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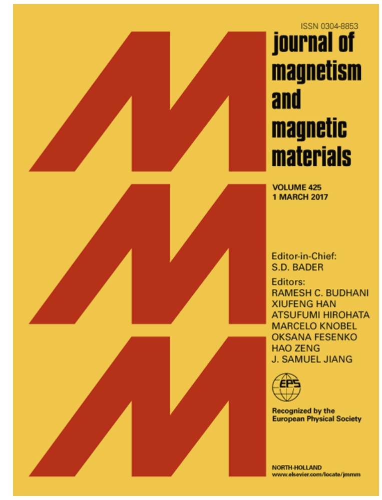

Longitudinal integration measure in classical spin space and its application to first-principle based simulations of ferromagnetic metals

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Longitudinal integration measure in classical spin space and its application to first-principle based simulations of ferromagnetic metals.

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The classical Heisenberg type spin Hamiltonian is widely used for simulations of finite temperature properties of magnetic metals often using parameters derived from first principles calculations. In itinerant electron systems, however, the atomic magnetic moments vary their magnitude with temperature and the spin Hamiltonian should thus be extended to incorporate the effects of longitudinal spin fluctuations (LSF). Although the simple phenomenological spin Hamiltonians describing LSF can be efficiently parameterized in the framework of the constrained Local Spin Density Approximation (LSDA) and its extensions, the fundamental problem concerning the integration in classical spin space remains. It is generally unknown how to integrate over the spin magnitude. Two intuitive choices of integration measure have been used up to date - the Murata-Doniach scalar measure and the simple three dimensional vector measure. Here we derive the integration measure by considering a classical limit of the quantum Heisenberg spin Hamiltonian under conditions leading to the proper classical limit of the commutation relations for all values of the classical spin magnitude and calculate the corresponding ratio of the number of quantum states. We show that the number of quantum states corresponding to the considered classical spin magnitude is proportional to this magnitude and thus a non-trivial integration measure must be used. We apply our results to the first-principles simulation of the Curie temperatures of the two canonical ferromagnets bcc Fe and fcc