Calculation scheme based on the exact diagonalization approach for solving the Extended DMFT equations

Ural Federal University
named after the first President of Russia B.N.Yeltsin

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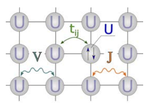
ABSTRACT

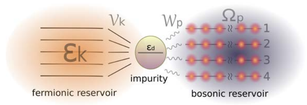
Here we propose a distinct numerical scheme based on the exact diagonalization approach to solve the equations of the Extended Dynamical Mean-Field Theory. We compare results to that of solver based on the CTQMC. The phase diagram U vs.V was constructed for the 1^{st} nearest neighbours in several correlation regimes. The influence of reservoirs discretization in the impurity model was analized. Also deep insulator regime was considered in case of charge interaction. Moreover magnetic interaction were considered too and main trend was determined.

EDMFT

Extended Hubbard model



Holstein-Anderson impurity model



$$H = \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{i\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} + \underbrace{\frac{1}{2}\left(\sum_{ij\sigma} V_{ij} n_{i\sigma} n_{j\sigma} + \sum_{ij} J_{ij} S_i S_j\right)}_{\text{nonlocal interactions}}$$

$$H_{imp} = \underbrace{\varepsilon_d \sum_\sigma c^\dagger_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}}_{\text{impurity}} + \underbrace{\sum_{k\sigma} \mathcal{V}_k (c^\dagger_{d\sigma} c_{k\sigma} + c^\dagger_{k\sigma} c_{d\sigma}) + \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}}_{\text{fermionic reservoir}} + \underbrace{\sum_p^4 \Omega_p \mathbf{b}^\dagger_p \mathbf{b}_p + \sum_p^4 \mathcal{W}_p \vec{\mathcal{O}}_p (\mathbf{b}^\dagger_p + \mathbf{b}_p)}_{\text{bosonic reservoir}}$$

TECHNICAL REALIZATION

Representation of bosons for computing

- The number of bosons on each orbital (in decimal system) is associated with a number in binary system.
- Bosonic part of basis vector consists of all possible configurations of occupansy on several orbitals.
- Boson part of a basis vector includes all possible combinations of number of bosons.

As a result we obtain a filling matrix of Hamiltonian for impurity model.

- Size of the matrix depends on totals number of orbitals: $[2^{2K+1}(N_1+1)(N_2+1)...(N_P+1)]^2$.
- Moreover, this matrix has sparce view. That gives us an opportunity to work with **SRC format**.

Matrix-matrix multiplication in iterative methods in case of big matrices should be avoided.

Krylov subspace methods.

Lanczos method → *ARPACK library*

IMPURITY SOLVER

In a basis of occupation numbers the vector looks as follow:

$$|\psi\rangle = \underbrace{|n_{b1}, n_{b2}, \ldots, n_{bp}, \ldots\rangle}_{\text{boson part}} \otimes \underbrace{|n^\uparrow_d, n^\uparrow_{c1}, \ldots, n^\uparrow_{ck} \ldots, n^\downarrow_d, n^\downarrow_{c1}, \ldots, n^\downarrow_{ck}, \ldots\rangle}_{\text{fermion part}}$$

consists of 0 and 1

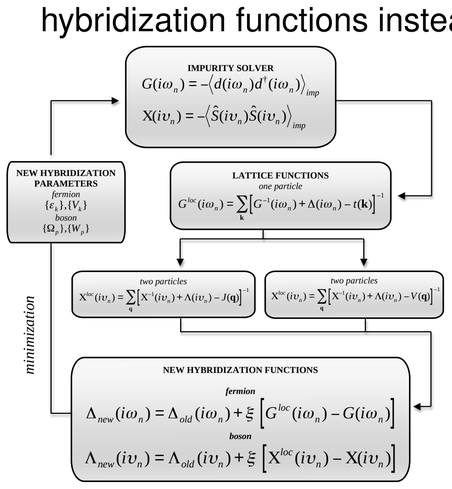
Hamiltonian has the following view:

$$\mathcal{H} = \mathcal{H}_F \otimes \mathcal{H}_B$$

here $\mathcal{H}_F$ is a fermionic Hamiltonian without boson part, $\mathcal{H}_B$ is a bosonic Hamiltonian.

SELF-CONSISTENT LOOP

In this scheme the main matched parameter is the hybridization functions instead of self-energy.



