Stuttgarter Physikalisches Kolloquium

Fachbereich Physik, Universität Stuttgart

Max-Planck-Institute für Festkörper- und Metallforschung

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Electron correlations in solids from the Dynamical Mean Field perspective and the dark matter of condensed matter physics

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Abstract

Materials with strong electronic correlations have long resisted *ab-initio* modeling due to their complexity arising from non-perturbative strength of the interaction. The Dynamical Mean Field Theory in combination with the Density Functional Theory has recently changed this position, and enabled detailed modeling of the electronic structure of complex heavy fermions, transition metal oxides and iron arsenides. Some of these materials exhibit subtle forms of self organization which are almost invisible to the available experimental tools, but which have dramatic physical consequences. One prominent example is provided by the actinide-based heavy fermion material URu_2Si_2. At high temperature, the U-5f electrons in URu_2Si_2 carry a very large entropy. This entropy is released at 17.5K via a second order phase transition to a state which remains shrouded in mystery, and which was termed a “hidden order“ state. The first principles calculation for URu_2Si_2 show that U-5f electrons undergo a Kondo effect below 70K, which is arrested at lower temperture by the crystal field splitting. At even lower temperatures, two broken symmetry states can be stabilized, characterized by a complex order parameter ψ. A real ψ describes the hidden order phase, and an imaginary ψ corresponds to the large moment antiferromagnetic phase, thus providing a unified picture of the two broken symmetry phases, which are realized in this material.