IMPLEMENTATION OF THE CALCULATION OF THE PRESSURE OF A ONE-COMPONENT PLASMA

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The electrostatic energy of an infinite electrically neutral system of charged particles is a conditionally convergent series, the sum of which depends on the summation order. Ewald proposed the solution to this problem for systems with translational symmetry. As a result, the expression for energy takes the form of a sum over all particles in a cell with some effective anisotropic interaction potential, the Ewald potential. In 2022 [1], G.S. Demyanov and P.R. Levashov completed the theoretical justification of the angular-averaged Ewald potential (AAEP), which was first introduced by E. Yakub and C. J. Ronchi [2, 3], and showed its effectiveness in calculating the energy of a one-component plasma (OCP) for a million particles [4].

In this work, we calculate the pressure for the equilibrium OCP obtained by the Monte Carlo method [5] in four ways. The first method is to differentiate the partition function with respect to volume. The expression for the derivative is obtained analytically by scaling the computational cell by some parameter and then differentiating with respect to it. The second method applies the virial theorem to a system whose particles interact in terms of a pair potential. In this work, we perform calculations using these two methods for the Ewald potential and AAEP, and analyze the differences in pressure results.

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