STRUCTURAL TRANSITION IN STRONGLY COUPLED COULOMB CLUSTERS

D.I. Zhukhovitskii and E.E. Perevoshchikov

Joint Institute for High Temperatures, RAS

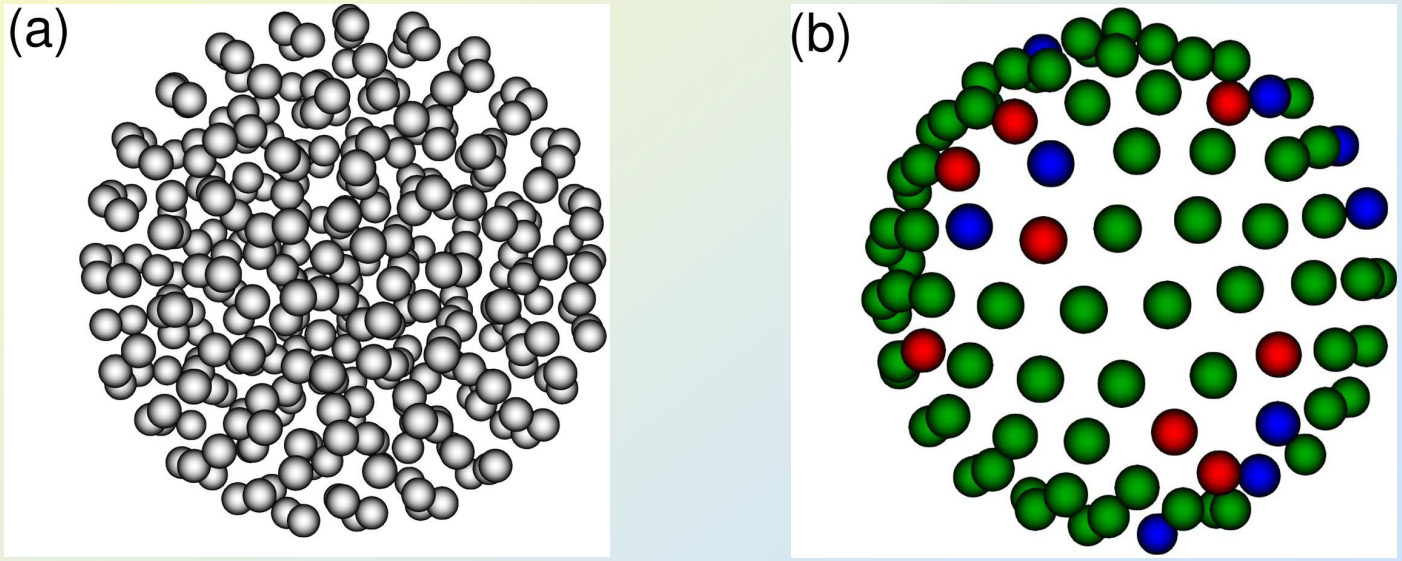
Scientific-Coordination Workshop on Non-Ideal Plasma Physics
December 4-5, 2024, Moscow, Russia

Motivation

1. Existence and threshold of the structural transition in the Coulomb clusters.

2. Crystallization and melting of the cluster core.

3. Particle pressure in the Coulomb cluster (limited one-component plasma).



E.S. Shpil'ko and D.I. Zhukhovitskii, Plasma Phys. Rep. **49**, 1207 (2023).
D.I. Zhukhovitskii and E.E. Perevoshchikov, High Temp. **62**, no.4 (2024).

Molecular dynamics of the Coulomb cluster

Dimensionless (Coulomb) quantities (*N* is the number of particles)

$$r_s = RN^{-1/3} \quad \varepsilon = Z^2 e^2 \,/\, r_s \quad \omega_0 = \frac{1}{\tau_0} = \frac{1}{r_s}\left(\frac{\varepsilon}{m}\right)^{1/2} = \frac{\omega_L}{\sqrt{3}}$$

