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First-Principle theory of Longitudinal Spin-Fluctuations at high temperatures for itinerant ferromagnets. SERGII KHMELEVSKYI, Center for Computational Material Science, Vienna University of Technology, ANDREI V. RUBAN, Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden, PETER MOHN, Center for Computational Material Science, Vienna University of Technology, BORJE JOHANSSON, Applied Material Physics, Royal Institute of Technology, Stockholm, Sweden — We have developed a framework for calculating parameters of effective magnetic Hamiltonian, which includes transverse as well as longitudinal spin fluctuations (LSF) on equal footing. The method is based on the set of constrained calculations within a Local Spin-Density Approximation and Coherent Potential Approximations. The used effective Hamiltonian is similar to those derived in Moriya-Takahashi theory approximating between local and weak itinerant limits of magnetism. The Curie temperatures, paramagnetic susceptibilities and magnetic specific heat have been calculated for bcc Fe and fcc Ni in good agreement with experiment. The importance of LSF contribution even for qualitatively correct description of magnetism of Ni is demonstrated. The first principles criteria for magnetic moment 'itineracy', based on fixed spin moment constrained calculations of a magnetic impurity in the Disordered Local Moment host, is established and applied to various magnetic systems. In particular, the famous Rhodes-Wohlfarth plot has been revisited. It is found that in some cases, like VAu_4, the magnetic moments have very local character in contrast to their long-standing interpretation as weak itinerant ferromagnets.

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