NPP 2021
NON-IDEAL PLASMA PHYSICS
Annual Moscow Workshop

Scientific–Coordination Workshop on
Non-Ideal
Plasma Physics

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

Chigvintsev A.Yu.[1], **Iosilevskiy I.L.**[1,2]

Cooperation: **Noginova I.Y.** [3], **Zorina I.G.**[4]

[1] *Moscow Institute of Physics and Technology, Dolgoprudny, Moscow Region, Russia*
[2] *Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow , Russia*
[3] *MISiS - National University of Science and Technology, Moscow, Russia*
[4] *Moscow State Technical University, Moscow, Russia*

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.

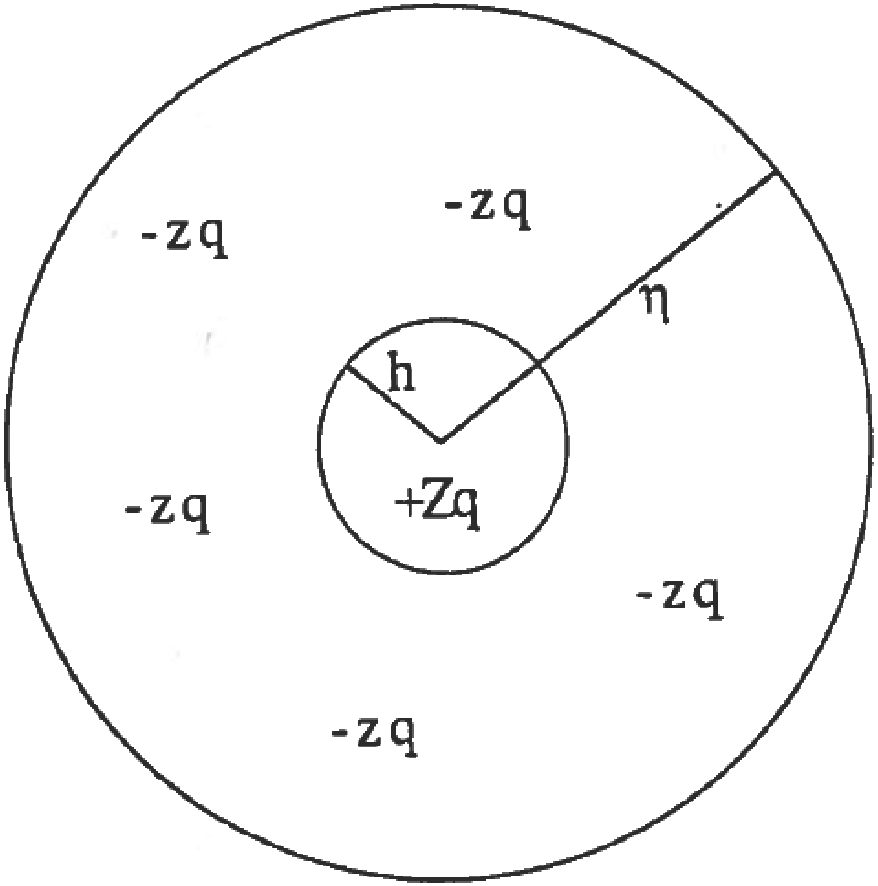
The simplest way to take into account of mean-particle correlations (**non-ideality**) in frames of **LDA** is using of improved **Thomas-Fermi-Dirac** or **Poisson-Boltzmann-Debye** approximations.

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 microions 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 ⇔ Variational approach

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

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

$\boxed{\int n_e(\bar{r})\, d\bar{r} = Z}$ *electroneutrality condition (Z – macroion charge)*

Correlation Functional in Local Density Approximation

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

$f_i(n,T)$ – reduced free energy of macroscopic uniform ion system

$$\boxed{f(n,T) \equiv \lim \left\{ \frac{F(N,V,T)}{N} \right\}_{(N\Rightarrow\infty;\, N/V=n)}}$$

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: = Sum of hard-core and electrostatic components(*): $F(V,N,T) = F_{HS} + F_{OCP}$

*****Brilliantov N, Malinin V., Netz R. // *Eur. Phys*. *J.* D **18,** 339 (2002)

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

*****Mulero A (Ed.) - *Theory and Simulation of Hard-Sphere Fluids and Related Systems*. (Berlin Heidelberg:Springer) (2008)

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. СОАН СССР, (1981)

****** Penfold R, Nordholm S et al. // *J. Chem. Phys*. **95** 2048 (1991)

Local EOS approximation

Hard- spheres component

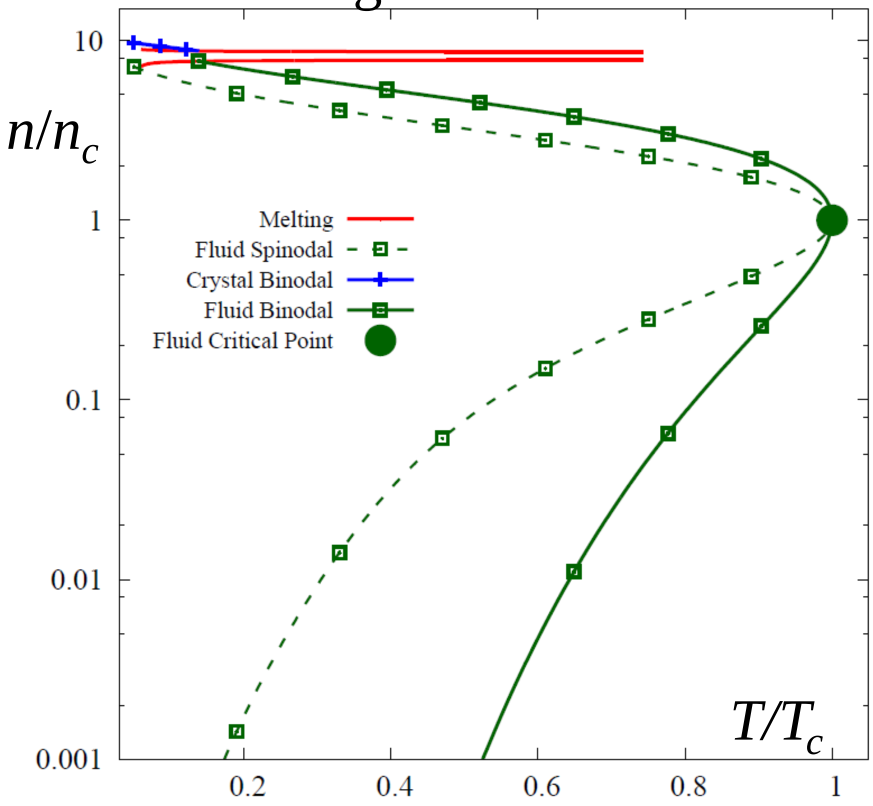
$$\eta \frac{\partial}{\partial \eta} \hat{f}_c^{\mathrm{hs}}(\mathrm{CS}) = \frac{2\eta(2-\eta)}{(1-\eta)^3};$$

