THEORETICAL CONSIDERATION OF ANGULAR–AVERAGED EWALD POTENTIAL TO CALCULATE TWO–COMPONENT PLASMA PROPERTIES ACCOUNTING FOR LONG–RANGE INTERACTION

Demyanov G.S., *[1,2] ***Levashov P.R.*** [1,2]

[1] *JIHT RAS, Moscow, Russia,* [2] *MIPT, Dolgoprudny, Russia*

**demyanov.gs@phystech.edu*

The long-range nature of the Coulomb potential originates difficulties during the numerical simulation and theoretical consideration of two-component plasmas. Often the simulation is performed in a cubic cell with periodic boundary conditions. Using the Ewald summation method, it is possible to obtain an expression for the energy of such a system in which the particles interact with the short-range Ewald potential only in the main cell.

Following the approach by E. Yakub and C. Ronchi [1], the Ewald potential can be averaged over directions to obtain the angular-averaged Ewald (AAE) potential (AAEP) and calculate the energy of a disordered system. The final expression for the potential was first presented in the original paper [1]; its detailed derivation and analysis are presented in our recent work [2].

From a physical point of view, the AAEP describes the interaction of two spheres; each sphere contains a point charge in the center and a uniformly distributed charge of the same value and opposite sign. The radius of each sphere is $r_m = (3/(4\pi))^{1/3}L$, where L is the side length of a cubic cell. The AAEP accounts for the long-range interaction between particles similar to the Ewald potential.

Due to its simple form, the AAEP can be used to obtain pseudopotentials accounting for quantum and long-range interaction effects. Following Kelbg [3], we obtained [4, 5] a generalized expression for the Kelbg pseudopotential in the case of AAEP. We call it the Kelbg-AAE pseudopotential; unlike the familiar Kelbg one, it rapidly decays at long distances. We believe that the Kelbg-AAE pseudopotential will be useful in path integral Monte Carlo methods.

---

1. E. Yakub, C. Ronchi // J. Chem. Phys. 2003, 119, 11556, https://doi.org/10.1063/1.1624364.
2. G. S. Demyanov, P. R. Levashov // J. Phys. A Math. Theor. 2022, 55, 385202, https://doi.org/10.1088/1751-8121/ac870b.
3. G. Kelbg // Ann. Phys. 1963, 467, 219, https://doi.org/10.1002/andp.19634670308.
4. G. S. Demyanov and P. R. Levashov // Derivation of the Kelbg poten-

tial/functional, https://arxiv.org/abs/2205.09885 (2022).
5. G. S. Demyanov and P. R. Levashov // Contrib. Plasma Phys. 2022, e202200100, https://doi.org/10.1002/ctpp.202200100.