

Abstract Submitted
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Ab-initio theory of spin fluctuations in magnets VLADIMIR ANTROPOV, LIQIN KE, Ames Laboratory, MARK VAN SCHILFGAARDE, Arizona State University, MIKHAEL KATSNELSON, Radboud University of Nijmegen — We propose a framework for a true ab initio theory of magnetism, based on many-body perturbation theory (MPBT). It fits in naturally with methods based MPBT such as the GW approximation; but the approach can be implemented as an extension to any existing static method for electronic structure such as the local spin density approximation to density functional theory, to include spin fluctuations. Initially we calculated the spin fluctuation contributions using random phase approximation. The self consistency procedure similar to the one used in Moriya-Kawabata theory can be naturally implemented. The fluctuation dissipation theorem is used to calculate the reduction of the mean field magnetic moment in itinerant magnets. The applications of the technique includes traditional 3d ferromagnetic metals, their alloys and compounds and 5f systems.

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