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

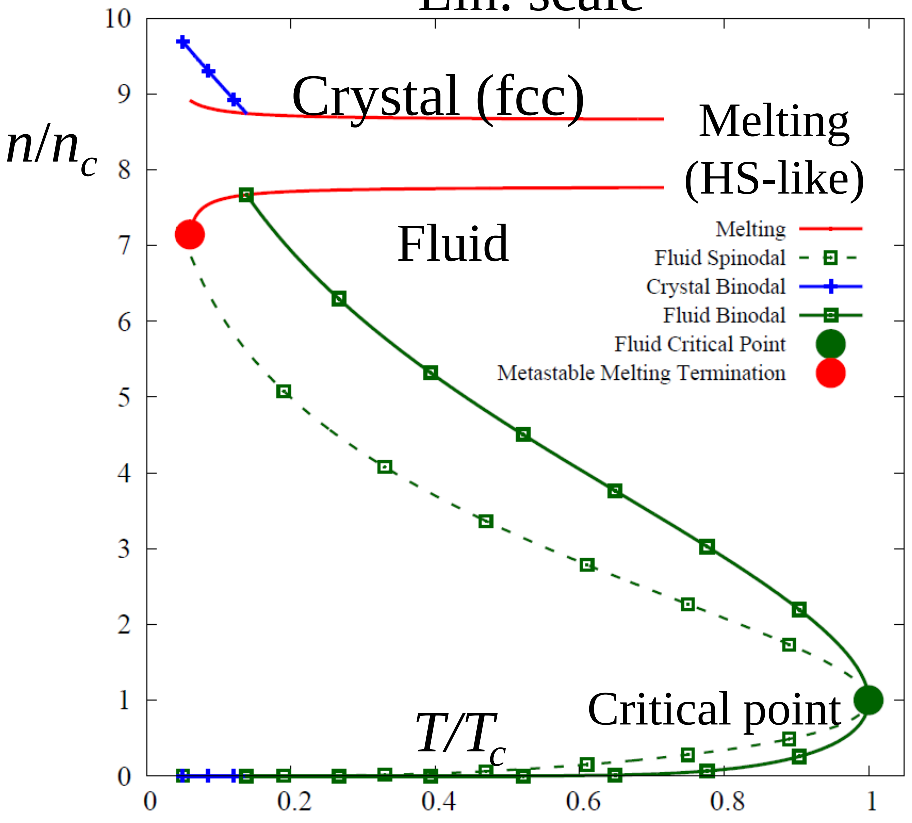
$$\begin{aligned}\eta \frac{\partial}{\partial \eta} \hat{f}_c^{\mathrm{msa}} = \frac{-\lambda}{24\eta}\Bigg(&\eta(1-2\eta/5)\lambda - (1-2\eta)\\ &+ \frac{(1-13\eta-6\eta^2)}{(1-\eta)}(Q-1) - \frac{2}{3\lambda}\left(\frac{1+2\eta}{1-\eta}\right)^3\\ &\times\left(1+\frac{9\eta}{(1-\eta)(1+2\eta)}\right)((Q-1)^3+1)\Bigg),\end{aligned}$$

Phase diagram for one-component model of charged hard spheres on *uniformly-compressible* background

Log. scale



Lin. scale



$T_c^* = (3.15 * z^2/d)$ (*z - microion charge, d - microion diameter in A*)

$\eta_c \equiv (\pi n_c \sigma^3/6) = 9.02*10^{-3}$ (critical packing fraction)

Chigvintsev A., Iosilevskiy I., Zorina I., Noginova L. // *J. of Phys. Conf. Ser.* **946**, (2018)

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:

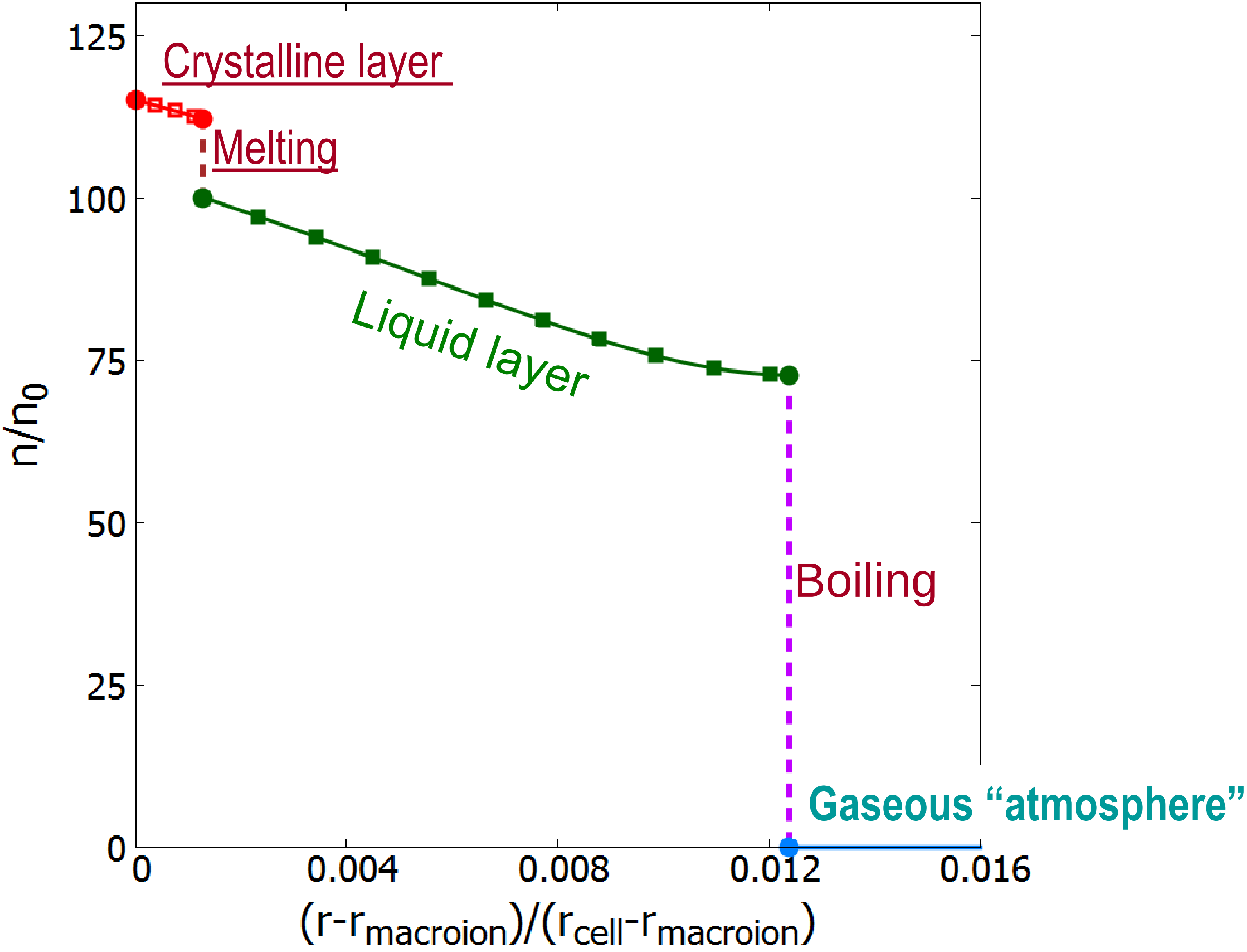
$$\mu_r' = -E(r), \quad n(0) = n_0$$

Electroneutrality condition :

