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Construction of a spin-density functional for models of strongly correlated systems: including spin improves the description of charge KLAUS CAPELLE, UFABC, DANIEL VIEIRA, Universidade do Estado de Santa Catarina, VIVIAN FRANCA, Albert Ludwigs Universität — An explicit spin-dependence is built into a class of previously developed density functionals for models of strongly correlated systems. As a side effect of accounting for the spin-degrees of freedom, the functional also provides an improved description of the charge-degrees of freedom. In particular, unlike earlier proposals, the present parametrization correctly predicts a positive Mott gap at half filling for any repulsive interaction. Applications to spatially inhomogeneous models, e.g. in the presence of impurities, external fields or trapping potentials are worked out and results are shown to be in excellent agreement with independent many-body calculations, at a fraction of the computational cost. See New J. Phys. 14 073021 (2012).

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