Electron-phonon interaction in heavy-fermion systems

J.Keller, R. Bulla, and Th. Höhn
Fakultät für Physik, Universität Regensburg, D-8400 Regensburg, Federal Republic of Germany

K.W. Becker
Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart, Federal Republic of Germany
(Received 23 May 1989)

A systematic theory of the electron-phonon interaction in heavy-fermion systems is developed on the basis of the mean-field approximation for the Kondo lattice. The electron-phonon interaction is introduced into the Anderson Hamiltonian by assuming that the hybridization between f electrons and conduction electrons depends on the local lattice strain. The interaction with conduction electrons is included by using a deformation-potential-type coupling. By solving the mean-field equations in the presence of lattice displacements, quasiparticle interactions described by Kondo bosons are included in the present theory. Using a random-phase-type approximation for the Kondo-boson propagators, the phonon self-energy and the elastic constants are calculated. The quasiparticle interaction mediated by phonons is derived, and its competition with the quasiparticle interaction by Kondo bosons is studied. The results of the present theory are compared with an effective static electron-phonon interaction. It is found that this is a reasonable approximation for interaction processes with large momentum transfer and small frequencies.

I. INTRODUCTION

In many heavy-fermion systems like $CeAl_3$, $CeCu_6$, $CeRu_2Si_2$, and UPt_3, anomalous effects in the temperature dependence of the elastic constants[1] and the magneto-acoustic properties[2] have been observed. These are attributed to the coupling between lattice vibrations and the heavy electrons. The physical origin of this coupling is probably the volume dependence of the hybridization between f electrons and conduction electrons. This leads to a strong dependence of the Kondo temperature T_K on the lattice strain ϵ_Ω, which can be characterized by a large Grüneisen parameter[3] $\eta = -d\ln(T_K)/d\epsilon_\Omega$. This type of electron-phonon interaction is of special interest as a possible source of a pairing interaction in heavy-fermion superconductors[4] like $CeCu_2Si_2$.

In this paper we want to develop a theory for the electron-phonon interaction that is based on a slave-boson mean-field approximation for the Anderson Hamiltonian.[5,6] Starting from the microscopic Anderson Hamiltonian we assume that the hybridization between conduction electrons and f electrons depends on lattice displacements. Here we consider only its dependence on a local lattice strain, i.e., we consider only the coupling to longitudinal phonons and neglect directional effects due to the anisotropy of the f-electron wave functions. We consider also the interaction between phonons and conduction electrons in the most simple form by introducing a volume-dependent shift of the conduction electron energies. Though this interaction is not essentially influenced by the Kondo effect, it is necessary for obtaining the correct total electronic compressibility.

By solving the mean-field equations in the presence of spatial and time-dependent perturbations induced by the lattice displacements we automatically include quasiparticle interactions described by the so-called Kondo bosons[5,7–9] in a random-phase approximation. With help of this approach we derive systematically the phonon self-energy and the quasiparticle interaction mediated by phonons. This allows us to check the validity of an effective electron-phonon interaction for quasiparticles, which we have introduced earlier.[4,6] The theory presented here is also an extension of other microscopic calculations[10] based on the mean-field approximation for the Anderson Hamiltonian.

Unfortunately the mean-field approximation is only good for $T \ll T_K$. Therefore many interesting properties that are related to the temperature dependence of the elastic properties and the ultrasonic attenuation cannot be studied accurately with this theory. To study these effects a more refined theory for the electronic properties of the Kondo lattice such as the perturbational approach[11] would be a better starting point. We also do not discuss here the hydrodynamic modes where density fluctuations mix with heat relaxation,[12] but instead concentrate on the lattice modes at larger frequencies.

In the following section we extend the well-known mean-field theory for heavy-fermion systems[5] to systems with external perturbations. Here the Kondo-boson propagator enters in a natural way as response of the

mean-field parameters on the external perturbation. The results are used in Sec. III to derive the electron-phonon interaction from which we calculate the phonon self-energy and the elastic properties in Sec. IV. Here we also present some numerical results for the phonon self-energy. Finally, in Sec. V we derive the interaction between quasiparticles mediated by phonons and study their interplay with the quasiparticle interaction mediated by Kondo bosons. Some details of the calculations are given in the Appendix.

II. MEAN-FIELD THEORY FOR HF SYSTEMS WITH EXTERNAL PERTURBATIONS

The starting point for the theoretical investigation of heavy-fermion systems is the Anderson Hamiltonian.[13] In the case of Ce compounds it contains a mixing interaction V between conduction electrons and f electrons (with energy ε_f far below the Fermi energy), and a large local Coulomb interaction U between f electrons, which suppresses a double occupancy of f states. In the limit $U \to \infty$ the Anderson Hamiltonian can be written in the slave-boson representation[5] as

$$H_0 = \sum_{k\alpha} \varepsilon_k c^\dagger_{k\alpha} c_{k\alpha} + \varepsilon_f \sum_{i\alpha} f^\dagger_{i\alpha} f_{i\alpha} + \sum_{i\alpha} V(b_i f^\dagger_{i\alpha} c_{i\alpha} + b^\dagger_i c^\dagger_{i\alpha} f_{i\alpha}) \ . \tag{1}$$

Here the large Coulomb interaction is eliminated formally by restricting the Hilbert space to empty and single occupied f states. In this restricted Hilbert space the operators for f electrons no longer fulfill the fermion commutation rules. This can be avoided by introducing additional (slave) boson operators b_i for each lattice site and replacing $f_{i\alpha}$ by $b^\dagger_i f_{i\alpha}$ and $f^\dagger_{i\alpha}$ by $b_i f^\dagger_{i\alpha}$ in the mixing interaction. The resulting Hamiltonian (1) is equivalent to the original Anderson Hamiltonian for states with $Q_i = \sum_\alpha f^\dagger_{i\alpha} f_{i\alpha} + b^\dagger_i b_i = 1$.

In the following we neglect for simplicity the dependence of V on the electron spin α and the momentum $\mathbf{k}$. This means that we treat the f electrons like s electrons with two spin directions. We also consider only one band of conduction electrons. In this case the relation between momentum representation and site representation is given by $c_{k\alpha} = (1/\sqrt{N}) \sum_i c_{i\alpha} \exp(-i\mathbf{k} \cdot \mathbf{x}_i)$, where N is the number of lattice sites.

For later use we also introduce external perturbations that couple to the electronic densities $H_{ex} = \sum_\nu H^{(\nu)}_{ex}$ with

$$H^{(1)}_{ex} = \sum_{i\alpha} \delta V_i (b_i f^\dagger_{i\alpha} c_{i\alpha} + b^\dagger_i c^\dagger_{i\alpha} f_{i\alpha}) \ , \tag{2}$$

$$H^{(2)}_{ex} = \sum_{i\alpha} \delta Z_i f^\dagger_{i\alpha} f_{i\alpha} \ , \tag{3}$$

$$H^{(3)}_{ex} = \sum_{i\alpha} \delta W_i c^\dagger_{i\alpha} c_{i\alpha} \ . \tag{4}$$

Here δV_i can be considered as a local change of the hybridization, δZ_i a shift of the energy of the f level, and δW_i a shift of the local potential for the conduction electrons.

In the mean-field approximation the boson operators are replaced by (real) expectations values r_i. The condition $Q_i = 1$ is replaced by the weaker condition $\langle Q_i \rangle = 1$. Technically this is achieved by adding a term $\sum_i \Lambda_i (Q_i - 1)$ to the Hamiltonian with an adjustable Lagrange parameter Λ_i. Then the total Hamiltonian is given by

$$H = H_0 + H_{ex} + \sum_i \Lambda_i (Q_i - 1) \ . \tag{5}$$

The resulting mean-field Hamiltonian (including the external perturbations) reads

$$H_{MF} = \sum_{k\alpha} \varepsilon_k c^\dagger_{k\alpha} c_{k\alpha} + \sum_{i\alpha} \delta W_i c^\dagger_{i\alpha} c_{i\alpha} + \sum_{i\alpha} (\varepsilon_f + \delta Z_i) f^\dagger_{i\alpha} f_{i\alpha} + \sum_{i\alpha} (V + \delta V_i) r_i (f^\dagger_{i\alpha} c_{i\alpha} + c^\dagger_{i\alpha} f_{i\alpha}) + \sum_i \Lambda_i \left(\sum_\alpha f^\dagger_{i\alpha} f_{i\alpha} + r_i^2 - 1 \right) + \sum_i \Lambda_i (b^\dagger_i - r_i)(b_i - r_i) \ . \tag{6}$$

It has the property $\langle H - H_{MF} \rangle_{MF} = 0$. The last term is added to enforce $\langle b^\dagger_i \rangle = \langle b_i \rangle = r_i$. The parameters r_i and Λ_i are determined by the condition $\langle Q_i \rangle_{MF} = 1$ and the minimum principle for the free energy, which in the present case leads to $\langle \partial H_{MF} / \partial r_i \rangle_{MF} = 0$. From these two relations the following self-consistency equations for the mean-field parameters are obtained:

$$V_i \langle A_i \rangle + 2\Lambda_i r_i = 0 \ , \tag{7}$$

$$\langle n^f_i \rangle + r_i^2 = 1 \ , \tag{8}$$

where

$$A_i = \sum_\alpha f^\dagger_{i\alpha} c_{i\alpha} + c^\dagger_{i\alpha} f_{i\alpha} \tag{9}$$

and

$$n^f_i = \sum_\alpha f^\dagger_{i\alpha} f_{i\alpha} \ . \tag{10}$$

These equations have to be fulfilled in the presence of perturbations. Note that only the perturbation in the hybridization, $V_i = V + \delta V_i$, enters directly. The other

perturbations are contained indirectly in the deviations $\delta\langle A_i\rangle$ and $\delta\langle n_i^f\rangle$ of these quantities from equilibrium.

