Two Impurities Anderson Model for Kondo Simulation in Boron-doped Graphene Nanorribons

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Recently, magnetic moments have been identified in graphene nanoribbons doped with heteroatoms, more specifically in the 2B-7AGNR [1] (see Fig. 1 a). Due to the low spin-orbit and hyperfine interactions, magnetic moments are expected to have long coherence times in these carbon-based systems. Thus, these spin-hosting graphene nanostructures are promising metal-free systems for elementary quantum spintronic devices. So far, the experimental identification of localized magnetic moments in nanographenes has been almost solely based on the observation of Kondo-like features in scanning tunneling spectroscopy (see Fig 1 b). In this context, this work aims at modeling and understanding the basic processes underlying this behaviour. We aim to simulate the Kondo physics of the two-boron center in the 2B-7AGNR. To this end, we propose and simulate a Two Impurities Anderson Model (TIAM) using the Slave-Boson method [2]. The Slave-Boson method is a conserving perturbative technique based in diagrammatic expansion. In this work, we present the theoretical basis of this method and its application to impurity problems. We develop the diagrammatic expansion to first order, named the Non-Crossing Approximation, for the Single Impurity and the Two Impurities Anderson Model. Parameters for the model are obtained from density functional theory (DFT) ab initio simulations.

References

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Figures

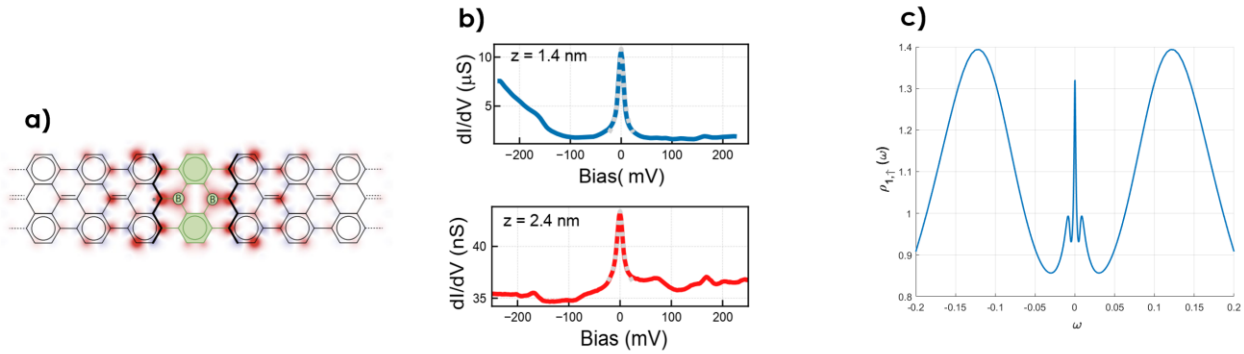

Figure 1: a) Schematic structure of the 2B-7AGNR. DFT computed spin densities in blue and red. **b)** Conductance against bias voltage for two STS measurements for 2B-7AGNR. **c)** Density of states of the TIAM for the simulated boron center in the 2B-7AGNR. The peak formed around ω=0 is the Kondo resonance. Parameters computed combining DFT calculations with ad-hoc substitutions. **a)** and **b)** extracted from [1]