MAR12-2011-005335

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Inelastic single-spin transport theory

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Spin-flip inelastic spectroscopy is a powerful tool for investigating the magnetic excitations of nano-scale magnets deposited on a metallic surface. In this talk I will present a perturbative approach to the calculation of the inelastic spin-flip spectra of magnetic adatoms, small magnetic clusters and magnetic molecules. The theory is based on the non-equilibrium Green's function formalism combined with a model spin Hamiltonian, where the conduction electrons are exchanged coupled to a system of quantum spins. By expanding the self-energy describing the electron-spin interaction to the third order we are able to capture both inelastic spin-flip events and the signature of Kondo resonances. Furthermore, when our approach is combined with a Master equation describing spin-relaxation, effects related to the spin-pumping at the single spin level can be described. In the talk I will demonstrate that the method offers an extremely good quantitative agreement with published experimental data. Importantly the formalism is amenable to be implemented together with highly accurate electronic structure methods.