MODELING REAL MAGNETIC IMPURITIES IN REAL METALS: APPLICATION TO TRANSPORT AND DEPHASING

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We construct and solve models of magnetic impurities in real metals by combining ab-initio density functional theory calculations with numerical renormalization group methods. Kondo atoms in bulk, on surfaces and in break junction geometries are considered. We apply our approach to resolve the longstanding problem of the correct low energy effective model of Fe impurities in Au and Ag, finding that a fully screened S=3/2 Kondo 3 channel model gives a consistent description of resistivity and decoherence measurements [1]

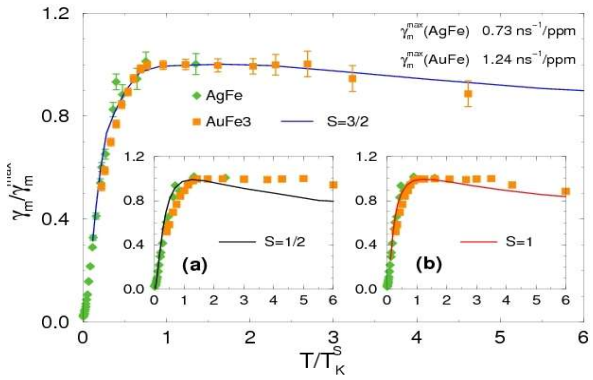

Figure. Calculated decoherence rates for S=1/2, 1, and 3/2 fully screened Kondo models compared to experimental data [1] for Fe impurities in Au and Ag showing that the S=3/2 Kondo model gives the best agreement.

[1] T.A.Costi,L.Bergqvist, A. Weichselbaum, J. von Delft, T. Micklitz, A. Rosch, P. Mavropoulos, P.H.Dederichs,F. Mallet, L.Saminadayar and C.Bauerle, Phys.Rev.Lett.102,056802(2009).