Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Density-Functional Theory description of transport in the single-electron transistor[1] KRISSIA ZAWADZKI[2], LUIZ N. OLIVEIRA[3], University of Sao Paulo — The Kondo effect governs the low-temperature transport properties of the single electron transistor (SET), a quantum dot bridging two electron gases. In the weak coupling limit, for odd dot occupation, the gate-potential profile of the conductance approaches a step, known as the Kondo plateau. The plateau and other SET properties being well understood on the basis of the Anderson model, more realistic (i. e., DFT) descriptions of the device are now desired. This poses a challenge, since the SET is strongly correlated. DFT computations that reproduce the conductance plateau have been reported, e. g., by Bergfield et al., Phys. Rev. Lett. **108**, 066801 (2012), which rely on the exact functional provided by the Bethe-Ansatz solution for the Anderson model. Here, sticking to DFT tradition, we employ a functional derived from a homogeneous system: the parametrization of the Lieb-Wu solution for the Hubbard model due to França et al., New J. Phys. **14**, 073021 (2012). Our computations reproduce the plateau and yield other results in accurate agreement with the exact diagonalization of the Anderson Hamiltonian. The prospects for extensions to realistic descriptions of two-dimensional nanostructured devices will be discussed.

[1]Luiz N. Oliveira thanks CNPq (312658/2013-3) and Krissia Zawadzki thanks CNPq (140703/2014-4) for financial support.
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Date submitted: 11 Nov 2016 Electronic form version 1.4