In the absence of perturbations (7) and (8) are easily solved, and one obtains in leading order in the Kondo temperature T_K

$$A = \langle A_i\rangle_0 = -2r\Lambda/V \ , \tag{11}$$

$$\Lambda = \tilde{\varepsilon}_f - \varepsilon_f = \mu + T_K - \varepsilon_f \ , \tag{12}$$

$$r^2 = 1 - \langle n_i^f\rangle_0 = T_K/2N(0)V^2 \ , \tag{13}$$

where

$$T_K = \mu \exp[-\Lambda/2N(0)V^2] \ . \tag{14}$$

Here μ is the chemical potential and $N(0)$ the density of states of the conduction electrons at the Fermi energy (in the absence of hybridization with f electrons). The mean-field Hamiltonian then describes hybridization of conduction electrons and f electrons with energy $\tilde{\varepsilon}_f$ slightly above the Fermi energy and a reduced mixing interaction $\tilde{V} = rV$.

In order to take into account the external perturbations we expand in (7) and (8) all quantities around their mean values:

$$A\delta V_i + V\delta\langle A_i\rangle + 2r\delta\Lambda_i + 2\Lambda\delta r_i = 0 \ , \tag{15}$$

$$2r\delta r_i + \delta\langle n_i^f\rangle = 0 \ . \tag{16}$$

The deviations $\delta\langle A_i\rangle$ and $\delta\langle n_i^f\rangle$ depend on the external perturbations $\delta V_l, \delta Z_l, \delta W_l$ (at the same and different lattice sites), and also on the values of the mean-field parameters r_l and Λ_l. We obtain for small perturbations approximately

$$\delta\langle A_i\rangle = \sum_l \ [\Pi_{11}(i,l)\delta\sigma_l + \Pi_{12}(i,l)(\delta\Lambda_l + \delta Z_l) + \Pi_{13}(i,l)\delta W_l \ ] \ , \tag{17}$$

$$\delta\langle n_i^f\rangle = \sum_l \ [\ \Pi_{21}(i,l)\delta\sigma_l + \Pi_{22}(i,l)(\delta\Lambda_l + \delta Z_l) + \Pi_{23}(i,l)\delta W_l \ ] \ . \tag{18}$$

Here $\delta\sigma_l = V\delta r_l + r\delta V_l$. The different response functions in (17) and (18):

$$\Pi_{11}(i,l) = \langle\langle A_i, A_l\rangle\rangle_0,$$

$$\Pi_{12}(i,l) = \langle\langle A_i, n_l^f\rangle\rangle_0,$$

$$\Pi_{13}(i,l) = \langle\langle A_i, n_l^c\rangle\rangle_0,$$

etc., have to be calculated in equilibrium, and are listed in the Appendix.

Using (17) and (18) in (15) and (16), and going over to Fourier-transformed quantities,

$$\delta V_{\mathbf{q}} = \left(1/\sqrt{N}\right)\sum_i \delta V_i \exp(-i\mathbf{q}\cdot\mathbf{x}_i) \ ,$$

we may write these equations as

$$K^{-1}(\mathbf{q})\begin{pmatrix} V\delta r_{\mathbf{q}} \\ \delta\Lambda_{\mathbf{q}}\end{pmatrix} = \frac{A}{V}\begin{pmatrix}\delta V_{\mathbf{q}} \\ 0\end{pmatrix} + \bar{\Pi}(\mathbf{q})\begin{pmatrix} r\delta V_{\mathbf{q}} \\ \delta Z_{\mathbf{q}} \\ \delta W_{\mathbf{q}}\end{pmatrix} \ . \tag{19}$$

Here

$$K^{-1}(\mathbf{q}) = K_0^{-1}(\mathbf{q}) - \Pi(\mathbf{q}) \ , \tag{20}$$

where

$$K_0^{-1}(\mathbf{q}) = -\begin{pmatrix} 2\Lambda/V^2 & 2r/V \\ 2r/V & 0\end{pmatrix} \ , \tag{21}$$

and $\Pi(\mathbf{q})$ is the 2×2 matrix,

$$\Pi(\mathbf{q}) = \begin{pmatrix}\Pi_{11}(\mathbf{q}) & \Pi_{12}(\mathbf{q}) \\ \Pi_{21}(\mathbf{q}) & \Pi_{22}(\mathbf{q})\end{pmatrix} \ . \tag{22}$$

The matrix $\bar{\Pi}(\mathbf{q})$ in (19) is a 2×3 matrix of the form

$$\bar{\Pi}(\mathbf{q}) = \begin{pmatrix}\Pi_{11}(\mathbf{q}) & \Pi_{12}(\mathbf{q}) & \Pi_{13}(\mathbf{q}) \\ \Pi_{21}(\mathbf{q}) & \Pi_{22}(\mathbf{q}) & \Pi_{23}(\mathbf{q})\end{pmatrix} \ . \tag{23}$$

From (19) we obtain as a response of the mean-field parameters on a perturbation coupling to the electronic densities,

$$\begin{pmatrix} V\delta r_{\mathbf{q}} \\ \delta\Lambda_{\mathbf{q}}\end{pmatrix} = \frac{A}{V}K(\mathbf{q})\begin{pmatrix}\delta V_{\mathbf{q}} \\ 0\end{pmatrix} + K(\mathbf{q})\bar{\Pi}(\mathbf{q})\begin{pmatrix} r\delta V_{\mathbf{q}} \\ \delta Z_{\mathbf{q}} \\ \delta W_{\mathbf{q}}\end{pmatrix} \ . \tag{24}$$

In $K(\mathbf{q})$ one can recognize the so-called Kondo-boson propagator, which is introduced in the functional-integral approach to describe amplitude and phase-fluctuations of the Kondo bosons.[5,7,8] The form given by (19) corresponds to the random-phase approximation (RPA) for the Kondo-boson propagator. Within the present treatment $K(\mathbf{q})$ appears as response of the mean-field parameters on a perturbation that couples to the mean-field variables. More precisely, if we add to the mean-field Hamiltonian an (artificial) perturbation of the form $\sum_i \sigma_i\delta\phi_i + \Lambda_i\delta\psi_i$ and solve the corresponding self-consistency equations in the same manner, the result for the induced fluctuations of $\delta\sigma_{\mathbf{q}}$ and $\delta\Lambda_{\mathbf{q}}$ are given by

$$\begin{pmatrix}\delta\sigma_{\mathbf{q}} \\ \delta\Lambda_{\mathbf{q}}\end{pmatrix} = K(\mathbf{q})\begin{pmatrix}\delta\phi_{\mathbf{q}} \\ \delta\psi_{\mathbf{q}}\end{pmatrix} \ . \tag{25}$$

The result of (24) can also be written in a more compact form, which will be useful later:

$$\begin{pmatrix}\delta\sigma_{\mathbf{q}} \\ \delta\Lambda_{\mathbf{q}} + \delta Z_{\mathbf{q}}\end{pmatrix} = K(\mathbf{q})M(\mathbf{q})\begin{pmatrix}\delta V_{\mathbf{q}} \\ \delta Z_{\mathbf{q}} \\ \delta W_{\mathbf{q}}\end{pmatrix} \ , \tag{26}$$

where $M(\mathbf{q})$ is the 2×3 matrix

$$M(\mathbf{q}) = \begin{pmatrix} -4\Lambda r/V^2 & -2r/V & \Pi_{13}(\mathbf{q}) \\ -2r^2/V & 0 & \Pi_{23}(\mathbf{q})\end{pmatrix} \ . \tag{27}$$

Later we will use (26) also for frequency-dependent perturbations, assuming that the self-consistency equations [(15) and (16)] also hold for time-dependent perturbations. This assumption is equivalent to the saddle-point approximation in the functional-integral approach.[5]

III. ELECTRON-PHONON INTERACTION

If we start from the Anderson Hamiltonian there are three possibilities where the coupling between lattice vibrations and electrons enters: (1) the influence on the hybridization between conduction electrons and f electrons, (2) the influence on the (unrenormalized) f-electron energy, and (3) the coupling to conduction electrons. The latter is present in all metals and can be described in the most simple and unspecific way by a deformation-potential coupling. The first effect is specific for intermediate valence and heavy-fermion systems. In the former it has been discussed already for many years.[14] Little is known about the influence of lattice vibrations on the unrenormalized f-electron energy. We include it here for completeness of the theory.

