European XFEL Theory Seminar

European XFEL

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Campus Schenefeld, main building (XHQ) room E1.172

Arata Tanaka

Hiroshima University, Japan

Metal-insulator transition and pseudo-gap formation in the two-dimensional Hubbard model at half-filling

Although numbers of studies have been devoted to the metal-insulator transition in the two-dimensional Hubbard mode, it is still a subject of debate. The difficulty mainly arises from the fact that long-range antiferromagnetic order cannot be stable at finite temperature in two dimensions because of the Mermin-Wagner theorem. Therefore, to describe the electronic state of the model, the theory must be taken into account not only the effects of the on-site Coulomb repulsion but also the long-range antiferromagnetic fluctuation properly. The dynamical mean field theory (DMFT) and its extension to the clusters are only capable for short-range correlation. However, the dual fermion approach (DFA), which is recently developed perturbative extension of DMFT, can incorporate the effects of long-range correlation.

In this talk the metal-insulator transition in the square-lattice Hubbard model at half-filling is discussed in relation to the spectral function by means of DFA. Although the continuous-time quantum Mote Carlo method is used to solve the effective Anderson impurity problem in the majority of previous DFA studies, the Lanczos exact-diagonalization technique is applied in this study. This technique is advantageous to access low temperatures and obtain accurate spectral functions on the real axis.

It is found that as temperature decreases pseudo-gap appears at Fermi energy in the DOS around the Néel temperature predicted by DMFT. For U/t <~6.5, this is followed by gradual destruction of the Fermi surface signaled by the formation of a dip at Fermi energy in the spectral function. For U/t <~5.5, the DOS inside the pseudo-gap gradually decreases with decreasing temperature but remain even at low temperatures (pseudo-gap phase). In contrast, for U/t >~5.5, a sharp reduction of the DOS at Fermi energy is found with decreasing temperature resulting in clear opening of the insulating gap at low temperatures (Mott insulator). These results are consistent with the previous study with the non-linear σ model.

Host: Evgeny Gorelov

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