Nonlocal orbital-free density functional theory for warm dense matter

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Accurate simulations of warm dense matter remain challenging in current research, while being motivated further as recent experiments probe more accurately into this regime. While the *de facto* standard is quantum molecular dynamics using Kohn-Sham DFT, this methods scales significantly with temperature due to the orbital dependence. From the other side, the orbital-free Thomas-Fermi approximation works well for hot dense systems, but loses accuracy at lower temperatures. Recently developed nonlocal orbital-free functionals for the noninteracting free energy [Phys. Rev. B 88, 195103], which show near Kohn-Sham accuracy for broad ranges of temperature and density are presented. The application of which are detailed in regards to pseudopotentials and molecular dynamics for various systems. Comparisons with local orbital-free methods as well as orbital-dependent Kohn-Sham calculations, including accuracy and computational cost are made.

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