The Triple Correlation Function of spherical dust clusters: structural analysis and phase transition

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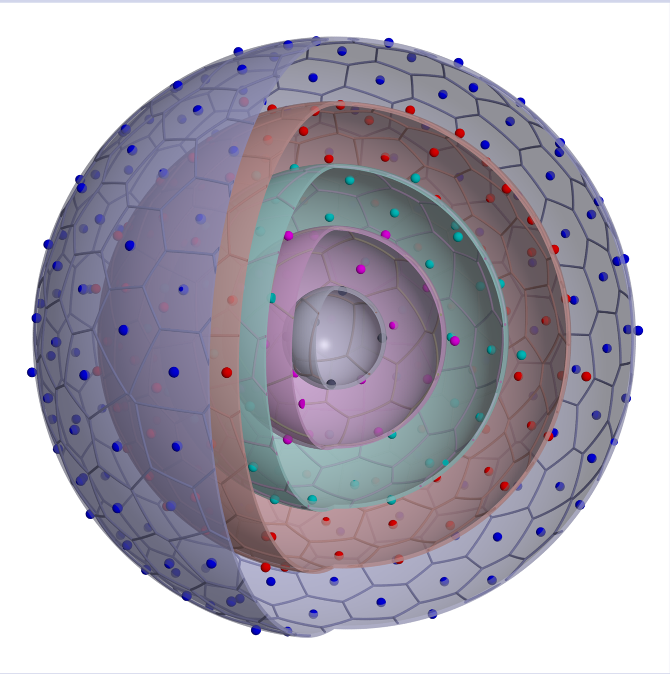
TR 24 complex plasmas

Abstract



Simulated Coulomb cluster with $N = 500$ particles

Dust particles in a complex plasma usually accumulate a high negative charge inside a plasma which is responsible for their strong repulsive interaction and high coupling. When confined in a parabolic trap, these particles form spherical clusters with a characteristic shell structure. In recent years the phase transition-like crossover from a crystal to a liquid-like state has attracted high interest, e.g. [1]. While the radial melting is now well understood, here we concentrate on the loss of intra- shell order. The radial pair correlation function $\rho(r_{ij})$ is well suited for homogeneous system but has to be adapted to the spherical symmetry for finite clusters. Here, we present the Triple Correlation function (TCF) as a sensitive tool for the investigation of intra-shell order. The TCF is calculated from the "bonding angles" of three particles, a particle triple. This quantity is particularly well suited to investigate the orientational order within spherical cluster shells. The intra-shell bond order of Coulomb balls with several hundreds of particles shows striking similarities with a flat 2D system. At the melting region, the 30°-peak in bond order between nearest and second-nearest neighbors shows a clear drop.

System of interest

The dimensionless total potential energy of N parabolically confined dust particles interacting via a *Coulomb potential* reads

$$E_{tot} = \sum_{i=1}^{N} \frac{r_i^2}{2} + \sum_{j<i} \frac{1}{r_{ij}}$$

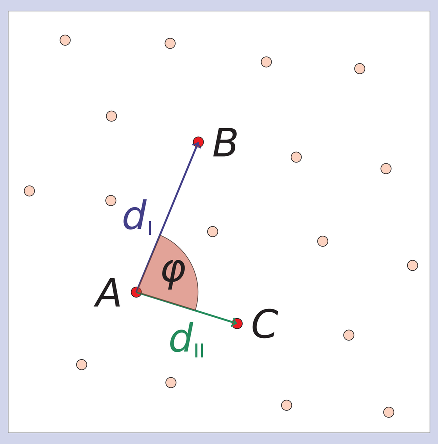
with $r_i = |\mathbf{r}_i|$ and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$.

- Distances are in units of $l_0 = \left(\frac{Q^2}{4\pi\epsilon_0 m\omega^2}\right)^{1/3}$
- The energy is given in units of $E_0 = \left(\frac{m\omega^2 Q^4}{16\pi^2\epsilon_0^2}\right)^{1/3}$
- The coupling parameter $\Gamma = \frac{E_{inter}}{E_{therm}}$ relates the typical interaction energy with the thermal energy

Triple Correlation Function

Flat 2D systems.

