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The Triple Correlation Function

as a Tool for Structural Analysis in Complex Plasmas

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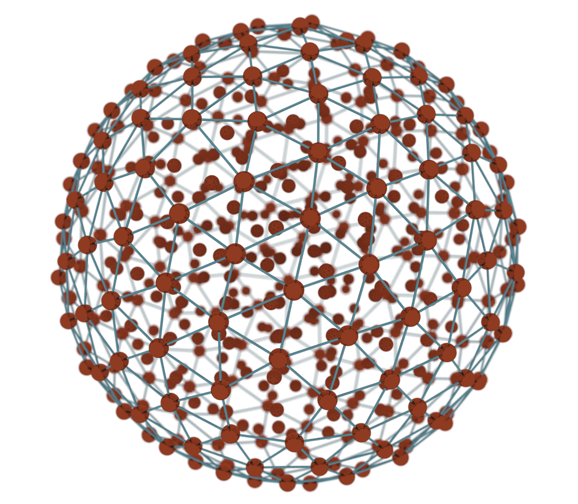
Abstract



Simulated Coulomb cluster with $N = 500$ particles

Dust particles in a plasma allow an analysis of strong correlations effects. The particles usually accumulate high negative charge inside a plasma which results in a strong repulsive interactions. In a parabolic trap, these particles form spherical clusters with a characteristic shell structure. Finite size effects play a major role here [1, 2].

When analyzing the cluster structure and its temperature behavior, it appears that radial distribution $\rho(r)$ and radial pair distribution $g_2(|\mathbf{r}_{ij}|)$ are often insufficient to describe the melting process. Therefore, we analyze the Triple Correlation Function (TCF), for which we sample all pairs of three particles and record two distances and one angle. This allows for an analysis beyond the pair distribution [3, 6]. In a second variant specifically adapted to the spherical shape of trapped dust clusters, we sample particle pairs and use the trap center as a reference points. This quantity resolves both correlation within one shell and angular correlations between different shells. Another advantage is, that the TCF is invariant under rotation of the cluster as a whole.

Using the TCF, furthermore, we study how the intra shell structure vanishes at a lower temperature than the radial structure and the dependence of intra shell structure and inter shell correlation on the screening length.

System of interest

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

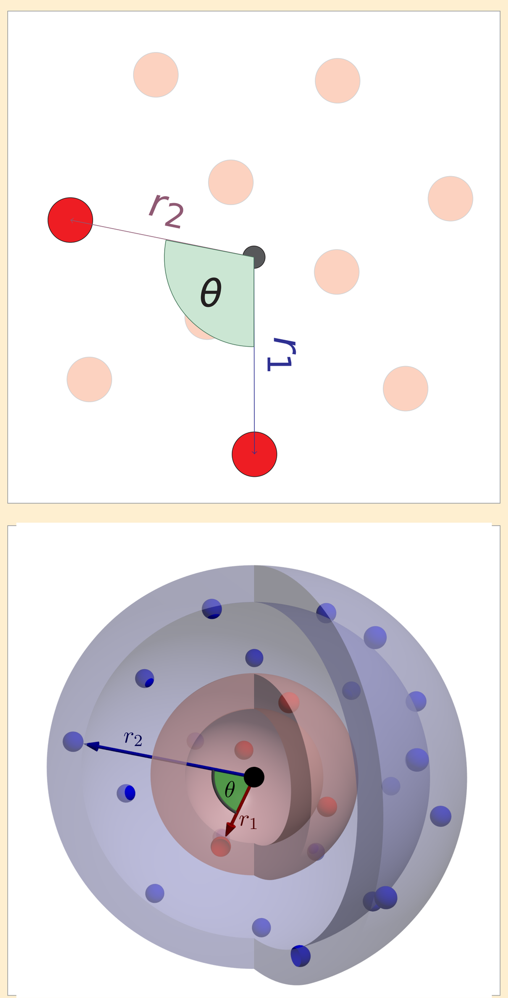
$$E_{tot} = \sum_{i=1}^{N} \frac{r_i^2}{2} + \sum_{j<i} \frac{1}{r_{ij}} \cdot e^{-\kappa \cdot r_{ij}}$$

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 screening constant κ is given by the inverse Debye length $\kappa = \lambda_D^{-1}$ in units of l_0
- The coupling parameter $\Gamma = \frac{E_{\text{inter}}}{E_{\text{therm}}}$ relates the typical interaction energy with the thermal energy

Definition of the TCF

The Three Particle Correlation Function (TPCF) is to extend the pair distribution function $g(r)$ by an angular component using pairs of three particles [5]. To investigate spherical Yukawa clusters, we replace one particle by the trap center. This takes the trap's symmetry into account. We call this quantity *Triple Correlation Function* (TCF).



