

# Local moment approach to multi-orbital Anderson and Hubbard models

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## Abstract

The local moment approach (LMA) of Logan *et al.* and its modification is summarized here. 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 LMA is used to solve a multi-orbital single impurity Anderson model. The method is also applied 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  
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## 1. Introduction

The single impurity Anderson model (SIAM) is one of the most investigated models in condensed matter physics [1]. This model is regarded as a prototype to understand and describe: i) properties of metals with magnetic atoms [2], ii) current transport through quantum dots [3], iii) Mott-Hubbard metal-insulator transitions (MIT) within the dynamical mean-field theory (DMFT) [4–9], and iv) a crossover between weak and strong coupling limits and confinement phenomena. The SIAM consists of a term describing band electrons coupled by hybridization to a term corresponding to a single impurity where the local Coulomb interaction is taken into account [1]. In the featureless hybridization limit the SIAM is solved exactly within the Bethe ansatz or conformal field theory techniques so the ground state and the whole excitation spectrum as well as thermodynamics is exactly known [2]. Un-

fortunately, these methods cannot in practice provide dynamical quantities, for example one-particle spectral functions or dynamical susceptibilities, for all interesting energies. Also the (asymptotic) exact solvability is not possible for a general hybridization term.

For practical applications of the SIAM one has to rely on either a numerically exact or an analytical but approximate solution. Numerically exact methods, like the numerical renormalization group (NRG) [10] or the determinant quantum Monte Carlo (QMC) [6] are very time (CPU) consuming. In particular, the CPU is very long when the number of orbitals is large in the NRG case and when the temperature is low in the QMC case. Also to extract dynamical quantities is a rather tricky task. Reliable analytical methods are therefore needed. One of such methods, which recovers properly both weak and strong coupling limits, is a *local moment approach* (LMA) invented recently by Logan *et al.* [11].

The LMA is a perturbative method around an unrestricted Hartree-Fock solution with broken symmetry, i.e. with a non-zero local magnetic moment. The broken symmetry is restored at the end by taking the average of the solutions corresponding to different di-

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rections of the local magnetic moment [11].

In the present contribution we describe the LMA method and our implementation of it, which is different from the original one [11] by the way of how the value of the local moment is determined. Namely, we use the variational principle demanding that the ground state energy should be minimized by the physical value of the local moment. Such a procedure allows us to easily generalize the LMA for multi-orbital models as well as for finite temperatures and systems with disorder [12–15]. We also discuss the Luttinger-Ward generating functional for the LMA and claim that this method belongs to the class of conserving approximations. The application of LMA for studying the electron flow through quantum dots and the Mott-Hubbard MIT is addressed at the end of the contribution.

## 2. Local moment method in one orbital SIAM

The single impurity Anderson model is given by the Hamiltonian

$$H_{\text{SIAM}} = H_c + H_{\text{imp}} + H_{\text{hyb}}, \quad (1)$$

where the conduction electrons are described by

$$H_c = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \quad (2)$$

where  $\epsilon_{\mathbf{k}}$  is an energy (a dispersion relation) for an electron in a state  $\mathbf{k}$  and spin  $\sigma = \pm 1/2$ , the impurity electrons with the local Coulomb interaction  $U$  are represented by

$$H_{\text{imp}} = \sum_{\sigma} (\epsilon_d + U n_{d-\sigma}) n_{d\sigma}, \quad (3)$$

with  $n_{d\sigma} = d_{\sigma}^\dagger d_{\sigma}$ , and the hybridization between conduction and impurity electrons is

$$H_{\text{hyb}} = \sum_{\mathbf{k}, \sigma} \left( V_{\mathbf{k}} d_{\sigma}^\dagger c_{\mathbf{k}\sigma} + h.c. \right). \quad (4)$$

All local (on impurity site) properties are expressed by the hybridization function

$$\Delta(\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{\omega - \epsilon_{\mathbf{k}}}, \quad (5)$$

and not by  $\epsilon_{\mathbf{k}}$  and  $V_{\mathbf{k}}$  separately.