$$\int n(\bar{r}, n_0)\, d\bar{r} = Z$$

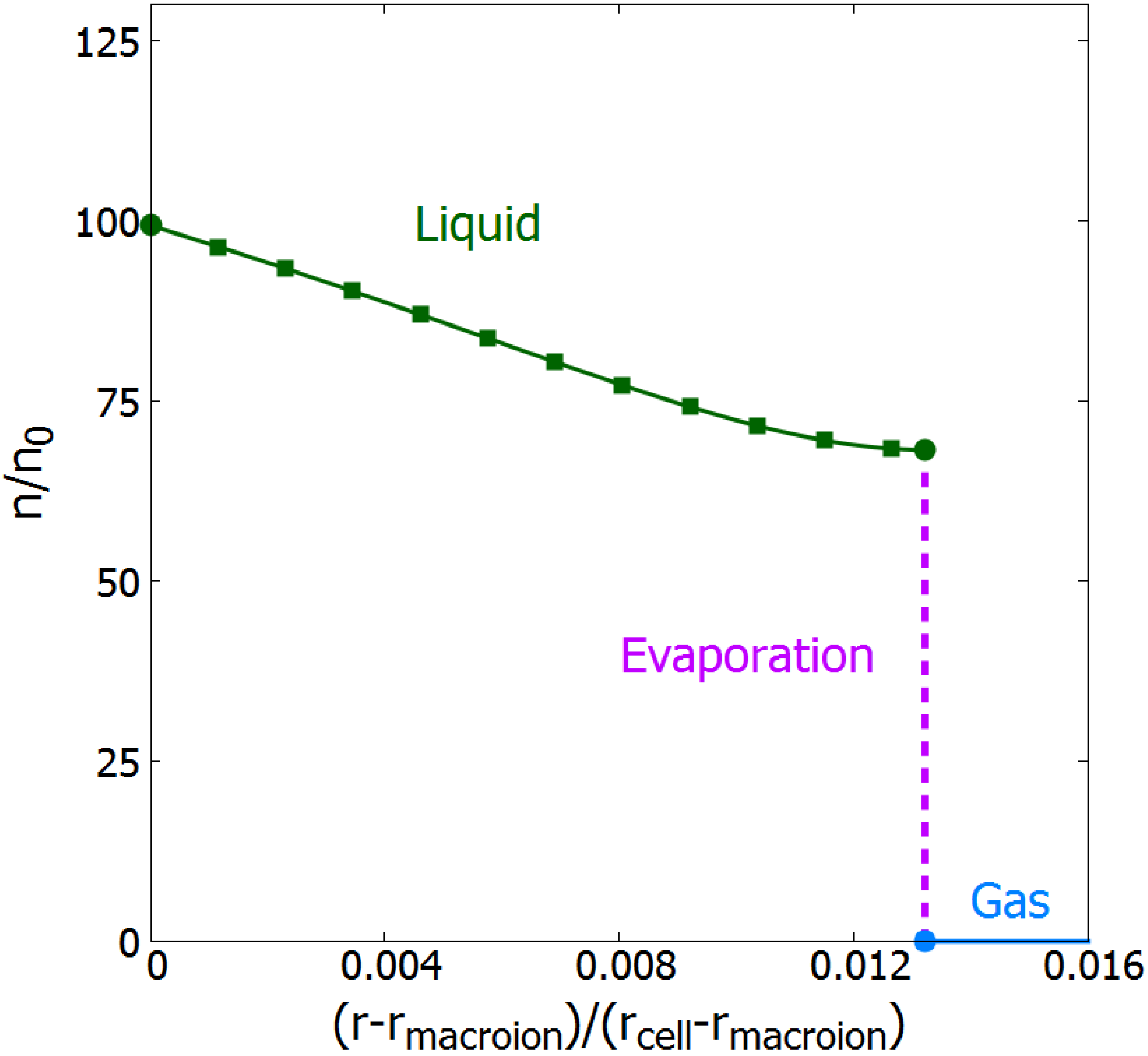
Application-1: Free microions distribution around Macroion in highly asymmetric complex plasmas

$Z_{\mathrm{MACRO}} = 10^5$ // $T = 0.35 T_{CR}$



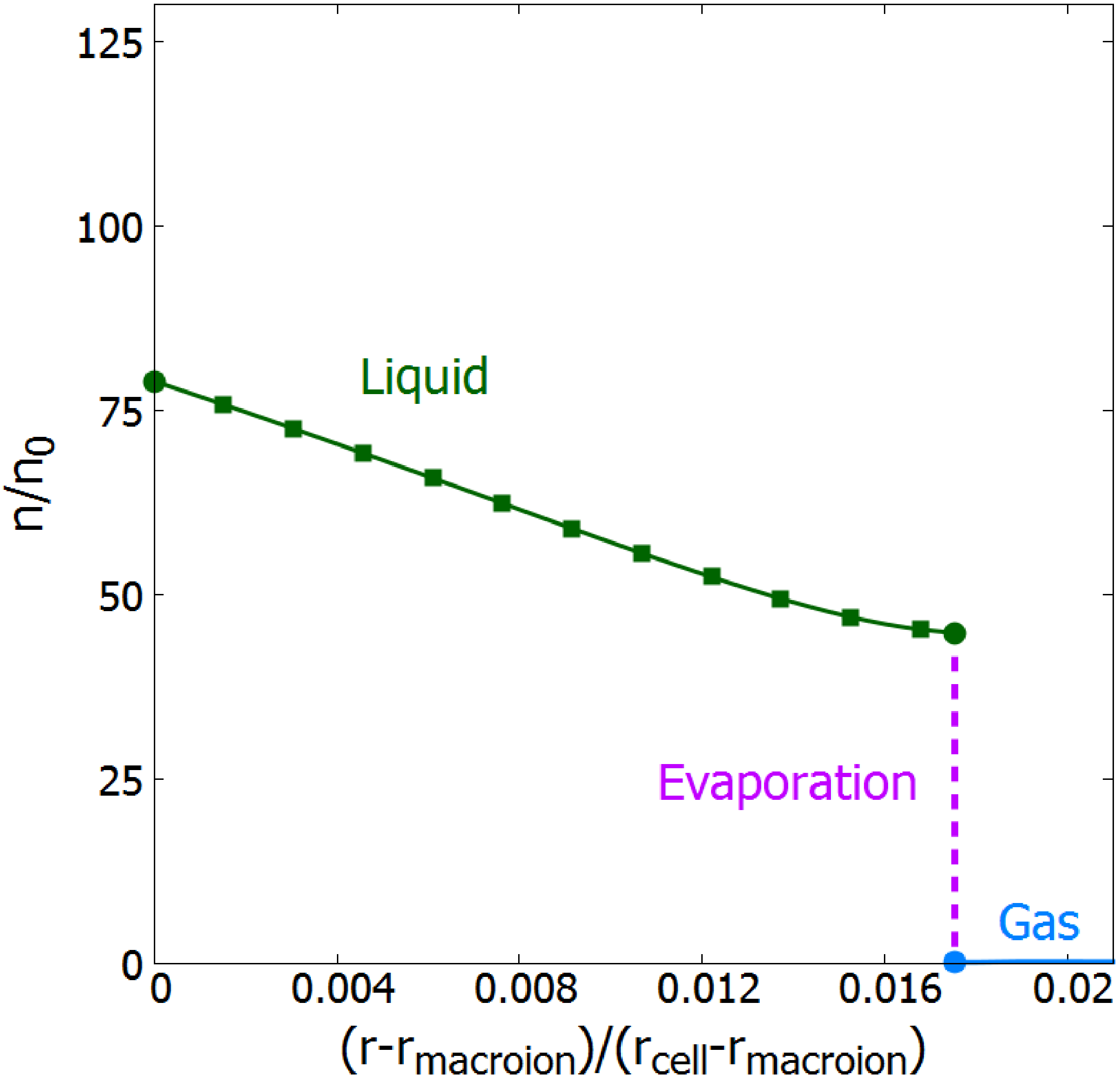
Free microions distribution around Macroion in WS-cell