The most simple form of an electron-phonon interaction is obtained if we assume that these three quantities depend only on the local volume strain $\epsilon_\Omega(i) = \delta\Omega_i/\Omega_c$, where Ω_c is the volume of a lattice cell. In that case the electron-phonon interaction is obtained from (2)–(4) by replacing the external perturbations by perturbations caused by the lattice strain: $\delta V_i = \epsilon_\Omega(i)\partial V/\partial\epsilon_\Omega$, etc. Then we find

$$H_{\rm int}^{(1)} = \sum_{i\alpha} \epsilon_\Omega(i) g_1 (b_i f_{i\alpha}^\dagger c_{i\alpha} + b_i^\dagger c_{i\alpha}^\dagger f_{i\alpha}) , \tag{28}$$

$$H_{\rm int}^{(2)} = \sum_{i\alpha} \epsilon_\Omega(i) g_2 f_{i\alpha}^\dagger f_{i\alpha} , \tag{29}$$

$$H_{\rm int}^{(3)} = \sum_{i\alpha} \epsilon_\Omega(i) g_3 c_{i\alpha}^\dagger c_{i\alpha} , \tag{30}$$

where $g_1 = \partial V/\partial\epsilon_\Omega$, $g_2 = \partial\varepsilon_f/\partial\epsilon_\Omega$, and $g_3 = \partial W/\partial\epsilon_\Omega$. As an order of magnitude estimate we may assume $g_1/V = -(1\text{–}5)$, $g_3/\varepsilon_F \simeq -1$, g_2 is unknown.

Let us first discuss $H_{\rm int}^{(1)}$. In the mean-field approximation the boson operators $b_i, b_i^\dagger$ in (28) are replaced by (real) expectation values $\langle b_i\rangle = \langle b_i^\dagger\rangle = r_i = r + \delta r_i$. In the case of small deviations from equilibrium we may linearize the electronic operators and we obtain [with $\delta A_i = A_i - A$ and A_i given by (9)]

$$H_{\rm int}^{(1)} = \sum_i \epsilon_\Omega(i) g_1 (rA + r\delta A_i + A\delta r_i) . \tag{31}$$

In the further treatment of $H_{\rm int}^{(1)}$ it is essential to consider not only the f-electron and conduction-electron excitations contained in A_i but also the local deviations δr_i of the mean-field values r_i from equilibrium. They are not quantum-mechanical operators, but nevertheless play the role of dynamical variables (the constant value rA is not relevant for the electron-phonon interaction).

Phonon coordinates can be introduced in all three interactions by using the following relation between the local volume strain and the field of lattice displacements $\mathbf{u}(i)$:

$$\epsilon_\Omega(i) = \nabla\cdot\mathbf{u}(i) . \tag{32}$$

The latter are expressed by phonon operators:

$$\mathbf{u}(i) = \sum_{\mathbf{q}} \left(\frac{1}{2\omega_{\mathbf{q}} MN}\right)^{1/2} \mathbf{e}(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{x}_i} (a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger) . \tag{33}$$

Here we have assumed, for simplicity, a monoatomic lattice with ionic masses M and have suppressed the polarization indices. The quantities $\mathbf{e}(\mathbf{q})$ are the phonon eigen- vectors. From (32) we then obtain

$$\epsilon_\Omega(i) = \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \gamma(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{x}_i} \phi_{\mathbf{q}} \tag{34}$$

with

$$\gamma(\mathbf{q}) = i(2\omega_{\mathbf{q}} M)^{-1/2} \mathbf{q}\cdot\mathbf{e}(\mathbf{q}) \tag{35}$$

and

$$\phi_{\mathbf{q}} = a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger . \tag{36}$$

Finally we may summarize all three types of interactions as

$$H_{\rm int} = \sum_{\mathbf{q}\nu} \gamma(\mathbf{q}) g_\nu B_{-\mathbf{q}}^{(\nu)} \phi_{\mathbf{q}} \tag{37}$$

with

$$B_{\mathbf{q}}^{(1)} = \frac{1}{\sqrt{N}} \sum_i e^{-i\mathbf{q}\cdot\mathbf{x}_i} (rA_i + A\delta r_i) = rA_{\mathbf{q}} + A\delta r_{\mathbf{q}} , \tag{38}$$

$$B_{\mathbf{q}}^{(2)} = \frac{1}{\sqrt{N}} \sum_{i\alpha} e^{-i\mathbf{q}\cdot\mathbf{x}_i} f_{i\alpha}^\dagger f_{i\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\alpha} f_{\mathbf{k}\alpha}^\dagger f_{\mathbf{k}+\mathbf{q}\alpha} , \tag{39}$$

$$B_{\mathbf{q}}^{(3)} = \frac{1}{\sqrt{N}} \sum_{i\alpha} e^{-i\mathbf{q}\cdot\mathbf{x}_i} c_{i\alpha}^\dagger c_{i\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}+\mathbf{q}\alpha} . \tag{40}$$

IV. CALCULATION OF THE PHONON SELF-ENERGY

Let us define the phonon Green's function by

$$D(\mathbf{q},\tau) = -\langle \mathcal{T}\phi_{\mathbf{q}}(\tau)\phi_{-\mathbf{q}}\rangle \tag{41}$$

and its Fourier transform ($\omega_s = 2\pi sT$) as

$$D(\mathbf{q}, i\omega_s) = \int_0^\beta d\tau D(\mathbf{q},\tau) e^{i\omega_s\tau} . \tag{42}$$

Then the phonon self-energy may be defined by the Dyson equation

$$D^{-1}(\mathbf{q},z) = D_0^{-1}(\mathbf{q},z) - \Sigma(\mathbf{q},z) \ , \tag{43}$$

where

$$D_0^{-1}(\mathbf{q},z) = (z^2 - \omega_{\mathbf{q}}^2)/2\omega_{\mathbf{q}} \tag{44}$$

is the phonon Green's function in the absence of electron-phonon interaction. In lowest order in the electron-phonon interaction we obtain for the (irreducible) phonon self-energy

$$\Sigma(\mathbf{q},z) = \sum_{\nu\nu'} |\gamma(\mathbf{q})|^2 g_\nu g_{\nu'} \langle\langle B_{\mathbf{q}}^{(\nu)} | B_{-\mathbf{q}}^{(\nu')} \rangle\rangle_z \ . \tag{45}$$

Here the electronic Green's functions on the right-hand side (rhs) of (45) have to be calculated with the full electronic interaction but further electron-phonon interaction can be neglected.

The most interesting contribution to the phonon self-energy comes from the hybridization interaction $H_{\rm int}^{(1)}$. Here we have to calculate the Green's function $\langle\langle B_{\mathbf{q}}^{(1)} | B_{-\mathbf{q}}^{(1)} \rangle\rangle_z$ of the variable $B_{\mathbf{q}}^{(1)}$ given by (38), which contains both electronic particle-hole excitations and fluctuations in the mean-field parameter r. Within the mean-field approach this Green's function can be evaluated with help of the following considerations (for the moment let us neglect the frequency dependence): we may regard $\langle\langle B_{\mathbf{q}}^{(1)} | B_{-\mathbf{q}}^{(1)} \rangle\rangle$ as the response of the variable $B_{\mathbf{q}}^{(1)}$ on a perturbation coupling to $B_{-\mathbf{q}}^{(1)}$, which in this case is the field $\delta V_{\mathbf{q}}$. Hence we have to calculate $\delta\langle B_{\mathbf{q}}^{(1)} \rangle$ in the presence of a perturbation $\delta V_{\mathbf{q}}$, and this can be done with help of the methods developed in Sec. II. From $\delta\langle B_{\mathbf{q}}^{(1)} \rangle = r\delta\langle A_{\mathbf{q}} \rangle + A\delta r_{\mathbf{q}}$, and using the results (17) and (24) we obtain

$$\begin{aligned} \langle\langle B_{\mathbf{q}}^{(1)} | B_{-\mathbf{q}}^{(1)} \rangle\rangle = {} & r^2 (\Pi(\mathbf{q}) K(\mathbf{q}) \Pi(\mathbf{q}))_{11} + r^2 (\Pi(\mathbf{q}))_{11} \\ & + \frac{rA}{V} (\Pi(\mathbf{q}) K(\mathbf{q}) + K(\mathbf{q}) \Pi(\mathbf{q}))_{11} \\ & + \left(\frac{A}{V}\right)^2 (K(\mathbf{q}))_{11} \ . \end{aligned} \tag{46}$$

Note that this result, which will be discussed further below, can also be obtained in a more direct way with help of the Kondo-boson formalism in the functional-integral approach[5] by evaluating

$$\langle\langle r\delta A_{\mathbf{q}} + A\delta r_{\mathbf{q}} | r\delta A_{-\mathbf{q}} + A\delta r_{-\mathbf{q}} \rangle\rangle = r^2 \langle\langle \delta A_{\mathbf{q}} | \delta A_{-\mathbf{q}} \rangle\rangle + rA(\langle\langle \delta A_{\mathbf{q}} | \delta r_{-\mathbf{q}} \rangle\rangle + \langle\langle \delta r_{\mathbf{q}} | \delta A_{-\mathbf{q}} \rangle\rangle) + A^2 \langle\langle \delta r_{\mathbf{q}} | \delta r_{-\mathbf{q}} \rangle\rangle \ . \tag{47}$$

The different terms in (47) correspond to the terms appearing in (46) in the order. In particular, in the expression $\langle\langle \delta A_{\mathbf{q}} | \delta A_{-\mathbf{q}} \rangle\rangle = (\Pi + \Pi K \Pi)_{11}$ the second term $\Pi K \Pi$ contains the quasiparticle interaction mediated by the Kondo-boson propagator.

