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Longitudinal spin fluctuations in itinerant ferromagnets

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Finite-temperature properties of magnetic materials strongly depend on their magnetic configuration given by relative orientation of local magnetic moments. In itinerant ferromagnets, an additional degree of freedom becomes important: the value of local magnetic moment, which is sensitive to the magnetic state and the local chemical environment of atoms as well as the thermal electronic excitations of different type, leading to the so-called longitudinal spin fluctuations (LSF). LSF play an important role in itinerant magnetic systems at high temperatures. In particular, they are responsible for the existence of finite local magnetic moments on atoms in the paramagnetic state, which affect different physical properties. At the same time, an ab initio based description of the LSF is problematic. The LSF are ignored in the local density and related approximations of density functional theory, which for instance leads into a substantial underestimation or complete disappearance of the local magnetic moments on atoms in the itinerant ferromagnets in the corresponding calculations at high temperature in the paramagnetic state. Although the LSF can be included in more elaborate schemes, such as the dynamical mean-field theory, the application of such techniques to real systems is too cumbersome in most cases. In this work a generalized form of classical magnetic Hamiltonian is suggested, which includes both transverse and longitudinal spin fluctuations on equal footing. Parameters of the Hamiltonian can be determined in the first-principles calculations, within the local spin density approximation. The method is applied to the calculations of high-temperature magnetic properties of Fe, Co and Ni, including the Curie temperature. The effect of the LSF in the high-temperature paramagnetic state on chemical interactions and other physical properties is demonstrated for several alloys, including fcc Fe-Cr-Ni alloys, which is the basis of austenitic stainless steels.