Semiclassical self-consistent and thermodynamically consistent average atom model

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Investigation of material properties at extremes, which are essential for high energy density physics development, requires the most advanced experimental facilities, theories, and computations. Nowadays it is possible to model properties of matter in such conditions using the state-of-the-art density functional theory (DFT) or path-integral Monte–Carlo approaches with remarkable precision. However, fundamental and computational limitations of these methods impede their practical usage while wide-range thermodynamic and transport models of plasma are required. As a consequence, an average atom (AA) framework is still relevant today and has been attracting more and more attention lately. The self-consistent field and electron density in an atomic cell is usually obtained using the Thomas–Fermi (TF), Hartree–Fock, Kohn–Sham approaches, or their extensions. In this study we present the AA model, where semiclassical wave functions are used for bound states, while free electrons are approximated by the TF model with a thermodynamically consistent energy boundary. The model is compared in various regions of temperatures and pressures with the reference data: Saha model for rarefied plasma, DFT for warm dense matter, and experimental shock Hugoniot data. It is demonstrated that a single AA model may provide a reasonable agreement with the established techniques at low computational cost and with stable convergence of the self-consistent field.