### 2.1. Mean field solution of the single impurity Anderson model

The Hartree-Fock mean-field solution of the SIAM is obtained by factorizing the interacting term  $n_{d\uparrow} n_{d\downarrow} \approx$

Fig. 1. The frequency dependent part of self-energy expressed as the RPA series around the broken symmetry Hartree-Fock solution. The transverse spin polarization bubbles constitute a geometric series which can be summed up to infinity.

$\langle n_{d\uparrow} \rangle n_{d\downarrow} + n_{d\uparrow} \langle n_{d\downarrow} \rangle - \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle$  [1]. For the interaction  $U$  above  $U_c$  and corresponding impurity electron densities  $\bar{n}_d$  the mean-field solution is unstable toward the local moment formation with non-zero moment  $\mu \equiv \langle n_{d\uparrow} \rangle - \langle n_{d\downarrow} \rangle$ . The solution is doubly degenerate because of two equivalent directions of the local moment  $\mu = \pm |\mu|$ , which give the same energy of the system. The local (impurity) Green function within the Hartree-Fock solution is

$$G_{\sigma}^{HF}(\omega) = \frac{1}{\omega - \epsilon_d - \Delta(\omega) - \Sigma^{HF} + i\delta \text{sgn}\omega} \quad (6)$$

where the static Hartree-Fock self-energy  $\Sigma_{\sigma}^{HF} = U \langle n_{\bar{\sigma}} \rangle$  and  $\delta \rightarrow 0^+$ . Since there are in principle two possible signs of the local moment, there are two different possible Hartree-Fock Green functions denoted by  $G_{\sigma}^A(\omega)^{HF}$  and  $G_{\sigma}^B(\omega)^{HF}$  that differ only by the sign of the local moment and depend parametrically on its value  $|\mu|$ .

The fundamental deficiency of the Hartree-Fock approximation is that it leads to a broken symmetry solution which cannot persist in the thermodynamic limit, i.e. a single impurity cannot lead to the magnetic solution in the infinite system. Also this solution does not recover the singlet ground state known from the exact Bethe ansatz solution. Nevertheless it turns out to be useful as a starting point in the further perturbative calculation combined with the symmetry restoration.

### 2.2. Two self-energy description

The two Hartree-Fock Green functions  $G_{\sigma}^{A,B}(\omega)^{HF}$  are used in the time-dependent many-body perturbation expansion. Within the random phase approximation (RPA) the polarization diagrams are

$$\Pi_{\sigma\bar{\sigma}}^{AA}(\omega) = \frac{{}^0\Pi_{\sigma\bar{\sigma}}^{AA}(\omega)}{1 - U {}^0\Pi_{\sigma\bar{\sigma}}^{AA}(\omega)} \quad (7)$$

and correspond to spin flip processes as represented by the Feynman diagrams in Fig. 1.

For each type of the mean-field solution  $G_{\sigma}^{A,B}(\omega)^{HF}$  we have the corresponding self-energy

$$\Sigma_{\sigma}^A(\omega) = \Sigma_{\sigma}^{HF} + U^2 \int \frac{d\omega'}{2\pi i} \Pi_{\sigma\bar{\sigma}}^{AA}(\omega') G_{\bar{\sigma}}^A(\omega - \omega')^{HF} \quad (8)$$

depending on frequency and parametrically on  $|\mu|$  as well. The full RPA-Green functions  $G_\sigma^{A,B}(\omega)$  are constructed by using the Dyson equation separately for A and B solutions. Note that  $G_\sigma^{A,B}(\omega)$  depends parametrically on still unknown  $|\mu|$ .

### 2.3. Symmetry restoration ansatz

To restore the spin-rotational symmetry Logan *et al.* [11] proposed the following ansatz for the full symmetrized Green function

$$G_\sigma(\omega) = \frac{1}{2} \left( G_\sigma^A(\omega) + G_\sigma^B(\omega) \right). \quad (9)$$

Within the LMA the physical Green function is an average of the two solutions with equal probabilities. Although each  $G_\sigma^{A,B}(\omega)$  are determined within the renormalized perturbation scheme the final Green function turns out to capture nontrivial non-perturbative physics as was shown by Logan *et al.* [11] and is also reproduced below. In particular, the LMA is able to recover the Kondo peak in the spectral function correctly with the exponential width.

