Correlated zero-bias transport in nanostructures

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In the recent years, scanning tunnelling microscope as well as break-junctions experiments have opened new routes in the study of the Kondo effect and how it affects the transport properties of nano-devices. Similarly,the Kondo effect in graphene and 2D topological insulators (TI) [1] has also attracted considerable interest because of to the peculiar electronic properties of these systems: while an impurity spin in graphene interacts with the Dirac fermions of the lattice, an impurity on the edge of a 2D-TI interacts with the helical edge liquid. Here we first describe (within the tight-binding formalism) the electronic structure of several graphene and 2D-TI model nanostructures, which incorporates magnetic impurities. In particular, we discuss how electron correlation effects on the transport properties of these systems can be studied by combining continuous time quantum Monte Carlo with the Green function transport theory and the existing schemes, which allows for the calculation of the electrodes hybridization function [2]. Then, we highlight how the same method can be combined with density functional theory in the Smeagol electronic transport code [3] in order to include material specific properties. Finally we present some preliminary results about our in-progress implementation.

[1] F. Goth et al., Phys. Rev. B 88, 075110 (2013).

[2] I. Rungger and S. Sanvito, Phys. Rev. B 78, 085414 (2006).

[3] A.R. Rocha et al., Phys. Rev. B. 73, 085414 (2006).