The Triple Correlation Function (TCF) is to extend the pair distribution function $g(r)$ by an angular component using pairs of three particles [2].



In the TCF, all pairs of three particles A, B and C are sampled. For each pair

- two inter particle distances d_{I} and d_{II} and
- the enclosed bond angle φ

are measured. Since none of the three particles is distinguished, each triple gives 6 contributions.

Distribution ↦ Correlation function.

The correlations $g_3(d_{\text{I}}, d_{\text{II}}, \varphi)$ can be calculated from the sampled distribution $\rho_3(d_{\text{I}}, d_{\text{II}}, \varphi)$ by dividing by the uncorrelated distribution $\rho_{\text{uncorr}}(d_{\text{I}}, d_{\text{II}}, \varphi)$:

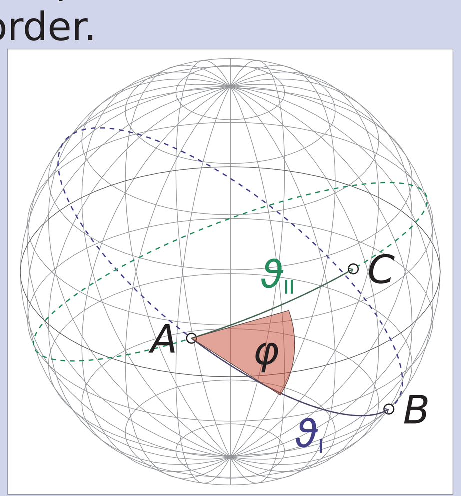
$$g_3(d_{\text{I}}, d_{\text{II}}, \varphi) = \frac{\rho(d_{\text{I}}, d_{\text{II}}, \varphi)}{\rho_{\text{uncorr}}(d_{\text{I}}, d_{\text{II}}, \varphi)}.$$

Uncorrelated three particle density in a homogeneous 2D system with $\rho_0 = \frac{N}{V}$:

$$\rho_{3,\text{uncorr}}(d_{\text{I}}, d_{\text{II}}, \varphi) = N \cdot 4\pi \cdot \rho_0 \cdot d_{\text{I}} \cdot d_{\text{II}}$$

Spherical 3D systems.

In spherical Coulomb clusters, we investigate the intra-shell order.



All possible pairs of three particles A, B and C within **one shell** are sampled. For each pair

- two angular pair distances ϑ_{I} and ϑ_{II} and
- the enclosed bond angle φ

are measured.

Distribution ↦ Correlation function.

Normalization by *uncorrelated* three-particle density

- consider homogeneous spherical shell with equal areal particle density $\rho_0^{sp} = \frac{N_S}{4\pi R_S^2}$

$$\rho_{3,\text{uncorr}}^{sp}(\vartheta_{\text{I}}, \vartheta_{\text{II}}, \varphi) = N_S^2 \cdot \rho_0^{sp} \cdot \sin(\vartheta_{\text{I}}) \cdot \sin(\vartheta_{\text{II}}) \qquad (1)$$

- integration over ϑ_{I} range ↦ $\tilde{\rho}_{3,\text{uncorr}}^{sp}(\vartheta_{\text{II}}, \varphi) \propto \sin(\vartheta_{\text{II}})$

Quasi-hexagonal lattice

The outer shells of large Yukawa balls ($N \gtrsim 100$) show similarities with an extended 2D system. The particles arrange themselves within the shell on lattice, which is hexagonal in wide areas [3]. But lattice positions with **five nearest neighbors always exist**, even for $\Gamma \to \infty$.