The result of (47) can be simplified further by using (20) as $\Pi(\mathbf{q}) = K_0^{-1}(\mathbf{q}) - K^{-1}(\mathbf{q})$ and $A = -2r\Lambda/V^2$. Then all the "bare" correlation functions $\Pi(\mathbf{q})$ can be eliminated in favor of the Kondo-boson propagator. The result can be written as

$$\langle\langle B_{\mathbf{q}}^{(1)} | B_{-\mathbf{q}}^{(1)} \rangle\rangle = (M^T(\mathbf{q}) K(\mathbf{q}) M(\mathbf{q}))_{11} + 6\frac{\Lambda r^2}{V^2} \ , \tag{48}$$

where the 2×3 matrix $M(\mathbf{q})$ is defined in (27). Note that in (48) only the first column of the matrix M enters, which is independent of $\mathbf{q}$. Therefore, this contribution to the phonon self-energy can be expressed completely by the Kondo-boson propagator.

So far we have considered only static perturbations. If we assume that the mean-field equations [(7) and (8)] also hold in the presence of time-dependent perturbations, then we arrive at

$$\langle\langle B_{\mathbf{q}}^{(1)} | B_{-\mathbf{q}}^{(1)} \rangle\rangle = (M^T(\mathbf{q},z) K(\mathbf{q},z) M(\mathbf{q},z))_{11} + 6\frac{\Lambda r^2}{V^2} \ , \tag{49}$$

where in the Kondo-boson propagator (20) and in the matrix M defined in (27) the electronic particle-hole propagators are replaced by the corresponding frequency dependent quantities. In the static limit ($z = 0$) and for $\mathbf{q} = 0$ the largest contribution comes from the component $K(0,0)_{11} = -[8N(0)]^{-1}$ (see the Appendix). From (47) we then obtain

$$\langle\langle B_0^{(1)} | B_0^{(1)} \rangle\rangle = -\tilde{\eta}^2 T_K/V^2 + 3\tilde{\eta} T_K/V^2 \ , \tag{50}$$

where $\tilde{\eta} = \Lambda/N(0)V^2$. Using the explicit dependence of the Kondo temperature T_K on the hybridization V given by (14) the rhs of (50) can also be written as $-(\partial^2 T_K/\partial V^2)$ plus terms of $O(T_K^2)$. Note that the quantity $\tilde{\eta}$ is related to the electronic Grüneisen parameter $\eta = -(\partial T_K/\partial \epsilon_\Omega)/T_K$ by $\eta = -\tilde{\eta}(\partial V/\partial \epsilon_\Omega)/V$. This will be used later, when we discuss the elastic properties.

In a similar manner also the other electronic Green's functions entering the phonon self-energy can be evaluated. For the Green's function of the conduction electron density $\langle\langle B_{\mathbf{q}}^{(3)} | B_{-\mathbf{q}}^{(3)} \rangle\rangle = \langle\langle n_{\mathbf{q}}^c | n_{-\mathbf{q}}^c \rangle\rangle$ we obtain

$$\begin{aligned} \langle\langle B_{\mathbf{q}}^{(3)} | B_{-\mathbf{q}}^{(3)} \rangle\rangle &= \Pi_{33}(\mathbf{q},z) + (\bar{\Pi}(\mathbf{q},z) K(\mathbf{q},z) \bar{\Pi}(\mathbf{q},z))_{33} \\ &= \Pi_{33}(\mathbf{q},z) + (M^T(\mathbf{q},z) K(\mathbf{q},z) M(\mathbf{q},z))_{33} \simeq -2N(0)[1 + O(T_K/\mu)] \end{aligned} \tag{51}$$

for $\mathbf{q} = 0$, $z = 0$. This is the other important contribution to the phonon self-energy and the electronic compressibility. The other contributions are

$$\langle\langle B_{\mathbf{q}}^{(2)} | B_{-\mathbf{q}}^{(2)} \rangle\rangle_z = (M^T(\mathbf{q},z)K(\mathbf{q},z)M(\mathbf{q},z))_{22} \simeq -T_K/[2N(0)V^2]^2 , \quad (52)$$

$$\langle\langle B_{\mathbf{q}}^{(1)} | B_{-\mathbf{q}}^{(2)} \rangle\rangle_z = (M^T(\mathbf{q},z)K(\mathbf{q},z)M(\mathbf{q},z))_{12} \simeq -\tilde{\eta}T_K/[2N(0)V^3] , \quad (53)$$

$$\langle\langle B_{\mathbf{q}}^{(1)} | B_{-\mathbf{q}}^{(3)} \rangle\rangle_z = (M^T(\mathbf{q},z)K(\mathbf{q},z)M(\mathbf{q},z))_{13} \simeq \tilde{\eta}T_K/(V\mu) , \quad (54)$$

$$\langle\langle B_{\mathbf{q}}^{(2)} | B_{-\mathbf{q}}^{(3)} \rangle\rangle_z = (M^T(\mathbf{q},z)K(\mathbf{q},z)M(\mathbf{q},z))_{23} \simeq T_K/[2N(0)V^2\mu] . \quad (55)$$

These results for the phonon self-energy can be expressed graphically by the diagrams shown in Fig. 1. Here a wavy and a double wavy line represent the unrenormalized and renormalized phonon propagator. The dashed and double dashed lines denote the bare quasiparticle interaction K_0 and the Kondo-boson propagator $K(\mathbf{q},z)$. The bubbles are electronic particle-hole propagators $\Pi(\mathbf{q},z)$. The dots denote the electron-phonon interactions g_ν. Note that the Kondo bosons couple to the phonons directly only for the coupling g_1.

A. Elastic constants

In the following we want to discuss in more detail the influence of the electron-phonon interaction on the elastic properties and the phonon damping. For small electron-phonon interaction one obtains for the renormalized (longitudinal) phonon frequency

$$\bar{\omega}_{\mathbf{q}} = \omega_{\mathbf{q}} + \Sigma'(\mathbf{q},\omega_{\mathbf{q}}) . \quad (56)$$

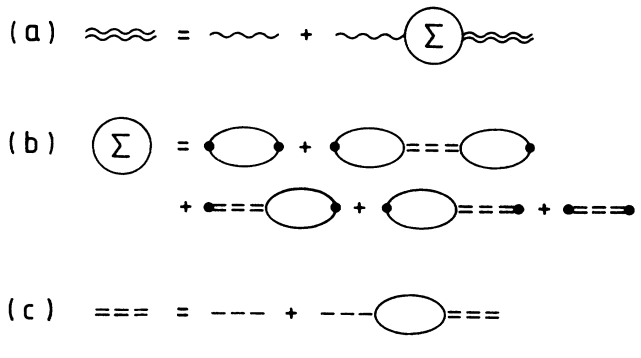

FIG. 1. Diagrammatic representation of (a) the phonon propagator (double wavy line), (b) the phonon self-energy Σ, and (c) the Kondo-boson propagator (double dashed line). The solid lines denote electronic quasiparticle Green's functions.

As $\Sigma'(\mathbf{q},\omega_{\mathbf{q}})$ is proportional to q for small $\mathbf{q}$, this leads to a renormalization of the (longitudinal) sound velocity v_s and the (longitudinal) elastic constant c. With $\omega_{\mathbf{q}} = v_s q$, $\bar{\omega}_{\mathbf{q}} = \bar{v}_s q$ and using the relation $c = v_s^2\rho$, where ρ is the mass density, one obtains

$$\left(\frac{\bar{v}_s}{v_s}\right) = \left(\frac{\bar{c}}{c}\right)^{1/2} = 1 + \Sigma'(\mathbf{q},0)/(v_s q) \quad (57)$$

for $q \to 0$. In a similar way the attenuation coefficient of longitudinal ultrasound is determined by the imaginary part of the phonon self-energy as

$$\alpha(\omega) = \Sigma''(\mathbf{q},\omega)/(2v_s) . \quad (58)$$

If we consider only the effect of the elastic strain on the hybridization we obtain from (50) and (57) in the present model:

$$\frac{\Delta c}{c} = -\frac{\eta^2 T_K}{M v_s^2} = -\frac{\eta^2 T_K}{c\Omega_c} , \quad (59)$$

where

$$\eta = -(\partial T_K/\partial\epsilon_\Omega) \simeq -\Lambda[N(0)V^3]^{-1}\partial V/\partial\epsilon_\Omega$$

is the electronic Grüneisen parameter and Ω_c the volume of a lattice cell.