In the Triple Correlation Function all possible pairs of two particles are sampled with respect to the trap center. The TCF depends on three coordinates:

- the distance r_1 from the trap center to the first particle
- the distance r_2 from the trap center to the second particle
- the angle θ between the two connections

Distribution $\mapsto$ Correlation Function.

The correlations $g_2(r_1, r_2, \theta)$ can be calculated form the sampled distribution $\rho_2(r_1, r_2, \theta)$ by dividing by the uncorrelated distribution $\rho_{\text{uncorr}}(r_1, r_2, \theta)$ and substracting 1

$$g_2(r_1, r_2, \theta) = \frac{\rho(r_1, r_2, \theta)}{\rho_{\text{uncorr}}(r_1, r_2, \theta)} - 1\,.$$

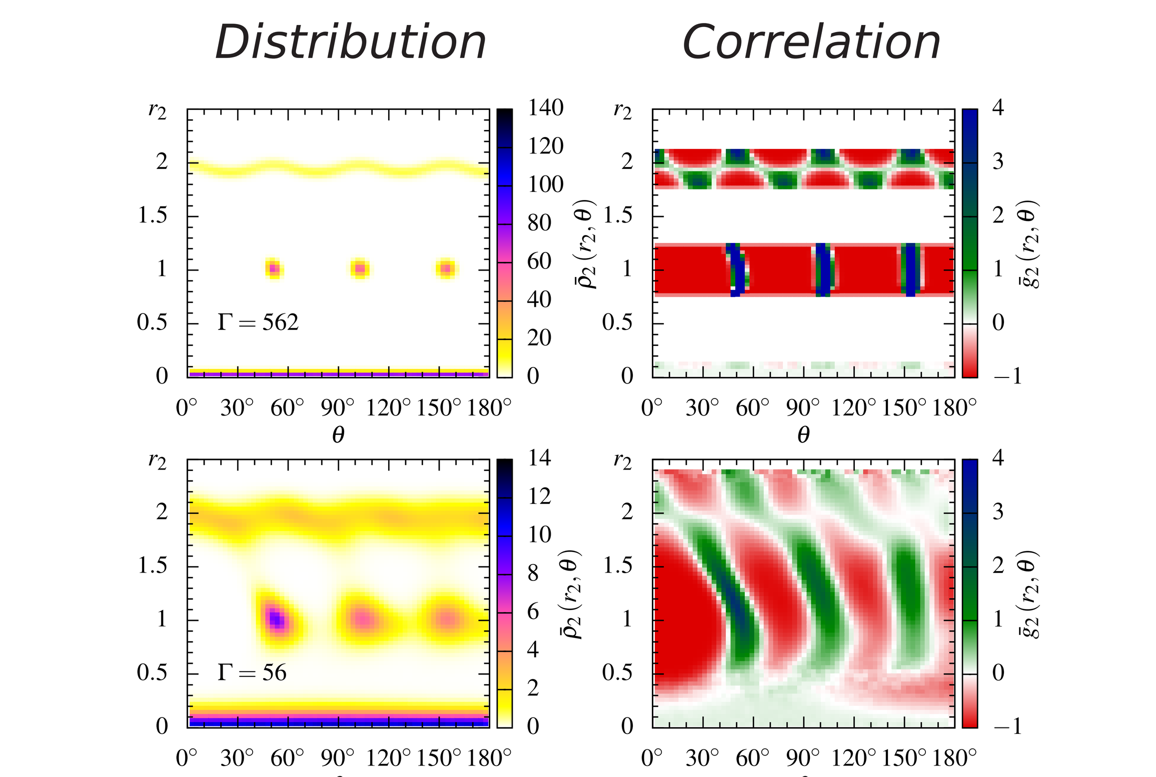
The uncorrelated two particle density in a radially symmetric system becomes

$$\rho_{2,\text{uncorr}}(r_1, r_2, \theta) = \rho(r_1) \cdot \rho(r_2) \cdot \frac{\sin\theta}{2} \qquad (3d)$$

$$\rho_{2,\text{uncorr}}(r_1, r_2) = \rho(r_1) \cdot \rho(r_2) \cdot \frac{1}{\pi} \qquad (2d)\,,$$

where $\rho(r)$ describes the radial one particle density.

