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Improved spherical atomic models for the opacity of warm/hot dense plasmas

In the recent decades, there is an increasing interest in the properties of material under extreme conditions of temperature and density (T-rho). The physical description of stars and planets formation and evolution, controlled fusion experiments and laser-material interaction requires the knowledge of the equation of state, opacity, ionization degree and some other physical quantities in a wide range of T-rho for many materials. Since there are no experimentally measured databases for these quantities, in such wide ranges of T-rho, these physical quantities are calculated, theoretically, using computational simulations. A popular theoretical approach for calculating the required quantities for plasmas relies on spherical models, like the ion-sphere average atom (ISAA) model [1]. In this simplified model, the electron-electron (e-e) interaction is approximated by the LDA/GGA exchange-correlation potential, and the interaction with the surrounding plasma ions is poorly described through the boundary condition of the ISAA's eigenfunctions. I will present an improved ISAA model which uses approximate optimized effective potentials, like KLI-SIC and KLI-EXX [2], for the e-e potential and the hyper-netted chain (HNC) [3] approximation for realistic description of the ion-plasma interaction. Also, improved opacity calculations, which are based on the improved potentials, will be presented for astrophysical systems and laser-plasma experiments, using the CRSTA code [4].

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