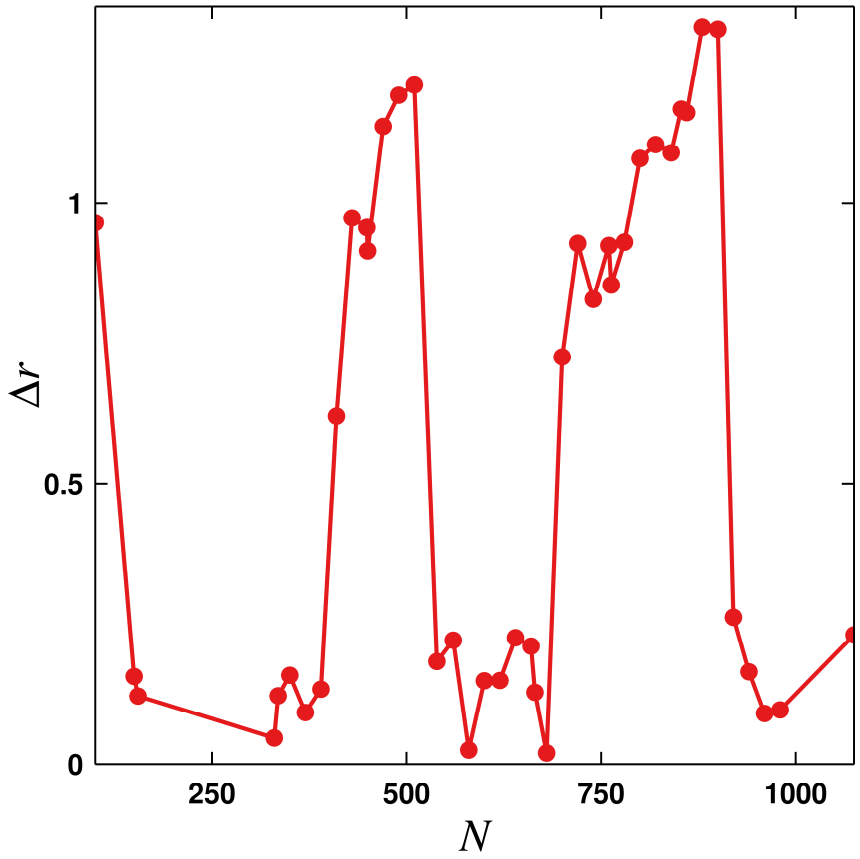
$$r_s = (3 \,/\, 4\pi n_Z)^{1/3} \qquad n_Z = 3N \,/\, 4\pi R^3 \qquad \Gamma = \varepsilon \,/\, T$$

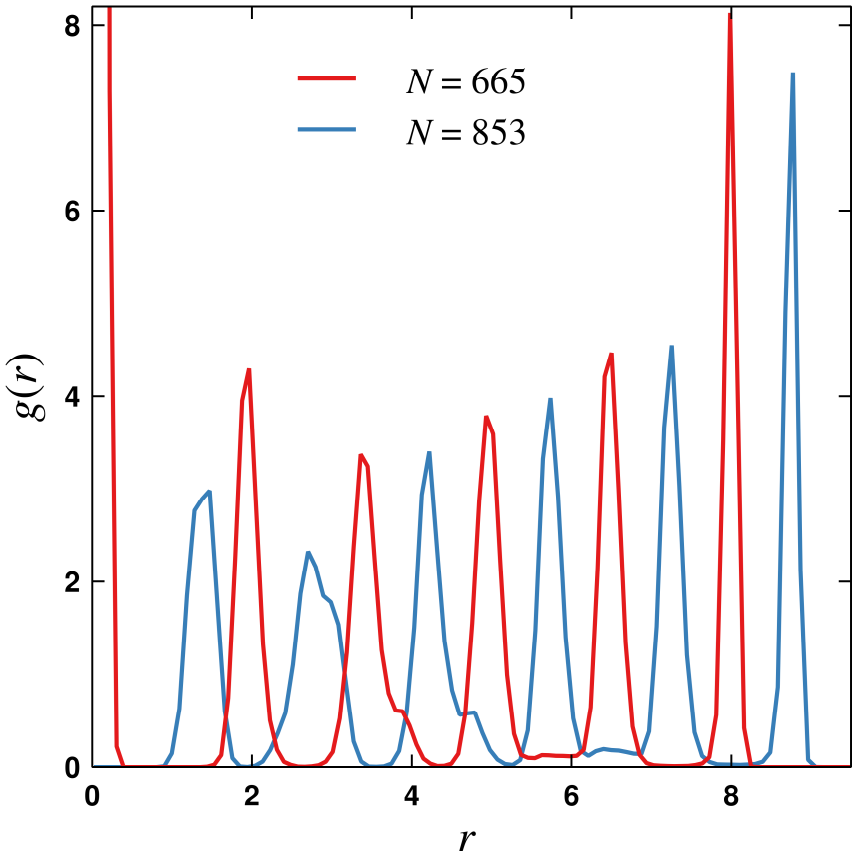
the Debye length $$l_D = \frac{1}{\sqrt{3\Gamma}} \quad (\Gamma \ll 1)$$