$Z_{\text{Macro}} = 10^5 \quad T = \mathbf{0.4}\,T\mathit{crt}.$



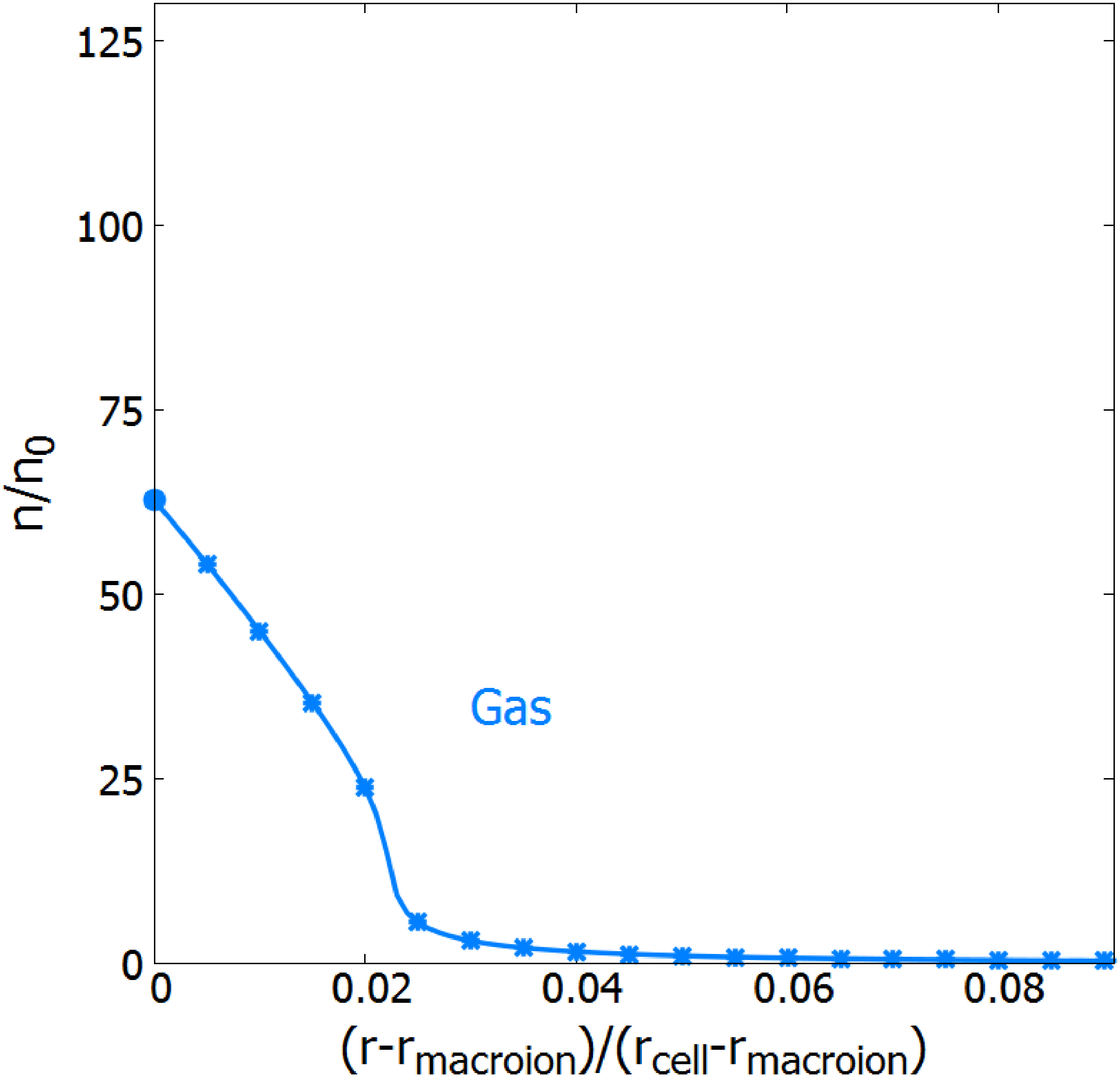
Free microions distribution around Macroion in WS-cell

$Z_{\mathrm{MACRO}} = 10^5$ // $T = 0.7T_{CR}$



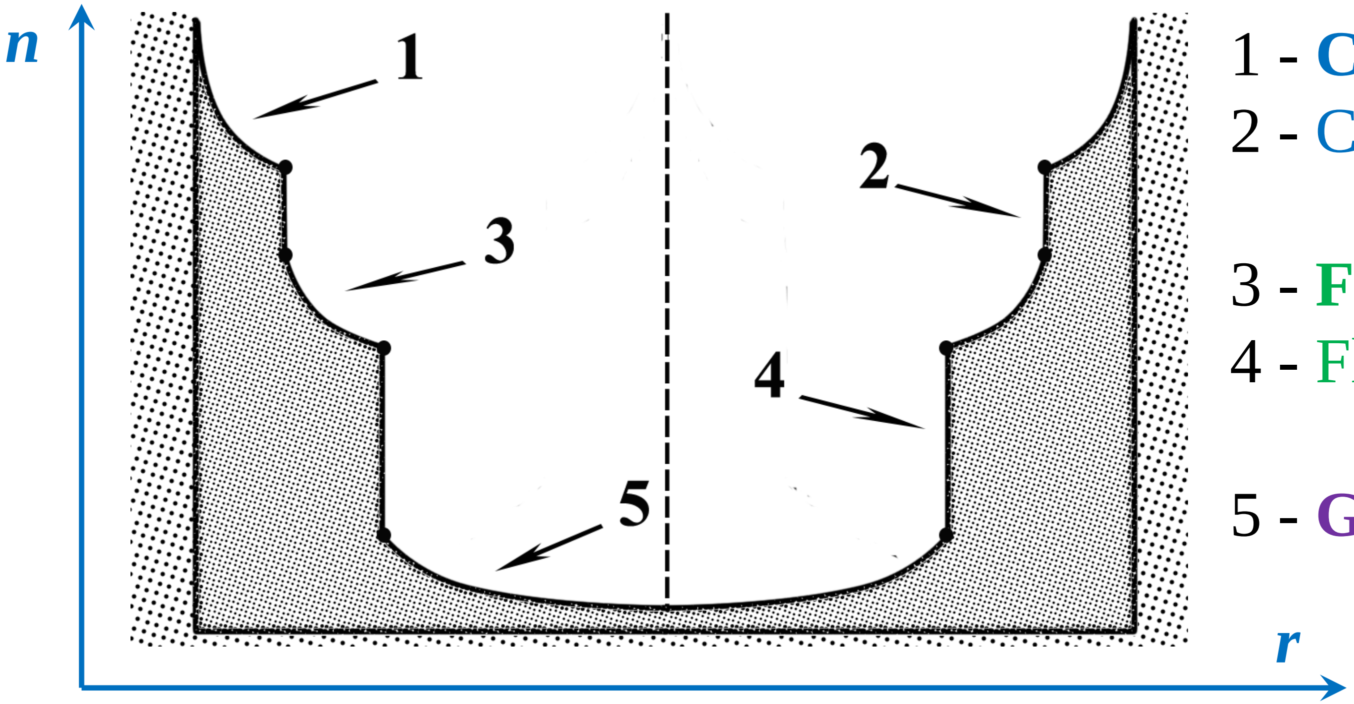
Free microions distribution around Macroion in WS-cell

