

Some Recent Results on Coulomb Manybody Systems

(Talk #11)

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Ewald summation method is popularly used in computer simulation of Coulomb many body systems. The periodic images used in this method are however unphysical and introduce artifacts in physical quantities. Furthermore, the constraint of charge neutrality inside the simulation box also leads to incorrect behaviors in correlation energy and charged distributions. In the first part of this talk, I will introduce a novel multi-scale Monte Carlo simulation method that are free of these artifacts.

In the second part of this talk, I will show that Poisson-Boltzmann theory breaks down in asymmetric electrolytes, due to strong correlations between ions. This leads to the following important consequences: 1) The Debye length receives corrections from electrostatic correlations; 2) A test ion may be attracted by a likely charged surface. I will also discuss some of further implications in the physics of charged membranes and of charged colloids.

References:

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- [4] The Poisson-Boltzmann Theory for Two Parallel Uniformly Charged Plates, Xiangjun Xing, Phys. Rev. E 83, 041410 (2011).