Equations of motion

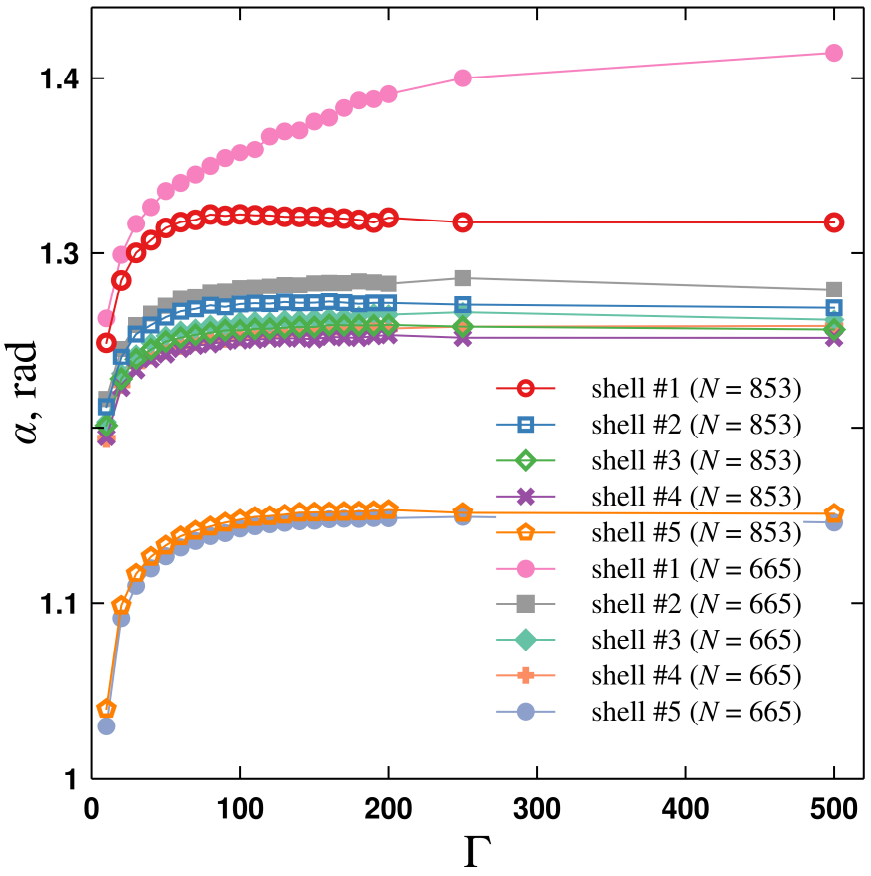
$$\ddot{\mathbf{r}}_i = \sum_{j \neq i} \frac{\mathbf{r}_i - \mathbf{r}_j}{\xi_{ij}^3} - \mathbf{r}_i - \gamma \dot{\mathbf{r}}_i + \mathbf{f}_{\mathrm{st}\,i}, \quad \xi_{ij} = \left| r_i - r_j \right|, \quad \left\langle f_{\mathrm{st}\,i}^2 \right\rangle = \frac{6\gamma}{\Gamma \tau_{\mathrm{st}}}.$$

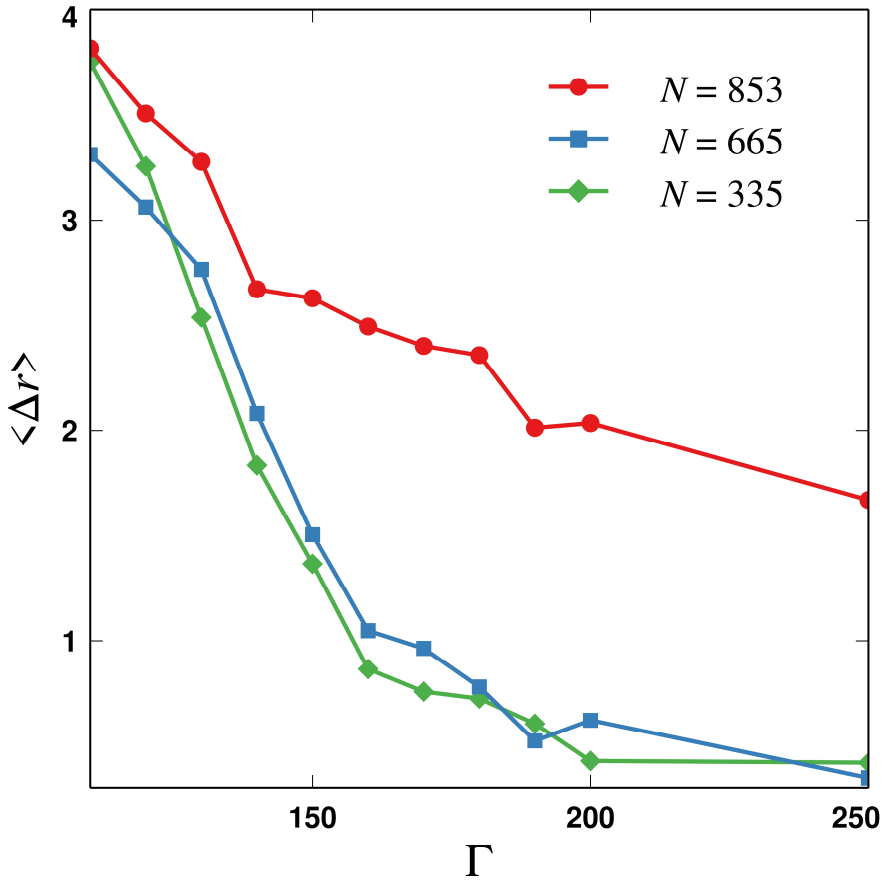
Shell structure of the moderate size Coulomb clusters ($N < 1100$), $\Gamma = 500$