$Z_{\mathrm{MACRO}} = 10^5$ // $T =$ **1.05**T_{CR}



Application-2: Free microions distribution in trap

The Simplest Trap Model - 1

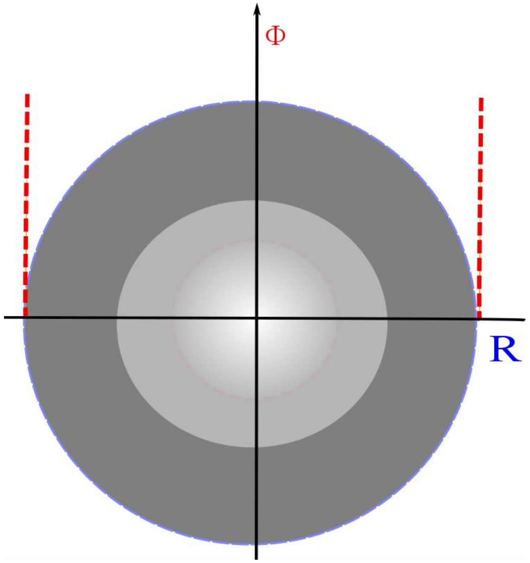


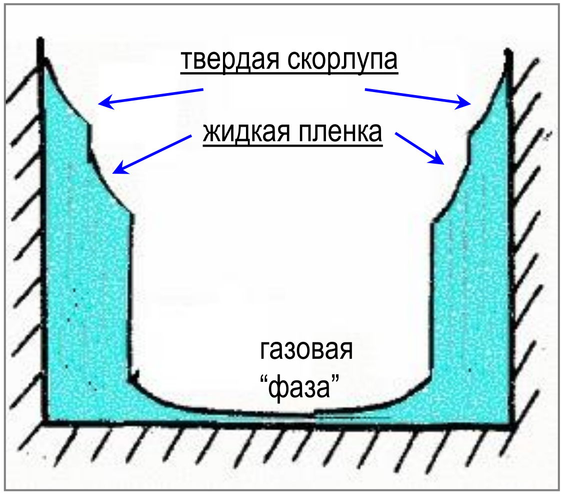
1 - **Crystal shell**
2 - Crystal-Fluid
phase transition
3 - **Fluid layer**
4 - Fluid-Gas
phase transition
5 - **Gas phase**

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

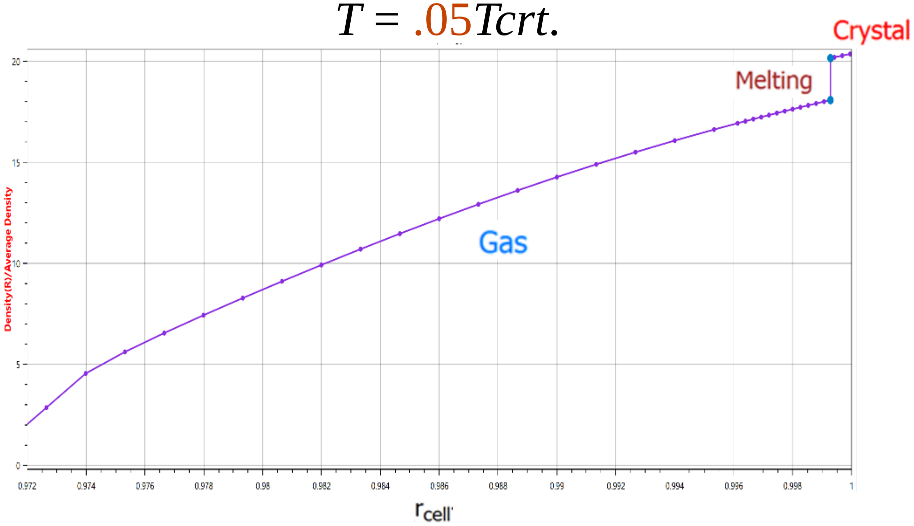
The simplest trap model - 1



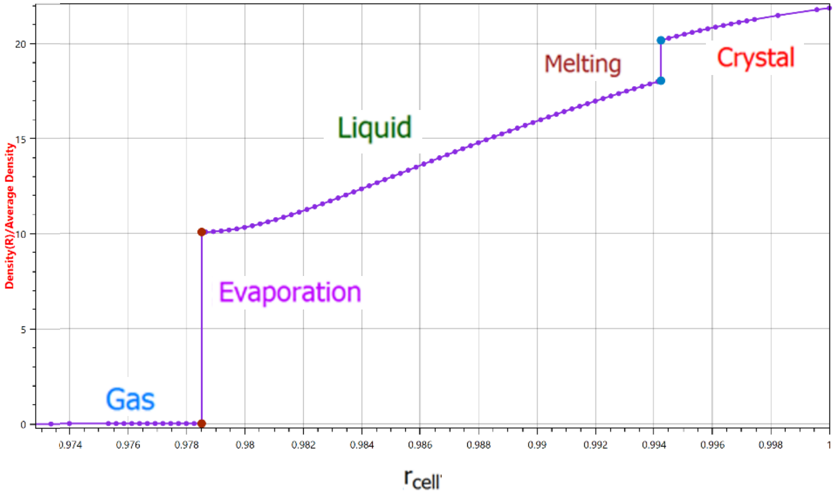


Iosilevskiy I. *High Temp* **23** 1041 (1985)

