Density-functional theory for the Hubbard model: numerical results for the Luttinger liquid and the Mott insulator

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We construct and apply an exchange-correlation functional for the one-dimensional Hubbard model. This functional has built into it the Luttinger-liquid and Mott-insulator correlations, present in the Hubbard model, in the same way in which the usual *ab initio* local-density approximation (LDA) has built into it the Fermi-liquid correlations present in the electron gas. An accurate expression for the exchange-correlation energy of the homogeneous Hubbard model, based on the Bethe Ansatz (BA), is given and the resulting LDA functional is applied to a variety of inhomogeneous Hubbard models. These include finite-size Hubbard chains and rings, various types of impurities in the Hubbard model, spin-density waves, and Mott insulators. For small systems, for which numerically exact diagonalization is feasible, we compare the results obtained from our BA-LDA with the exact ones, finding very satisfactory agreement. In the opposite limit, large and complex systems, the BA-LDA allows to investigate systems and parameter regimes that are inaccessible by traditional methods.