*34th EPS Conference on Plasma Phys. Warsaw, 2 - 6 July 2007 ECA Vol.**31F**, P-5.038 (2007)*

Density profile of strongly correlated spherical Yukawa plasmas

C. Henning[1], H. Baumgartner[1], A. Piel[2], P. Ludwig[1,3], M. Bonitz[1]

[1] *ITAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany*

[2] *IEAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany*

[3] *Institut für Physik, Universität Rostock, D-18051 Rostock, Germany*

Abstract

The ground state of an externally confined one-component Yukawa plasma is derived analytically using the mean-field approximation (MF) [1] as well as the local density approximation (LDA) [2]. In particular, the radial density profiles are computed. By comparison with first-principle simulations for three-dimensional spherical Yukawa crystals we demonstrate that both approximations complement each other. Together they accurately describe the density profile in the full range of screening parameters.

Introduction

The recent discovery of 3D dust crystals, so-called "Yukawa balls" [3], which allow precision measurements and direct observation of strong correlation phenomena, excited intensive experimental and theoretical activities [4, 5, 6]. The shell structure of these crystals, including details of the shell radii and the particle distribution over the shells has been very well explained theoretically by a simple model involving an isotropic Yukawa-type pair repulsion and an external harmonic confinement potential [5, 6]. An open question is the average particle distribution, i.e. how does the radial density profile look. It is well known that in the case of Coulomb interacting particles in a harmonic potential the answer is given by a constant density.

Here, we extend this analysis to a Yukawa plasma based upon a continuum approach in a non-local mean-field approximation. We show that screening has a dramatic effect on the density profile, which we derive analytically for the ground state [1] and which is found to agree very well with first principle computer simulations for Yukawa crystals. However, when the screening is increased deviations in the trap center keep growing which is attributed to correlation effects missing in the MF model.

To remove these discrepancies we also analyze correlations by applying the local density approximation (LDA) [2]. By comparison with molecular dynamics simulations, we find that the results obtained by the MF and by LDA complement one another to accurately describe the average particle distribution of shell structured spherical crystals within the full range of the screening parameter. We find that LDA agrees very well with simulations of Yukawa crystals in the limit of strong screening. On the other hand, for weak screening, the previous MF result turns out to be more accurate. Interestingly, for intermediate values of the screening parameter both methods are accurate, so a combination of both allows one to quantitatively describe the density profile in the whole range of screening parameters.

Ground state of a confined plasma within MF

We consider a finite one-component plasma (OCP) in its ground state containing N identical particles with mass m and charge Q in an external potential Φ with pair interaction potential $V(r) = (Q^2/r)\exp(-\kappa r)$ described by the ground-state energy functional

$$E[n] = \int d^3r\, u(\mathbf{r}), \tag{1}$$

with energy density contributions from the confinement, and interaction separated in its mean-field and correlation parts $u(\mathbf{r}) = u^{\text{conf}}(\mathbf{r}) + u^{\text{mf}}(\mathbf{r}) + u^{\text{cor}}(\mathbf{r})$. To obtain the MF result, we neglect the correlation contribution u^{cor}, which will be discussed below by means of the LDA, and use

$$u^{\text{conf}}(\mathbf{r}) = n(\mathbf{r})\Phi(\mathbf{r}), \tag{2a}$$

$$u^{\text{mf}}(\mathbf{r}) = n(\mathbf{r})\frac{N-1}{2N}\int d^3r_2\, n(\mathbf{r}_2)V(|\mathbf{r}-\mathbf{r}_2|). \tag{2b}$$

From the variation of the resulting mean-field energy functional $E^{\text{MF}}[n]$ with respect to the density regarding the constant particle number an explicit expression for the mean-field density profile $n^{\text{MF}}(\mathbf{r})$ in an arbitrary confinement potential can be derived (for details see Ref. [1])

$$n^{\text{MF}}(\mathbf{r}) = \frac{N}{4\pi(N-1)Q^2}\Big(\Delta\Phi(\mathbf{r}) - \kappa^2\Phi(\mathbf{r}) + \kappa^2\mu\Big), \tag{3}$$

where the chemical potential μ ensures the constant particle number.

