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Finite temperature orbital-free density functional theory MD for warm dense matter systems[1] TRAVIS SJOSTROM, JEROME DALIGAULT, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Warm dense systems present significant challenges for ab initio simulations. In order to incorporate the quantum nature of these systems, state of the art approaches use Kohn-Sham DFT. The number of orbitals required in this approach however scales with the temperature, making it computationally prohibitive. In recent years attention has been given to orbital-free (OF) DFT, which depends only on the density and does not suffer the same scaling issue. For the most part the finite temperature Thomas-Fermi approximation has been used, with some efforts making use of the gradient expansion, or a generalized gradient form. Interestingly, zero temperature OF DFT efforts have made use of non-local functionals based upon linear response theory, with marked improvement over gradient methods. Here we explore extension of this approach to finite temperature. We have implemented the new approximations in both an average atom scheme and for extended systems in OF MD, and will present here the results for system in the warm dense matter regime.

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