Local moment approach to multi-orbital Anderson and Hubbard models

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Abstract The variational local moment approach (V-LMA), being a modification of the method due to Logan et al., is presented here. The existence of local moments is taken from the outset and their values are determined through variational principle by minimizing the corresponding ground state energy. Our variational procedure allows us to treat both fermi- and non-fermi liquid systems as well as insulators without any additional assumptions. It is proved by an explicit construction of the corresponding Ward functional that the V-LMA belongs to the class of conserving approximations. As an illustration, the V-LMA is used to solve the 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.

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 [16], ii) charge transport through quantum dots [24], iii) Mott-Hubbard metal-insulator transitions (MIT) within the dynamical mean-field theory (DMFT) [23,6,14,28,30,27], and iv) a crossover between weak and strong coupling limits and confinement phenomena. The SIAM consists of a term describing band electrons coupled by hybridiza-
tion 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 are exactly known [16]. Unfortunately, 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) [5] or the determinant quantum Monte Carlo (QMC) [14] 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 [17]. 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. [26].

The LMA is a perturbative method around an unrestricted Hartee-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 directions of the local magnetic moment [26].

In the present contribution we describe the LMA method and our implementation of it, which is different from the original one [26] 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 is minimized by the physical value of the local moment. Therefore we use the name variational local moment approach (V-LMA) for this method. Such a procedure allows us to easily generalize the V-LMA for multi-orbital models as well as for finite temperatures and systems with disorder [8, 7, 9, 10]. We also discuss the Luttinger-Ward generating functional for the V-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

\[ H_{\text{SIAM}} = H_c + H_{\text{imp}} + H_{\text{hyb}}, \]  

where the conduction electrons are described by

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

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

(3)

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

$$H_{hyb} = \sum_{k,\sigma} (V_k d_{\sigma}^\dagger c_{k\sigma} + h.c.).$$

(4)

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

$$\Delta(\omega) = \sum_k \frac{|V_k|^2}{\omega - \epsilon_k},$$

(5)

and not by $\epsilon_k$ and $V_k$ separately. This can be proved by tracing out the non-interacting conducting electrons.

### 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 $n_{d\uparrow} n_{d\downarrow} \approx \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle$ for the interaction $U$ above $U_c$ and corresponding impurity electron densities $\bar{n}_{\sigma}$ 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

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

(6)

where the static Hartree-Fock self-energy $\Sigma^{HF}_{\sigma} = U \langle n_{\sigma} \rangle$ 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 $G^A_{\sigma}(\omega)^{HF}$ and $G^B_{\sigma}(\omega)^{HF}$ 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

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

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

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.

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

\[
\Sigma_{\sigma}^{A}(\omega) = \Sigma_{\sigma}^{HF} + U^2 \int \frac{d\omega'}{2\pi i} \Pi_{\sigma\bar{\sigma}}^{AA}(\omega') G_{\sigma}^{A}(\omega - \omega')^{HF}
\] (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. proposed the following ansatz for the full symmetrized Green function

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

Within the LMA the physical Green function is an average of the two solutions with equal probabilities. Although each \( G_{\sigma}^{A,B}(\omega) \) is 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. 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. [26] 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 $|\mu|$. At zero temperature the relevant potential is just the ground state energy of the system, i.e.

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

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

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

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 [3] 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 re-
spect to $G_\sigma(\omega)$ which is by definition equal to the self-energy of the system. It can be shown that the LMA is a conserving approximation and we can construct explicitly the Luttinger-Ward functional

$$
\Phi[G] = \Phi[G^A, G^B] = \frac{1}{2} (\Phi^A_{RPA} + \Phi^B_{RPA}) + \frac{1}{2} Tr \log G_\sigma^A G_\sigma^B + Tr \log \left( \frac{1}{2} (G_\sigma^A + G_\sigma^B) \right)
$$

(12)

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

$$
\Omega[G] = \Phi[G] + Tr \log G - Tr \Sigma
$$

(13)

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

The fact that the LMA is a conserving approximation, as we proved above, makes this theory reliable in describing correlated electron systems, in particular in the intermediate regimes of parameters.

