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The theory of far-infrared properties of heavy-fermion compounds

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Abstract. We investigate optical properties starting from the Anderson model using the slave-boson method in a mean field and random phase approximation (RPA) method. It is shown that the structure of the low-frequency optical spectrum persists up to a temperature which is higher than the Kondo temperature.

1. Introduction

Recently far-infrared optical measurements on heavy-fermion compounds [1–4] have been performed.

The optical data have shown the existence of two plasma edges, one for light normal electrons at about a few eV, and one for heavy electrons at a few hundred meV. Moreover, anomalies at energies of the order a few meV were observed in the reflectivity and in the real parts of the optical conductivity spectra. These anomalies were associated with the observed optical transitions across a gap in the density of states and were identified as electronic transitions between strongly hybridized f bands, with the Fermi level in one of these bands. The gap was related to the hybridization gap which, as was verified in [5, 6], is at lower energies than the optical phonons. In addition, it was found that the characteristic shape of the low-frequency spectrum (e.g. $CeCu_6$ [2]) disappeared only at relatively high temperatures which were an order of magnitude larger than the Kondo temperature.

In this paper we shall discuss the existence of an energy gap at the same temperature as that at which quasiclassical thermodynamics is observed. We shall start from the Anderson lattice Hamiltonian and consider the case $U = \infty$ using the slave-boson approach [7] in the mean field. This procedure leads to two hybridizing bands. We obtain and discuss an expression for the complex dielectric constant (including interband terms), applicable to a metal. We have considered phenomenological damping so that we obtain the proper RPA results when the relaxation times tend to infinity [8].

2. Model and method

We start from the Anderson lattice Hamiltonian

$$H = \sum_k \sum_{m=1}^{N} \varepsilon_{km} c_{km}^{+} c_{km} + \sum_i \sum_{m=1}^{N} E_{0m} f_{im}^{+} f_{im}$$

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$$+\sum_i \sum_k^N \sum_{m=1} (V_{km} e^{ik\cdot R_i} c_{km}^+ f_{im} + \text{HC}) + U \sum_i \sum_{m\neq m'}^N n_{im} n_{im'}. \tag{1}$$

Here ε_{km} are the band energies for the hybridizing conduction electrons. E_{0m} is the bare f electron energy—it is assumed to be independent of m, V_{km} is the hybridization term and U is the on-site Coulomb repulsion. The large local Coulomb repulsion can be eliminated by introducing the slave-boson technique in which the f electron occupation n_{if} is restricted to be less than or equal to one (for cerium systems) by including the following constraint in the Lagrangian $n_{if} + b_i^+ b_i = 1$, where b^+ (b) is the creation (annihilation) operator of the slave boson. The mean field approximation yields $\langle b_i^+ \rangle = \langle b_i \rangle = (1 - n_f)^{1/2}$. This leads to the following mean field Hamiltonian:

$$H_{mf} = \sum_{m=1,k}^N \varepsilon_k c_{km}^+ c_{km} + \sum_{m=1,i}^N \varepsilon_f f_{im}^+ f_{im} + \tilde{V} \sum_{m=1,k}^N (c_{km}^+ f_{km} + \text{HC}) + \text{constant} \tag{2}$$

where ε_f is the renormalized f energy and $\tilde{V} = V(1 - n_f)^{1/2}$ is the renormalized hybridization. The Hamiltonian (2) can be easily diagonalized to give two hybridized bands with quasiparticle energies

$$E_\pm(k) = \frac{1}{2}\left(\varepsilon_k + \varepsilon_f \pm \sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4\tilde{V}^2}\right).$$

As we shall discuss interband contributions to the optical conductivity we have to estimate the indirect gap E_g between the hybridization bands, the threshold E_t for interband transitions and the direct gap E_{dir}. E_t is assumed to result from the excitations of the quasiparticles at the Fermi surface to the higher quasiparticle band (E_+) (in the following we shall consider only direct transitions). $E_g = N\tilde{V}^2/[W(N-1)]$ (NW is the bandwidth of conduction electrons). At $T = 0$ K

$$E_g = \frac{N}{(N-1)} T_K$$

(T_K—the Kondo temperature at $T = 0$ K).

$E_t \approx \tilde{\varepsilon}_f + \tilde{V}^2/W$, where $\tilde{\varepsilon}_f$ is the renormalized 4f level measured relative to the Fermi energy μ. We have calculated E_g and E_t as a function of temperature (see figure 1). E_g is approximately equal to the Kondo temperature. The direct gap is defined as a minimum of the difference $\Delta E = [(\varepsilon_k - \varepsilon_f)^2 + 4\tilde{V}^2]^{1/2}$ between the higher and lower bands for the same value of ε_k. Thus $E_{\text{dir}} = 2V(1-n_f)^{1/2}$. ΔE changes from about 50 eV to $E_{\text{dir}} \approx 370$ meV (at $T = 0$ K) and $\approx$300 meV (at $T = 100$ K). In figure 2 ΔE is plotted in a narrow range of ε_k in order to see its temperature dependence more clearly.