$\Delta c/c$ has been estimated for several heavy-fermion systems from the temperature dependence of the elastic constants below T_K. Here in fact a depression of some of the elastic constants of a few percent has been observed.[1] In the analysis of the experimental data it is assumed that at high temperatures ($T \gg T_K$) the influence of the Kondo effect on the elastic constants vanishes, while the maximum depression is reached for $T \to 0$. Here one has to subtract in some cases first the much larger effect of the magnetoelastic coupling between the lattice and the quadrupolar moments of the rare-earth ions. Using the experimental data listed in Ref. 10 for $\Delta c/c$, the Kondo temperature T_K, and $c\Omega_c$ we obtain the following results for the Grüneisen parameter η: $CeAl_3$ ($\eta = 60$), $CeCu_6$ ($\eta = 15$), and $CeRu_2Si_2$ ($\eta = 40$). These values are a factor of 3–4 smaller than those reported in Ref. 10, and those obtained from thermodynamic relations between the elastic constants, specific heat, and the thermal expansion.[1,3] These relations can be derived from scaling relations for the free energy.[15,6] The origin of this discrepancy is not quite clear. There may be several reasons: the present one-band model may be too simple; we did not take into account the other contributions to the phonon self-energy, and we neglected higher-order derivatives $\partial g_\nu/\partial\epsilon_\Omega$ and a $\mathbf{k}$ dependence of this coupling.

We also have to consider that the elastic constant calculated here by the phonon self-energy corresponds to the isothermal elastic constant at constant chemical potential, while the measured quantity is more like the adiabatic elastic constant at constant particle number. Neglecting the difference between adiabatic and isothermal processes, which is not relevant at low temperatures, we

obtain for the difference between elastic constant Δc_μ at constant chemical potential and elastic constant Δc_{N_e} at constant electron number[6] N_e at $T = 0$:

$$\Delta c_{N_e} = \Delta c_\mu + \frac{1}{\Omega}\left(\frac{\partial^2 \mu}{\partial \epsilon_\Omega^2}\right)_{N_e}^2 \left(\frac{\partial N_e}{\partial \mu}\right)_{\epsilon_\Omega} . \tag{60}$$

If we assume that the influence of lattice strain on the conduction electrons can be approximated by $g_3 = \partial W/\partial \epsilon_\Omega = \partial \mu/\partial \epsilon_\Omega$ the contribution to the phonon self-energy (51) from the coupling of the phonons to the conduction electrons just cancels the additional term in (60). Therefore this effect cannot explain the discrepancy in the results for the Grüneisen parameters mentioned previously.

Let us note finally that the result (59) for the elastic constant can also be obtained directly from the defining relation

$$\Delta c_{N_e} = \frac{1}{\Omega}\left(\frac{\partial^2 E_e}{\partial \epsilon_\Omega^2}\right)_{N_e} , \tag{61}$$

where E_e is the electronic ground-state energy. Since in our simple model the reduction of the electronic ground-state energy due to the Kondo effect (per rare-earth ion) is given by[6]

$$(E_e - E_e^{(0)})/N = -T_K , \tag{62}$$

we obtain immediately the result of (59) for the electronic contribution to the elastic constant depending on the Kondo effect.

B. Numerical results for the phonon self-energy

We have also investigated the phonon self-energy at finite $\mathbf{q}$ and ω. If we take into account only the contribution from the strain dependence of the hybridization, we may write for the phonon self-energy

$$\frac{\Sigma(\mathbf{q},\omega)}{\omega_\mathbf{q}} = \frac{\eta^2 T_K}{2c\Omega_c}\left(\frac{v_s q}{\omega_\mathbf{q}}\right)^2 \frac{K_{11}(\mathbf{q},\omega)}{|K_{11}(0,0)|} . \tag{63}$$

Here we have split off the prefactor, which also appears in the elastic constant $\Delta c/c$ in (59). Let us note that $K_{11}(\mathbf{q},\omega)$ is directly proportional to the density correlation function of the f electrons:

$$\begin{aligned}\tilde{\Pi}_{22}(\mathbf{q},z) &= (\Pi(\mathbf{q},z) + \Pi(\mathbf{q},z)K(\mathbf{q},z)\Pi(\mathbf{q},z))_{22} \\ &= [2N(0)T_K\tilde{\eta}^2/V^2]K_{11}(\mathbf{q},z) .\end{aligned} \tag{64}$$

This means that the sound attenuation processes are produced primarily by density fluctuations of the heavy fermions.

Some numerical results for the phonon self-energy are shown in Fig. 2, where

$$X(\mathbf{q},\omega) = K_{11}(\mathbf{q},\omega)/|K_{11}(0,0)|$$

is plotted as function of ω for two different q values. These results, which are discussed in more detail in Ref. 9, were calculated with a dispersion $\varepsilon_\mathbf{k} = k^2/2m$ for the conduction electrons. Parameters are chosen such that $m^*/m = 200$ and $T_K/\varepsilon_F = 3 \times 10^{-3}$. In Fig. 2 for $qv_F^* \ll T_K$, structure is seen in the self-energy at the zero-sound frequency[8,9] $\omega = qv_F^*(m^*/3m)^{1/2}$ and at the interband transition energy $2\tilde{V}$. For $q = k_F$, where $qv_F^* > T_K$, the self-energy is real and constant up to $\omega = T_K$. For $\omega > T_K$ the real part falls off gradually to zero, while the imaginary part increases up to the charge excitation energy Λ. The results for $qv_F^* \ll T_K$ should not be taken too seriously because the finite lifetime of the quasiparticles, which is not yet taken into account, will damp the zero-sound mode. Furthermore, if we take into account the Coulomb interaction between conduction electrons, we will find an additional mode at $\omega = \sqrt{6}T_K$, which corresponds to plasma oscillations in the heavy-fermion band.[8] These effects, which are important primarily in the hydrodynamic limit for the ultrasonic attenuation, are discussed in more detail in Refs. 6, 8, 12, and 16. How the electron-phonon interaction influences the phonon spectrum in the energy range of in-

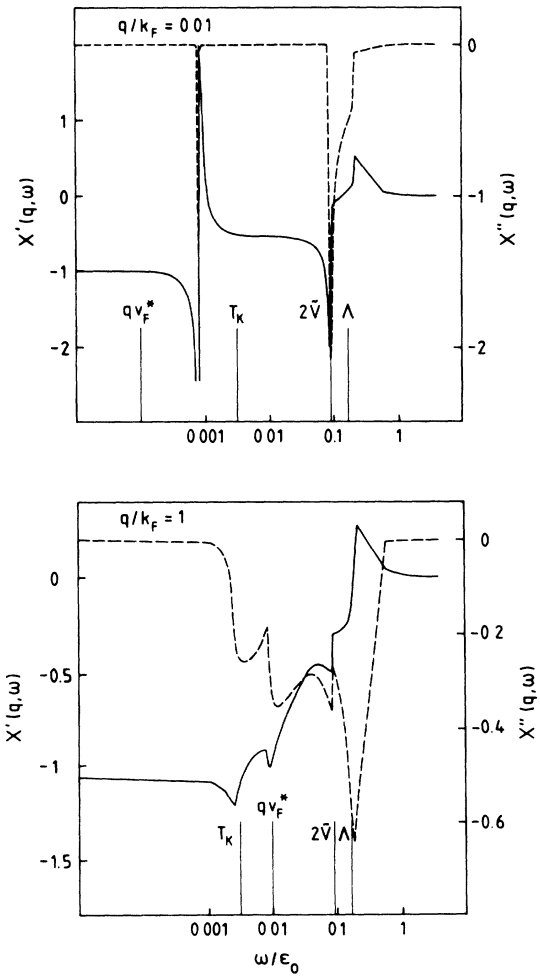

FIG. 2. Normalized Kondo-boson propagator $X(\mathbf{q},\omega) = K_{11}(\mathbf{q},\omega)/|K_{11}(0,0)|$ as function of frequency ω for two different values of the wave vector q. The solid curve shows the real part $X'(\mathbf{q},\omega)$ (left scale); the dashed curve shows the imaginary part $X''(\mathbf{q},\omega)$ (right scale).

elastic neutron scattering depends, of course, very much on the coupling constant $\eta^2 T_K/c\Omega_c$. If it is as small as obtained from the estimates of the elastic constants, the effect on the phonon spectrum would be negligible except, maybe, when one of the electronic density modes coincides with one of the lattice modes. If, however, we insert the values for the Grüneisen parameters as measured from the thermodynamic relations, the effect should be observable in the phonon spectrum.

