

Thermodynamic limit of the Coulomb system in the model of a bounded one-component plasma

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The classical one-component plasma (OCP) bounded by a spherical surface (BOCP) is studied using molecular dynamics (MD). A series of simulations performed for BOCP containing large number (up to 50,000) of ions allowed us to establish the size dependences of the investigated quantities and extrapolate them to the thermodynamic limit. In particular, the total electrostatic energy per ion was estimated in the thermodynamic limit of OCP over a wide range of the Coulomb coupling parameter Γ from 0.03 to 1000 with a relative error not exceeding 0.1%. The calculated energies for $\Gamma < 30$ are approximately 0.5% lower than those obtained previously in the Monte Carlo (MC) simulation of OCP with periodic boundary conditions and in the MD simulation of OCP using the LAMMPS software package, carried out in this work, and for $\Gamma > 174$, they almost coincide with the MC and MD results. The excess interionic and ion-background interaction energies are introduced. These energies allow calculation of the ionic compressibility factor, which is inaccessible in ordinary MC and MD simulations of OCP. The resulting wide-range ionic equation of state can be recommended for testing the correctness of OCP simulations with various effective interaction potentials, which is especially important when studying the transport properties of OCP. Based on this equation of state, the cutoff parameter used in LAMMPS was calculated, ensuring reproduction of a correct state equation. The importance of choosing an accurate cutoff parameter is illustrated by LAMMPS simulation of the fluid–solid transition in OCP, which shows that the position of metastable region depends significantly on this parameter.