The complex dielectric constant was derived using the a RPA procedure for the quasiparticle density correlation function, but with the introduction of collision terms by adding relaxation times both for intra- and interband transitions into the Liouville equation [8, 9].

As we shall not discuss the widths of the observed peaks in the optical spectra, all the relaxation times are assumed to be independent of frequency [4].

Therefore, the relaxation times describe only broadening effects and have been introduced so that the expression for the dielectric constant is simple, leads to proper limits of high and low frequencies, and reduces to the RPA result when the relaxation times tend to infinity. Then the dielectric constant $\varepsilon(\omega)$ consists of a free quasiparticle and interband contributions, and in the long-wavelength limit

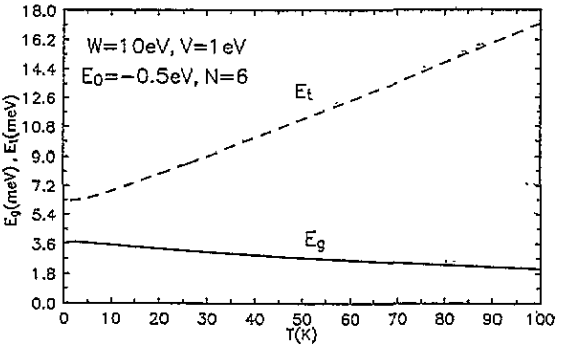

Figure 1. The hybridization gap E_g and the threshold energy E_t versus temperature.

$$\varepsilon(\omega) = 1 - \frac{4\pi e^2 n}{m^*}\frac{1}{\omega(\omega + \mathrm{i}/\tau_1)} - \left(\frac{e}{\pi}\right)^2 \frac{1}{m^*}\int \mathrm{d}^3k \sum_{l,l'=\pm}{}' F_{ll'}(k) f(E_l(k)) \times \frac{1}{(\omega + \mathrm{i}/\tau_{ll'})^2 - \omega_{ll'}^2}. \tag{3}$$

Here m^* is the quasiparticle mass in mean field, τ_1 is the relaxation time in the lower quasiparticle band (intraband relaxation time), n is the electron density $\tau_{ll'}$ is the interband relaxation time, $f(E)$ is the Fermi distribution function, $\omega_{ll'} = E_l - E_{l'}$, and $F_{ll'}$ is the oscillator strength as defined in [8]. The oscillator strengths obey the sum rule $\sum F_{ll'}(k) \approx n$ (n is the total number of electrons in the bands). The plasma frequency of the heavy fermion is obtained from the real part of the intraband term of equation (3) in the limit $\tau_1 \longrightarrow \infty$.

In this paper we concentrate on the problem of interband transitions; we analyse the optical conductivity spectrum at finite energy. Therefore, because there were only very small changes in the structure of the huge zero-energy peak for a wide range of the intraband relaxation time τ_1, we neglected any temperature dependence τ_1. However, we take into account the temperature dependence of the electron– phonon scattering rate. For temperatures much lower than the Debye temperature the interband relaxation time ($\tau_{ll'} = \tau_2$) has the following form:

$$1/\tau_2 = 1/\tau_0 + cT^3$$

where τ_0 is the temperature-independent relaxation time coming from electron–impurity scattering and c is a constant. The finite-frequency part of the optical conductivity is shown in figure 3.

In the mean field approximation we obtain the following relation between the plasma frequencies, ω_p^* and ω_p, for the quasiparticle and the conduction electrons respectively: $\omega_p/\omega_p^* = (1 + \tilde{V}^2/\tilde{\varepsilon}_f^2)^{1/2}$. We find that the value of ω_p/ω_p^* changes from about 10 at $T = 0$ K to about 35 at $T = 100$ K. This is qualitatively consistent with the reflectivity data (cf. [2]) which give $\omega_p/\omega_p^* \approx 20$ (for $CeCu_6$) and ≈ 15 (for UPt_3).

