Reliable thermodynamic limit of a one–component plasma energy using angular–averaged Ewald potential

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A one–component plasma (OCP) is a simple model of a substance under extreme conditions in which ions can be considered classical and electrons are highly degenerated. Commonly, the Ewald summation technique is used to model such long–range disordered Coulomb plasmas. However, the anisotropic Ewald potential can be redundant and computationally expensive. In 2003, Yakub and Ronchi introduced an angular–averaged Ewald potential (AAEP) for a two–component plasma (TCP) [1] that can be used to efficiently simulate two–component Coulomb systems [2,3]. This potential for an OCP is not the same as that of a TCP; besides, the expression for the OCP energy in Yakub and Ronchi's paper [4] is incorrect. In our work [5], we present a rigorous derivation of the AAEP OCP as well as the correct expression for the energy and perform Monte Carlo (MC) simulations of OCP in the range of coupling parameter from 0.1 to 100; up to a *million* particles is used in the calculations to obtain a reliable thermodynamic limit. We find the simulation method to be much more efficient compared to other known methods [6, 7] and useful for MC simulations of the "jellium" model, the quantum mechanical analog of an OCP.

[1] Yakub E and Ronchi C 2003 *J. Chem. Phys.* **119** 11556–11560
[2] Demyanov G S and Levashov P R 2022 *J. Phys. A Math. Theor.* **55** 385202
[3] Demyanov G S and Levashov P R 2022 *Contrib. Plasma Phys.* **62** e202200100
[4] Yakub E and Ronchi C 2005 *J. Low Temp. Phys.* **139** 633–643
[5] Demyanov G S and Levashov P R 2022 *Phys. Rev. E* **106** 015204
[6] Caillol J M 1999 *J. Chem. Phys.* **111** 6538–6547
[7] Caillol J M and Gilles D 2010 *J. Phys. A: Math. Theor.* **43** 105501