T = .05$Tcrt.$



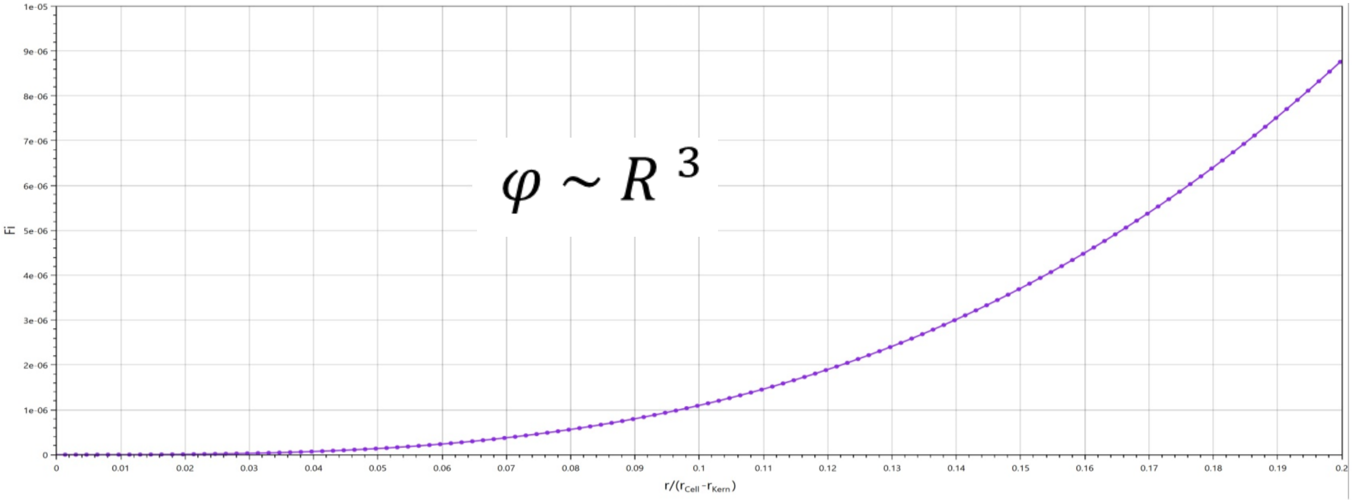
T = .55$Tcrt.$



Application-3: Ionic Trap with Cubic Potential

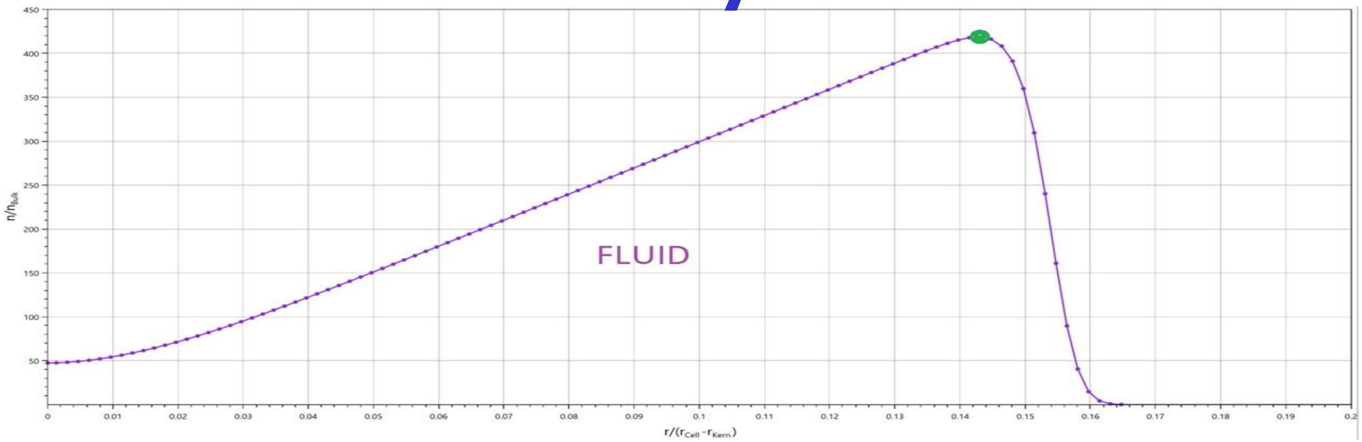
External (Trap) Potential

$T/T_c = 0.99$



$\varphi \sim R^{3}$

