Real-space dynamical mean-field theory approach to the Hubbard model on finite honeycomb lattices

Models of correlated electrons on the honeycomb lattice are currently under intense theoretical and experimental investigation. One motivation is certainly the discovery of graphene that won the 2010 Nobel prize in physics. This realization of the Dirac physics on the honeycomb lattice is not only exciting from a fundamental point of view, but owing to the many unusual properties of this one-atom thin layer of carbon atoms bears also great promise for applications (see, e.g., [1–4]). One key feature is the existence of gapless edge states in the non-interacting system that give rise to a magnetic instability in the presence of interactions [5–9]. The typical tool used in this context is a mean-field decoupling of the Hubbard model [5–9]. While this mean-field decoupling is surprisingly accurate for certain quantities including dynamic ones [7, 9], the mean-field results for the stability range of the semi-metallic region at weak coupling [10] are known to underestimate its value as obtained by more accurate numerical methods [11–14].

During the one-month visit of Thomas Pruschke we plan to investigate if inclusion of dynamical fluctuations in the framework of dynamical mean-field theory (DMFT) [15] improves the accuracy the approximation, in particular for dynamical quantities. To be precise, we plan to employ a real-space version of DMFT (see, e.g., [16]) with the numerical renormalization group (NRG) [17] as solver for the associated impurity problem. The concrete problems that we plan to study include hexagonal "dots" as well as nanoribbons with zig-zag edges.

Thomas Pruschke is an internationally recognized expert on DMFT and its cluster generalizations [18] as well as the NRG [19]. In particular, we plan to use his NRG program. The one-month stay of Thomas Pruschke at the Université de Cergy-Pontoise is therefore essential to the success of the project.

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