### 2.4. Determining the value of local moment

The value of the local moment is a free parameter and must still be determined. In the original approach, Logan *et al.* [11] imposed the Fermi liquid condition to determine  $|\mu|$  at zero temperature. This condition might be too restrictive at finite temperatures or in the multi-orbital cases. Therefore we decided to find the physical solution to the problem by minimizing the relevant thermodynamical potential with respect to  $|\mu|$  [16]. At zero temperature the relevant potential is just the ground state energy of the system, i.e.

$$E_{\text{physical}} = \min_{\{\mu, n\}} E_G(\mu, n), \quad (10)$$

where in the case away of half-filling the particle density  $n$  must also be determined. The variational method reproduces the Fermi liquid properties where they are expected.

### 2.5. Ground state energy in the Anderson impurity model

The ground state energy of the SIAM is given by  $E_G = \langle 0|H|0\rangle$ . This quantum-mechanical average consists of two parts: the bulk, which is proportional to the system volume and is independent of the local moments, and the impurity part, which depends explicitly on  $|\mu|$ . The impurity part of the ground state energy, expressed by the local Green function  $G_\sigma(\omega)$  and the hybridization function  $\Delta(\omega)$ , is equal to [17]

$$E_{\text{imp}} = \frac{1}{2\pi i} \sum_\sigma \oint_C d\omega \left[ \frac{\omega + \epsilon_d + \Delta(\omega)}{2} - \omega \frac{\partial \Delta(\omega)}{\partial \omega} \right] G_{\text{imp}}^\sigma(\omega), \quad (11)$$

where the contour integral is over the half circle in the upper complex plane.

### 2.6. LMA as a conserving approximation

According to Kadanoff and Baym [18] any approximate theory is conserving if there exists a Luttinger-Ward functional  $\Phi[G]$  for this theory. It is necessary that this functional: i) is universal, i.e. it depends only on the full propagator  $G_\sigma(\omega)$  and not on the atomic properties of the system and ii) has a functional derivative with respect to  $G_\sigma(\omega)$  which is by definition equal to the self-energy of the system. It turns out [16] that the LMA is a conserving approximation and we can construct explicitly the Luttinger-Ward functional

$$\Phi[G] = \Phi[G^A, G^B] = \frac{1}{2} \left( \Phi_{RPA}^A + \Phi_{RPA}^B \right) + \frac{1}{2} \text{Tr} \log G_\sigma^A G_\sigma^B - \text{Tr} \log \left( \frac{1}{2} \left( G_\sigma^A + G_\sigma^B \right) \right), \quad (12)$$

where  $\text{Tr} = T \sum_\sigma \sum_{i\omega_n} e^{i0^+}$  and the functionals  $\Phi_{RPA}^{A,B}$  are represented diagrammatically by the RPA diagrams with  $G_\sigma^{A,B}(\omega)$  respectively. The constraint that  $G = \frac{1}{2} (G_A + G_B)$  must be satisfied. Finally, the free energy functional is given by

$$\Omega[G] = \Phi[G] + \text{Tr} \log G - \text{Tr} \Sigma G \quad (13)$$

and the stationarity condition  $\delta\Omega[G]/\delta G$  gives the Dyson equation and the physical solution for  $G$ .

