Quasizone model of hot dense matter

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There exists a problem in dense plasma simulations known as density effects, and it is yet far from being solved. For instance, all the recent conferences on opacity calculations hold the discussions on the influence of high density and pressure effects on energy spectra and opacity coefficients. The same situation exists in simulation of thermodynamic properties of plasma. In every-day calculations there are used old empiric formulas, such as by Inglis-Teller or Pryatt, along with methods of cutting off bound levels according to orbit’s radius. These methods allow to describe the density effects qualitatively, but don’t provide the understanding of the physical processes. The considered methods work only within small density range solving the problem just partially.

One of the simplest, but at the same time pretty much effective method to account for density effects is the Thomas-Fermi (TF) model for high density plasma. Once improved with exchange and correlation corrections, the TF model becomes quite adequate over wide range of high density and temperature.

But there are some drawbacks in the TF model and the major one is that the electron energy spectrum is presumed to be continuous, which is very rough approximation. Thus the TF model is incapable to describe the very important aspect of ionized matter – the shell structure of ions. In order to describe the shell structure, the self-consistent field models can be applied, and one of the well known representatives of such methods is the Hartree-Fock-Slater (HFS) model [1]. We use the average atom approximation in order to describe the ensemble of ions in different states. As a result, we get one ion with average occupation numbers inside electrically neutral spherical cell. Energy spectrum of this ion is divided into three groups of states – bound, continuous and intermediate. For simulation of intermediate (weakly coupled) states, the model of averaged spherical cells with quasi-periodical boundary conditions is being used and concept of “quasizone” is implied. This approach brings out unified model, that allows to perform calculations for various substances at arbitrary density and temperature. As a result, we can get detailed information about energy spectrum of electrons in studied substance, smooth thermodynamic functions within wide region of temperatures and densities (the actual calculations have been done for densities from 10^{-4} g/cm^3 up to 10^4 g/cm^3 and for temperatures from 1 eV up to 10 keV).

During growth of density, bound levels in energy spectrum evolve through intermediate states into continuum. Proper description of this process is very important for development of physically adequate model of matter. The offered quasizone model seems to meet this requirement quite satisfactorily in comparison with other models.

The calculations are being made using numerical wave functions for all groups of states of electrons. As an example, equation of state and shock adiabats for He, Be, Al, Fe, Sn and Pb are presented.

References

[1] *Nikiforov A.F., Novikov V.G., Uvarov V.B.*, Quantum-Statistical Models of Hot Dense Matter. Methods for Computation Opacity and Equation of State. Birkhäuser, 2005.