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Double-exchange mechanism in rare-earth compounds

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ABSTRACT

We show that double-exchange mechanism is responsible for ferromagnetism in low dimensional rare-earth compounds. We use the bosonized version of the one-dimensional Anderson lattice model in Toulouse limit to characterize the properties of the emerging ferromagnetic phase. We give a comprehensive description of the ferromagnetic ordering of the correlated electrons which appears at intermediate couplings and doping. The obtained ferromagnetic phase transitions have been identified to be an order–disorder transition of the quantum random transverse-field Ising type.

1. Introduction

It is well known that the competition between the Kondo effect and magnetism plays a very important role in anomalous rare-earth and also actinide compounds [1]. In fact, the 4*f*-electrons are well localized and many rare-earth compounds are either Kondo or mixed-valence ones. Indeed, many valence transitions are accompanied by substantial changes in the magnetic behaviour of the system. This is due to the fact that the localized f orbitals responsible for the mixed-valence behaviour are also responsible for the intrinsic magnetic moment of the ion. When the occupation of these orbitals changes, modification of the compound's magnetic properties is expected. Specifically, the valence anomalies may occur due to the superposition of different magnetic states of the mixed-valence ions. Furthermore, many of the elements (mostly Ce and Yb) that form mixed-valence compounds (e.g. $CeSn_3$, $CePd_3$, YbInAu) also form other compounds (e.g. $CeAl_2$, CeSb, YbCuAl) which are not in

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a mixed-valence state but instead display well-defined magnetic behaviour consistent with integer-valence states. A convincing model of rare earth compounds should be able to interpolate between these limits.

Although it is clearly a very important feature of the physics of rare-earth compounds, the large orbital degeneracy of the $4f$ states makes a theoretical description challenging. Years of theoretical investigation of actinide impurities have demonstrated that there exists general features of such systems that can be studied using generic models; more sophisticated treatments only become necessary when attempting to make contact with actual physical systems. One of the most popular of the "generic models" is the Anderson impurity model, which neglects all but the most gross features of the impurity orbital structure [2].

Because of its success in explaining the physics of the isolated rare-earth ion, the Anderson impurity model has been extended to the lattice limit by Varma and Yafet [3]. The so-called Anderson lattice model is defined

$$\mathcal{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \epsilon_f \sum_{j,\sigma} n^f_{j\sigma} + U \sum_{j} n^f_{j\uparrow} n^f_{j\downarrow} + V \sum_{j,\sigma} (f^{\dagger}_{j\sigma} c_{j\sigma} + \text{H.c.}). \tag{1}$$

The first term on the right-hand side (RHS) of Eq. (1) describes a non-interacting tight-binding conduction electron band with $t > 0$. The next two terms describe the atomic structure of the ions: it is assumed a simplified two-level structure with the f^1-level at ϵ_f and the f^2-level at $\epsilon_f + U$. The on-site Coulomb repulsion U can be large (i.e. $U \gg t$) due to the small radius of the $4f$ orbitals. The last line of Eq. (1) is the hybridization potential V between the f orbitals and the conduction electrons. The concentration n of electrons is constant, fixed at $n = (1/N) \sum_{j\sigma} (n^f_{j\sigma} + n^c_{j\sigma})$, $0 \leq n \leq 2$.

Since its introduction, the theoretical interest in the Anderson lattice has been very intense. The different theoretical and numerical approaches to the model are too numerous to summarize here [1]. Instead, we direct our attention to describing the two most important regimes of behaviour demonstrated by the Anderson lattice: the Kondo and the mixed valence regimes.

As is well known, in the limit when $\epsilon_f \ll e_F$, $\epsilon_f + U \gg e_F$ and $|\epsilon_f - e_F|$, $|\epsilon_f + U - e_F| \gg \Gamma$ (the effective width of the f-levels due to hybridization), the single-impurity Anderson model can be perturbatively mapped onto the Kondo impurity [4,5]. As the f^1-level lies far below the Fermi energy and the f^2-level lies far above, the ion is always singly-occupied, thus maintaining a spin-$\frac{1}{2}$ moment. Charge fluctuations on the f^1 state due to the hybridization may be treated as virtual processes, which lead in second-order perturbation theory to antiferromagnetic effective exchange interactions between the conduction electrons and the localized moment. In analogy to the charge screening cloud, the conduction electrons form a spin screening cloud around this local moment, leading to anomalous behaviour of the susceptibility.

A similar analysis can of course be carried out for the Anderson lattice, with a local moment regime being realized for the same parameter values as in the impurity model: the f^1 level lies far below the Fermi energy (located in the conduction band) while the f^2 level lies far above. As such, the f orbitals are singly occupied and maintain a magnetic moment. The effective Hamiltonian in this regime is the weak-coupling Kondo lattice model (KLM), where the f orbitals at each site are replaced by a localized spin-$\frac{1}{2}$ that interacts via antiferromagnetic exchange with the conduction electrons. The KLM has been extensively studied as a model of heavy fermion materials [1]. Magnetically-ordered phases have also been observed within the KLM: this indicates that similarly non-trivial ordering behaviour can be found in the Anderson lattice. The knowledge of the KLM's behaviour is particularly advanced in 1D, with both theoretical and numerical studies forming a complete picture of the phase diagram [4,6]. The 1D KLM will be discussed in more detail in Section 1.

The other easily-identifiable regime of the Anderson lattice is the mixed-valence regime: here the f^1-level lies close to the Fermi energy, acquiring a finite width due to the hybridization with the conduction electron band. The f^2-level lies far above the Fermi energy and so it may be regarded as (permanently) unoccupied. We hence see that a mixed-valence state involving the f^1 and f^0 configurations is realized. The mixed-valence regime of the Anderson lattice is very poorly understood. In contrast to the Kondo regime, there exists no simple effective model onto which the mixed-valence can be mapped. For $n = 2$ (i.e. half-filling) and $U = 0$, Eq. (1) describes an insulator with band gap of width $\sim \Gamma$. In the case where $U \ll \Gamma$, a perturbation series in U converges for the ground state at