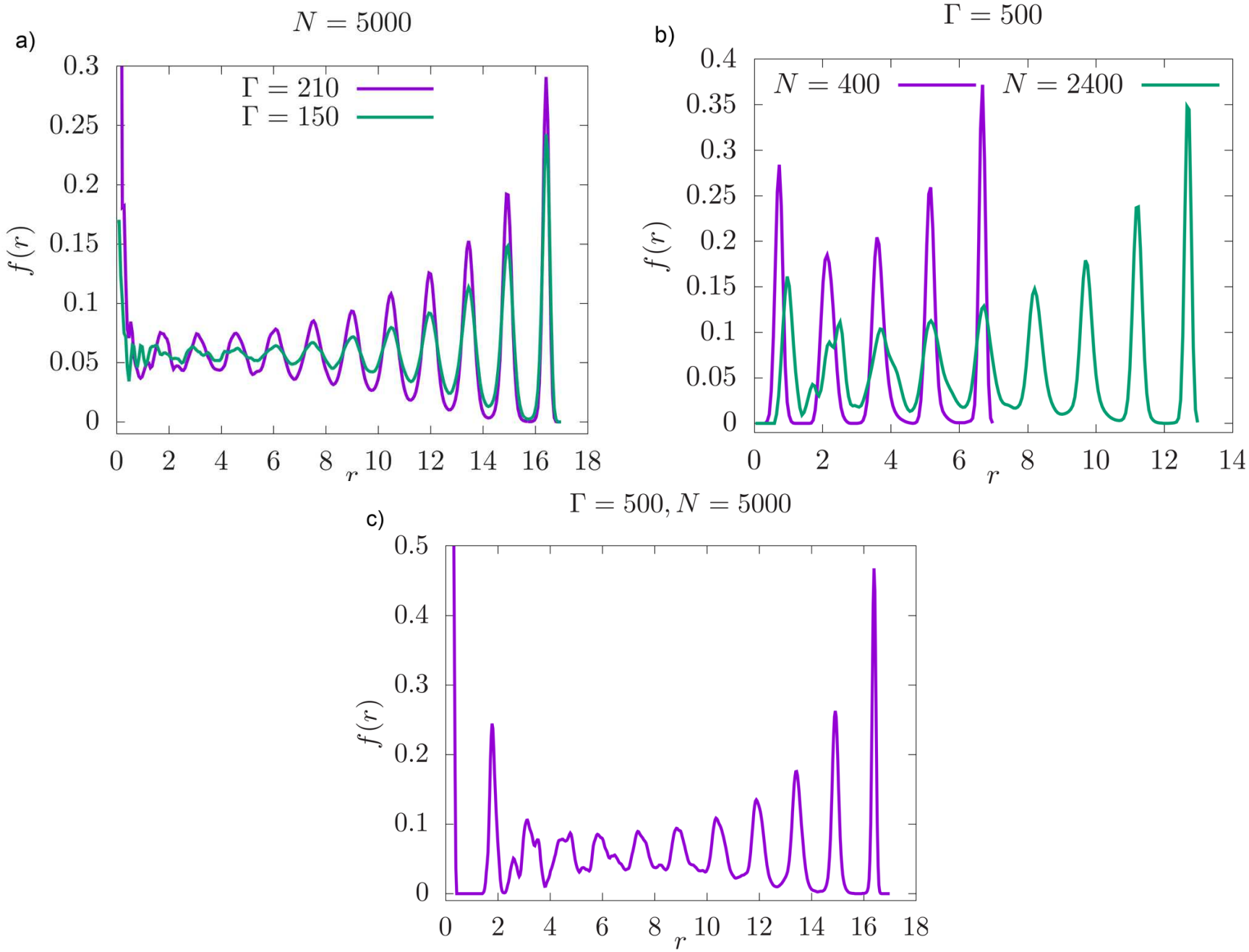


Melting of the shells (2D) and “melting” of a central particle (3D); $N < 1100$

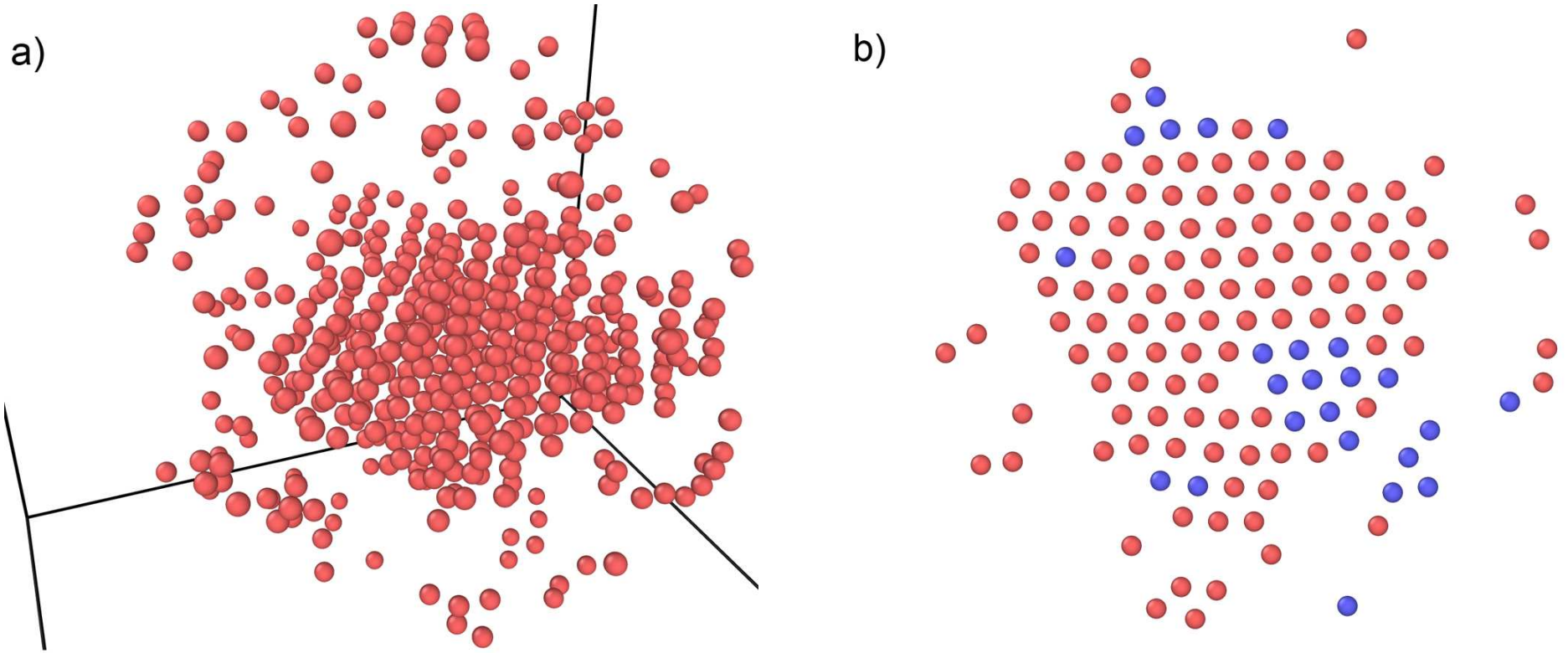




