U(1)×SU(2) Gauge Invariance Made Simple for Density Functional Approximations

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A semi-relativistic density-functional theory that includes spin-orbit couplings and Zeeman fields on equal footing with the electromagnetic potentials, is an appealing framework to develop a unified first-principles computational approach for non-collinear magnetism, spintronics, orbitronics, and topological states. The basic variables of this theory include the paramagnetic current and the spin-current density, besides the particle and the spin density, and the corresponding exchange-correlation (xc) energy functional is invariant under local U(1)×SU(2) gauge transformations. The xc-energy functional must be approximated to enable practical applications, but, contrary to the case of the standard density functional theory, finding simple approximations suited to deal with realistic atomistic inhomogeneities has been a long-standing challenge. Here, we propose a way out of this impasse by showing that approximate gauge-invariant functionals can be easily generated from existing approximate functionals of ordinary density-functional theory by applying a simple *minimal substitution* on the kinetic energy density, which controls the short-range behavior of the exchange hole. Our proposal opens the way to the construction of approximate, yet non-empirical functionals, which do not assume weak inhomogeneity and should therefore have a wide range of applicability in atomic, molecular and condensed matter physics.