

Abstract Submitted  
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**Generalized Gradient Approximation for Exchange-Correlation Free Energy**<sup>1</sup> VALENTIN KARASIEV, Physics and QTP, Univ. Florida, JAMES DUFTY, Physics, Univ. Florida, SAMUEL TRICKEY, Physics and QTP, Univ. Florida — The exchange-correlation (XC) free-energy is an essential ingredient of density functional theory (DFT). Use of a ground-state functional completely misses the explicit T-dependence. Depending on state conditions, that dependence can be important for warm dense matter (WDM)[2]. The local density approximation [1] XC free-energy functional has the proper T-dependence for the homogeneous electron gas. Here we analyze the finite-T gradient corrections for the X and C contributions to identify the appropriate T-dependent dimensionless density gradient variables. We then introduce a generalized gradient approximation (GGA) for the XC free energy with correct limits [3]. The result, together with the VT84F finite T GGA for the non-interacting free energy [4] provides a non-empirical GGA free-energy functional for WDM. 1. V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. 112, 076403 (2014). 2. V.V. Karasiev, L. Calderin, and S.B. Trickey, Phys. Rev. E 93, 063207 (2016). 3. V.V. Karasiev, J. Dufty, and S.B. Trickey, manuscript in preparation. 4. V.V. Karasiev, D. Chakraborty, O.A. Shukruto, and S.B. Trickey, Phys. Rev. B 88, 161108(R) (2013).

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