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

$$\Lambda(\Omega) = \sum_p \frac{2W_p^2 \Omega_p}{(i\nu_n)^2 - \Omega_p^2}$$

PHASE TRANSITIONS

MI → FL

- Check a sign of $\Delta\Sigma = \Sigma(1) - \Sigma(0)$
- Check the quasiparticle weight.

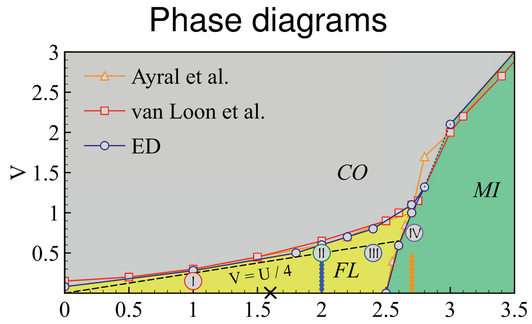
$$Z = \left[1 - \frac{Im\Sigma(i\omega_0)}{\omega_0}\right]^{-1}$$

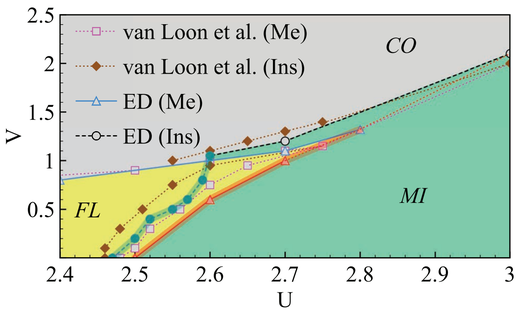
MI/FL → CO

- Change sign in the $\chi^{NN}(i\nu_0; \mathbf{q} = (\pi, \pi))$.

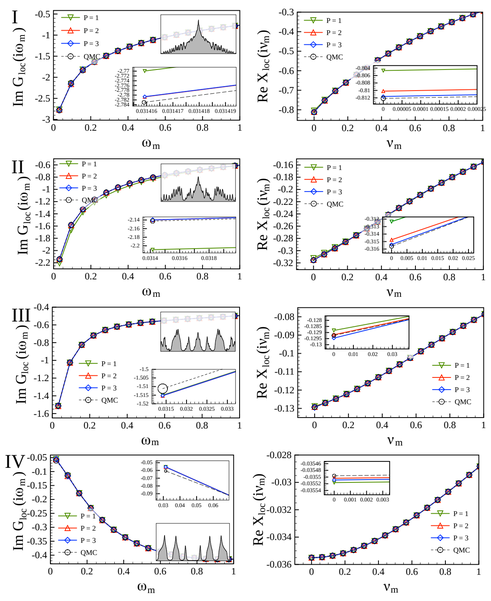
RESULTS FOR CHARGE INTERACTIONS

Phase diagrams

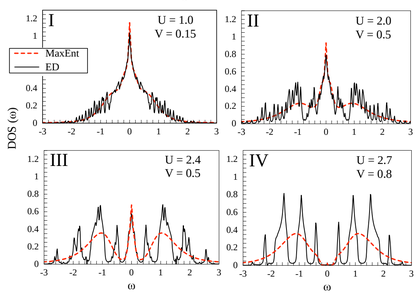




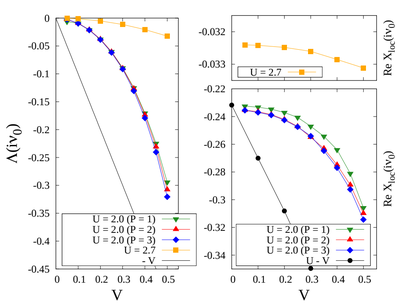
Benchmark ED / CTQMC



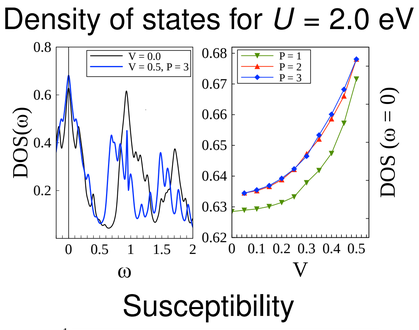
Density of states



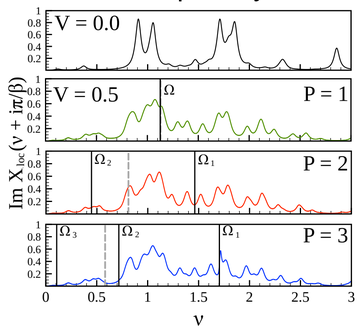
Hybridization function



Density of states for U = 2.0 eV



Susceptibility



Grey line denotes a screening frequency.