## 3. Local moment approach for the multi-orbital SIAM

### 3.1. Multi-orbital SIAM and LMA generalization

Single impurity Anderson model with many orbital levels is given by the Hamiltonian:

$$H_{\text{SIAM}} = \sum_{\alpha, \sigma} (\epsilon_\alpha + U_\alpha n_{\alpha, \bar{\sigma}}) n_{\alpha, \sigma} + \sum_{\sigma, \sigma' \alpha \neq \beta} \sum_{\sigma, \sigma'} (U'_{\alpha\beta} - J\delta_{\sigma\sigma'}) n_{\alpha\sigma} n_{\beta\sigma'} + \sum_{\mathbf{k}, \sigma, \alpha} V_{\mathbf{k}\alpha} \left( d_{\alpha\sigma}^\dagger c_{\mathbf{k}\sigma} + c_{\mathbf{k}\sigma}^\dagger d_{\alpha\sigma} \right) + \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}, \quad (14)$$

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

In the mean field approximation of the multi-orbital SIAM we also encounter a doubly degenerate solution, where the two possible Green functions differ only by the sign of the impurity magnetic moment. Within the LMA, we introduce for each pair of orbital indices  $\alpha$  and  $\beta$  the two Green functions  $G_{\sigma}^{\alpha\beta,A}(\omega)^{HF}$  and  $G_{\sigma}^{\alpha\beta,B}(\omega)^{HF}$  that correspond to the two possible directions of the total magnetic moment on the impurity. These Hartree-Fock Green functions depend now parametrically on values of local moments on each of the orbitals  $\mu_{\alpha}$ . Next we use the RPA approximation to obtain two Green functions  $G_{\sigma}^{\alpha\beta,A}(\omega)$  and  $G_{\sigma}^{\alpha\beta,B}(\omega)$ , which are parametrically dependent on the local moments on each orbitals  $\mu_{\alpha}$ .

### 3.2. Symmetry restoration and determining the local moment values

The symmetry restoration in the multi-orbital case is a straightforward generalization of the previous ansatz, i.e.

$$G_{\sigma}^{\alpha\beta}(\omega) = \frac{1}{2} \left( G_{\sigma}^{\alpha\beta,A}(\omega) + G_{\sigma}^{\alpha\beta,B}(\omega) \right), \quad (15)$$

except that now the symmetrized Green functions  $G_{\sigma}^{\alpha\beta}(\omega)$  depend explicitly on local moments on all of the orbitals, i.e.  $|\mu_{\alpha}|$ . The parameters  $|\mu_{\alpha}|$  have to be determined independently. They are found by the minimization of the ground state energy of the impurity with respect to both local moment values on orbitals  $\mu_{\alpha}$  and particle number on each of the orbitals  $n_{\alpha}$

$$E_{\text{physical}} = \min_{\{\mu_{\alpha}, n_{\alpha}\}} E_G(\mu_{\alpha}, n_{\alpha}). \quad (16)$$

As mentioned above, the variational procedure allows us to extend the LMA on the multi-orbital cases, where the Luttinger (Fermi liquid) condition for each orbital is absent. Also the possibility of non-Fermi liquid solution is naturally included within present generalization of the LMA [16].

## 4. Application to multilevel quantum dots

### 4.1. The model of a multilevel quantum dot

A single quantum dot with many atomic-like levels coupled to leads are described by a multi-orbital single impurity Anderson model:

$$H = H_{\text{dot}} + H_{\text{leads}} + H_{\text{dot-leads}},$$

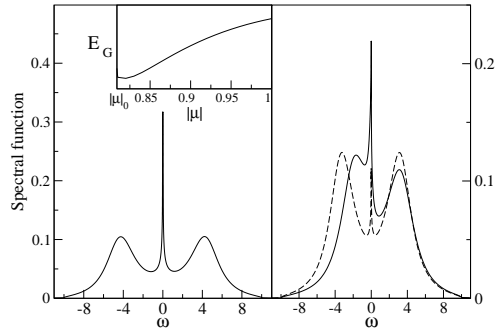


Fig. 2. Spectral functions for one level (left panel) and two level (right panel) quantum dots. Left panel: spectral function at half-filling and  $U = 6$  (inset: the ground state energy as a function of the absolute value of local moment  $|\mu|$ ; the axis starts at the Hartree-Fock value  $|\mu| = |\mu_0|$ ). Right panel: orbitally resolved spectral functions in the dot for  $U = 3$ ,  $J = 0.25U$ ,  $|\epsilon_1 - \epsilon_2| = 0.1U$ , and the total filling  $n_d = 1.95$ . All curves are for semi-elliptic hybridization function with the width  $W = 20$ . The Fermi level is at zero.

where  $H_{\text{dot}}$  is the local impurity part of the SIAM Hamiltonian,  $H_{\text{leads}}$  corresponds to the conduction electron part of the SIAM Hamiltonian, and  $H_{\text{dot-leads}}$  is equal to the hybridization term in SIAM [3].