For metallic systems it is convenient to introduce the reflectivity, which can be expressed in terms of the complex dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + \mathrm{i}\varepsilon_2(\omega)$:

$$R(\omega) = \left|\frac{1 - \sqrt{\varepsilon(\omega)}}{1 + \sqrt{\varepsilon(\omega)}}\right|^2. \tag{4}$$

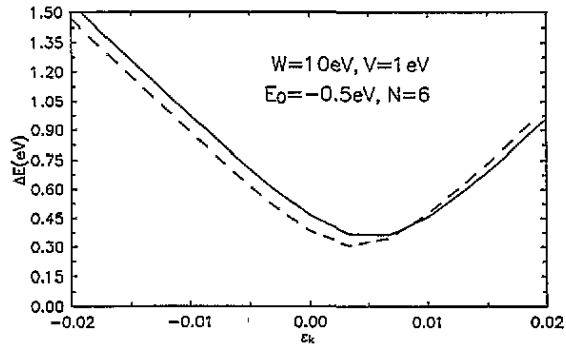

Figure 2. The interval ΔE between the higher and lower bands versus ε_k in units of the bandwidth NW. Solid line: $T = 0$ K; broken line: $T = 50$ K.

When $\omega\tau \ll 1$ we obtain the Hagen–Rubens law, $R(\omega) = 1 - (2\omega/\pi\sigma(\omega))^{1/2}$, where $\sigma(\omega)$ is the real part of the optical conductivity and Im $\varepsilon(\omega) = 4\pi \mathrm{Re}\,\sigma(\omega)/\omega$. In the limit $\omega \to 0$ we get $R(\omega) = 1$.

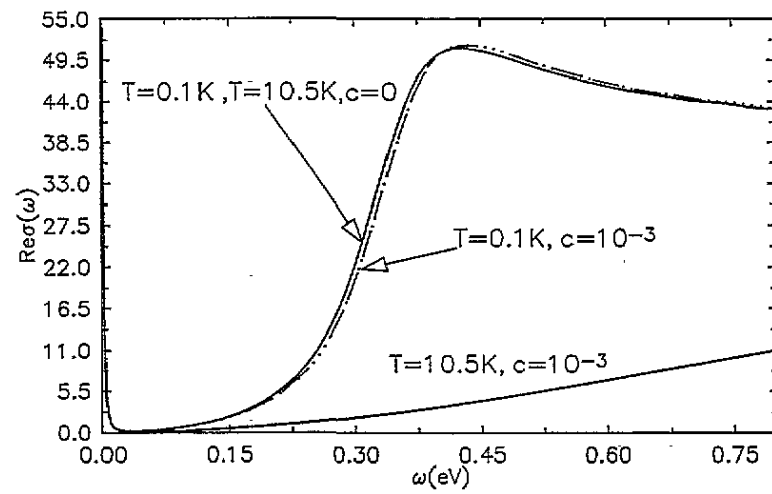

Figure 3. The optical conductivity at two temperatures. $1/\tau_0 = 0.08$ eV.

3. Final remarks

We can see in figuress 1 and 2 that both E_{dir} and E_g weakly depend on temperature and persist to a temperature higher than the Kondo temperature. This is consistent with the mean field results for other thermodynamical properties of heavy-fermion systems [10, 11]. Moreover, E_{dir} is always much greater than E_g and E_t (by approximately a factor of 50 times). The calculated values of E_g and E_t are in agreement with the observed peaks in the reflectivity (e.g. 4 meV for UPt_3 and 5 meV for $CeCu_6$ [2]). This can indicate that the indirect gap or interband threshold (for a metal) are responsible for the observed far-infrared optical absorption At very low temperatures the peak in the optical conductivity occurs only at the frequency corresponding the direct interband transitions. Therefore this peak can be related to the hybridization gap. This agrees with the infrared experimental data [2]. The

temperature dependence of the optical conductivity indicates that the structure of the peak strongly depends on the temperature dependence of the interband relaxation time τ_2. For the temperature-independent τ_2, i.e. for $c = 0$, the peak persists up to a temperature many times higher than the Kondo temperature. On the other hand, for finite c the peak may disappear, depending on the value of c (see figure 3). Thus the temperature dependence of τ_2 plays a crucial role in explaining of the disapppearance of a finite frequency peak such as that observed in the optical conductivity of $CeCu_6$ [12]. At the mean field level the excitations are not damped. In a theory which included fluctuations beyond mean field theory the relaxation times would not have to be 'put in by hand'. Electron–phonon interactions would also need to be included. The hope is that this procedure will not change a reasonably good description of the optical properties of the heavy-fermion systems obtained within the phenomenological approach to the damping processes. From the numerical calculations one can conclude that the interpretation of the low-energy dynamics in terms of our simple relaxation times leads to results in accordance with the position and height of the peak (at least qualitatively). However, an explanation for other very small structures observed in the experiments needs to include frequency and temperature dependences coming from Fermi-liquid behaviour due to electron–electron interactions.

Acknowledgments

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