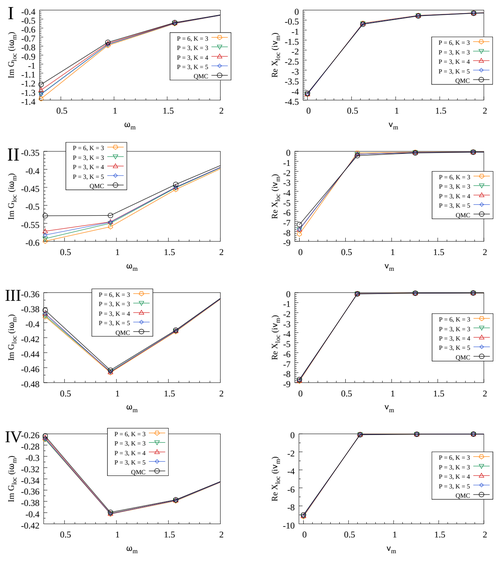
RESULTS FOR MAGNETIC INTERACTIONS

Discretization of the bosonic reservoir in case of magnetic interaction accounting is based on the representation of the vector boson projections in a spin space as effective orbitals $\mathbf{S} = \{S^z, S^x, S^y\}$ with equal energy Ω and hybridization parameter $\mathcal{W}_p$, where p is an index of bosonic orbital.

Calculated points parameters:

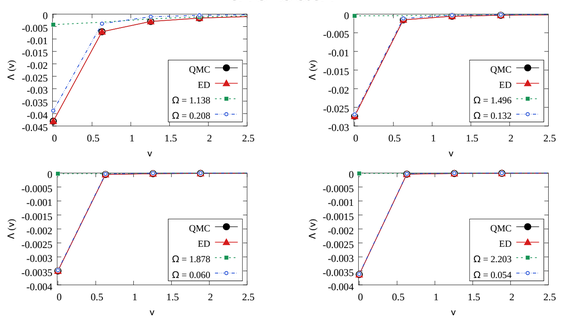
U = 1.0 eV, J = 0.05 eV	U = 2.0 eV, J = 0.03 eV
U = 2.4 eV, J = 0.01 eV	U = 2.7 eV, J = 0.01 eV

Benchmark ED / CTQMC

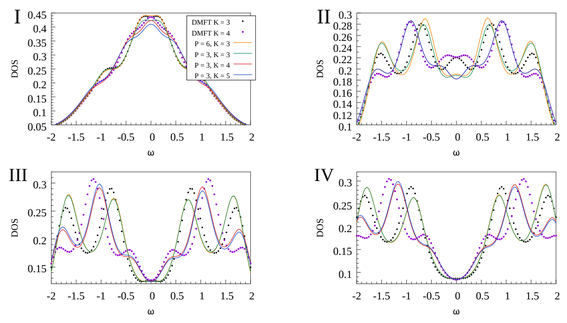


Hybridization function

for different numbers of bosonic orbitals in the bath



Density of states



CONCLUSIONS

- The discretization of fermionic and bosonic hybridization functions is necessary in ED. Benchmarks with a CTQMC solver in different regimes show in most cases two screening modes suffice for the discretization of the bosonic bath.
- An exception is the boundary between an insulating and a charge-ordered phase, where more than two modes are needed due to the broad spectrum of charge excitations near the transition.
- More significant than the discretization of the bosonic bath are unavoidable and familiar artifacts due to the discretization of the fermionic bath.
- We find that deep in the half-filled insulator ED can be well applied as a solver for the EDMFT equations, while it becomes difficult to converge the CTQMC schemes there due to the singular behavior of the self-energy.
- EDMFT seems to ignore the screening effect of the local by the nonlocal interaction in the Mott insulator phase and predicts nonlinear effect in Fermi liquid phase.
- We suppose to achieve a different local screening mechanism, a self-consistent renormalization of the dynamically screened local interaction is needed.

ACKNOWLEDGEMENT

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