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Kondo effect of magnetic impurities on nanotubes[1] PIER PAOLO BARUSELLI, SISSA, Via Bonomea, 265 34136 Trieste (Italy), CNR-IOM Democritos, ALEXANDER SMOGUNOV, SISSA, CEA Saclay, MICHELE FABRIZIO, ERIO TOSATTI, SISSA, ICTP, CNR-IOM Democritos — The effect of magnetic impurities on the ballistic conductance of nanocontacts is, as suggested in recent work, amenable to ab initio study [1]. Our method proceeds via a conventional density functional calculation of spin and symmetry dependent electron scattering phase shifts, followed by the subsequent numerical renormalization group solution of Anderson models – whose ingredients and parameters are chosen so as to reproduce these phase shifts. We apply this method to investigate the Kondo zero bias anomalies that would be caused in the ballistic conductance of perfect metallic (4,4) and (8,8) single wall carbon nanotubes, ideally connected to leads at the two ends, by externally adsorbed Co and Fe adatoms. The different spin and electronic structure of these impurities are predicted to lead to a variety of Kondo temperatures, generally well below 10 K, and to interference between channels leading to Fano-like conductance minima at zero bias.

[1] P. Lucignano, R. Mazzarello, A. Smogunov, and E. Tosatti, Nature Materials 8, 563 (2009).

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Pier Paolo Baruselli
SISSA, Via Bonomea, 265 34136 Trieste (Italy), CNR-IOM Democritos

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