

A variational atomic model of plasma accounting for ion radial correlations and electronic structure of ions (VAMPIRES)

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We propose a model of ion-electron plasma (or nucleus-electron plasma) that accounts for the electronic structure around nuclei (i.e. ion structure) as well as for ion-ion correlations. The model equations are obtained through the minimization of an approximate free-energy functional, and it is shown that the model fulfills the virial theorem. The main hypotheses of this model are 1) nuclei are treated as classical indistinguishable particles 2) electronic density is seen as a superposition of a uniform background and spherically-symmetric distributions around each nucleus (system of ions in a plasma) 3) free energy is approached using a cluster expansion 4) resulting ion fluid is modeled through an approximate integral equation.

In this presentation we will describe the set of hypotheses of this model, sketch the derivation of the model equations and comment on them. We will show how this model fulfills the virial theorem, allowing a sound definition of the related thermodynamic quantities. Finally, we will show results from numerical calculations, comparison with other models such as VAAQP or INFERN0, and discuss the limitations of the model.

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