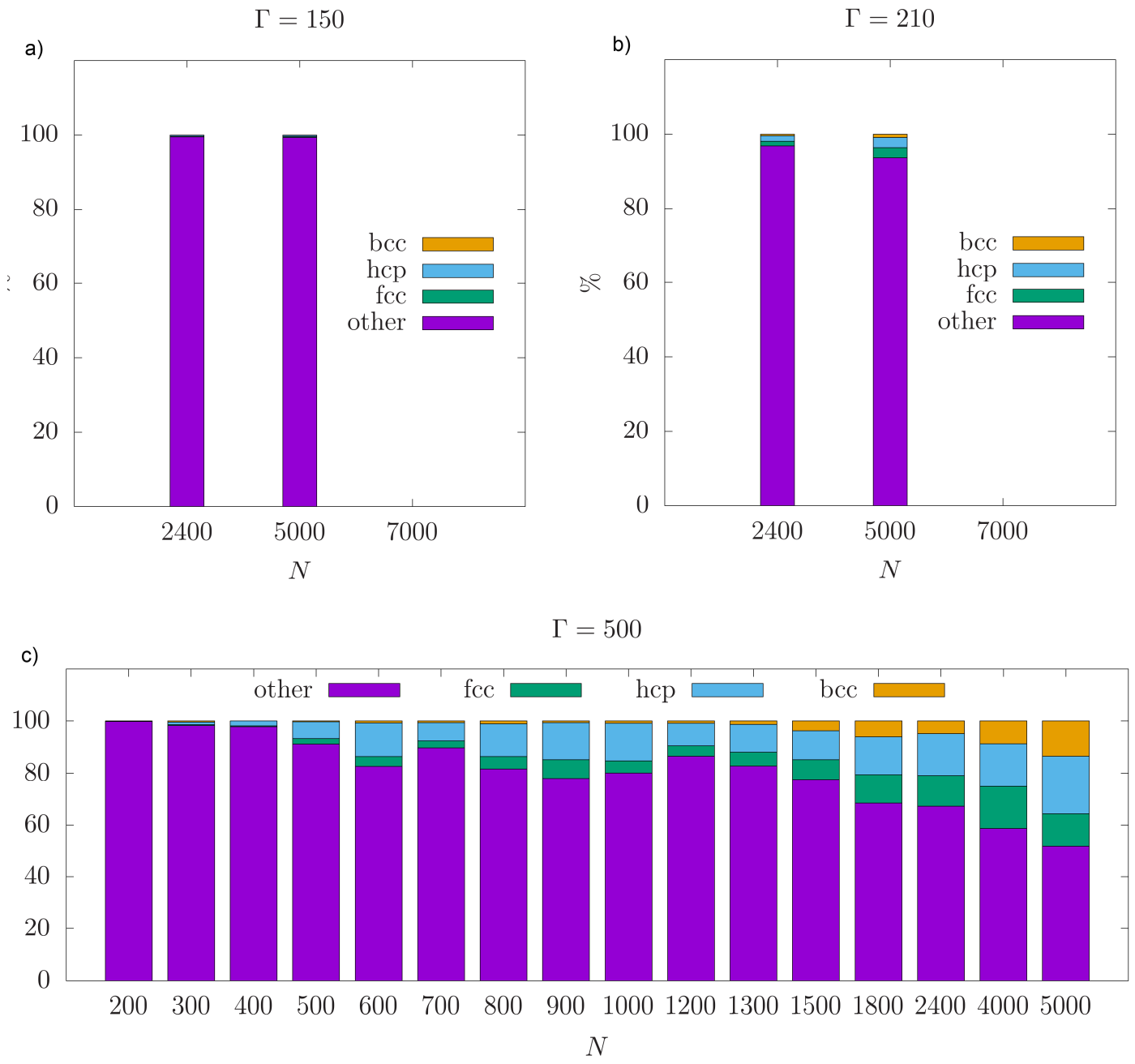
Radial distribution functions in the region of cluster core formation and melting



