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Berry phase Chern number spin Hamiltonians for nanomagnets using DFT techniques¹

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We will present a formalism capable of describing the low-energy spin dynamics of ferromagnetic metal nanoclusters consisting of up to a few tens of atoms[1]. Our procedure is based on a quantum action with a single magnetization-orientation degree of freedom corresponding to the direction of the Kohn-Sham spin- density functional theory wave-function. Besides the magnetic anisotropy energy functional, the action contains a Berry phase term arising when the fast electronic degrees of freedom are integrated out. The associated Berry curvature has a nontrivial dependence on magnetization orientation when spin-orbit interactions are included; its average over all magnetization directions is a topological invariant known as Chern number, which can only be a multiple of half integers. From the magnetic anisotropy energy and Berry curvature functionals, it is possible to construct an effective quantum Hamiltonian for the nanomagnet, in terms of a single giant-spin degree of freedom whose magnitude is equal to the Berry phase Chern number. We illustrate this procedure by computing within DFT the anisotropy energy and Berry curvature for small clusters of transition metal atoms, from which we extract the corresponding spin Hamiltonians. We show that the Berry phase term can profoundly alter the dynamics of the spin degree of freedom. Our approach can address the spin dynamics of small nanomagnets, which is now accessible experimentally in STM-engineered magnetic clusters[2]. [1] C.M. Canali, A. Cehovin and A.H. MacDonald, Phys. Rev. Lett. **91**, 046805 (2003); [2] C.F. Hirjibehedin et al., Science **312**, 1021 (2006); D. Kitchen et al., Nature **442**, 436 (2006).

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