Revised Thomas-Fermi Functional for Singular Potentials[1] JAMES
DUFTY, SAMUEL TRICKEY, Univ. Florida — Approximations to the non-
interacting free energy density functional that include the Thomas-Fermi (TF) func-
tional, or a local density approximation, lead to singular densities for singular exter-
nal potentials (e.g. Coulomb). We address this limitation of the TF approximation
by a formal map of the exact functional for a given external potential onto a fic-
titious TF functional for an effective external potential. The latter functional is
found to be a "regularized" version of the external singular potential, tempered by
convolution with the finite temperature Lindhard response function. The result is
a Thomas-Fermi approximation but with the singularity removed. Applications at
high and low temperatures are described, including comparison with the Parr-Ghosh
cusp-condition procedure for a non-singular TF density at zero temperature.

Samuel Trickey
Univ. Florida