Local and non-local correlation effects in nanoscopic systems

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We discuss how to apply many-body methods to correlated nanoscopic systems. First the criteria of validity for a treatment at the dynamical mean field theory (DMFT) approximation level, in which only local correlations are taken into account, are discussed. We then present the first results beyond the DMFT-level, i.e. taking into account nonlocal correlations via the Dynamical Vertex Approximation ("DΓA"). In order to test our scheme we consider one of the most difficult cases for DMFT, namely, for a quasi-one-dimensional molecule such as a benzene ring. The comparison against a numerically exact solution shows that nonlocal spatial correlations are relevant only in the limit of weak coupling between the molecule and the metallic leads and of low inter-atomic connectivity, otherwise DMFT provides a quantitative description of the system. As applications we investigate the role of correlations on electronic transport in quantum junctions, and we show that a local Mott-Hubbard crossover is a robust phenomenon in sharp nanoscopic contacts. Furthermore we analyze the effect of size reduction in Mn-nanoclusters.

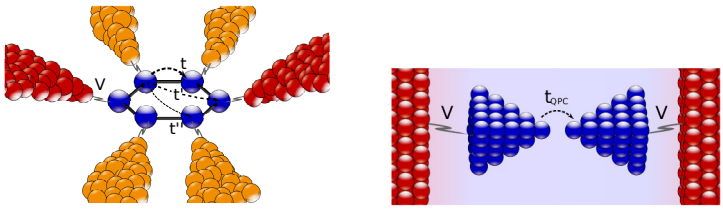

Figure 1: Schematic nanostructures considered in *Phys. Rev. Lett.* **104**, 246402 (2010)

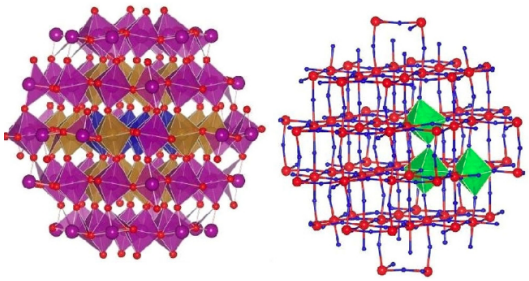

Figure 2: Realistic Mn-nanocluster considered in *Phys. Rev. Lett.* **107**, 197202 (2011)