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Temperature dependence of Thomas-Fermi errors¹ AURORA PRIBRAM-JONES, Department of Chemistry, University of California, Irvine, KIERON BURKE, Departments of Physics and Chemistry, University of California, Irvine — Finite temperature Thomas-Fermi theory, in addition to its success in systems dominated by classical behavior, can also form the basis for development of a finite temperature local density approximation and its leading corrections. It is therefore imperative that we fully understand its limitations and strengths. To this end, the temperature dependence of Thomas-Fermi errors in densities and integrated quantities for simple models is explored. Behavior of finite-temperature Thomas-Fermi theory in limiting cases will be discussed in the contexts of traditional DFT and its semiclassical foundations. Analysis of finite temperature Thomas-Fermi as a potential functional will be presented.

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