Project Title:

Analysis of f-electron superlattices

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Background:

Phenomena observed in f-electron materials are still at the focus of many research groups. This is so, because of the intriguing properties of these systems such as quantum criticality and unconventional superconductivity. Furthermore, recent progress in experimental techniques made it possible to build artificial f-electron superlattices, which consists of different f-electron materials. These artificial superlattices exhibit novel properties: The properties of the magnetic and superconducting phase can be easily tuned by changing the superlattice structure; the quantum critical behavior can be changed; novel two-dimensional superconductivity was observed.

Method:

Using inhomogeneous dynamical mean field theory, I have studied the magnetic properties of these f-electron systems. Dynamical mean field theory maps the system on a quantum impurity model, which has to be solved self-consistently. By mapping different atoms or layers on different impurity calculations, inhomogeneities like a superlattice structure can be taken into account.

Firstly, I focused directly on these novel f-electron superlattices. The advantage of my calculations is that I can take the superlattice structure of the system exactly into account. This is a big difference to other theoretical studies for these systems, where the superlattice structure was strongly approximated. Because the self-energies of different layers are independent from each other, the calculation can be very efficiently parallelized on the MPC-cluster of RICC. Thus, I could calculate the magnetic properties and the quantum critical behavior for large f-electron superlattices. Secondly, because this method is able to analyze large inhomogeneous structures, I also studied inhomogeneous spin- and charge-density waves in heavy fermion systems.

Results:

I have found that the magnetic transition temperature and the quantum critical point strongly depend on the superlattice structure. This is completely in accordance with the experimental observations. Decreasing the spacer layers between different f-electron layers increases the RKKY interaction and thus increases the magnetic transition temperature. I furthermore observed an unexpected dependence of the Kondo-temperature on the superlattice structure. This dependence is due to an interference of the Kondo effect occurring simultaneously in different f-electron layers. A similar effect has been recently found in NMR experiments for such superlattices. As mentioned above, I have used the same method to analyze spin-density waves in heavy fermion systems. I have shown the existence of a combination of spin- and charge-density waves in the two-dimensional Kondolattice model. I could distinguish four different phases in this model; two phases have been unknown until now. These phases show long-range spin-density waves, which combine antiferromagnetic and ferromagnetic correlations.

Future directions:

The results are currently prepared for publication. Furthermore, recent experiments suggest that the Rashba-interaction might become important at the interface between different f-electron materials in the superlattice. Therefore, I plan to include this kind of interaction in future calculations.

Fiscal Year 2014 List of Publications Resulting from the Use of RICC

[Oral presentation at an international symposium]

1. International workshop at the ISSP: “Recent Developments in the Kondo problem”: **Invited talk** “Explaining STM-measurements for impurities and heavy fermions via the Kondo proximity effect”, 10.01.2015
2. International conference “New Horizons of Strongly Correlated Physics” at the ISSP (Kashiwa): contributed talk “Spin density waves in heavy fermion systems”, 30.06.2014
3. International conference of Young Researchers on Advanced Materials: **Invited talk** “Dynamical mean field theory for layered f-electron systems”, 26.10.2014