Dynamical Mean-Field Theory for Electronic Structure and Transport Properties of Nanoscopic Conductors

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Dynamic correlations due to strong electron interactions can play a crucial role in determining the electronic structure and transport properties of nanostructures containing magnetic atoms. This has been most impressively demonstrated by the recent observation of Kondo effect in *ferromagnetic* nanocontacts [1]. Other recent examples demonstrating the importance of dynamic correlations in nanoscopic systems are the observation and manipulation of the Kondo effect in magnetic adatoms and molecules on metal surfaces [2-4].

We present a novel approach that allows to predict the electronic structure and transport properties of nanoscopic conductors taking fully into account the strong dynamic correlations arising from the strong electron-electron interactions of d- or f-electrons of transition metal atoms. Our approach combines *ab initio* electronic structure calculations with the Dynamical Mean-Field Theory (DMFT) in order to treat the dynamic correlations originating from the strongly interacting d- and f-electrons properly. This work extends upon our previous work considering a single magnetic impurity in a nanocontact [5] to the case of several magnetic atoms.

We demonstrate the importance of dynamic correlations for several experimentally relevant systems: A single magnetic impurity in a nanocontact (Fig. 1a), a single magnetic atom adsorbed on a graphene sheet (Fig. 1b), and a magnetic nanocontact consisting of several magnetic atoms (Fig. 1c). The examples show that dynamic correlations in these systems are indeed important and can give rise to Kondo effect which shows up as Fano features in the conductance vs. bias voltage characteristics similar to those observed in experiments. In contrast, conventional *ab initio* transport calculations based on density functional theory (DFT) cannot describe the dynamic correlations that lead to Kondo effect and the corresponding Fano features in the conductance as can be seen in Fig. 2.

References

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Figures

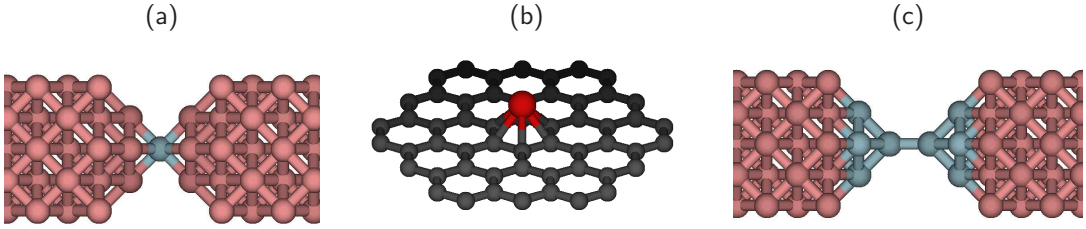

Fig. 1: (a) Single magnetic impurity in the contact region of a Cu nanocontact. (b) Single Co atom adsorbed at the hollow site of graphene sheet. (c) Ni nanocontact bridging two semi-infinite Cu nanowires.

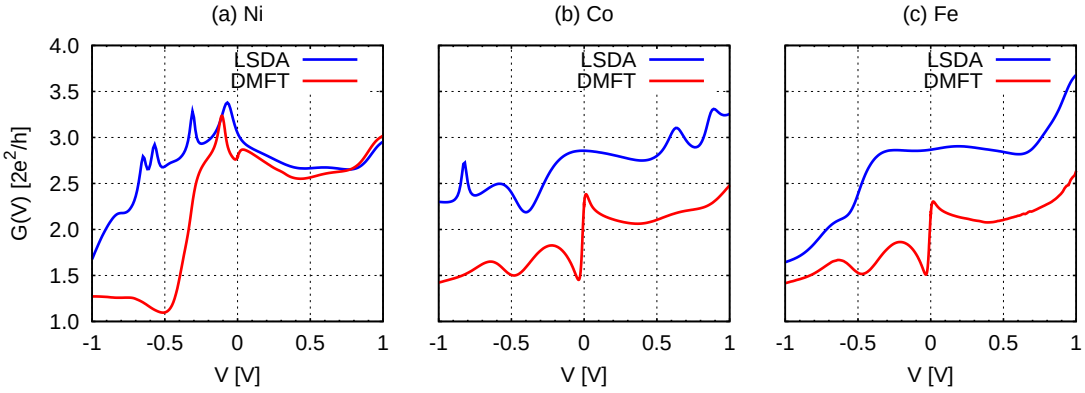

Fig. 2: Conductance vs. bias voltage of a Cu nanocontact hosting a single magnetic impurity calculated with the novel DMFT nanotransport method (red curves) on the one hand and with the conventional DFT based transport method (blue curves) within the local spin density approximation (LSDA) on the other hand.