V. EFFECTIVE ELECTRON-ELECTRON INTERACTION

The result of Sec. II, which describes the response of the mean-field parameters on the external perturbation, can also be used to derive an effective interaction between electrons mediated by phonons. This interaction is of particular importance as a possible mechanism for superconducting pairing.

Let us note first that within the mean-field approach the external perturbations couple either directly to the electronic densities (in the case of conduction-electron states) or indirectly via the mean-field parameters (in the case of f-electron states or mixed states). Consequently the lattice vibrations, which can be considered as a special type of external perturbation, couple either directly to the electronic densities or indirectly via a Kondo-boson propagator.

The different possible kinds of effective electron-electron interactions are shown in the diagrams of Figs. 3(a)–3(e) [in Fig. 3(a) the general form of the momentum and frequency dependence of the effective interaction is defined]. As in Fig. 1, a double dashed line denotes a Kondo-boson propagator, and a double wavy line denotes a phonon propagator (which contains Kondo bosons as self-energy corrections). The total interaction is obtained as the sum of the contributions 3(a)–3(e).

The interaction mediated by the Kondo-boson propagator that is shown in Fig. 3(a) is given by

$$I^a_{\rho\rho'}(\mathbf{q}, i\omega_s) = K_{\rho\rho'}(\mathbf{q}, i\omega_s) \ . \tag{65}$$

Here the indices $\rho = 1, 2$ refer to vertices with electronic operators of the form $f^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}+\mathbf{q}\alpha}$ or $c^\dagger_{\mathbf{k}\alpha} f_{\mathbf{k}+\mathbf{q}\alpha} (\rho = 1)$, and $f^\dagger_{\mathbf{k}\alpha} f_{\mathbf{k}+\mathbf{q}\alpha} (\rho = 2)$, respectively. At vertices with electronic operators of the form $c^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}+\mathbf{q}\alpha} (\rho = 3)$ the phonon couples directly; therefore, the effective interaction mediated by a phonon shown in Fig. 3(e) is given by

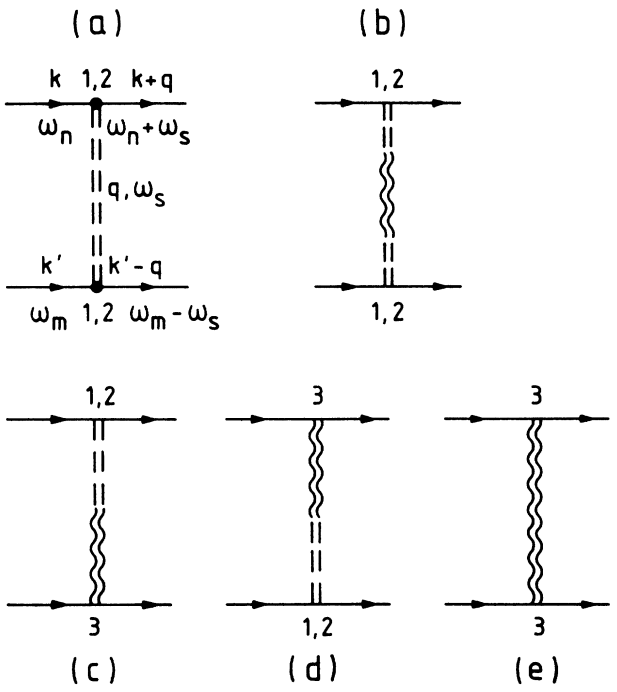

FIG. 3. Diagrammatic representation of the effective electron-electron interaction mediated by phonons (double wavy line) and Kondo bosons (double dashed line). The numbers at the vertices refer to a coupling to the mixed cf density ($\rho = 1$), the f electron density ($\rho = 2$), and the conduction electron density ($\rho = 3$).

$$I^e_{33}(\mathbf{q}, i\omega_s) = |\gamma(\mathbf{q})|^2 g_3 D(\mathbf{q}, i\omega_s) g_3 \ . \tag{66}$$

In order to derive the indirect interaction between electrons and phonons we note that as in (17) and (18) the electronic operators $c^\dagger_{\mathbf{k}\alpha} f_{\mathbf{k}+\mathbf{q}\alpha}$ and $f^\dagger_{\mathbf{k}\alpha} c_{\mathbf{k}+\mathbf{q}\alpha}$ couple to the combination $\delta\sigma_\mathbf{q} = r\delta V_\mathbf{q} + V\delta r_\mathbf{q}$, while $f^\dagger_{\mathbf{k}\alpha} f_{\mathbf{k}+\mathbf{q}\alpha}$ couples to $\delta\Lambda_\mathbf{q} + \delta Z_\mathbf{q}$. We can therefore use the compact result of (26) describing the response of these parameters on external perturbations. The coupling to the phonons is obtained if we replace the external perturbations $\delta V_\mathbf{q}$, etc., by the perturbations $\delta V_\mathbf{q} = \epsilon_\Omega(\mathbf{q}) g_1$, etc. For the interaction shown in Fig. 3(b) we then obtain (a summation over repeated indices is implied and $\rho, \rho' = 1, 2$)

$$I^b_{\rho\rho'}(\mathbf{q}, i\omega_s) = K_{\rho\beta}(\mathbf{q}, i\omega_s) M_{\beta\nu}(\mathbf{q}, i\omega_s) |\gamma(\mathbf{q})|^2 g_\nu D(\mathbf{q}, i\omega_s) g_{\nu'} M^T_{\nu'\beta'}(\mathbf{q}, i\omega_s) K_{\beta'\rho'}(\mathbf{q}, i\omega_s) \ . \tag{67}$$

Finally the interactions of the type shown in Figs. 3(c) and 3(d), where at one vertex the phonons couple directly to conduction electron states, are given by

$$I^c_{3\rho}(\mathbf{q}, i\omega_s) = |\gamma(\mathbf{q})|^2 g_3 D(\mathbf{q}, i\omega_s) g_\nu M^T_{\nu\beta}(\mathbf{q}, i\omega_s) K_{\beta\rho}(\mathbf{q}, i\omega_s) \ , \tag{68}$$

$$I^d_{\rho 3}(\mathbf{q}, i\omega_s) = K_{\rho\beta}(\mathbf{q}, i\omega_s) M_{\beta\nu}(\mathbf{q}, i\omega_s) |\gamma(\mathbf{q})|^2 g_\nu D(\mathbf{q}, i\omega_s) g_3 \ . \tag{69}$$

The most important contribution to the electron-electron interaction mediated by phonons are the terms in M that contain the large factor $\tilde{\eta} = \Lambda/N(0)V^2$ and result from fluctuations in the hybridization V induced by lattice vibrations. If we consider only this interaction, and furthermore approximate the Kondo-boson propagator by its static value at $\mathbf{q} = 0$, we may define an effective electron-phonon coupling $(KM)_{\rho 1}\partial V/\epsilon_\Omega$. Comparing these quantities with (26) we find

$$(KM)_{11}\partial V/\partial\epsilon_\Omega = \partial\sigma/\partial\epsilon_\Omega = \partial\tilde{V}/\partial\epsilon_\Omega \ , \tag{70}$$

$$(KM)_{21}\partial V/\partial\epsilon_\Omega = \partial\Lambda/\partial\epsilon_\Omega = \partial T_K/\partial\epsilon_\Omega \ . \tag{71}$$

Such an effective electron-phonon interaction has been introduced in Refs. 4 and 6. There it was assumed that the effective hybridization $\tilde{V}$ and the effective position of the f level $\tilde{\varepsilon} = \mu + T_K$ fluctuate under the influence of lattice vibrations. Now we see that such a description of the electron-phonon interaction corresponds to a special limit of the more general theory presented here. Taking the results shown in Fig. 2 for the Kondo-boson propagator $K_{11}(\mathbf{q},\omega)$ [the numerical results for $K_{21}(\mathbf{q},\omega)$ are quite similar] we see that such an approximation of using a constant effective electron-phonon interaction is not too bad for large q values as long as $\omega < T_K$. For larger frequencies this approximation fails, and the phonons mix with the dynamics of the Kondo bosons. For small q values with $qv_F^* \ll T_K$ we have to take into account the zero-sound mode and the low-frequency plasma oscillation of the Kondo boson.[8,15] In Ref. 6 the mean-field Hamiltonian was expanded up to second order in the lattice displacements, which was necessary to obtain the correct value for the electronic compressibility. This is no longer necessary in the present treatment because here quasiparticle interactions are included within our dynamic mean-field approach.

