Mott physics and long-range fluctuations : A unified framework

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Electronic correlations – the effect of interactions between electrons in a system – raise deep challenges to theoretical physics. While dynamical mean field theory (DMFT) and its cluster extensions are best suited for handling strong local interactions and aptly describe the resulting local and short-ranged correlations, extensions are needed when the feedback of nonlocal correlation effects beyond the cluster size needs to be taken into account.

In this presentation, I will describe a new method which unifies the Mott physics description of strongly-correlated materials with spin fluctuation theory or the *GW* approximation, which are designed to better capture long-range fluctuations. This method, dubbed 'TRILEX', is based on a local approximation of the three-particle irreducible vertex function. [1] [2] This vertex is self-consistently computed by solving a quantum impurity model with dynamical interactions in the charge and spin channels, using a continuous-time quantum Monte-Carlo algorithm. The electronic self-energy and the polarization constructed from this vertex are both frequency- and momentum- dependent. TRILEX incorporates local correlations as well as feedback from some long-range spin and charge fluctuations, at a comparatively low computational expense compared to existing cluster methods, making it a potentially useful tool for realistic computations in materials with both sizable interactions and long-ranged fluctuations.

I will show that in the two-dimensional Hubbard model at half-filling on a square lattice, the frequency-dependence of the three-leg vertex, as well as the momentum-dependence of the self-energy and polarizations, strongly depend on the correlation regime. Upon doping, this leads to a Fermi arc in the one-particle spectral function, which is one signature of the pseudo-gap state.

1. TA, Olivier Parcollet, Phys. Rev. B. 92, 115 109 (2015)
2. TA, Olivier Parcollet, arXiv 1512.06719