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

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DATE / TIME: Monday, December 12th 2016, 4:00 p.m.
LOCATION: Seminar Room DB gelb 09, TU Wien, "Freihaus"-building, 9th floor

A non-relativistic density-functional approach that includes spin-orbit couplings self-consistently is an appealing framework to develop a unified first-principles computational approach for non-collinear magnetism, spintronics, and spinorbitronics. The basic variables of this framework include the (paramagnetic) particle- and spin-currents besides the particle- and spin-densities. The corresponding exchange-correlation energy functional is invariant under local U(1)×SU(2)-gauge transformations. This functional must be approximated to enable practical applications but, contrary to the standard case, it has been a long-standing challenge to find simple building blocks ideally suited to deal with realistic atomistic inhomogeneities. Here, we propose a non-empirical resolution based on the analysis of the short-range behavior of the exchange-hole function and related quantities. Novel prototypical approximations will be outlined.