2D - Results

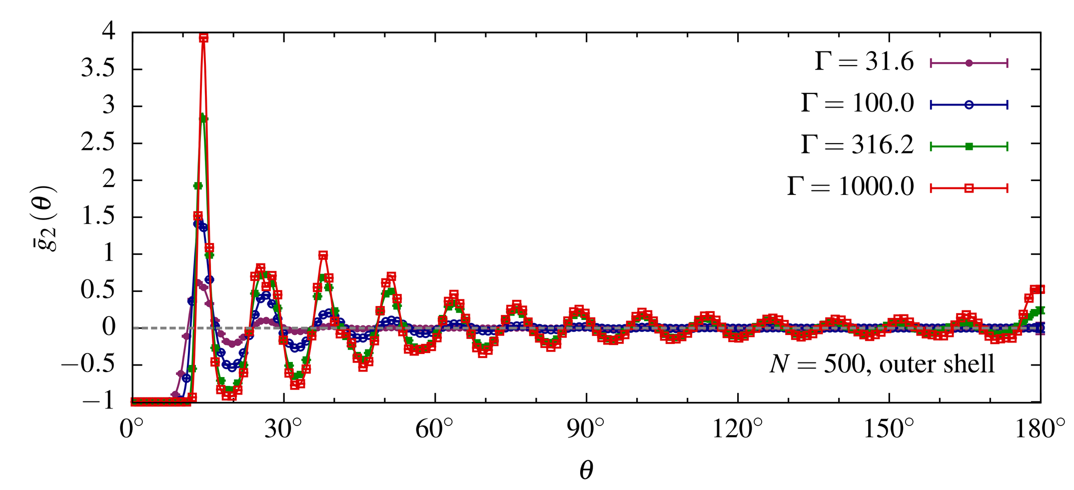


TCF of a 2D Yukawa ($\kappa = 1.0$) cluster with $N = 19$ particles: By averaging r_1 over the inner shell, the reference particle is always chosen from this shell. We find correlation between particles in the same shell ($r_2 \approx 1$) and with those on the outer shell ($r_2 \approx 2$). Although, particles on the outer shell appear as a continuous line in ρ_2, their angular positions are correlated with the inner shell.

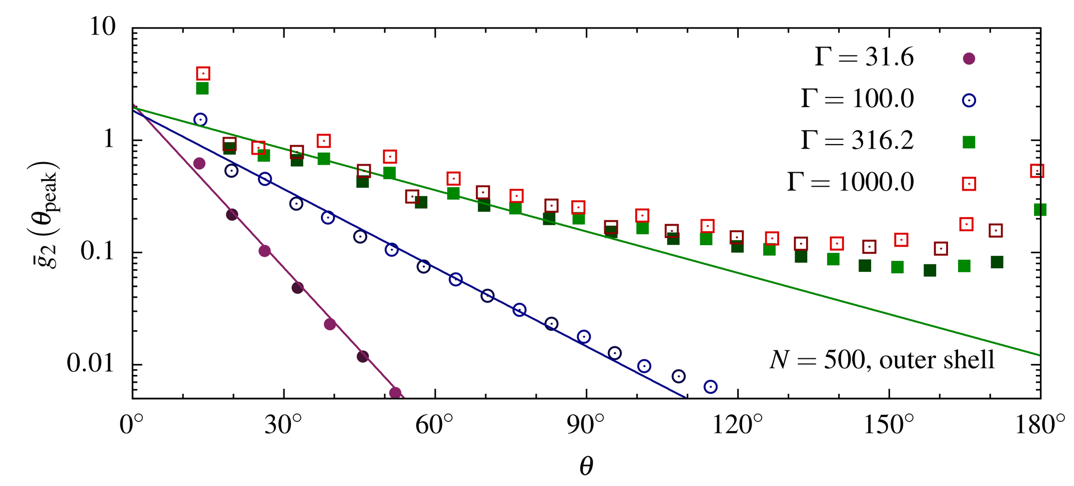
3D - Results

Large 3D Coulomb ball (N=500).