Snapshots of the hcp Coulomb cluster core and its cross section (hcp+bcc)
$N = 5000$, $\Gamma = 500$



Formation of a crystalline core upon cluster solidification and growth



Two-parameter model (TPM) for the Coulomb cluster

$$N = 3\lambda N_{\rm cr}^{2/3} + 3\lambda^2 N_{\rm cr}^{1/3} + \lambda^3 + N_{\rm cr}$$

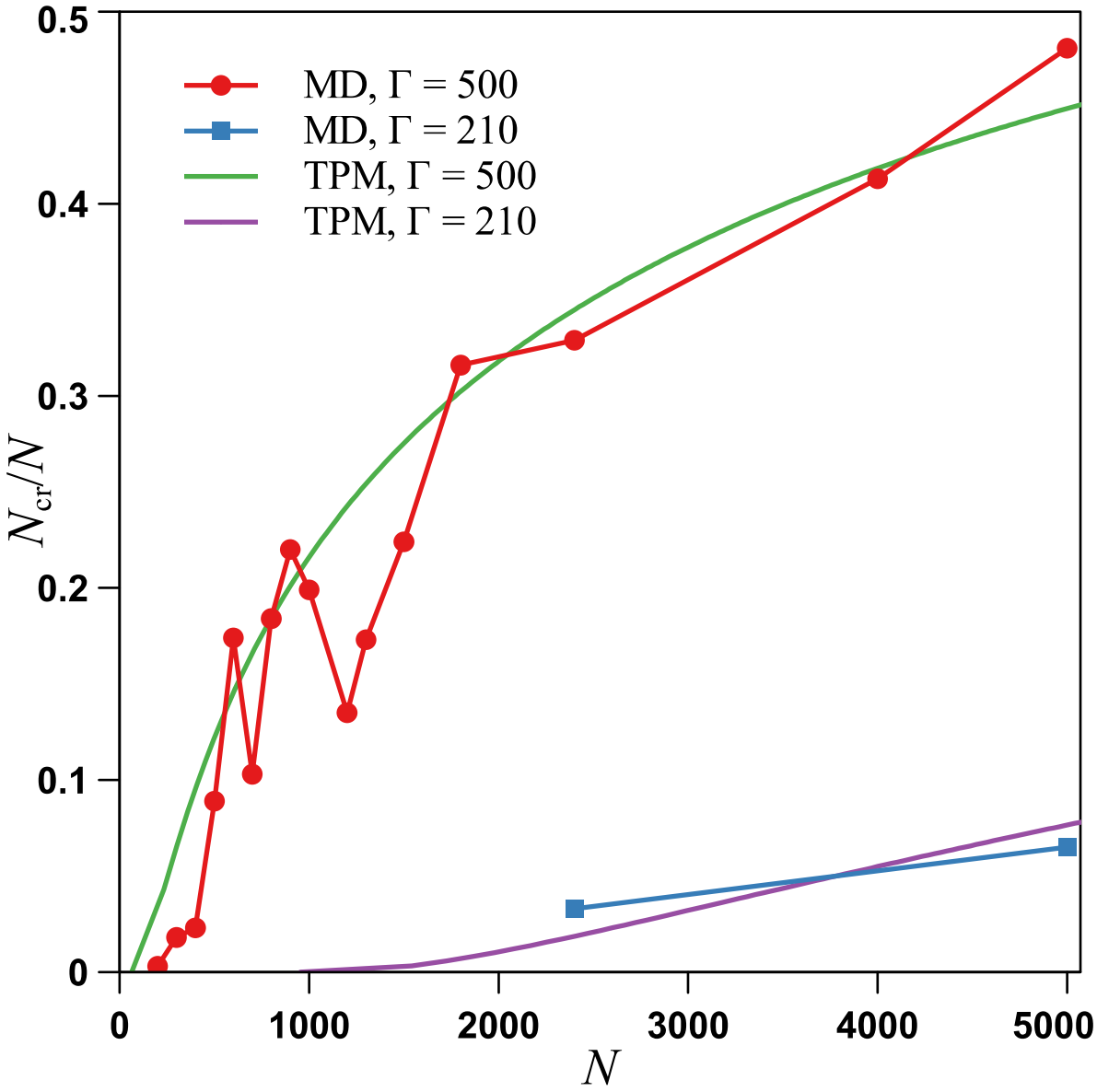
A crystal core first emerges at $N > \lambda^3$.

