Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Local and non-local correlations in nanoscopic systems GIORGIO SANGIOVANNI, A. VALLI, G. ROHRINGER, A. TOSCHI, K. HELD, Vienna University of Technology, H. DAS, Cornell University, T. SAHA-DASGUPTA, Bose National Centre for Basic Sciences — Tools for reliably treating nanoscopic systems, like coupled quantum-dots, ad-atoms on surfaces, macromolecules, etc., in the presence of electronic correlations are either missing or prohibitively expensive. We have implemented a new computational scheme based on a self-consistently defined set of local problems [1]. Our method scales linearly with the number of sites and allows us to perform large-scale sign-problem free Quantum Monte-Carlo simulations. We have studied the behavior of a single-atom junction formed upon stretching a metallic wire and found that a metal-insulator crossover is induced when the wire is about to break up. The combination with ab-initio techniques allowed us to study size-dependent properties of Manganite nano-clusters [2]. The simplest implementation of our method includes only local self-energy effects. We recently went beyond this and applied the resulting more sophisticated version of our method to an exactly solvable model finding results in remarkable agreement with the exact solution.

[1] A. Valli, G. Sangiovanni, O. Gunnarsson, A. Toschi and K. Held, PRL **104**, 246402 (2010)
[2] H. Das, G. Sangiovanni, A. Valli, K. Held and T. Saha-Dasgupta, PRL **107**, 197202 (2011)

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Date submitted: 11 Nov 2011 Electronic form version 1.4