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Local Density Approximation Exchange-correlation Free-energy Functional[1] VALENTIN KARASIEV, University of Florida, TRAVIS SJOSTROM, LANL, JAMES DUFTY, S.B. TRICKEY, University of Florida — Restricted path integral Monte-Carlo (RPIMC) simulation data for the homogeneous electron gas at finite temperatures [1] are used to fit the exchange-correlation free energy as a function of the density and temperature. Together with a new finite-T spin-polarization interpolation, this provides the local spin density approximation (LSDA) for the exchange-correlation free-energy functional required by finite-T density functional theory. We discuss and compare different methods of fitting to the RPIMC data. The new function reproduces the RPIMC data in the fitting range of Wigner-Seitz radius and temperature, satisfies correct high-density, low- and high-T asymptotic limits and is applicable beyond the range of fitting data.

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