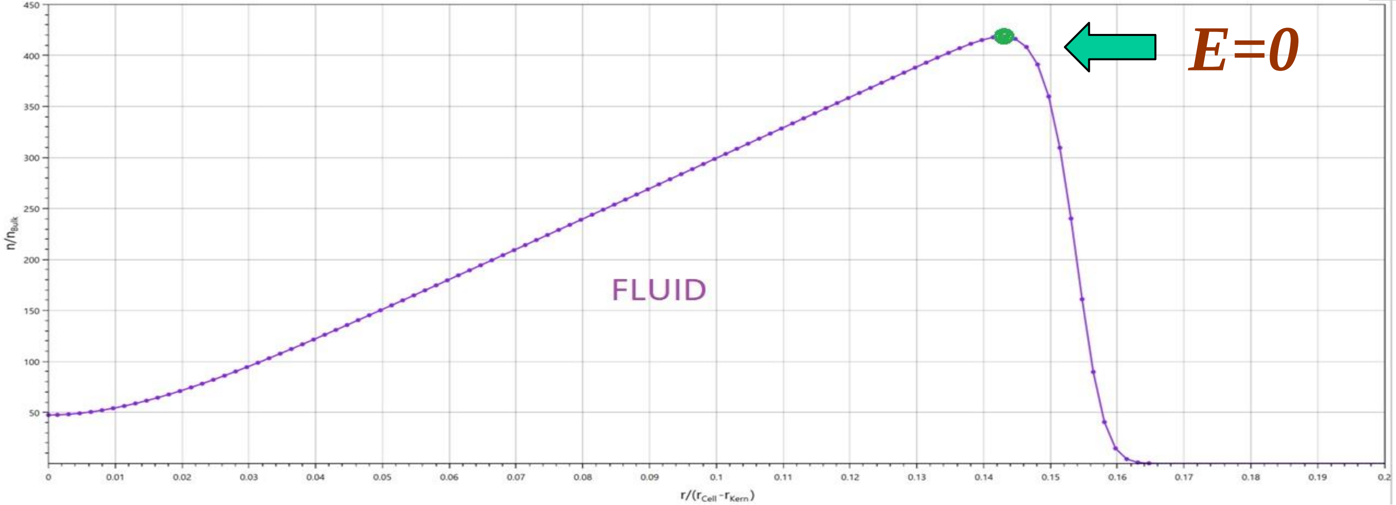
Density Profile



Ionic Profile and Electrostatic Filed via Variational Approach

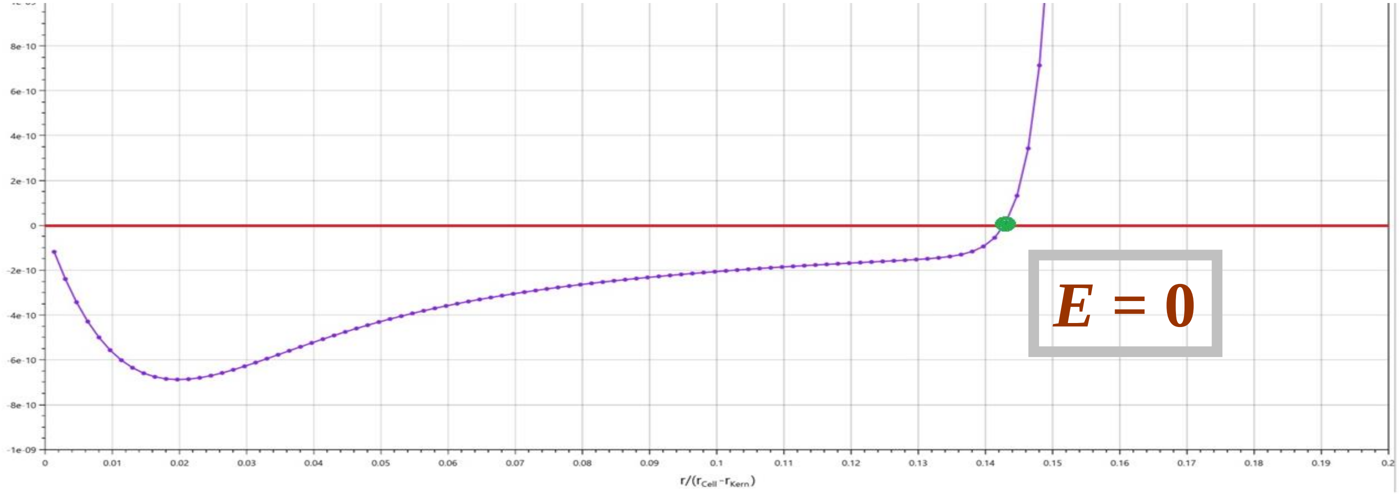
$T/T_c = 0.99$

Ion Density Profile in Cubic Trap



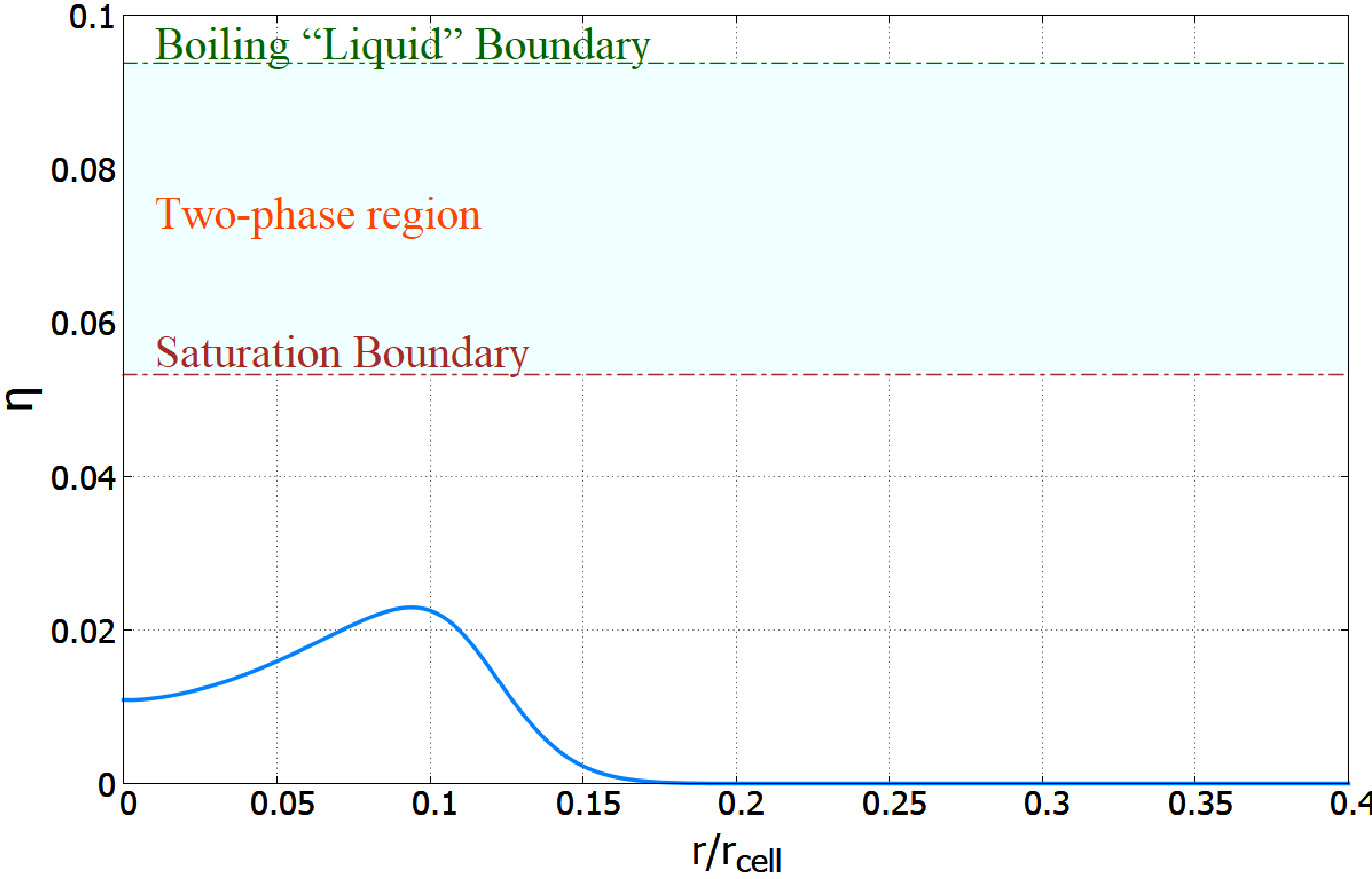
