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Density-functional theory of interacting electrons in inhomogeneous quantum wires SAEED H. ABEDINPOUR, MARCO POLINI, GAO XI-ANLONG, MARIO P. TOSI, NEST-CNR-INFM and Scuola Normale Superiore, I-56126 Pisa, Italy — Motivated by the experimental evidence of electron localization in cleaved edge overgrowth quantum wires and by the recent interest in the development of density-functional schemes for inhomogeneous Luttinger and Luther-Emery liquids, we present a novel density-functional study of a few interacting electrons confined by power-law external potentials into a short portion of a thin quantum wire. The theory employs the quasi-one-dimensional (Q1D) homogeneous electron liquid as the reference system and transfers the appropriate Q1D ground-state correlations to the confined inhomogeneous system through a suitable local-density approximation (LDA) to the exchange and correlation energy functional. The LDA describes accurately "liquid-like" phases at weak coupling but fails in describing the emergence of "Wigner molecules" at strong coupling. A local spin-density approximation allowing for the formation of antiferromagnetic quasi-order with increasing coupling strength is proposed as a first step to overcome this problem.

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