3 Local moment approach for the multi-orbital SIAM

In reality the magnetic impurities in metals are atoms with partially field d- or f-orbitals. Such orbitals have degenerate levels. Even when a particular environment which decrease the symmetry and leads to $e_g$ and $t_{2g}$ split levels, partial degeneracy between orbitals remains. The appropriate model to describe such situations is the multi-orbital single impurity Anderson model. It describes a single impurity with many orbital levels $\alpha$, which can be degenerate or split depending on the single-body matrix element $\epsilon_\alpha$. In this case the electrons can interact via direct (density-density) type of the interaction and via the exchange (Hund) interaction. Microscopically, the single impurity Anderson model with many orbital levels is given by the Hamiltonian:

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

(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.

This multi-orbital version of the SIAM is also of interest in quantum dot physics, where dots with a few orbitals can be prepared and investigated experimentally.
One of the interesting aspects of such system is the possibility to observe the orbital Kondo effect \[18\].

### 3.1 LMA generalization

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 \( G_{\sigma}^{\alpha \beta A}(\omega) \) and \( G_{\sigma}^{\alpha \beta B}(\omega) \) 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.

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

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 \( n_\alpha \)

\[
E_{\text{physical}} = \min_{\{\mu_\alpha, n_\alpha\}} E_G(\mu_\alpha, n_\alpha).
\]

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 \[20\], i.e. the variational local moment approach.
4 Application to multilevel quantum dots

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

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

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 [24].

4.1 V-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 orbitals 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 multilevel quantum dots including transport properties will be presented elsewhere [20].

![Fig. 2](image.png)

*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.
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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.

5 Application to the multi-orbital Hubbard model

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

$$H_{\text{Hubb}} = \sum_{ij} \sum_{\alpha, \sigma} t_{i\alpha}^0 d_{i\alpha\sigma}^\dagger d_{j\alpha\sigma} + H_{\text{local}},$$

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 [14]. 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.

5.1 V-LMA method in DMFT

In the recent few years the orbital-selective Mott-Hubbard metal-insulator transition has been the subject of extensive studies [22, 25, 13, 4, 2].

Using the V-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.

At the end we discuss the V-LMA in perspective to other methods used to solve the impurity problem and DMFT equations. The V-LMA belongs to the class of approximate, analytical methods like for example the iteration perturbation theory (IPT) [15], the non-crossing approximation (NCA) [12], or slave-boson theory (SB) [29], and various extensions of these methods. As we showed here, the V-LMA is a conserving approximation, contrary for example to the IPT, and correctly describes
high- and low-energy parts of the spectra, recovering the Kondo peak and Luttinger pinning. We tested this theory at zero temperature but there is no conceptual obstacle why the V-LMA should not work at finite temperatures as well.

The V-LMA is not numerically exact like the quantum Monte Carlo method \cite{14}, the numerical renormalization group (NRG) \cite{5}, dynamical matrix renormalization group (DMRG) \cite{31}, or exact diagonalization (ED) \cite{11}. However, each of the numerically exact methods suffers from principal obstacles in practical applications, in particular when the temperature is too low (QMC) or too high (NRG), or number of orbitals increases (NRG, DMRG, ED).

Therefore we conclude that the V-LMA is a method of choice for solving the DMFT equations and can be used as a relatively fast and accurate impurity solver. The only technical difficulty in the variational LMA is to compute with high accuracy the system energy and to find its minimum. This should be performed with a great care.

**Summary**

The generalized variational 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 \cite{19}. 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.

**Acknowledgements** We thank dr. R. Bulla and prof. D. Vollhardt for the discussions. The hospitality at Augsburg University is also acknowledged. This work is supported by Sonderforschungsbereich 484 of the Deutsche Forschungsgemeinschaft (DFG) and by the European Commission under the contract No MRTN-CT-2003-504574.

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