Anomalous spatial charge profiles of plasma in trap as manifestation of phase transitions in local EOS approximation

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**Introduction**

**LDA** (or “jellium”... or “pseudo-liquid“ approximation – it is replacing system of discrete particles (electrons and/or ions) by hypothetical “fluid” with pure local thermodynamic properties (i.e. *depending on local density only*) - is widely used in calculation of equilibrium charged particles distribution near a source of non-uniformity

In most cases **LDA** uses **ideal-gas** EOS! It leads to well-known “correlationless” Thomas – Fermi or Poisson – Boltzmann approximations.

The simplest way to take into account of mean-particle correlations (non-ideality) in frames of **LDA** is using of improved **Thomas-Fermi-Dirac** or **Poisson-Boltzmann-Debye** approximations.
Applications

There are great number applications where Poisson- Boltzmann approximation can be replaced by model of charged hard (or soft) spheres (HS-OCP or SS-OCP):

• Equilibrium counterions distribution around a polyions in highly asymmetric electrolyte;

• Equilibrium ions distribution around macroions in highly asymmetric complex plasma;

• Spatial ionic profile in Z-pinch – i.e. equilibrium quasistationary ensemble of classical “cold” ions around contracted "string" of relativistic electrons;

• etc.
Simplified Model – Macro- and micro ions in WS cell

Macro and micro ions – are charged hard spheres

+Z and D – charge and diameter of macroions
(Z >> 1)

- z and σ – charge and diameter of microions
Thermo-electrostatics $\Leftrightarrow$ Variational approach

$$F_{\text{Equilibrium}}(N,V,T) = \min_{n(\cdot)} (F\{n(\cdot)\}) = U_{Ze} + U_{ee} + F\{n(\cdot)\} \equiv$$

$$-\int \frac{Ze^2}{\bar{r}} n(\bar{r}) d\bar{r} + \frac{e^2}{2} \int \frac{n(\bar{x}) \cdot n(\bar{y})}{|\bar{x} - \bar{y}|} d\bar{x} d\bar{y} + F^*[n(\cdot)]$$

$$\int n_e(\bar{r}) d\bar{r} = Z \quad \text{electroneutrality condition (} Z - \text{macroion charge)}$$

**Correlation Functional in Local Density Approximation**

$$F^*[n(\cdot)] = \int f(n(\bar{x})) \cdot n(\bar{x}) d\bar{x}$$

$f_i(n,T) - \text{reduced free energy of macroscopic uniform ion system}$

$$f(n,T) \equiv \lim \left\{ \frac{F(N,V,T)}{N} \right\}^{(N \rightarrow \infty; N/V = n)}$$
Local EOS approximation choice

To take into account ion-ion correlation in the Local EOS approximation correctly - we should use exact EOS of non-ideal OCP of classical charged hard spheres system (HS-OCP) on uniformly-compressible electrostatic background.

We use for this purpose Model EOS: $F(V, N, T) = F_{HS} + F_{OCP}$


**Hard-spheres component** – a wide range of choice(*)


**Electrostatic component** – Modified Mean Spherical Approximation (MSA)(*)

* Иосилевский И.Л., Фазовые переходы в кулоновских системах “Уравнение состояния в экстремальных условиях” Ред. Г.В. Гадияк // ..Новосибирск: Изд. COAH CCCP, (1981)

Local EOS approximation

Hard-spheres component

\[ \eta \frac{\partial}{\partial \eta} \hat{f}_{\text{hs}}^{c}(CS) = \frac{2\eta(2 - \eta)}{(1 - \eta)^3} \]

Electrostatic component – Modified Mean Spherical Approximation (MSA)

\[ \eta \frac{\partial}{\partial \eta} \hat{f}_{\text{msa}}^{c} = \frac{-\lambda}{24\eta} \left( \eta(1 - 2\eta/5)\lambda - (1 - 2\eta) \right) + \frac{(1 - 13\eta - 6\eta^2)}{(1 - \eta)}(Q - 1) - \frac{2}{3\lambda} \left( \frac{1 + 2\eta}{1 - \eta} \right)^3 \times \left( 1 + \frac{9\eta}{(1 - \eta)(1 + 2\eta)} \right)((Q - 1)^3 + 1) \]
Phase diagram for one-component model of charged hard spheres on uniformly-compressible background

**Equation:**

\[ T_c^* = \frac{(3.15 z^2/d)}{d} \] (\( z \) - microion charge, \( d \) - microion diameter in Å)

\[ \eta_c = \frac{\pi n_c \sigma^3}{6} = 9.02 \times 10^{-3} \] (critical packing fraction)

Numerical Calculation Scheme

From Functional:

\[ \mu'_r = -E(r) \]

\( E(r) \) - electrostatic field strength
\( \mu(n(r),T) \) – reduced chemical potential of unified ion system

Cauchy problem:

\[ \mu'_r = -E(r), \quad n(0) = n_0 \]

Electroneutrality condition:

\[ \int n(\tilde{r}, n_0) d\tilde{r} = Z \]
Application-1: Free microions distribution around Macroion in highly asymmetric complex plasmas

\[ Z_{\text{MACRO}} = 10^5 \quad \text{//} \quad T = 0.35 T_{\text{CR}} \]
Free microions distribution around Macroion in WS-cell

\[ Z_{\text{Macro}} = 10^5 \quad T = 0.4 T_{\text{crt.}} \]
Free microions distribution around Macroion in WS-cell

\[ Z_{\text{MACRO}} = 10^5 \quad /\!\!/ \quad T = 0.7 T_{\text{CR}} \]
Free microions distribution around Macroion in WS-cell

\[ Z_{\text{MACRO}} = 10^5 \quad // \quad T = 1.05T_{CR} \]
Application-2: Free microions distribution in trap

