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A Kinetic Energy Functional From the Airy Gas Model ALEXANDER LINDMAA, Linkoping University, ANN MATTSSON, Sandia National Laboratories, RICKARD ARMIENTO, Linkoping University — We present a density functional for the kinetic energy derived from the Airy gas model, which is a model system for an edge electron gas. Electronic edges are the regions in a system where the electronic density changes to become exponentially decaying, and the electron physics requires special consideration. The Airy model describes an electron gas around the classical turning point, where the electrons interact with a uniform force-field, i.e., an effective linear potential along one of the spatial coordinates. A formally exact energy density is derived in terms of Airy functions and is parametrized to behave correctly in the Thomas-Fermi and von Weizsäcker limits. In contrast to already existing kinetic energy functionals derived from the Airy gas, starting from a closed-form expression yields greater freedom in the choice of parametrization. Comparative tests between our and previous functionals are presented. Improved kinetic energy functionals are highly relevant in the context of orbital-free DFT (OF-DFT) as well as for applications at very high temperature.

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