(TD)DFT for noncollinear spins: orbital functionals, semilocal approximations, and xc torques

Carsten A. Ullrich
University of Missouri

Most commonly used approximations in (TD)DFT for noncollinear magnetism are based on reference systems with collinear spins and fail to capture exchange-correlation (xc) torque effects. We present a semilocal exchange-correlation energy functional for noncollinear spin density functional theory based on short-range expansions of the spin-resolved exchange hole and the two-body density matrix [1]. Our functional is explicitly derived for noncollinear magnetism, is U(1) and SU(2) gauge invariant, and gives rise to nonvanishing xc torques. Testing the functional for the ground state of frustrated antiferromagnetic chromium clusters, a delicate interplay between exchange and correlation torques is uncovered. We then consider small Hubbard clusters, including spin-orbit coupling induced geometric spin frustrations, and find that xc torques make a significant contribution to the noncollinear spin dynamics [2].

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[1] Nicolas Tancogne-Dejean, Angel Rubio, and Carsten A. Ullrich, Phys. Rev. B **107**, 165111 (2023)
[2] Daniel Hill, Justin Shotton, and Carsten A. Ullrich, Phys. Rev. B **107**, 115134 (2023)