$$\lambda = 9.84 \quad \text{for} \quad \Gamma = 210$$

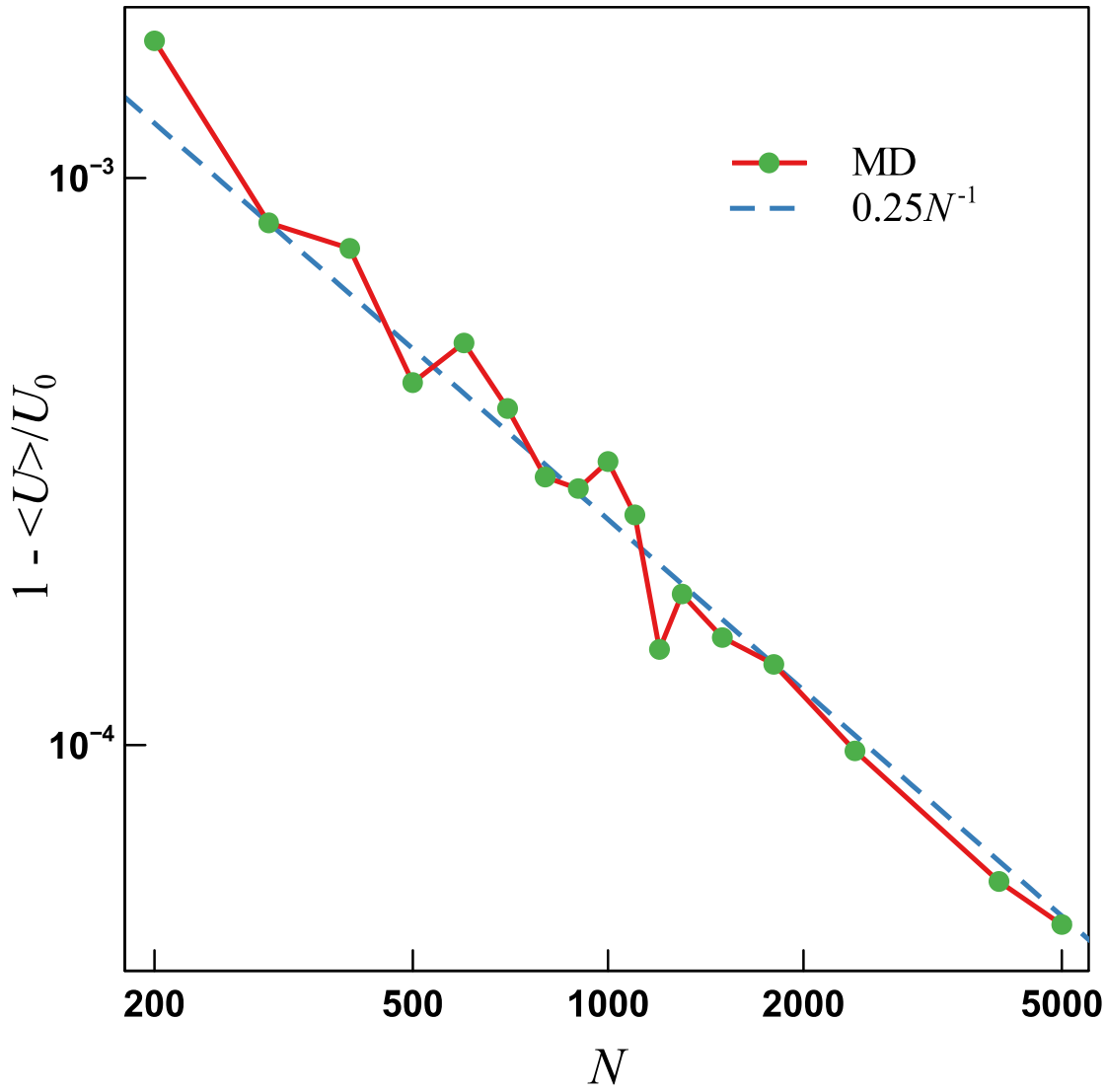
$$\lambda = 4.0 \quad \text{for} \quad \Gamma = 500$$

D.I. Zhukhovitskii, J. Chem. Phys **114**, 184701 (2016).

Size dependence of the crystallized particle fraction



Size dependence of the Coulomb cluster formation energy.
<U> is the LOC potential energy and U_0 is the hcp optimum crystal energy



Compressibility factor for the particle subsystem in LOCP

From the virial theorem for the forces

$$Z_c = \frac{pV}{NT} = 1 + \frac{1}{3NT}\sum_{i=1}^{N}\left\langle \mathbf{r}_i \mathbf{f}_i \right\rangle$$