The Simplest Trap Model - 1

1 - Crystal shell
2 - Crystal-Fluid phase transition
3 - Fluid layer
4 - Fluid-Gas phase transition
5 - Gas phase

Иосилевский И.Л., Фазовые переходы в кулоновских системах
Сб. “Уравнение состояния в экстремальных условиях”
Ред. Г.В. Гадияк // Новосибирск, Изд. СОАН СССР, (1981)
High Temperature, 23, 1041 (1985)
Application-2: Free microions distribution in trap

The simplest trap model - 1

Iosilevskiy I. *High Temp* 23 1041 (1985)

\[ T = 0.05T_{crt}. \]

\[ T = 0.55T_{crt}. \]
Application-3: Ionic Trap with Cubic Potential

External (Trap) Potential

\[ \phi \sim R^3 \]

Density Profile

\( T/T_c = 0.99 \)
Ionic Profile and Electrostatic Filed via Variational Approach

Ion Density Profile in Cubic Trap

$T/T_c = 0.99$

Total Electrostatic Filed

$E = 0$
Toward the Mixed Phase Appearance

Boiling "Liquid" Boundary

Two-phase region

Saturation Boundary

$r/r_{cell}$
Toward the Mixed Phase Appearance ($Z < Z_1$)

**Boiling “Liquid” Boundary**

**Two-phase region**

**Saturation Boundary**

![Graph showing the transition from one phase to another, with labeled boundaries and a plot of $r/r_{cell}$ vs. $r$]
Toward the Mixed Phase Appearance ($Z < Z_1$)

Boiling “Liquid” Boundary

Two-phase region

Saturation Boundary
Ionic “Vapor” Saturation Moment ($Z = Z_1$)

$$T/T_c = 0.99$$
“Mixed Phase” Concept

- “Mixed phase” – *Ultra-fine* dispersion limit of *mesoscopic structure* (*mist, emulsion, suspension, foam* etc) for *two-phase mixture* in the limit of zero-size fragments for both mixed phases in *Coulomb systems* (!)

- Mixed phase concept is well known and very popular in *astrophysical applications* – e.g. in theoretical description of structure for dense nuclear matter in interiors of so-called *compact stars* (neutron stars, strange (quark) stars, hybrid stars etc)

- Mixed phase is the zero surface tension limit of more realistic form – so-called *Structured Mixed Phase* (“Pasts Plasma”) – equilibrium mesoscopic mixture of *non-spherical charged microfragments* of coexisting phases (bubbles, rods, plates etc.)

See e.g.
*etc*
Ionic “Vapor” Saturation Moment ($Z = Z_1$)

- Boiling “Liquid” Boundary
- Two-phase region
- Saturation Boundary

Graph showing the relationship between $\frac{r}{r_{cell}}$ and $\mu$. The graph includes curves representing different phases and boundaries.
“Mixed Phase” Layer Appearance ($Z_1 < Z < Z_2$)

- Boiling “Liquid” Boundary
- Two-phase region
- Saturation Boundary
- Ionic “Vapor”
- $\mu = \text{const}$
- $E = 0$

$E = 0$
Mixed Phase Layer Growth \( (Z_1 < Z < Z_2) \)

- Boiling "Liquid" Boundary
- Two-phase region
- Saturation Boundary
- Ionic "Vapor"
Mixed Phase Layer Growth ($Z_1 < Z < Z_2$)

Boiling “Liquid” Boundary

Two-phase region

Saturation Boundary

μ = const

$E = 0$

Mixed Phase

Ionic “Vapor”

Ionic “Vapor”

$r/r_{cell}$
Liquid Layer Appearance \((Z = Z_2)\)

- Boiling “Liquid” Boundary
- Two-phase region
- Saturation Boundary
- Ionic “Vapor”
- Mixed Phase
- \(\mu = \text{const}\)
- \(E = 0\)
Liquid Layer Growth ($Z > Z_2$)

- **Boiling “Liquid” Boundary**
- **Saturation Boundary**
- **Two-phase region**
- **Mixed Phase**
- **Ionic “Vapor”**

$\mu = \text{const}$

$E = 0$

$r/r_{\text{cell}}$
Liquid Layer Growth ($Z > Z_2$)

- Boiling “Liquid” Boundary
- Saturation Boundary
- Two-phase region
- Mixed Phase
- Ionic “Vapor”

$\mu = \text{const}$

$E = 0$

$r/r_{cell}$
Liquid Layer Growth ($Z > Z_2$)

- **Boiling “Liquid” Boundary**
- **Saturation Boundary**
- **Two-phase region**
- **Mixed Phase**
- **Ionic “Vapor”**

- $E = 0$
- $\mu = \text{const}$
CONCLUSION

• In spite of the repulsion of like charges, taking into account correlations of individual charges within the Local Density Approximation is equivalent to an effective Additional Attraction, and therefore, the resulting charge profiles will be steeper in comparison with the profile calculated in "correlationless" (Poisson-Boltzmann or Thomas-Fermi) approximation.

• At sufficiently low temperatures (even at small coupling parameter $\Gamma$) this effect could lead to dramatic change in the charged particles profile.

• The fact of the discontinuity appearance, as well as the parameters under which this discontinuity appearance takes place, receive a natural interpretation in terms of a phase transition in modified One-Component Plasma models (OCP($\sim$)), which EOS replaces ideal gas Equation of State in Local Density Functional when we take into account correlations of charged particles.