Thermodynamic theory of a strongly correlated confined Yukawa plasma

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What are crystals in dusty plasmas?

- Dusty plasma: micrometer-sized particles immersed in a gaseous plasma environment
- Dust particles are of high charge ($\approx 10^4$ elementary charges)
- 3D-Crystallization of dust particles due to strong interaction
Coulomb balls have interesting internal structure

- Consists of shells with definite occupation number
- Explanation by Yukawa interacting particles within isotropic parabolic confinement

\[^{a}M.\ Bonitz,\ D.\ Block,\ O.\ Arp,\ V.\ Golubnychiy,\ H.\ Baumgartner,\ P.\ Ludwig,\ A.\ Piel,\ and\ A.\ Filinov,\ Phys.\ Rev.\ Lett.\ 96,\ 075001\ (2006)\]
Average Properties

- Interesting question of average density
- Consider **Coulomb** interacting particles
- Textbook result
  - Homogeneous density leads to parabolic potential within

\[ \rho(r) \quad E(r) \quad \Phi(r) \]

- Parabolic confinement leads to homogeneous density
Average Properties

Question

Density profile of Yukawa interacting particles?
Ground state density of Coulomb balls

<table>
<thead>
<tr>
<th>Energy functional</th>
</tr>
</thead>
<tbody>
<tr>
<td>Classical ground state energy (mean-field)</td>
</tr>
</tbody>
</table>

\[
E[n] = \int d^3 r \ u(r) \\
\]

\[
u(r) = n(r) \left\{ \Phi(r) + \frac{N - 1}{2N} \int d^3 r_2 \ n(r_2) V(|r - r_2|) \right\}
\]

<table>
<thead>
<tr>
<th>Explicit solution of density for Yukawa interacting particles</th>
</tr>
</thead>
</table>

\[
n(r) = \frac{N}{4\pi(N-1)Q^2} \left( \Delta \Phi(r) - \kappa^2 \Phi(r) + \kappa^2 \mu \right) \quad \forall r : n(r) \neq 0
\]
Results for isotropic parabolic confinement

Density for $N = 2000$

\[
\kappa r_0 = 0
\]
Results for isotropic parabolic confinement

Density for $N = 2000$

- $\kappa r_0 = 0$
- $\kappa r_0 = 0.3$
Results for isotropic parabolic confinement

Density for $N = 2000$

Motivation
Mean-field approximation
LDA
Outlook
Conclusion

Density $n(r) [r_0^{-3}]$ as a function of $r [r_0]$. The graph shows three curves for different values of $\kappa r_0$: red for $\kappa r_0 = 0$, yellow for $\kappa r_0 = 0.3$, and green for $\kappa r_0 = 0.6$. The density decreases as $r$ increases for all values of $\kappa r_0$.
Results for isotropic parabolic confinement

Density for $N = 2000$

$n(r) [r_0^{-3}]$ vs $r [r_0]$

- $\kappa r_0 = 0$
- $\kappa r_0 = 0.3$
- $\kappa r_0 = 0.6$
- $\kappa r_0 = 1$
Comparison with simulation results for Coulomb crystals

- Correlation between continuous density and discrete shell-like structure?
- Comparison: Continuous density ↔ averaged shell densities
Comparison with simulation results for Coulomb crystals

Comparison with MD simulation for $N = 2000$
Local Density Approximation

- Inclusion of correlations possible due to LDA
- Avoidance of non-local expressions within the energy density by means of homogeneous system results \(^1\)

**Energy functional**

- Classical ground state energy (LDA including correlations)

\[
E[n] = \int d^3 r \ u(r)
\]

\[
u(r) = n(r) \Phi(r) + \frac{N - 1}{N} \ n(r)^2 \frac{2\pi Q^2}{\kappa^2}
\]

\[
- \gamma_1 Q^2 n(r)^{\frac{4}{3}} \exp\left(-\gamma_2 \kappa n(r)^{-\frac{1}{3}} + \gamma_3 (\kappa n(r)^{-\frac{1}{3}})^4\right)
\]

Mean-field vs. LDA with correlations

Comparison with simulation results

\[ n(r) [r_0^{-3}] \]

\[ r [r_0] \]

\[ \kappa r_0 = 2.0 \]
\[ \kappa r_0 = 1.0 \]
\[ \kappa r_0 = 0.0 \]

\[ N = 1000 \]
Mean-field vs. LDA with correlations

Comparison with simulation results

\[
\kappa r_0 = 5.0, \quad \kappa r_0 = 3.0, \quad N = 1000
\]
Outlook: Finite temperature

- Approach to finite temperature by BBGKY-Hierarchy

Differential equation of the density

\[
4\pi \frac{N-1}{N} Q^2 n(r) = (\Delta - \kappa^2) \left[ \Phi(r) - \mu + k_B T \ln \left( \frac{n(r)}{\bar{n}} \right) \right] \]

\[ \forall r : n(r) \neq 0 \]
Outlook

- Access to equation of state
- Derivation of other quantities, like
  - pressure
  - compressibility
  - specific heat capacity
- Analysis of \((\kappa, \Gamma)\)-dependence
Conclusion

- Calculation of ground state density of Yukawa particles in arbitrary confinement (mean-field)
- Comparison with simulated Coulomb balls yields good agreement, but also discrepancies for strong screening
- LDA remedies the discrepancies by including correlations but fails for weak screening
- Both models complement one another in describing the density profile within the full screening range
- An ansatz how to include temperature dependence was shown
Conclusion

Thank you for your attention.
Mean-field vs. LDA with correlations

Comparison with simulation results

$n(r) [r_0^{-3}]$

\[ \kappa r_0 = 3.0 \]

\[ \kappa r_0 = 1.0 \]

\[ N = 10000 \]