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

Zhukhovitskii D. I.[1] **and Perevoshchikov E. E.**[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, 141701, Russia

[@] perevoshchikyy@jiht.ru

We present a molecular-dynamics study of a bounded one-component plasma (BOCP): identical classical ions embedded in a uniform neutralizing background and confined by a rigid, specularly reflecting spherical wall. By simulating a sequence of sufficiently large BOCP systems and quantifying finite-size trends, we extrapolate key quantities to the thermodynamic limit. In particular, we obtain the electrostatic energy per ion over a wide range of the Coulomb coupling parameter $0.03 \leq \Gamma \leq 1000$ with a typical relative uncertainty of $\sim 10^{-3}$. The resulting energies are systematically lower than several modern periodic-boundary Monte Carlo datasets at $1 \lesssim \Gamma \lesssim 30$ (by roughly 0.5%), while converging to the same weak- and strong-coupling limit at low and high Γ, respectively. Beyond the conventional total energy, we introduce two separately convergent quantities — the excess interionic energy and the excess ion–background energy — which together yield the ionic compressibility factor and thus an ionic equation of state not directly accessible in standard periodic OCP simulations. Using this EOS as a reference, we propose an improved Γ-dependent real-space cutoff for interionic forces in LAMMPS workflow, and demonstrate that kinetic and interfacial measures can depend sensitively on cutoff choice. These results provide a high-precision benchmark for validating plasma simulation methods and for calibrating approximate free-energy models across weak to strong coupling. The BOCP framework also offers a controlled route to extract thermodynamic derivatives from particle simulations without relying on periodic-image conventions.