For the frequently encountered case of a parabolic external potential, $\Phi(r) = \frac{\alpha}{2}r^2$, the results are shown in Fig. 1 for three particle numbers between $N = 100$ and $N = 2000$ using the Coulomb length scale $d_c = (2Q^2/\alpha)^{1/3}$ and Coulomb density scale $n_c = (3\alpha)/(4\pi Q^2)$. The graph reveals that the curvature of the density profile changes dramatically, when the plasma screening is increased.

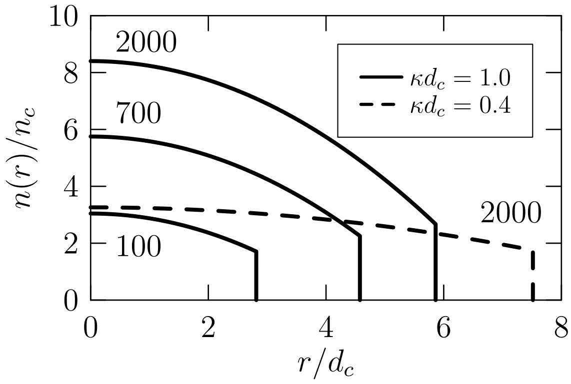

Figure 1: Radial density profile for a parabolic confinement potential $\Phi(r) = \alpha r^2/2$ and a constant screening parameter $\kappa d_c = 1$ and three different particle numbers N shown in the figure. For comparison, the result for $\kappa d_c = 0.4$ and $N = 2000$ is shown by the dashed line.

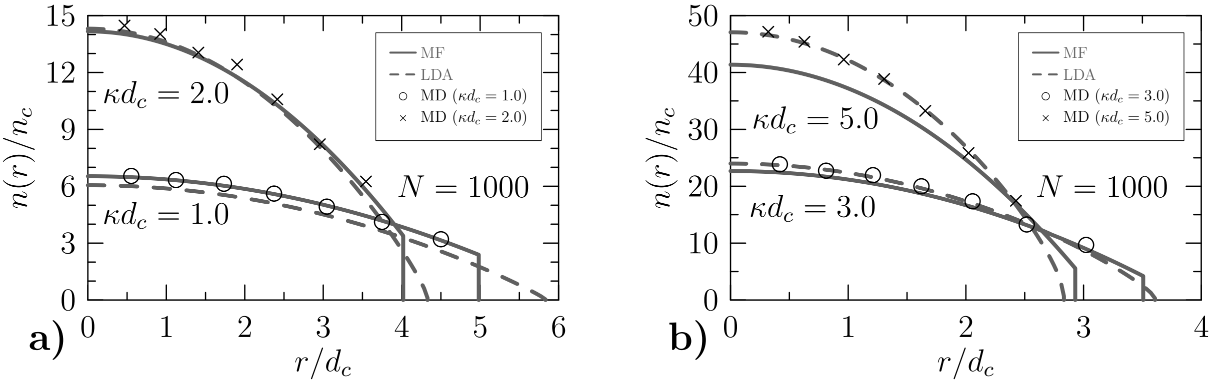

Figure 2: Radial density profiles of a three-dimensional plasma of $N = 1000$ particles calculated with the exact mean-field model (solid lines) and with LDA including correlation contributions (dashed lines) for four different screening parameters: a) $\kappa d_c = 1.0, 2.0$, b) $\kappa d_c = 3.0, 5.0$. Averaged shell densities of molecular dynamics results of a plasma crystal for the same parameters are shown by the symbols.

