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

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The dynamical mean-field theory (DMFT) is a 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 $J_{ij}S_i S_j$. The corresponding impurity Hamiltonian is given by

$$H_{imp} = \epsilon_d \sum_{\sigma} c_{d\sigma}^+ c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_k V_{dk}(c_{d\uparrow}^+ c_{k\uparrow} + c_{d\downarrow}^+ c_{k\downarrow}) + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \sum_p \Omega_p b_p^+ b_p + \sum_p W_p \hat{S}(b_p^+ + b_p)$$

where $\epsilon_d$ and $\epsilon_k$ are energies of the correlated impurity and fermionic bath states, $c_{d\sigma}^+$ ($c_{d\sigma}$) and $c_{k\sigma}^+$ ($c_{k\sigma}$) are the creation (annihilation) operators for impurity and bath electrons, $V_{dk}$ is the hopping integral between impurity and fermionic bath states, $\mu$ is the chemical potential and $U$ is the on-site Coulomb interaction, $b_p^+$ ($b_p$) - creation (annihilation) operator of $p^{th}$ boson, $\Omega_p$ - 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, $\chi(q, \omega)$ 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

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, $\beta$ is the inverse temperature.