- analysis of the structure within the outer shells
- average both radial coordinates r_1 and r_2 over this shell
- resulting quantity describes probability to find two particles under a certain angle



Angular correlations on the outer shell : Strongest correlations are found for neighbored particles within the shell. Significant correlations of particles at $\theta = 180°$ are found strong coupling $\Gamma \gtrsim 300$.



Decay of the peak heights : The absolute heights correlation maxima (bright symbol) and anti-correlation minima (dark symbols) are shown in this plot. For weak coupling, exponential fits (straight lines) show good agreement.

References

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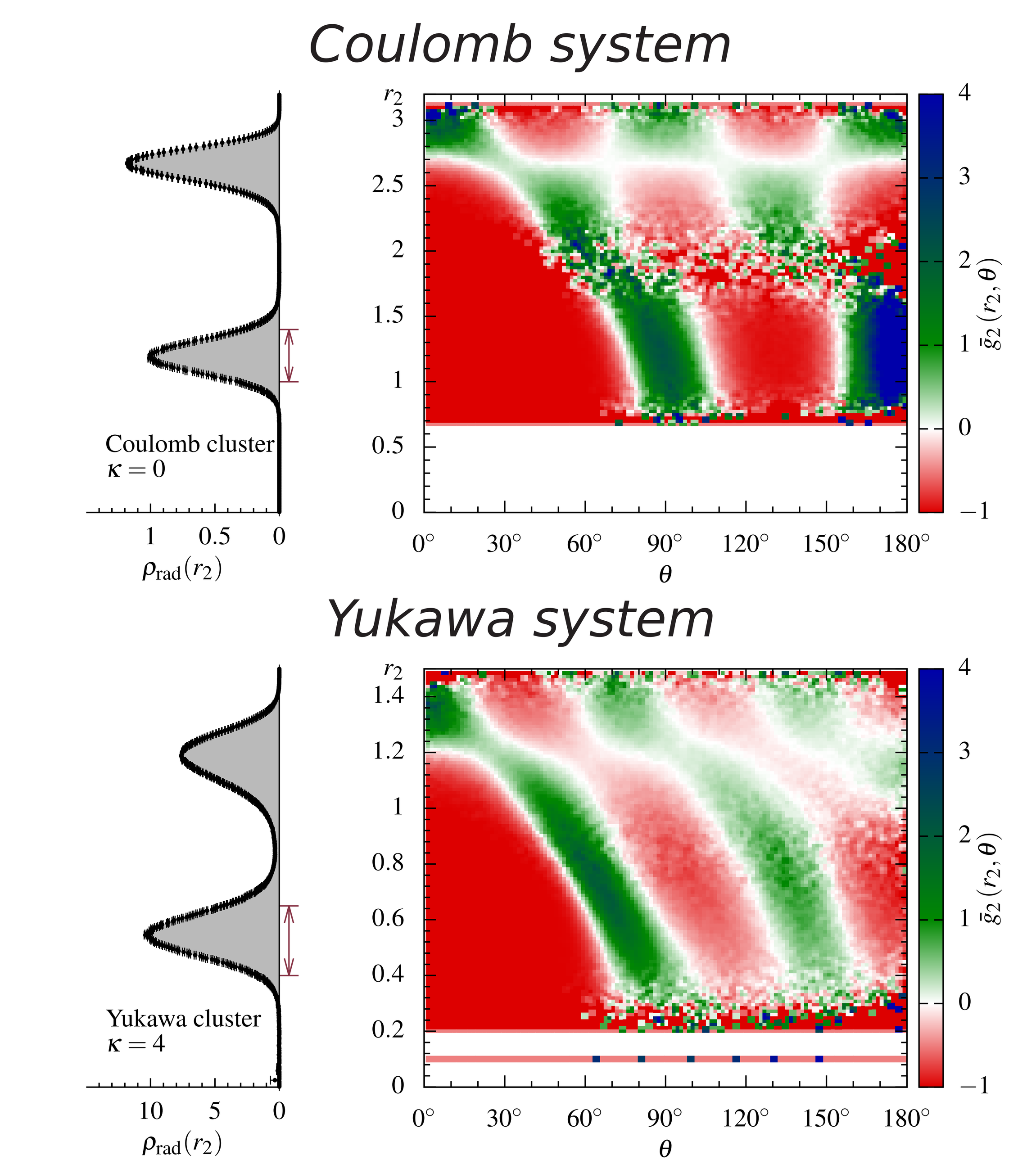
Coulomb vs. Yukawa



TCF of a cluster with $N = 38$ particles: Both plots show a cluster with moderate coupling strength $\Gamma = 100$. The first radial coordinate is integrated over the inner shell (red arrow).

