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QUASIPARTICLE BAND STRUCTURE OF Ce-BASED HEAVY-FERMION COMPOUNDS

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Abstract. - We study the influence on the Fermi surface topology of many-body corrections beyond LDA. A Renormalized Band method is used to calculate the quasiparticle band structures of both CeAl₃ and Ce₃Al compounds. We discuss the conditions under which the LDA is expected to predict the correct Fermi surface.

Band structure effects play an important role in determining the low-energy excitations-quasiparticles in heavy-fermion materials. Coherence effects resulting from the periodicity of the lattice are observed in many transport properties. The most direct evidence, however, is given by the recent de Haas van Alphen experiments [1] where well-defined Fermi surfaces for the heavy quasiparticles are observed and determined. The effective masses are very high and of the same order of magnitude as the values inferred from specific heat data.

Realistic theoretical studies of the electronic structure of heavy-fermion systems in general, and of the Fermi surface in particular, were mainly based on the Local Density Approximation (LDA) which has been very successful in describing conventional weakly-correlated systems. There has been a general consensus that the LDA would not be able to predict the high effective quasiparticle masses which reflect the strong correlations among f-electrons at the U or rare earth (RE) sites. However the Fermi surface (FS) topology of UP₃ which can be derived from the fully-relativistic LDA band structure [2] turned out to be in excellent agreement with experiment.

The central question we focus on in the present paper is how the calculated (FS) topology is influenced by many-body corrections beyond LDA. We adopt the Renormalized Band (RB) method [3] to calculate the quasiparticle band structures of the classical Ce-based heavy-fermion compound CeAl₃ and its isostructural homologue Ce₃Al [4]. The results lead us to speculate under which conditions we can expect the LDA to predict the correct FS topology.

Before we present our results we wish to emphasize that the calculations should be considered as model studies. Firstly, a full RB calculation must take crystalline electric field (CEF) effects properly into account. The necessary experimental information, however, is not available for Ce₃Al. Since we do not want to rely on point charge models, and because we want to treat both Ce-Al systems on equal footing we neglect CEF effects in our calculations. A second point is more subtle: The compounds CeₙM (M = Al, Sn, In) are probably at the border line of the range of validity of the RB concept. The formalism only accounts for the heavy masses of the quasiparticles. Magnetic interactions between the Ce sites which seem to be rather strong in this new class of compounds are ignored here. Thirdly, for Ce₃Al, only transport and magnetic susceptibility measurements are available. We cannot extract the quasiparticle density of states at $E_F$ at 0 K from the data since the system undergoes an antiferromagnetic phase transition at low temperatures.

The RB formalism focuses on coherence effects introduced by the periodic arrangement of the U or RE ions. The low-energy excitations are calculated from an effective Hamiltonian for independent electrons moving in a periodic potential. The quasiparticle bands can therefore be determined by solving a band structure problem. The actual computations were performed by means of the Linearized Muffin Tin Orbital method adopting the Atomic Sphere Approximation [5]. The effective LDA potentials were determined from a fully relativistic approach. We refer to the results of this calculation as "LDA results".

The strong correlations between f-electrons at the Ce sites are accounted for by reducing the probability that a conduction electron can hop into an f-orbital. The reduction factor for the effective hybridization is related to the probability that the f-orbital is empty. It is treated as a phenomenological parameter which can be estimated from fits to the low-temperature specific heat coefficient. This step of reducing the effective hybridization is referred to as "renormalization". Technically, it is performed by modifying the potential function $P(E)$ [5] for the spin-orbit ground state multiplet $j = 5/2$ at the Ce site for which we adopt the linearized form

$$P_{j=5/2}^{Ce}(E) = (E - C) / T^*.$$  \(1\)

The two parameters, $C$ and $T^*$, are the center and the width of the renormalized f-states, respectively. We impose the additional condition that the Fermi energy is not changed upon renormalization, i.e.

$$E_F^{LDA} (C, T^*) = E_F^{LDA}.$$  \(2\)

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In order to satisfy condition (2) the energy difference between the center $C$ and $E_F$ must be proportional to $T^*$. The results of the present calculation are summarized in figure 1 (CeAl$_3$) and figure 2 (Ce$_3$Al). The FS topologies calculated within LDA (Fig. 1a) and RB method (Fig. 1c) agree remarkably well. The majority of states at $E_F$ are derived from the $j = 5/2$ ground state multiplet. The remaining differences between LDA and RB results arise from the fact that the spin-orbit splitting is comparable in magnitude to the LDA f-band width, whereas it is much larger than the characteristic energy $T^*$. As a result there are tails from the $j = 7/2$ multiplet in the LDA. These states, however, appear on separate parts of the Fermi surface which are missing in the RB calculation. This connection is illustrated in figure 1b which shows the Fermi surface obtained from LDA self-consistent potentials but with the $j = 7/2$ shifted away. Increasing thus the spin-orbit splitting does not dramatically alter the $j = 5/2$ bands. Their dispersion does not result from direct hybridization between f-states at different Ce sites but rather from the coupling to conduction states. The situation is different in Ce$_3$Al as can be seen from the band dispersions shown in figure 2. In this compound the Ce-Ce distance is much smaller than in CeAl$_3$. Within LDA there is appreciable hybridization between f-states at different Ce-sites and the resulting f-bands contain strong admixtures of $j = 7/2$ states in the vicinity of $E_F$. Shifting away the $7/2$-states and renormalizing the $j = 5/2$ band width leads to dramatic changes in the band structure. We expect similar difficulties for all densely packed heavy-fermion or mixed valence compounds.

Our investigations lead us to conjecture that LDA calculations will predict the correct FS topology provided the following two conditions are satisfied: (1) CEF splitting can be neglected i.e. the associated energy splitting is small compared to the characteristic energy $T^*$; (2) spin-orbit splitting is large compared to the LDA f-band width. Let us conclude by mentioning that these two criteria are satisfied in UPt$_3$ where the LDA has been shown to predict the correct FS topology [2]. An estimate for the characteristic energy is $T^* \geq 100$ K and no pronounced CEF splittings have been reported so far. In CeAl$_3$, however, condition (1) is not satisfied. The characteristic energy derived from fits to the specific heat data ($T^* \approx 5$ K) is much smaller than the CEF excitation energies (60 K and 88 K). The FS topologies derived from LDA and RB calculations have been done and will be published.