### 4.2. LMA in quantum dots

The properties of transport in a quantum dot in equilibrium, i.e. with infinitesimally small bias voltage between the leads, are determined by the spectral functions on each of the orbitals. Examples of the spectral functions are presented in Fig. 2 for the one-orbital case (left panel) and for the two orbital case (right panel). In the two orbital case the atomic levels are shifted such that one of the orbital is at half filling (dashed line) and the other is away of half filling (solid line). The Kondo peak in the symmetric case is suppressed by the exchange (Hund) interaction ( $J \neq 0$ ), which favors parallel spin orientations. In the asymmetric case the Kondo peak survives due to the presence of uncompensated magnetic moment and is shifted toward the lower Hubbard band. Further investigation of multi-level quantum dots including transport properties will be presented elsewhere [16].

## 5. Application to the multi-orbital Hubbard model

### 5.1. Multi-orbital Hubbard model

The generalized LMA is also applied to solve the multi-orbital Hubbard model

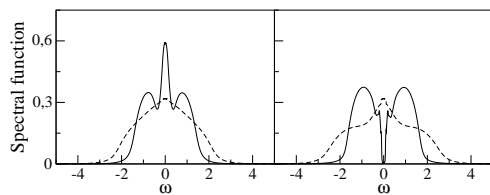


Fig. 3. Spectral functions for two-orbital Hubbard model with different band widths  $W = 2$  (solid line) and  $W = 4$  (dashed line) on Bethe lattice with infinite coordination number. Left panel:  $U = 1.2$ ,  $J = 0.1U$ . Right panel:  $U = 2$ ,  $J = 0.1U$ . The inter-band interaction  $U' = U - 2J$  is fixed preserving  $SU(4)$  symmetry. In both cases the Fermi level is at zero energy and the bands are half filled.

$$H_{\text{Hubb}} = \sum_{ij} \sum_{\alpha, \sigma} t_{ij}^{\alpha} d_{i\alpha\sigma}^{\dagger} d_{j\alpha\sigma} + H_{\text{local}},$$

where the local part is a lattice sum of the 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 [6]. In this way the lattice problem is mapped onto the Anderson impurity problem which has to be solved for different hybridization functions until self-consistency is achieved. In order to solve the Hubbard model within DMFT we need to solve the SIAM for arbitrary hybridization functions. The self-consistency condition simplifies greatly for the Bethe lattice which is used in this contribution.

## 5.2. LMA method in DMFT

In the recent few years the orbital-selective Mott-Hubbard metal-insulator transition has been the subject of extensive studies [19–23].

Using the LMA to obtain the solution of the SIAM in each of the DMFT loops the spectral functions for two-orbital Hubbard model at zero temperature were found. As an example, Fig. 3 shows the results for the case with different bandwidths and non-zero Hund coupling  $J$ . Since one of the spectral function is metallic-like (finite at  $\omega = 0$ ) and the other is insulating-like (vanishes at  $\omega = 0$ ) we conclude that the orbital selective MIT occurs in this model system.

## Summary

The generalized LMA to the multi-orbital SIAM allows us to efficiently solve the problems of correlated electron systems such as multilevel quantum dots and the Hubbard model within the DMFT. In particular it is relatively easy to address the problems of different band widths and also the removing of the orbital degeneracy [24]. We experienced that the local moment

approach is an efficient method in studying these problems, in particular, when the number of the orbitals is larger than two.

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