Local moment approach to multi-orbital single impurity Anderson model; application to dynamical mean-field theory

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Abstract

Using a local moment approach of Logan et al. we developed a solver for a multi-orbital single impurity Anderson model. The existence of the local moments is taken from the outset and their values are determined through variational principle by minimizing the corresponding ground state energy. The method is used to solve the dynamical mean-field equations for the multi-orbital Hubbard model. In particular, the Mott-Hubbard metal–insulator transition is addressed within this approach.

Key words: Lattice fermion models, Metal-insulator transitions, Local magnetic moment, Kondo effect

PACS: 71.10.Fd; 71.30.+h; 75.20.Hr

The problem of a magnetic impurity in a metallic host, i.e. the Kondo problem, plays a major role in many branches of modern condensed matter physics. This problem of coupling degenerate spin degrees of freedom to gapless fermionic excitations is essential in the dynamical mean–field theory (DMFT) of strongly correlated electron systems [1]. The DMFT is a self–consistent method, where in each iteration loop the Kondo problem is solved numerically. The application of the DMFT to investigate real systems, in particular with many orbitals, is difficult because of the necessity to solve the Kondo problem for arbitrary parameters. Numerically exact methods, like numerical renormalization group [2] or determinant quantum Monte Carlo [3] are very time (CPU) consuming, in particular when the number of orbitals is large. Reliable analytical methods are therefore needed. One of such methods, which recovers Luttinger property and Kondo exponential scale as well as Hubbard satellites has been recently invented by Logan et al. [4] and named a local moment approach (LMA). In this contribution we generalize this method to investigate multi-orbital systems at zero temperature. Within the DMFT framework supplemented with the LMA we analyze the problem of Mott–Hubbard metal–insulator transition (MIT) in orbitally degenerate and non–degenerate systems.

We start with the generalization of the LMA to solve the single impurity Anderson model (SIAM) with many orbital levels:

\[
H_{\text{SIAM}} = \sum_{\alpha,\sigma} (\epsilon_\alpha - U \sigma n_{\alpha,\sigma}) n_{\alpha,\sigma} + \sum_{\sigma,\sigma', \alpha \neq \beta} (U'_{\alpha\beta} - J \delta_{\sigma\sigma'}) n_{\alpha\sigma} n_{\beta\sigma'} + \sum_{k,\sigma,\alpha} V_{k\alpha} (d_{\alpha\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger d_{\alpha\sigma}) + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma},
\]

where the direct \(U\) and \(U'\) as well as exchange \(J\) interactions between electrons of spin \(\sigma\) and on orbitals \(\alpha\) or \(\beta\) are taken into account.

In the unrestricted Hartree–Fock approximation to the SIAM the local Green functions \(G_{\sigma}^{\alpha\beta}(\mu_\alpha, \mu_\beta; \omega)^{HF}\) depend explicitly on the local magnetic moments \(\mu_\alpha\) on each orbital. These local Green functions are used in the random phase approximation (RPA) to determine the polarization diagrams \(\Pi_{\sigma}^{\alpha\beta}(\mu_\alpha, \mu_\beta; \omega)\), cor-

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Preprint submitted to Elsevier Science 20 July 2018
responding to spin flip processes, and hence the self-
energies $\Sigma^\alpha_{\sigma}(\mu_\alpha, \mu_\beta; \omega)$. The Green functions calculated in this way depend now on the local moments $\mu_\alpha$. However, in a single impurity problem the spin-
rotational symmetry cannot be spontaneously broken.

To restore this symmetry within the approximate so-



eral orbital moments and $N_{\text{orb}}$ is the number of orbitals. In this method the existence of the local moments is assumed from the beginning.

The lengths of the local moments $|\mu_\alpha|$ and the num-
ber of particles on each orbital $n_\alpha$ are determined by minimizing the ground state energy function, i.e. $E_{\text{physical}} = \min(\mu_\alpha, n_\alpha) E(\mu_\alpha, n_\alpha)$. In this work we also adjust the Fermi energy of the electrons in the impu-

rity atom to have the proper total number of electrons.

This generalized LMA is used to solve multi-orbital

Hubbard model $H_{\text{Hubb}} = \sum_{ij} \sum_{\alpha,\sigma} t_{ij} \alpha \sigma d_{i\alpha \sigma}^\dagger d_{j\alpha \sigma} + H_{\text{local}}$, where the local part is a sum over all lattice site terms which are of the same form as the atomic part in the SIAM. This model is solved within the DMFT where the self-consistency condition relates the local matrix Green functions with the matrix of the self-
energies [3]. This condition simplifies for the Bethe lattice that is used in this contribution. The band width $W_\alpha = 2$ for each orbital $\alpha$ sets the energy units.

In Fig. 1 the spectral functions for two–orbital Hub-

bard model are shown for degenerate case $\epsilon_\alpha = \epsilon_B$ (upper panel) and for nondegenerate (asymmetric) case $|\epsilon_\alpha - \epsilon_B| = 0.3$ (lower panel). Also the cases with $(J = U/4)$ and without $(J = 0)$ Hund exchange coupling are compared. The inter-band interaction $U' = U - 2J$ is fixed preserving $SU(4)$ symmetry. In all cases the average number of electrons is fixed to $n_e = 2$ per lattice site.

In the first case $\epsilon_\alpha = \epsilon_B$ when $U$ is sufficiently large the correlation gap is opened and the system is a Mott insulator. At smaller $U$, when the system is on the metallic side, the Kondo–like peak is seen at $J = 0$ and is destroyed at $J > 0$. When the orbital degeneracy is removed, as in $|\epsilon_\alpha - \epsilon_B| = 0.3$ case, the system for a given $U$ is metallic on one of the orbitals, whereas on the other it is insulating. The number of electrons per site on each orbital level is no longer equal and the spectral functions on different orbitals begin to differ qualitatively. At larger $U$ the system is insulating in both orbitals. So we find an orbital selective Mott-Hubbard MIT in asymmetric case. Increasing further the difference $|\epsilon_\alpha - \epsilon_B|$ would lead to the appearance of the band insulator possessing a gap between bands.

Initially the orbital selective Mott-Hubbard MIT was found in a two-orbital symmetric case, where orbitals had the same energies but different bandwidths [5,6,7].

The present contribution extends this investigation on a case where this orbital degeneracy is removed. The crystal level splitting can be tuned in some extend by the axial pressure and thereby there is a practical oppor-
tunity to search experimentally for the orbital select-
ive MIT.

The generalized LMA to multi–orbital SIAM allows us to efficiently study the correlated electron systems within DMFT. In particular it is relatively easy to address the problems where the degeneracy of orbital levels is removed, and hence the Fermi energy has to be determined self–consistently in each iteration loop. Also the local moment approach is much more efficient in studying problems with more then two orbitals [8]. This regime is hardly accessible in numerically exact approaches.

This work is supported by Polish Committee of Sci-
entific Research through grant KBN-2 P03B 08 224. Partial support of the Sonderforschungsbereich 484 of the Deutsche Forschungsgemeinschaft (DFG) is also acknowledged.

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