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Transport properties of the Hubbard - Kondo lattice model

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In some materials with complex crystal structure the strong correlation effects can be associated with several atoms within the unit cell. Two such examples are the cuprate $Nd_{2-x}Ce_xCuO_4$, and the quadruple perovskites ruthenate $CaCu_3Ru_4O_{12}$ and iridate $CaCu_3Ir_4O_{12}$. In the latter case, for instance, Cu site hosts a $S = 1/2$ localized spin degree of freedom, whole the itinerant electrons experience strong Coulomb interaction on the Ru/Ir sites. These materials show heavy fermion behvior at low temperatures. An appropriate model for such compounds is a combination of (multiorbital) Hubbard model and the periodic Anderson model. To capture the essential physics, this model can be further simplified to a single-band Hubbard model with an additional spin degree of freedom on each site, exchange coupled to the conduction-band orbital, i.e., a "Hubbard - Kondo lattice model" or, alternatively, the "correlated Kondo lattice model", which can be considered as the minimal model for this class of compounds.

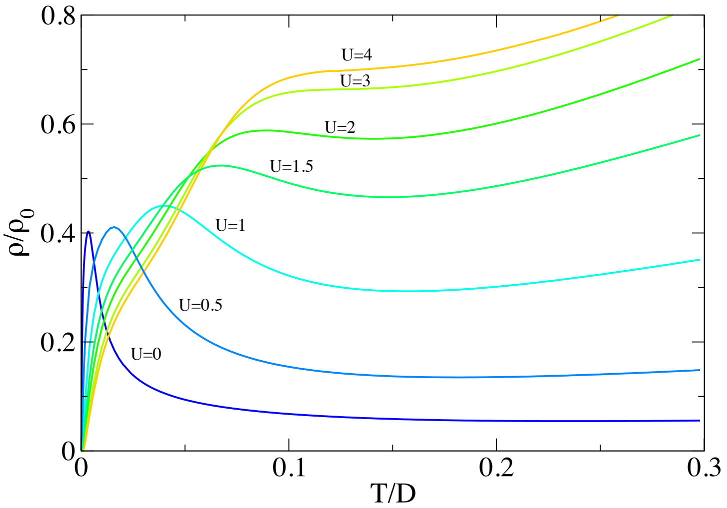

Figure 1: Resistivity of the "correlated Kondo lattice model" at fixed Kondo coupling constant $J = 0.3$ and conduction band filling $n = 0.8$, for a range of the Hubbard repulsion U. ρ_0 is the Mott-Ioffe-Regel resistivity, D is the half-bandwidth of the non-interacting conduction band.

In this work we study the transport properties of the correlated Kondo lattice model from the perspective of the dynamical mean field theory (DMFT). We focus on the paramagnetic phase and we discuss all temperature ranges, including the asymptotical high temperature limit. We provide some technical remarks on calculating the integrated transport quantities using the numerical renormalization group (NRG) technique to solve the DMFT self-consistency equations in the high temperature range where the method was previously believed to be wholly inapplicable [1, 2].

We consider how the transport properties of the correlated Kondo model evolve from the limits of pure Hubbard model and pure Kondo lattice model. In particular, we find strong enhancement of T_{max}, the temperature of the resistivity peak, as the Hubbard U is increased from zero in the limit of pure Kondo lattice model. The peak transforms into an inflection point at high U, and the temperature of the inflection point saturates in the large U limit. Starting from the limit of pure Hubbard model, a low-temperature resistivity peak is generated for small J. With increasing J, this peak broadens into a plateau shape. For large J, the resistivity curve has a complex form with two very clear cross-over scales. We find that at constant electron density n the resistivity curves from a family of universal curves parametrized by the product UJ: after rescaling the temperature axis by T_{max}, the resistivity curves for constant UJ overlap for low and intermediate temperatures. This implies that the resistivity maximum at $T = T_{\mathrm{max}}$ is a function of two parameters only, n and UJ.

For any values of U and J, we find that at high temperature the resistivity asymptotically increases linearly with T. The temperature dependence is due to the $1/T$ dependence of the charge susceptibility, while the diffusion constant saturates, similar to what had been found in the pure Hubbard model [1]. The same behavior is, surprisingly, also observed in the pure Kondo lattice model: the decreasing resistivity after $T = T_{\mathrm{max}}$ is eventually followed by an upturn to a T-linear high-temperature regime. This cross-over occurs on the temperature scale of $\approx \sqrt{JD}$. At temperatures in excess of the bandwidth the downward renormalization of the exchange coupling constant with increasing T is terminated, and the spins are not completely decoupled from the conduction band. Hence the resistivity at high temperatures is due to the conduction-band electrons scattering on thermally fluctuating spins.

The spectral function of the correlated KLM can be understood as the quasiparticle peak of the pure Hubbard model undergoing hybridization to form a pseudogap structure with the chemical potential lying in the subband of heavy fermions, similar to the low-energy behavior of the spectral function in the pure KLM.

The thermopower (Seebeck coefficient) of the hole-doped correlated KLM features two positive peaks: the one at lower temperature is associated with the heavy quasiparticles (and is related to the thermopower peak close to T_{max} in the pure KLM), while the one at higher temperature is associated with the charge degrees of freedom in the conduction band (and is related to the high-energy peak in the pure Hubbard band of the same origin).

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