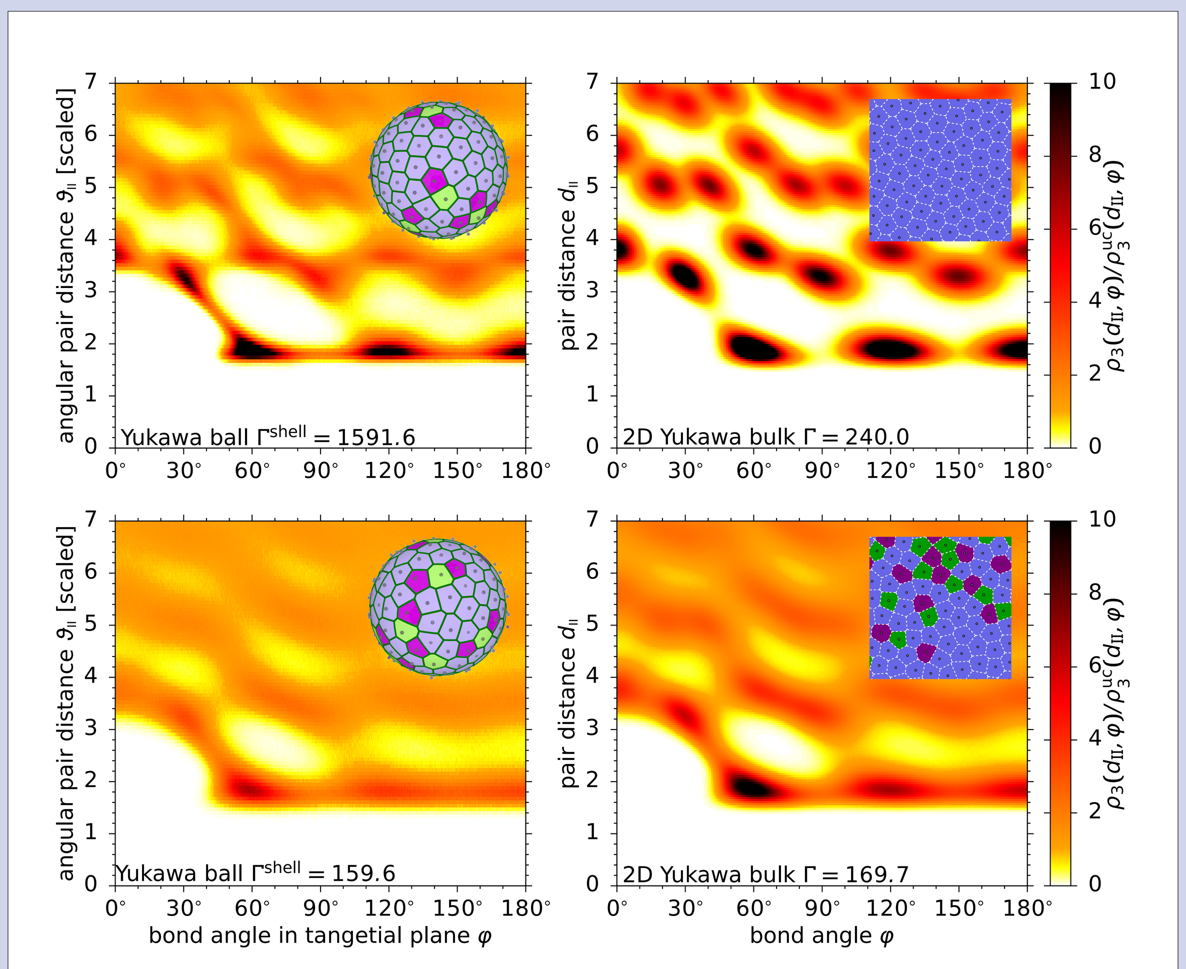


Fig. 1: *TCF of a Yukawa ball (left) and a flat 2D system (right) The outer shell of $N = 500$ Yukawa ball carries $\langle N_S \rangle = 193$ on average. d_{I} and ϑ_{I} respectively is integrated over the nearest neighbor distance. Both system show clear peaks at $\varphi = 60°$ indicating an hexagonal lattice.*

The intra-shell coupling strength calculated as

$$\Gamma^{shell} = \frac{Q^2}{4\pi\epsilon_0\, a_{WS}^{shell}\, k_B T}, \qquad (2)$$

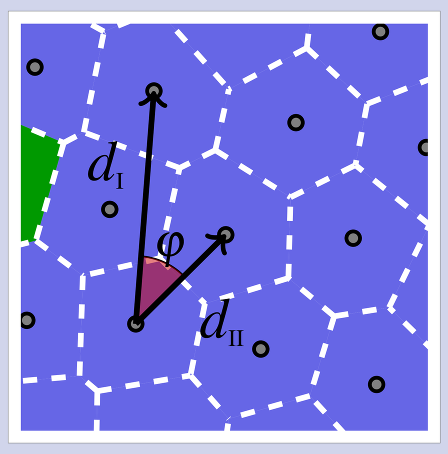
with the intra-shell Wigner-Seitz radius

$$a_{WS}^{shell} = \frac{2}{\sqrt{N^{shell}}} R^{shell} \qquad (3)$$

- Similar angular order in flat an spherical system
- Peaks are separated more clearly in the flat system.

