Screening and Friedel oscillations in inhomogeneous systems with correlated fermions

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ABSTRACT

The thesis presents theoretical and numerical studies on electronic screening and Friedel Oscillations (FO) in correlated fermionic systems in the presence of external inhomogeneity. These spatial oscillations in the electronic densities appear in the neighbourhood of the impurity due to quantum scattering from the impurity. They are observed in metals at low temperatures. The interacting system has been modeled by the Hubbard Hamiltonian which has been further solved numerically using the Real space Dynamical Mean-Field Theory (R-DMFT). We study one-, two-, and three-dimensional finite lattice systems with periodic boundary conditions. The inhomogeneous potential has been modeled by a single impurity, two impurities and an extended inhomogeneity. Different approximations accounting for the electronic correlations have also been discussed in the course of the thesis. The effects of electronic correlations, particularly at the Mott metal to insulator transition, on the behaviour of FO have been explored. According to our numerical studies, the oscillations are damped with the interactions, disappear at the Mott transition and completely beyond it. At finite temperature the oscillations are damped and slowly disappear as we increase the temperature of the system. At half-filling the period and phase of the oscillations remain unaltered by the interactions. The Friedel sum rule for the interacting system has been investigated. The variation of the screening charge around the neighbourhood of the impurity called ``Neighbourhood screening charge" or ``N-screening charge" with interaction, temperature is studied for different impurity potentials. It is further seen that the interactions weaken the screening effects. The spectral functions in the presence of an external inhomogeneity and electronic interactions have been studied at different lattice sites. In the presence of the interaction a sign of resonance appears in the spectral function at the impurity site. In the presence of two impurities interaction weakens the interference effects on the oscillations. Finally the one-body scattering formalism is modified to describe analytically the effects of correlations in many body systems modeled by a momentum independent self-energy with semi circular density of states. Effects of electronic correlations in the scattering phase-shift and spectral functions are obtained in our calculations. The thesis provides predictive numerical results which can motivate future experiments.