New gradient functional for SDFT derived from spin spirals in the uniform electron gas F.G. EICH, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Halle, Germany — The development of functionals in SDFT depending on gradients of the spin magnetization is a long standing challenge. We present a new functional based on the spin-spiral state of the uniform electron gas. Comparing the principal idea of the new functional to the LSDA and GGAs, we highlight the intrinsic way non-collinearity is built into the proposed approximation. As key feature the functional yields exchange-correlation magnetic fields that are non-collinear w.r.t. the spin magnetization, while obeying the zero-torque theorem by construction. This means that an adiabatic application of the functional within TD-SDFT accounts for the local torque exerted by the exchange-correlation field and retains the numerical simplicity of explicit density functionals. An implementation of the functional based on the RPA-treatment of spin spirals in the electron gas is shown.

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