Test: Extended 2D system

Bond angle distribution $p(\varphi)$.



Different averages of the TCF can be computed by integration of ρ_3 and $\rho_{3,\text{uncorr}}$ over one or more coordinates.

- d_{I} is integrated over nearest neighbors
- d_{II} is integrated over second neighbors

⇒ bond angle distribution $p(\vartheta)$

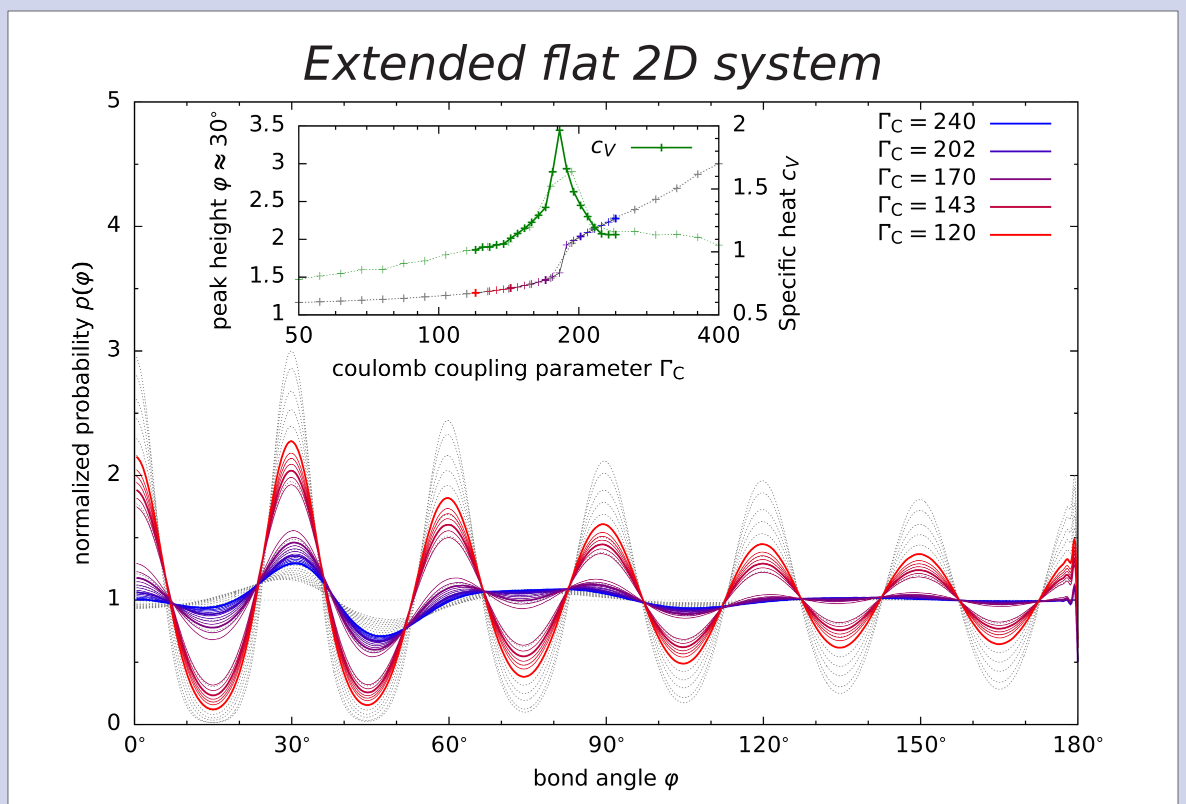
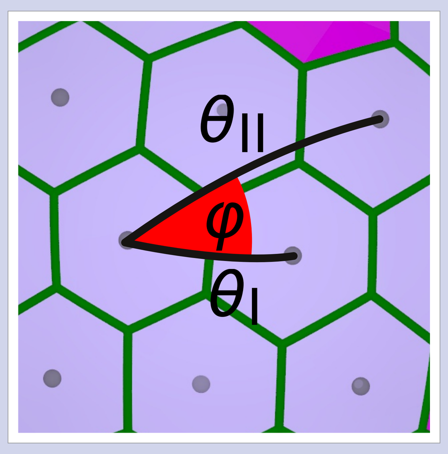