The electron-electron interaction can also be written in terms of quasiparticle operators corresponding to the two bands that are obtained if we diagonalize the mean-field Hamiltonian (6) in equilibrium. For the lower band crossing the Fermi surface the quasiparticle operator is given by [see the Appendix, (A3)]

$$d_{1\mathbf{k}\alpha} = u_{\mathbf{k}} f_{\mathbf{k}\alpha} - v_{\mathbf{k}} c_{\mathbf{k}\alpha} \tag{72}$$

and (near the Fermi surface) has primarily f character:

$$u_{\mathbf{k}}^2 \simeq 1, \quad v_{\mathbf{k}}^2 \simeq m/m^* \simeq N(0)/N^*(0) \ll 1 \ .$$

Here m^* and $N^*(0)$ are the effective mass and the density of states of the quasiparticles at the Fermi energy. The effective interaction mediated by Kondo bosons between quasiparticles at the Fermi surface is obtained, if we multiply I^a given by (65) with the appropriate weight factors $u_{\mathbf{k}}, v_{\mathbf{k}}$ with $k = k_F$. At $\mathbf{q} = 0$, $\omega_s = 0$ we find, using the results (A12) of the Appendix,

$$I_{\mathrm{qp}}^a = 4u_{\mathbf{k}}^2 v_{\mathbf{k}}^2 K_{11} - 4u_{\mathbf{k}}^3 v_{\mathbf{k}} K_{12} + u_{\mathbf{k}}^4 K_{22} \simeq 1/[2N^*(0)] \simeq T_K \ . \tag{73}$$

This interaction is repulsive, which is due to the second term on the rhs of (73). Note that the $(-)$ sign in (73) comes from the $(-)$ sign in (72).

If we define in a similar manner an effective quasiparticle-phonon interaction g_{qp} by

$$H_{\mathrm{int}}^{\mathrm{qp}} = \frac{1}{N}\sum_{\mathbf{q}\mathbf{k}\alpha} \epsilon_\Omega(\mathbf{q}) g_{\mathrm{qp}} d_{\mathbf{k}\alpha}^\dagger d_{\mathbf{k}+\mathbf{q}\alpha} \ , \tag{74}$$

then we find from (70) and (71)

$$g_{\mathrm{qp}} = -2u_{\mathbf{k}}v_{\mathbf{k}}\partial\tilde{V}/\partial\epsilon_\Omega + u_{\mathbf{k}}^2\partial T_K/\partial\epsilon_\Omega \simeq -\frac{4r\Lambda}{V^2}\frac{\partial V}{\partial\epsilon_\Omega}(-2u_{\mathbf{k}}v_{\mathbf{k}}K_{11} + u_{\mathbf{k}}^2 K_{21}) \ . \tag{75}$$

Using the results (A12) of the Appendix, the two contributions in the parentheses of (75) cancel in the leading order in T_K near the Fermi surface; therefore the total expression (74) is only of the order of T_K^2. This, however, is an artifact of the simple model for the conduction electrons. If we use a quadratic dispersion for the conduction-electron energies, we find a contribution that is proportional to T_K. The size of the effective quasiparticle-phonon interaction therefore depends very much on the details of the quasiparticle band structure.

If we compare the relative size of the different contributions I^{a-e} of the effective electron-electron interaction, in particular, if we compare the effective interaction I^a mediated by the Kondo boson and the one mediated indirectly by a phonon I^b, we find

$$|I_{11}^b/I_{11}^a| = O(\eta^2 T_K/c\Omega_c) \ , \tag{76}$$

which is small. From this one might conclude that the phonons can play only a minor role in a pairing interaction. This may be different if we consider multiple bands crossing the Fermi energy and take into account the anisotropy of the hybridization and pairing in real space at different lattice sites. Finally we would like to mention that a quasiparticle phonon interaction of similar nature has also been derived within the perturbation theory for heavy-fermion systems.[17]

VI. CONCLUSION

In this paper we have developed a systematic theory for the electron-phonon interaction in heavy-fermion systems based on the slave-boson mean-field approximation for the Anderson lattice. We have calculated the phonon self-energy and have derived the effective electron-electron interaction mediated by phonons. Our theory includes quasiparticle interactions in a manner equivalent to the random-phase approximation for the Kondo-boson interaction in the functional-integral approach. In our treatment the Kondo-boson propagators enter naturally as response of the mean-field parameters on a perturbation, which can be either an external perturbation or a perturbation induced by lattice displacements. It is interesting to note that phase fluctuations of the boson field, which are introduced in the functional-

integral approach, never occur within the present RPA-type treatment. Instead one obtains fluctuations of the two real mean-field parameters r, corresponding to the amplitude of the boson field, and the Lagrange parameter Λ introduced to fulfill the condition $\langle Q_i \rangle = 1$. These fluctuations do not appear as additional dynamical variables, but are tied to the perturbations induced by phonons or electronic density fluctuations.

We have estimated the strength of the electron-phonon interaction from the measured depression of the elastic constants at $T \ll T_K$ compared to their values above T_K. We derived electronic Grüneisen parameters that are large, but are a factor 3–4 smaller then those obtained from a thermodynamic relation between thermal expansion and elastic constant. The reason for this discrepancy is not clear; however, we have to keep in mind that our calculations are performed with a very simple model for the conduction electrons (one band with constant density of states). We also neglected all momentum and spin dependence of the hybridization, treating the f electrons like s electrons. Furthermore, we used the most simple form of the electron-phonon interaction: momentum-independent shifts of the energy levels and a change of the hybridization depending only on the volume strain.

We also calculated the effective electron-electron interaction mediated by Kondo bosons and by phonons. We found that in those interaction terms that contain the large Grüneisen parameter the phonons do not couple directly to the electrons but are coupled via a Kondo-boson propagator. This tells us that it is not possible to study the interaction with phonons while ignoring the quasiparticle interaction. Within the simple model we found that the attractive interaction mediated by phonons is weak compared to the repulsive interaction by Kondo bosons, at least for quasiparticle states that are close to the Fermi surface. Again this may be different if we consider nonlocal and directional effects in the electron-phonon interaction and consider interband transitions. The present theory serves as a good basis for treating such interaction processes with finite frequency and momentum transfer. It also allows us to study nonlinear elastic effects, and, finally, may be useful for the investigation of the electron-phonon interaction in high-T_c superconductors, if one starts from a quasiparticle description based on a slave-boson approximation.

ACKNOWLEDGMENTS

We would like to thank W. Brenig and P. Fulde for helpful discussions. This work was supported by a grant from the Deutsche Forschungsgemeinschaft.

APPENDIX

In this appendix we want to summarize some results obtained in the mean-field theory that are needed to calculate the phonon self-energy and the quasiparticle interaction. Most of these results can be found in the literature.[5,6] They are presented here in a unified notation. For the practical calculations in this appendix we use a single conduction band with a constant density of states, i.e., we replace $\sum_{\mathbf{k}}$ by $N(0)\int d\varepsilon$. We confine ourselves to a spin degeneracy of two for the conduction electrons and the f electrons and neglect all spin dependence and $\mathbf{k}$ dependence of the hybridization V.

Diagonalization of the mean-field Hamiltonian (6) in equilibrium leads to

$$H_{\mathrm{MF}} = \sum_{\mathbf{k}l\alpha} E_l(\mathbf{k}) d^{\dagger}_{l\mathbf{k}\alpha} d_{l\mathbf{k}\alpha} \ . \tag{A1}$$

One obtains two bands of quasiparticles [$l = (1,2) = (-,+)$] with energies

$$E_l(\mathbf{k}) = \tfrac{1}{2}(\varepsilon_{\mathbf{k}} + \tilde{\varepsilon}_f) \pm \tfrac{1}{2} W_{\mathbf{k}} \ , \tag{A2}$$

where $W_{\mathbf{k}} = [(\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f)^2 + 4\tilde{V}^2]^{1/2}$, $\tilde{V} = rV$, and $\tilde{\varepsilon}_f = \varepsilon_f + \Lambda = \mu + T_K$. The last relation is used as a definition of the Kondo temperature of the lattice. We assume that the Fermi energy is close to the top of the lower band ($l = 1$).

