Spin fluctuations in nearly magnetic metals from ab-initio dynamical spin susceptibility calculations

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Abstract

We describe our theoretical formalism and computational scheme for making *ab-initio* calculations of the dynamic paramagnetic spin susceptibilities of metals and alloys at finite temperatures. Its basis is Time-Dependent Density Functional Theory within an electronic multiple scattering, imaginary time Green function formalism. Results receive a natural interpretation in terms of overdamped oscillator systems making them suitable for incorporation into spin fluctuation theories. Following a study of the nearly ferromagnetic metal Pd, we go on to describe the incommensurate and commensurate anti-ferromagnetic spin fluctuations in paramagnetic Cr and the compositionally disordered $Cr_{95}V_5$ and $Cr_{95}Re_5$ alloys together with the connection to the nesting of their Fermi surfaces. We compare and contrast the spin dynamics of these systems and identify those fluctuations with relaxation times much longer than typical electronic 'hopping times'.