Fig. 2: *TCF of 2D Yukawa ($\kappa = 1.0$) cluster: By integration of ϑ_{I} and ϑ_{II}, one pair of nearest neighbors and one pair of second neighbors are selected. The resulting bond angle distribution $p(\varphi)$ shows pronounced peaks at multiples of 30°. Inset: The height of the 30°-peak shows a step-like increase at the melting point.*

- bond angle distribution of distant neighbors: similar behavior

3D - Results

Bond angle distribution $\rho(\varphi)$.



As for 2D, averages of the TCF are computed by integration of ρ_3 and $\rho_{3,\text{uncorr}}$.

- ϑ_{I} is integrated over nearest neighbors
- ϑ_{II} is integrated over second neighbors

⇒ bond angle distribution $p(\vartheta)$

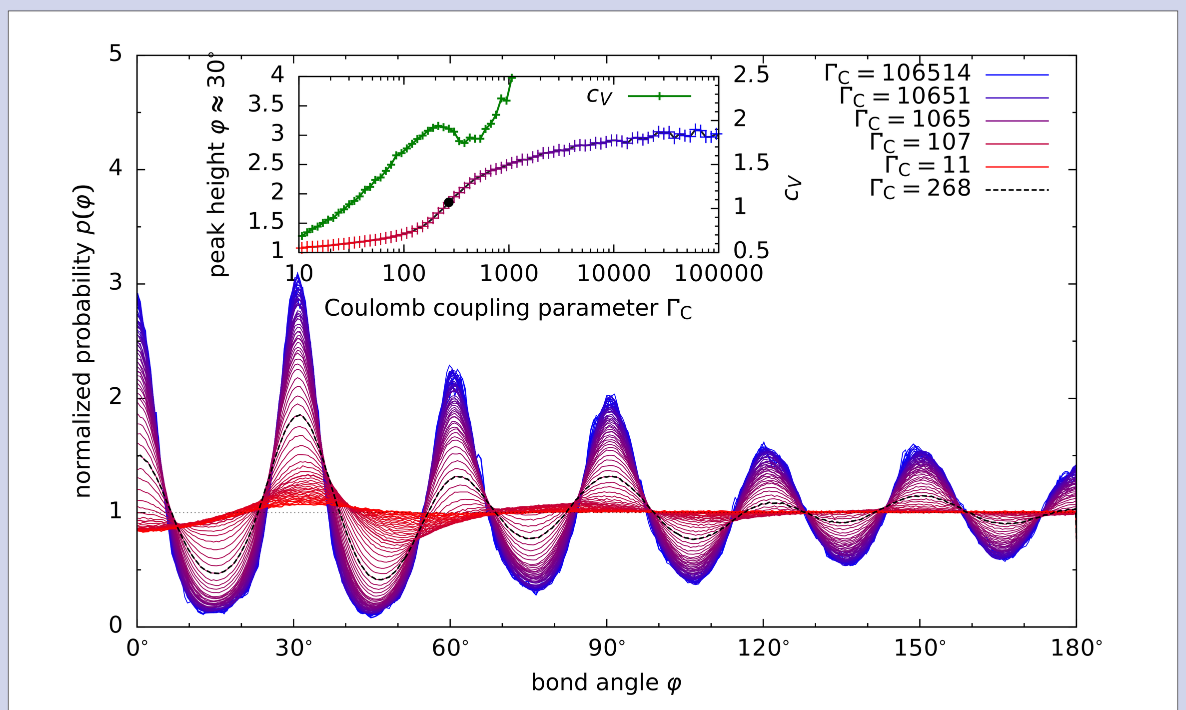


Fig. 3: *TCF of 3D Coulomb ball with $N = 500$ particles: By integration of ϑ_{I} and ϑ_{II}, one pair of nearest neighbors and one pair of second neighbors are selected. The resulting bond angle distribution $p(\varphi)$ again shows pronounced peaks at multiples of 30°. Inset: The height of the 30°-peak shows an increase at the melting region.*

Angular intra-shell pair correlation $g(\vartheta_{\text{I}})$.

