \tfrac{1}{2}\left((N-1)W + \tilde{\varepsilon}_f - \sqrt{[(N-1)+\tilde{\varepsilon}_f]^2 + 4\tilde{V}^2}\right) \tag{A2}$$

and n, n_f, N, ρ_0, are the total number of the electrons, the number of f electrons, the degeneracy factor and the conduction electron density of states, respectively. Hence

$$\frac{\partial\mu}{\partial V} = -\frac{1}{N\rho_0}X_V \tag{A3}$$

$X_V = \partial n_f/\partial V$ and

$$X_V = \frac{2n_f^2(1-n_f)(E_0-\tilde{\varepsilon}_f)}{N\rho_0 V^3(1+K)} \tag{A4}$$

where

$$K = \frac{n_f^2(1-n_f)}{N^2\rho_0^2V^2}. \tag{A5}$$

The same result can be obtained from the approximate formula $\mu = W(1-n_f)$.

Using two equivalent definitions of the Kondo temperature

$$T_K = \tilde{\varepsilon}_f - \mu \tag{A6}$$

and

$$T_K = W\exp[(\tilde{\varepsilon}_f)/N\rho_0V^2] \tag{A7}$$

we get

$$\frac{\partial\tilde{\varepsilon}_f}{\partial V} = \frac{1-n_f}{2-n_f}\left(\frac{2(E_0-\tilde{\varepsilon}_f)}{V} + \frac{1}{N\rho_0}X_V\right) - \frac{1}{N\rho_0}X_V. \tag{A8}$$

Similarly, evaluating $\partial\tilde{V}/\partial V$ we obtain

$$\frac{\partial\tilde{V}}{\partial V} = r\left(1 - \frac{n_f}{1+K} - \frac{n_f^2(E_0-\tilde{\varepsilon}_f)}{N\rho_0V^2(1+K)}\right) \tag{A9}$$

where $r = \sqrt{(1-n_f)}$.

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