From the virial theorem for the energy

$$K = -E + 3(pV + U_b + N^{5/3})$$

$$E = K + U_p + U_b$$

where U_p is the particle pair interaction energy

$$U_p = \sum_{i<j} \frac{1}{\left|\mathbf{r}_i - \mathbf{r}_j\right|}$$

U_b is the energy of particle interaction with the background

$$U_b = \sum_{i=1}^{N} \frac{r_i^2}{2} - 1.5N^{5/3}$$

Compressibility factor for the particle subsystem in LOCP

Thus,

$$Z_c = \frac{pV}{NT} = 1 + \frac{\Gamma}{3}(u_p - 2u_b - 3N^{2/3})$$

where

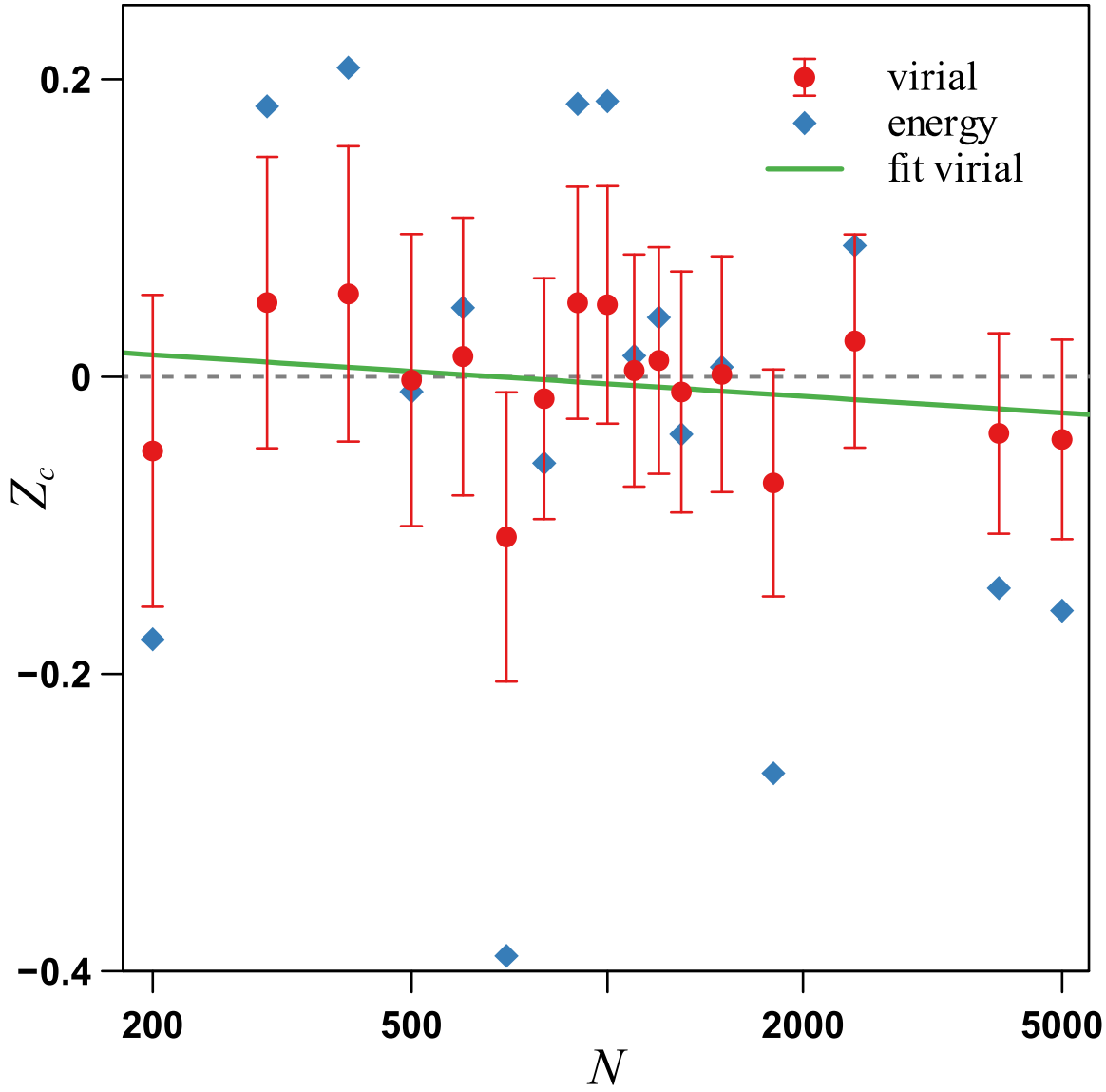
$$u_p = U_p / N \qquad u_b = U_b / N$$

Interpolation of MD data

$$Z_c = a + b \ln N \qquad Z_c(N = 10^6, \Gamma = 500) = -0.0885$$

$$|Z_c| \ll 1$$

Size dependence of the LOCP particle compressibility factor, Γ = 500



$$Z_c(N = 10^6, \Gamma = 500) = -0.0885$$

Compressibility factor in the ion sphere model

The model reduces dynamics of the treated system to the motion of a single particle:

$$Z_c = 1 + \frac{\langle \mathbf{rf} \rangle}{3T}$$

Since $\langle \mathbf{rf} \rangle = -m \langle v^2 \rangle = -3T$, we obtain $\boxed{Z_c \equiv 0}$

in accordance with MD simulation.

From this model, the total potential energy per one particle is a sum of

(1) the work of separation of the neutral ion spheres, contribution = 0;

(2) the work of separation of an ion from its sphere, contribution = $-1/2 - 1$;

(3) the energy of uniformly charged sphere background, contribution = $3/5$.

Then the sum is

$$u = u_p + u_b + 0.6N^{2/3} = -0.9,$$

which is the Lieb–Narnhofer lower bound.

Thank you for your attention!