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Kondo decoherence: from ab-initio calculations to many-body Hamiltonians and beyond ...

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Understanding decoherence, the process by which a quantum system loses phase coherence by getting entangled with its environment, is important in the context of quantum computation. Here we show how decoherence, induced by dilute magnetic impurities and studied via weak antilocalization, can be harnessed to resolve a longstanding question concerning the classic Kondo systems of Fe impurities in the noble metals gold [1] and silver: which Kondo-type model yields a realistic description of the relevant multiple bands, spin and orbital degrees of freedom ? In order to answer this question we follow a three-pronged strategy: (i), we perform spin-resolved density functional theory calculations that suggest an $n = 3$ channel fully screened ($S = 3/2$) Kondo model, (ii), we solve this model for dynamic and transport properties using the numerical renormalization group method [2] within the complete basis set [3] and full density matrix approach [4], and, (iii), we compare the predictions to previous and new measurements of both the resistivity and decoherence rate in quasi 1-dimensional wires. We also compare the experimental data to $n = 1$ and 2 channel fully screened Kondo models (underscreened and overscreened models were previously shown to be incompatible with the data [5]). Excellent agreement is found for $n = 3$ with a *single* Kondo scale for *both* the resistivity and decoherence rate. This contrasts to previous comparisons [5] for an $n = 1$ fully screened Kondo model which could fit either the resistivity or the decoherence rate with a given Kondo scale, but not both. Our results set a new benchmark for the level of quantitative understanding attainable for the Kondo effect in real materials.

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