The fermion operators of f electrons and conduction electrons can be expressed by the quasiparticle operators as

$$\begin{aligned} f_{\mathbf{k}\alpha} &= u_{\mathbf{k}} d_{1\mathbf{k}\alpha} + v_{\mathbf{k}} d_{2\mathbf{k}\alpha} \\ c_{\mathbf{k}\alpha} &= -v_{\mathbf{k}} d_{1\mathbf{k}\alpha} + u_{\mathbf{k}} d_{2\mathbf{k}\alpha} \ , \end{aligned} \tag{A3}$$

where

$$\begin{aligned} u_{\mathbf{k}}^2 &= \frac{1}{2}\left(1 + \frac{\varepsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}}\right), \quad v_{\mathbf{k}}{}^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}} - \tilde{\varepsilon}_f}{W_{\mathbf{k}}}\right) , \\ u_{\mathbf{k}} v_{\mathbf{k}} &= \frac{\tilde{V}}{W_{\mathbf{k}}} \ . \end{aligned} \tag{A4}$$

Using the simple model for the conduction electrons mentioned earlier one obtains

$$T_K = \mu \exp\{-\Lambda/[2N(0)V^2]\} \tag{A5}$$

and the results (11)–(13). Furthermore, in this model the quasiparticle density of states at the Fermi energy $N^*(0)$ (for one spin direction) that determines the electronic specific heat and defines the effective mass $m^*/m = N^*(0)/N(0)$ of the heavy fermions is obtained as

$$\begin{aligned} N^*(0) &= N(0)/[dE_1(\mathbf{k})/d\varepsilon_{\mathbf{k}}]|_{k_F} = N(0)/v_{k_F}^2 \\ &\simeq N(0) + \tfrac{1}{2}\{1/T_K - 1/[2N(0)V^2] + 1/\mu\} \ . \end{aligned} \tag{A6}$$

For the calculation of the correlation functions we need the single-particle Green's functions. Using the notation

$$\langle\langle A|B\rangle\rangle_{i\omega_n} = -\int_0^{\beta} d\tau \, e^{i\omega_n \tau} \langle T A(\tau) B\rangle \ , \tag{A7}$$

we find, with $i\omega_n \to z$,

$$G_{ff}(\mathbf{k},z) = \langle\langle f_{\mathbf{k}\alpha}|f^{\dagger}_{\mathbf{k}\alpha}\rangle\rangle_z = u^2_{\mathbf{k}}/[z-E_1(\mathbf{k})] + v^2_{\mathbf{k}}/[z-E_2(\mathbf{k})] ,$$

$$G_{cc}(\mathbf{k},z) = \langle\langle c_{\mathbf{k}\alpha}|c^{\dagger}_{\mathbf{k}\alpha}\rangle\rangle_z = v^2_{\mathbf{k}}/[z-E_1(\mathbf{k})] + u^2_{\mathbf{k}}/[z-E_2(\mathbf{k})] , \tag{A8}$$

$$G_{fc}(\mathbf{k},z) = \langle\langle f_{\mathbf{k}\alpha}|c^{\dagger}_{\mathbf{k}\alpha}\rangle\rangle_z = -(\tilde{V}/W_{\mathbf{k}})/[z-E_1(\mathbf{k})] + (\tilde{V}/W_{\mathbf{k}})/[z-E_2(\mathbf{k})] ,$$

$$G_{cf}(\mathbf{k},z) = G_{fc}(\mathbf{k},z) .$$

We then obtain for the Green's function of the f density

$$\Pi_{22}(\mathbf{q},i\omega_s) = \langle\langle n^f_{\mathbf{q}}|n^f_{-\mathbf{q}}\rangle\rangle_{i\omega_s} = \frac{2}{N}\sum_{\mathbf{k}}\frac{1}{\beta}\sum_{\omega_n} G_{ff}(\mathbf{k},i\omega_n)G_{ff}(\mathbf{k}+\mathbf{q},i\omega_n+i\omega_s) . \tag{A9}$$

Using for this expression the abbreviated notation $\Pi_{22} = G_{ff}G_{ff}$ the different Green's functions $\Pi_{\rho\rho'}$ of the f density ($\rho = 2$), conduction-electron density ($\rho = 3$), and mixed density ($\rho = 1$) can be written as

$$\begin{aligned}
\Pi_{11} &= G_{cf}G_{cf} + G_{fc}G_{fc} + G_{ff}G_{cc} + G_{cc}G_{ff} ,\\
\Pi_{12} &= G_{ff}G_{cf} + G_{fc}G_{ff} ,\\
\Pi_{13} &= G_{cf}G_{cc} + G_{cc}G_{fc} ,\\
\Pi_{22} &= G_{ff}G_{ff} ,\\
\Pi_{23} &= G_{cf}G_{fc} ,\\
\Pi_{33} &= G_{cc}G_{cc} .
\end{aligned} \tag{A10}$$

With help of the simple model for the conduction electrons with a constant density of states these functions are easily evaluated at $\mathbf{q} = 0$, $i\omega_s = 0$. Writing down only the leading terms in an expansion in T_K we find

$$\begin{aligned}
\Pi_{11} &\simeq -2\Lambda/V^2 - 8N(0)\tilde{V}^2/\mu^2 \simeq -2\Lambda/V^2 - 4T_K/\mu^2 ,\\
\Pi_{12} &\simeq 4N(0)/\sqrt{2N(0)T_K} - T_K/[V^2\sqrt{2N(0)T_K}] - \sqrt{2N(0)T_K}/\mu \simeq 4[N(0)N^*(0)]^{1/2} ,\\
\Pi_{13} &\simeq 4N(0)\tilde{V}/\mu \simeq 2\sqrt{2N(0)T_K}/\mu \simeq 2[N(0)/N^*(0)]^{1/2}/\mu ,\\
\Pi_{22} &\simeq -1/T_K + 1/[2N(0)V^2] - 1/\mu \simeq -2N^*(0) ,\\
\Pi_{23} &\simeq -2N(0)\tilde{V}^2/\mu^2 \simeq -T_K/\mu^2 ,\\
\Pi_{33} &\simeq -2N(0) .
\end{aligned} \tag{A11}$$

In the same approximation the results for the matrix elements of the Kondo boson propagator are

$$\begin{aligned}
K_{11} &\simeq -1/[8N(0)] ,\\
K_{12} &\simeq -1/\{4[N(0)N^*(0)]^{1/2}\} ,\\
K_{22} &\simeq -T_K^2/[8N(0)\mu^2] .
\end{aligned} \tag{A12}$$

[1] M. Niksch, B. Lüthi, and K. Andres, Phys. Rev. B **22**, 5774 (1980); D. Weber, M. Yoshizawa, I. Kouroudis, B. Lüthi, and E. Walker, Europhys. Lett. **3**, 827 (1987); M. Yoshizawa, B. Lüthi, and K. D. Schotte, Z. Phys. B **64**, 169 (1986).

[2] I. Kouroudis, D. Weber, M. Yoshizawa, B. Lüthi, L. Puech, P. Haen, J. Flouquet, G. Bruls, U. Welp, J. J. M. Franse, A. Menovsky, E. Bucher, and J. Hufnagel, Phys. Rev. Lett. **58**, 820 (1987); D. Weber, I. Kouroudis, B. Lüthi, G. Bruls, M. Yoshizawa, P. Haen, J. Flouquet, E. Bucher, and J. Hufnagel, J. Magn. Magn. Mater. **76&77**, 315 (1988); T. Goto, T. Suzuki, Y. Ohe, T. Fujimura, and A. Tamaki, J. Magn. Magn. Mater. **76&77**, 305 (1988).

[3] R. Takke, M. Niksch, W. Assmus, B. Lüthi, R. Pott, R. Schefzyk, and D. K. Wohlleben, Z. Phys. B **44**, 33 (1981); B. Lüthi, J. Magn. Magn. Mater. **52**, 70 (1985).

[4] H. Razafimandimby, P. Fulde, and J. Keller, Z. Phys. B **54**, 111 (1984).

[5] For a review and introduction to the mean-field approach and the Kondo-boson formalism see P. Coleman, Phys. Rev. B **35**, 5072 (1987).

[6] For a review of the theory of heavy-fermion systems see P. Fulde, J. Keller, and G. Zwicknagl, Solid State Phys. **41**, 1 (1988).

[7] Z. Tesanovic and O. T. Valls, Phys. Rev. B **34**, 1918 (1986); A. J. Millis and P.A. Lee, *ibid.* **35**, 3394 (1987); A. Auerbach and K. Levin, Phys. Rev. Lett. **57**, 877 (1986); A. Auerbach, Ju H. Kim, K. Levin, and M. R. Norman, *ibid.* **60**, 623 (1988).

[8] A. J. Millis, M. Lavagna, and P. A. Lee, Phys. Rev. B **36**, 864 (1987).

[9] Th. Höhn and J. Keller, J. Magn. Magn. Mater. **76&77**, 343 (1988).

[10] P. Thalmeier, J. Phys. C **20**, 4449 (1987).

[11] N. Grewe, Z. Phys. B **67**, 323 (1987); H. Keiter, J. Magn. Magn. Mater. **76&77**, 65 (1988); C.-I. Kim, Y. Kuramoto, and T. Kasuya, Solid State Commun. **62**, 627 (1987).

[12] K. W. Becker and P. Fulde, Z. Phys. B **65**, 313 (1987); **67**, 35 (1987).

[13] P. W. Anderson, Phys. Rev. **124**, 41 (1961).

[14] P. Entel, N. Grewe, M. Sietz, and K. Kowalski, Phys. Rev. Lett. **43**, 2002 (1979).

[15] P. Thalmeier and P. Fulde, Europhys. Lett. **1**, 367 (1986).

[16] W. Brenig and K. W. Becker, J. Magn. Magn. Mater. **76&77**, 252 (1988).

[17] N. Grewe, Z. Phys. B **56**, 111 (1984); N. Grewe, T. Pruschke, and H. Keiter, *ibid.* **71**, 75 (1988).