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Generalized-gradient approximations with non-vanishing exchange-correlation magnetic torque GIOVANNI SCALMANI, Gaussian, Inc., STEFANO PITTALIS, Department of Physics and Astronomy, University of Missouri-Columbia, MICHAEL J. FRISCH, Gaussian, Inc., GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri-Columbia — The description of systems of interacting electrons in the presence of magnetic fields, within spin-density functional theory (SDFT), requires the non-collinear magnetization density vector $\mathbf{m}(\mathbf{r})$ to be used as basic variable, along with the particle density $n(\mathbf{r})$. Futhermore, for a meaningful description of spin-dynamics, the magnetization density and its conjugate exchange-correlation (xc) field $\mathbf{B_{xc}}(\mathbf{r})$ must not be constrained to be locally parallel at every point in space. It is well known that the local density approximation (LDA) cannot, by construction, provide such a non-collinear configuration of the two vector fields. Here we show how popular generalized gradient approximations (GGAs), developed assuming collinear spin-density, can be used to describe non-collinear magnetization states, including the presence of non-vanishing local torque between $\mathbf{m}(\mathbf{r})$ and $\mathbf{B_{xc}}(\mathbf{r})$. Unlike previous attempts to extend the use of collinear GGAs to the domain of non-collinear magnetization densities, the approach we introduce is invariant with respect of spin-rotations, globally satisfies the *zero-torque theorem*, reduces to the proper collinear limit and is numerically stable.

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