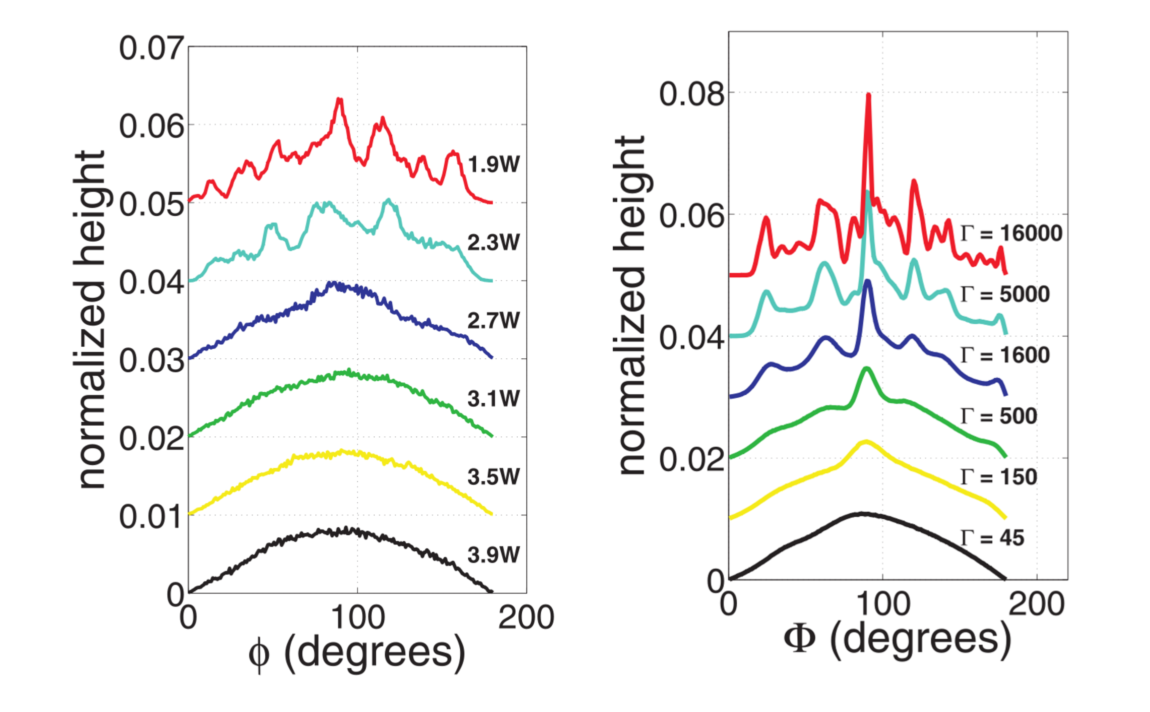
- Strong angular correlations with particles on the same shell
- Correlation with particles on the outer shell depends on the outer particles radius (sub-shells)
- Although rare transitions between shells: transition-channels visible

Experiment vs. Simulation

In the experiment, the temperature of a 3d Yukawa ball with $N = 32$ particles is controlled by the plasma power. The TCF is calculated as **distribution** $\rho(r_1, r_2, \Phi)$ ($\Phi = \theta$) without dividing by the uncorrelated two-particle distribution.

- r_1 is integrated over the inner shell (one particle is always from the inner shell)
- r_2 is integrated over the whole cluster

$\Rightarrow$ angular distribution $\tilde{\rho}(\Phi)$



The radially integrated TCF from experiment [6] (left) and MC simulation (right) show good qualitative agreement.

Summary

- The *intra shell configuration* and the radial structure can be analyzed in detail by the TCF during dynamic processes, e.g. melting, excitation
- *Angular correlations* between different shells can be resolved (r_1 and r_2 averaged over different shells)
- The TCF is not affected by a rotation of the entire cluster
- The TCF is calculated by an histogram and is hence fully compatible with Monte Carlo simulation, especially with the Parallel Tempering method
- Full Three Particle Correlations useful for extended systems: calculate $\rho_{3,\text{uncorr}}(r_I, r_{II}, \theta)$ from radial pair distribution

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