Ground state of a confined plasma within LDA

One way to include the correlation contribution u^{cor} is to apply LDA using the corresponding contribution of the homogeneous system [7] which yields the LDA energy functional (for details see Ref. [2])

$$E^{\text{LDA}}[n] = \int d^3r \left\{ n(\mathbf{r})\Phi(\mathbf{r}) + \frac{N-1}{N} Q^2 n(\mathbf{r})^2 \frac{2\pi}{\kappa^2} \right. \\ \left. - 1.444 Q^2 n(\mathbf{r})^{\frac{4}{3}} \times \exp\Big(-0.375 \kappa n(\mathbf{r})^{-\frac{1}{3}} + 7.4 \cdot 10^{-5} (\kappa n(\mathbf{r})^{-\frac{1}{3}})^4 \Big) \right\}. \tag{4}$$

As before, variation of this energy at constant particle number yields the ground state density profile, but now with correlation effects included. In this case the strong non-linear character of the energy density does not allow for an explicit solution. Just an implicit solution is possible and is given by the following equation for $z^3(\mathbf{r}) = \kappa^{-3} n^{\text{LDA}}(\mathbf{r})$

$$0 = \frac{N-1}{N} z^3(\mathbf{r}) + \frac{\Phi(\mathbf{r}) - \mu}{4\pi Q^2 \kappa} - \big(c_1 z(\mathbf{r}) + c_2 - c_3 z(\mathbf{r})^{-3} \big) \exp\Big(-c_4 z(\mathbf{r})^{-1} + c_5 z(\mathbf{r})^{-4} \Big), \tag{5}$$

with the constants $c_1 = 0.153$, $c_2 = 0.0144$, $c_3 = 1.134 \cdot 10^{-5}$, $c_4 = 0.375$, $c_5 = 7.4 \cdot 10^{-5}$.

The solution of Eq. (5) can be obtained numerically. For the case of a parabolic external potential $\Phi(r) = (\alpha/2) r^2$ results are given in Fig. 2 by the dashed lines for $N = 1000$ and four different screening parameters between $\kappa d_c = 1.0$ and $\kappa d_c = 5.0$.

Comparison with simulation results for finite Yukawa crystals

In order to compare the density profiles $n(r)$ of our continuous models with the density of discrete spherical Yukawa crystals, we performed molecular dynamics simulations of the ground state of a large number of Yukawa balls, for details, see refs. [5, 6]. As an example, Fig. 2 shows the comparison with a Yukawa ball of 1000 particles. The symbols denote the average particle density of the shell, while the lines represent the MF (solid) and the LDA (dashed) densities.

For small values of the screening parameter $\kappa d_c < 2$ the simulation results are very well reproduced by the analytical density profile of the non-local mean-field model (MF), whereas the LDA underrates the results (lower lines in Fig. 2 (a)). On the other hand, for larger values of the screening parameter $\kappa d_c > 2$ the simulation results are reproduced by LDA, whereas MF underestimates these results in the center. This underestimation is accompanied by a wrong prediction of the profile curvature (Fig. 2 (b)). For intermediate values of the screening parameter $\kappa d_c \approx 2$ both methods are very close to the simulation results (upper lines in Fig. 2 (a)).

Summary and discussion

We have presented a theoretical analysis of the ground state density profile of spatially confined one-component Yukawa plasmas using the mean-field approximation as well as the local density approximation with inclusion of correlations. Closed equations, Eqs. (3, 5), for the density profile for an arbitrary confinement potential have been derived.

Comparisons with first-principle simulation results of strongly correlated Yukawa crystals with varying screening parameter have shown that the MF results are more accurate for weak screening whereas LDA yields the proper description for large screening. Therefore, MF together with LDA complement one another in the description of strongly correlated spatially confined one-component Yukawa plasmas.

Acknowledgments

This work is supported by the Deutsche Forschungsgemeinschaft via SFB-TR 24 projects A3, A5 and A7.

References

[1] C. Henning et al., Phys. Rev. E 74, 056403 (2006)

[2] C. Henning, P. Ludwig, A. Filinov, A. Piel, and M. Bonitz, submitted to Phys. Rev. E

[3] O. Arp, D. Block, A. Piel, and A. Melzer, Phys. Rev. Lett. 93, 165004 (2004)

[4] H. Totsuji, C. Totsuji, T. Ogawa, and K. Tsuruta, Phys. Rev. E 71, 045401 (2005)

[5] P. Ludwig, S. Kosse, and M. Bonitz, Phys. Rev. E 71, 046403 (2005)

[6] M. Bonitz et al., Phys. Rev. Lett. 96, 075001 (2006)

[7] H. Totsuji, J. Phys. A **39**, 4565 (2006)