A wide-range model of metal plasmas based on semiclassical average atom model with self-consistent field

Polyukhin A S^{1,2,@}, Dyachkov S A^{1,3} and Levashov P R^{1,2}

- 1 Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
- 2 Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia
- 3 Dukhov Research Institute of Automatics (VNIIA), Sushchevskaya 22, Moscow 127055, Russia

Fluid dynamic simulations of complex phenomena in high energy density physics should be supplied with a high quality equation of state for matter. The approaches based on the density functional theory (DFT) [1] allow us to calculate various properties of substances in a wide range of temperatures and pressures, but they usually have high computational complexity and require significant supercomputer resources. The simple theoretical models [2] agree with experimental data only in some regions of the phase diagram, which limits their application. The purpose of this study is to develop a relatively simple, but reasonable wide-range model for thermodynamic properties evaluation. In contrast to the conventional Thomas–Fermi model and its extensions [3], we use the semiclassical approach in the average atom framework to estimate the self-consistent density of electrons and their energy levels. The resulting model is similar to the Hartree–Fock–Slater one, but with the reduced complexity and enhanced convergence properties due to the predefined form of the wave functions. We demonstrate the wide-range thermodynamic consistency of the model and the proper asymptotic behavior compared to Saha model, DFT, and the Thomas–Fermi model. Supported by RSF grant No. 20-42-04421.

- [1] Kohn W and Sham L J 1965 Phys. Rev. A. 140 1133–1141
- [2] Feynman R P, Metropolis N and Teller E 1949 Phys. Rev. 75 1561–1573
- [3] Nikiforov A F, Novikov V G and Uvarov V B 2005 Quantum-Statistical Models of Hot Dense Matter (Basel: Birkhäuser)

[®] polyukhinas@gmail.com