An exact-diagonalization-based scheme for solving the extended DMFT equations

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The dynamical mean-field theory (DMFT) is successful route for description of strongly correlated systems, which can exhibit some of the most intriguing features known to condensed matter physics, including high-temperature superconductivity, heavy fermion behavior, metal-insulator transitions and others [1]. However, there are many examples when one should overcome the main limitation of the DMFT that is neglect of the non-local magnetic and charge correlations. This is the case for graphene-based systems for which strong inter-site Coulomb correlations[2] and magnetic couplings [3] were found. To solve this problem one can use different extensions and modifications of the single-site DMFT approach that are cluster DMFT [4], dual fermions approach [5] and others.

Here we propose a distinct numerical scheme based on the exact diagonalization approach to solve the equations of the extended dynamical mean-field theory. In contrast to the single-site DMFT we deal with the impurity problem where the correlated site interacts with fermion and boson baths. The latter gives us opportunity to simulate the non-local magnetic fluctuations in the system describing by the Heisenberg-type term $J_{ij}\mathbf{S}_i\mathbf{S}_j$. The corresponding impurity Hamiltonian is given by

$$H_{imp} = \varepsilon_d \sum_\sigma c^\dagger_{d\sigma} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_k V_{dk}(c^\dagger_{d\sigma} c_{k\sigma} + c^\dagger_{k\sigma} c_{d\sigma}) + \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_p \Omega_p \mathbf{b}^\dagger_p \mathbf{b}_p + \sum_p W_p \hat{\mathbf{S}}(\mathbf{b}^\dagger_p + \mathbf{b}_p)$$

where ϵ_d and ϵ_k are energies of the correlated impurity and fermionic bath states, $c^\dagger_{d\sigma}$ ($c_{d\sigma}$) and $c^\dagger_{k\sigma}(c_{k\sigma})$ are the creation (annihilation) operators for impurity and bath electrons, V_{dk} is the hopping integral between impurity and fermionic bath states, μ is the chemical potential and U is the on-site Coulomb interaction, $\mathbf{b}^\dagger_p(\mathbf{b}_p)$ - creation(anihillation) operator of p^{th} boson, Ω_p - boson frequency, W_p - fermion-boson interaction. Within the self-consistency cycle the hybridizations with each type of the reservoirs are recalculated.

The developed scheme gives us opportunity to provide a complete description of the magnetic properties of a low-dimensional system, since the momentum- and frequency-dependent magnetic susceptibility of the system, $\chi(\mathbf{q},\omega)$ can be calculated. Fig.1 gives the EDMFT results obtained by using the developed scheme for the Hubbard model with half-filling on the square lattice. One can see that the account of the non-local magnetic interactions, J leads to the formation of the low-energy excitations in the local magnetic susceptibility.

References

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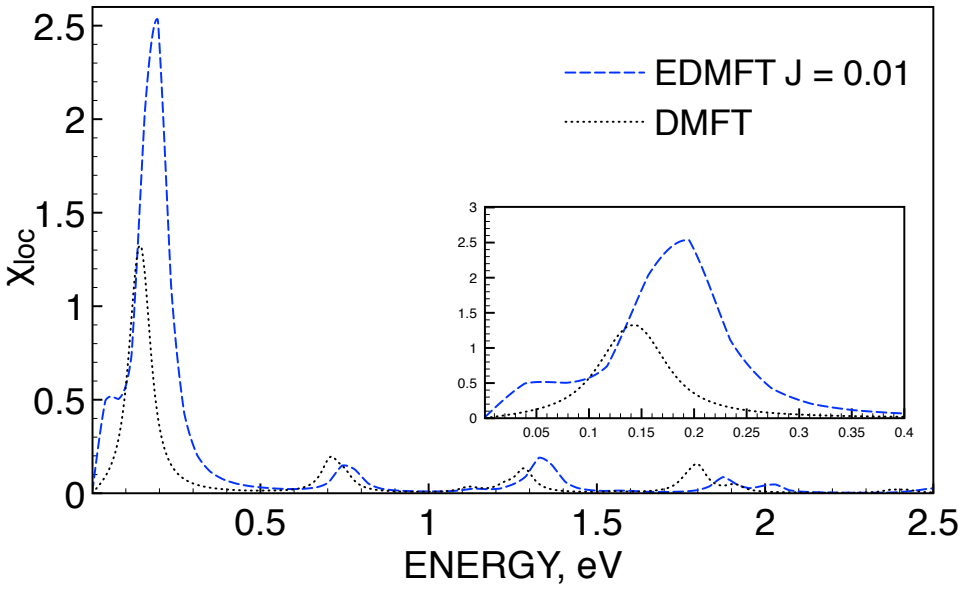

Figure 1: Comparison of the local susceptibilities calculated by using DMFT and EDMFT solvers for $J = 0.01$ eV with $\beta = 10$ and $U = 2$ eV, β is the inverse temperature.