CELOÚSTAVNÍ SEMINÁŘ
Ústavu fyziky materiálů AV ČR

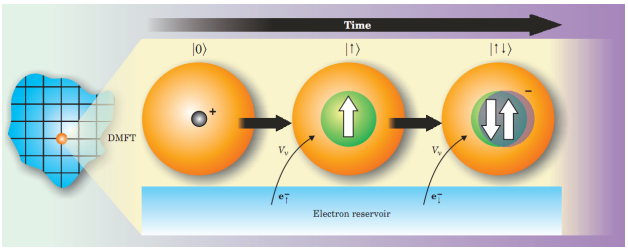
dne **1.3.2011** (úterý) v **10:00 h**
v přednáškovém sále (4. patro)
Ústavu fyziky materiálů AV ČR, Žižkova 22, Brno

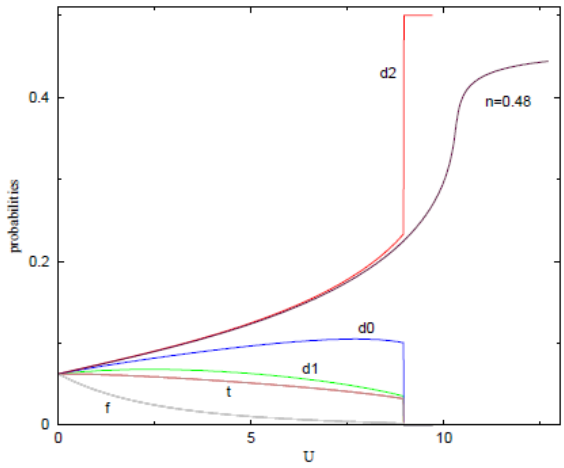
Prof. Jean-Pierre Julien
CNRS - Institut Néel, Grenoble, France

Electronic structure of strongly correlated electrons materials: I. Concepts and applications

Except for small molecules, it is impossible to solve many electron systems without imposing severe approximations. Generalization of Quantum Chemistry approaches usefull for molecules, like configuration interaction approaches (CI) or Coupled Clusters techniques, is difficult for solids. For materials with a kinetic energy greater than the Coulomb interaction, first principles calculations based on the density functional theory (DFT), within the local density approximation (LDA), give satisfying results to describe ground state properties. However, application of LDA to systems where the wave functions are more localized (*d* or *f*-states) such as transition metals oxides, heavy fermions, rare earths or actinides is more questionable and can even lead to unphysical results.

Using a density matrix approach to Gutzwiller method, I will present a formalism to treat multiband Tight-Binding-like Hamiltonians (i.e. with a LMTO basis or a Wannier basis) including local Coulomb interaction in a solid. Starting from the density matrix of the non-interacting state, a multi-configurational variational wave function is built. The probabilities of atomic configurations are the variational parameters. This method can be performed from ab-initio level and can be seen as an improvement beyond a standard mean field approach of the more popular LDA+U method in which the density-density correlations are treated. First application to plutonium will be presented with peculiar attention to the equilibrium volume, and investigations for other densities will be discussed.





Kontakt: Dr. Roman Gröger (tel. 532 290 448, e-mail: groger@ipm.cz)

CELOÚSTAVNÍ SEMINÁŘ
Ústavu fyziky materiálů AV ČR

dne **2.3.2011** (středa) v **10:00 h**
v přednáškovém sále (4. patro)
Ústavu fyziky materiálů AV ČR, Žižkova 22, Brno

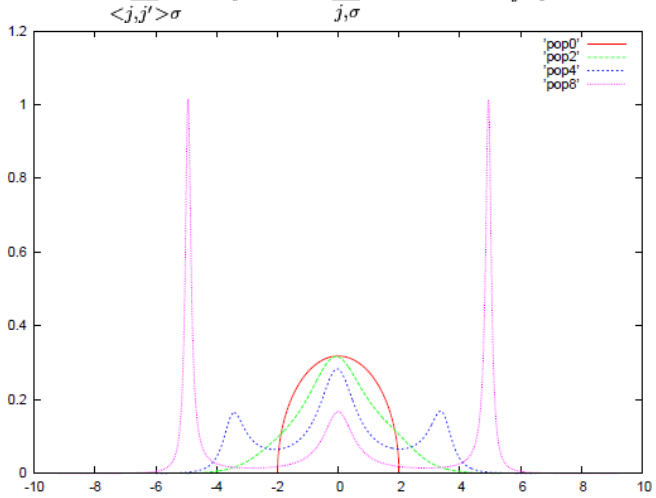
Prof. Jean-Pierre Julien
CNRS - Institut Néel, Grenoble, France

Electronic structure of strongly correlated electrons materials: II. New efficient solver of the Anderson impurity model

The Gutzwiller method being restricted to the low energy physics and missing the higher energy excitations (the so-called "Hubbard sub-bands) legitimates the seek for a method handling on an equal footing low and high energy excitations: this can be achieved by the Dynamical Mean Field Theory (DMFT).

In this talk, I will present a new efficient and accurate impurity solver for the single impurity Anderson model (SIAM), which is a central problem in the DMFT method. This solver is based on a non-perturbative recursion technique in a space of operators and involves expanding Green functions and self-energy as a continued fraction. The method has no special occupation number or temperature restrictions; the only approximation is the number of levels of the continued fraction retained in the expansion. We also show how this approach can be used as a new approach to the DMTF and illustrate this with the Hubbard model. The three lowest orders of recursion give the Hartree-Fock, Hubbard I, and Hubbard III approximations. A higher level of recursion is able to reproduce the expected 3-peak structure in the spectral function and Fermi liquid behavior.

$$H = \sum_{\sigma} \epsilon_f f_\sigma^\dagger f_\sigma + \sum_{<j,j'>\sigma} t_{jj'} c_{j\sigma}^\dagger c_{j'\sigma} + \sum_{j,\sigma} (V_j f_\sigma^\dagger c_{j\sigma} + V_j^* c_{j\sigma}^\dagger f_\sigma) + U f_\uparrow^\dagger f_\uparrow f_\downarrow^\dagger f_\downarrow$$



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