Finite-size effects in one-component plasma with and without long-range interactions

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The dependence of thermodynamic properties upon the number of particles N is one of the main problems of atomistic simulation for calculating properties in the thermodynamic limit [1]. Usually, to reduce finite-size effects, periodic boundary conditions are imposed on the computational cell [2]. In Coulomb systems, the influence of periodic images should be taken into account, leading to a finite-range Ewald potential. However, simulations of Coulomb systems are often performed with the truncated Coulomb potential, i.e. without taking long-range effects into account [3].
Using a one-component plasma as an example, we study the effect of long-range interactions on the N-convergence of the plasma potential energy by calculating the energy dependence on the number of particles for the truncated Coulomb, Ewald and angular-averaged Ewald potentials [4]. It turns out that taking into account long-range interaction effects with the Ewald technique significantly improves the convergence of the energy with the number of particles in the medium- and strong-coupling regimes.
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