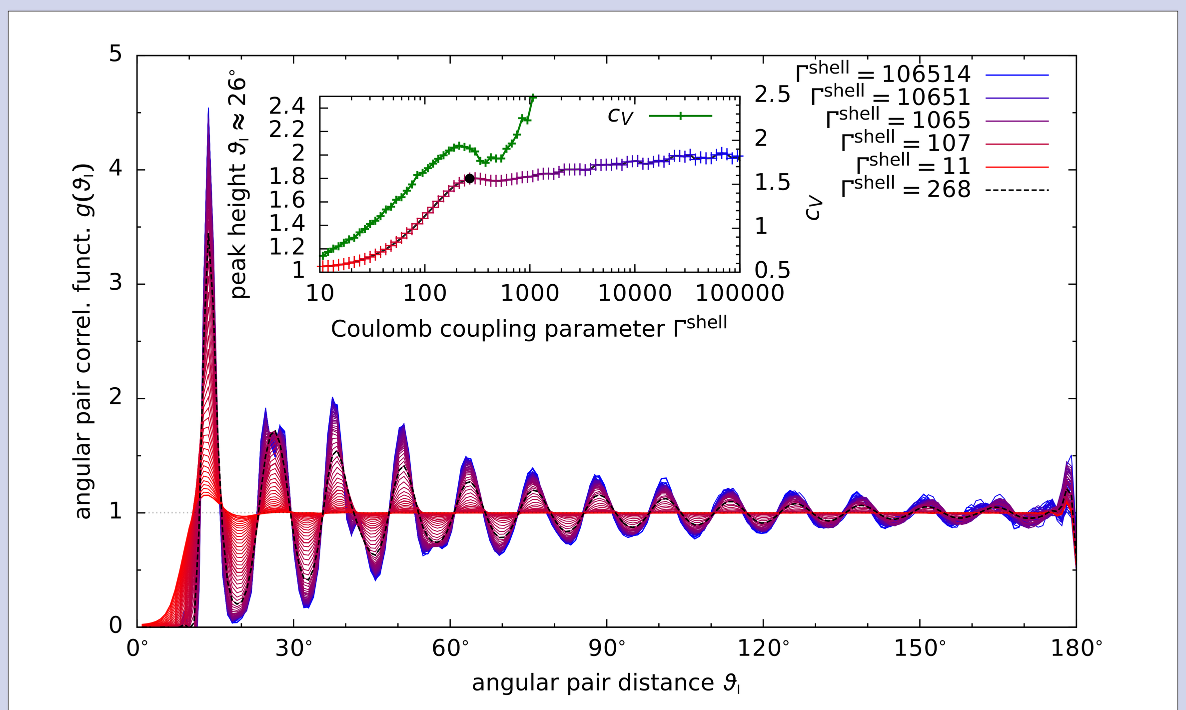


Fig. 4: *Angular pair correlation function (PCF) on the outer shell: By full integration of ϑ_{I} and φ, the inter-shell angular PCF is extracted. This function $g(\varphi)$ corresponds to $g(r_{ij})$ in flat systems. Inset: The height of the 2nd neighbor peak saturates at the melting region.*

Summary

It is shown that the three-particle correlation function is a powerful and sensitive tool for structural analysis in strongly correlated matter

- The *intra shell configuration* and the radial structure can be analyzed in detail by the TCF during dynamic processes, e.g. melting, excitation
- The TCF is not affected by a rotation of the entire cluster
- In contrast to other bond order parameters, *no fixed reference direction* is *required*
- The TCF is not restricted to discrete particles, also applicable to density function, e.g. discharge filaments [4]

Outlook

- Calculate and subtract two-particle contributions to obtain pure three-particle correlations
- Derivation of criteria for phase boundaries from the TCF
- Promising candidate: height of the 30°-peak in bond angle distribution

References

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[3] M. Bonitz *et al.*(Eds.), Complex Plasmas: Scientific Challenges and Technological Opportunities, Springer (2014)
[4] R. Wild and L. Stollenwerk, *Eur. Phys. J. D* **66**, 214 (2012)

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