E=0

Total Electrostatic Filed

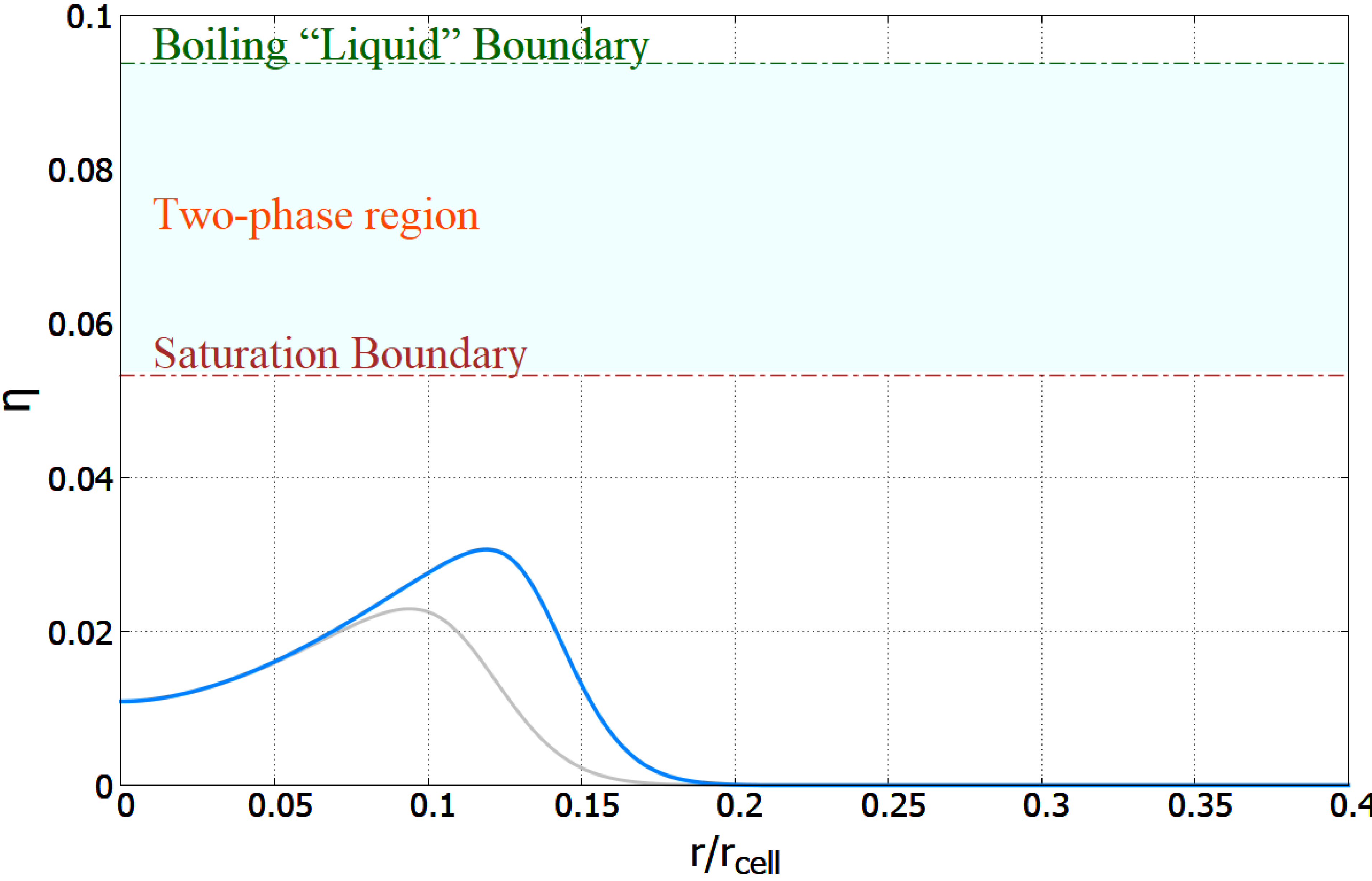


$E = 0$

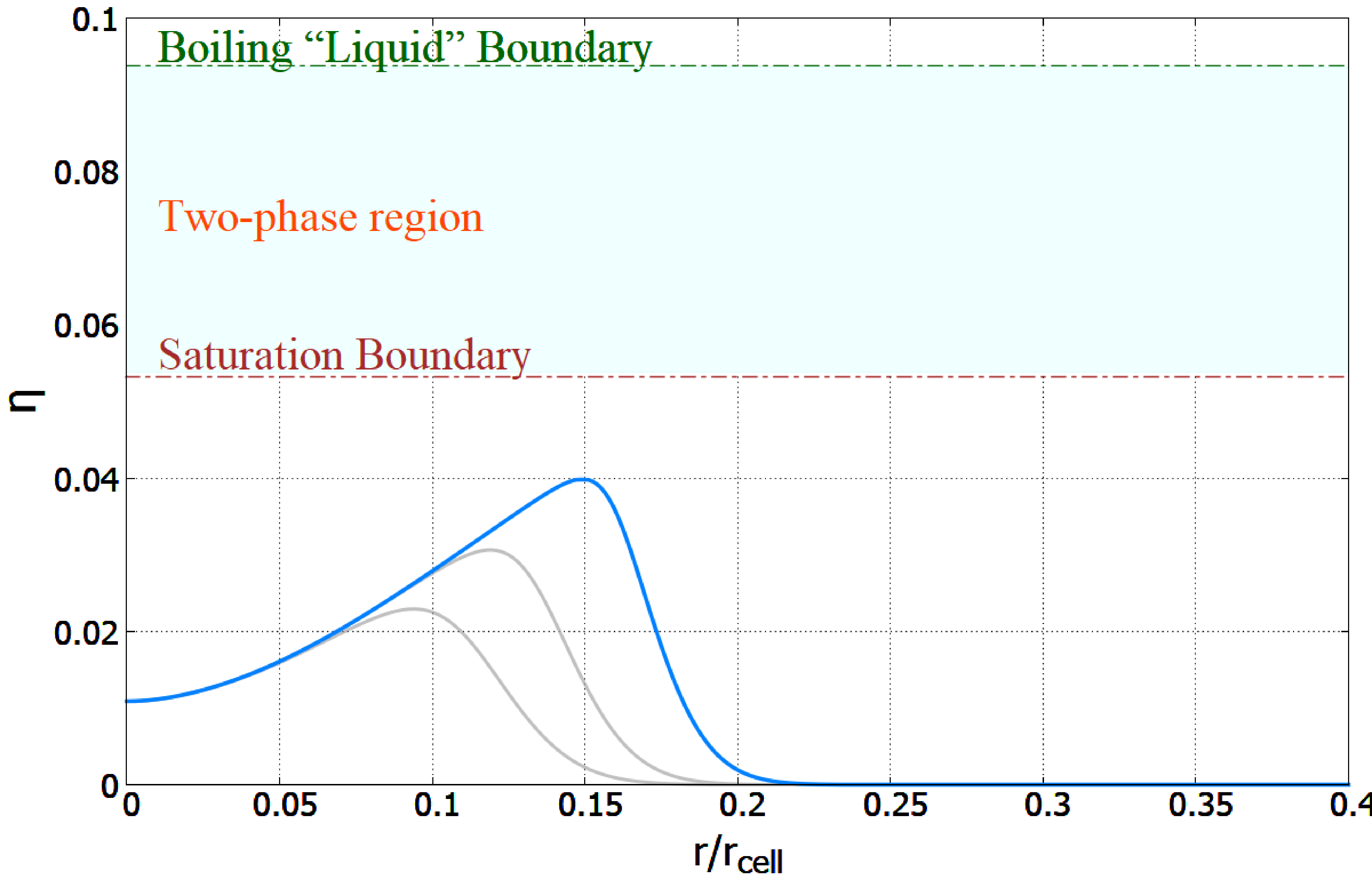
Exotics - Mixed Phase Appearance



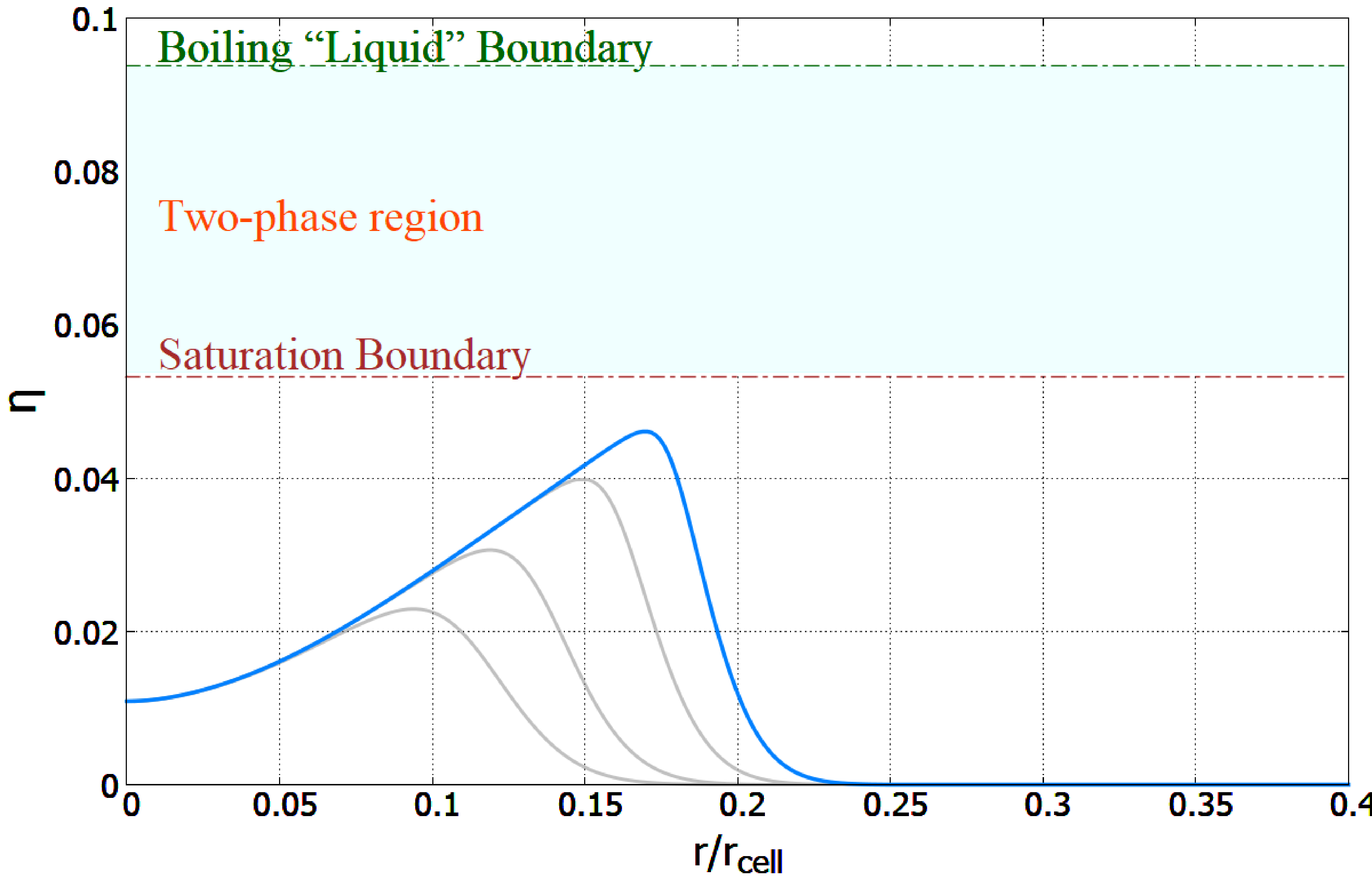
Toward the Mixed Phase Appearance



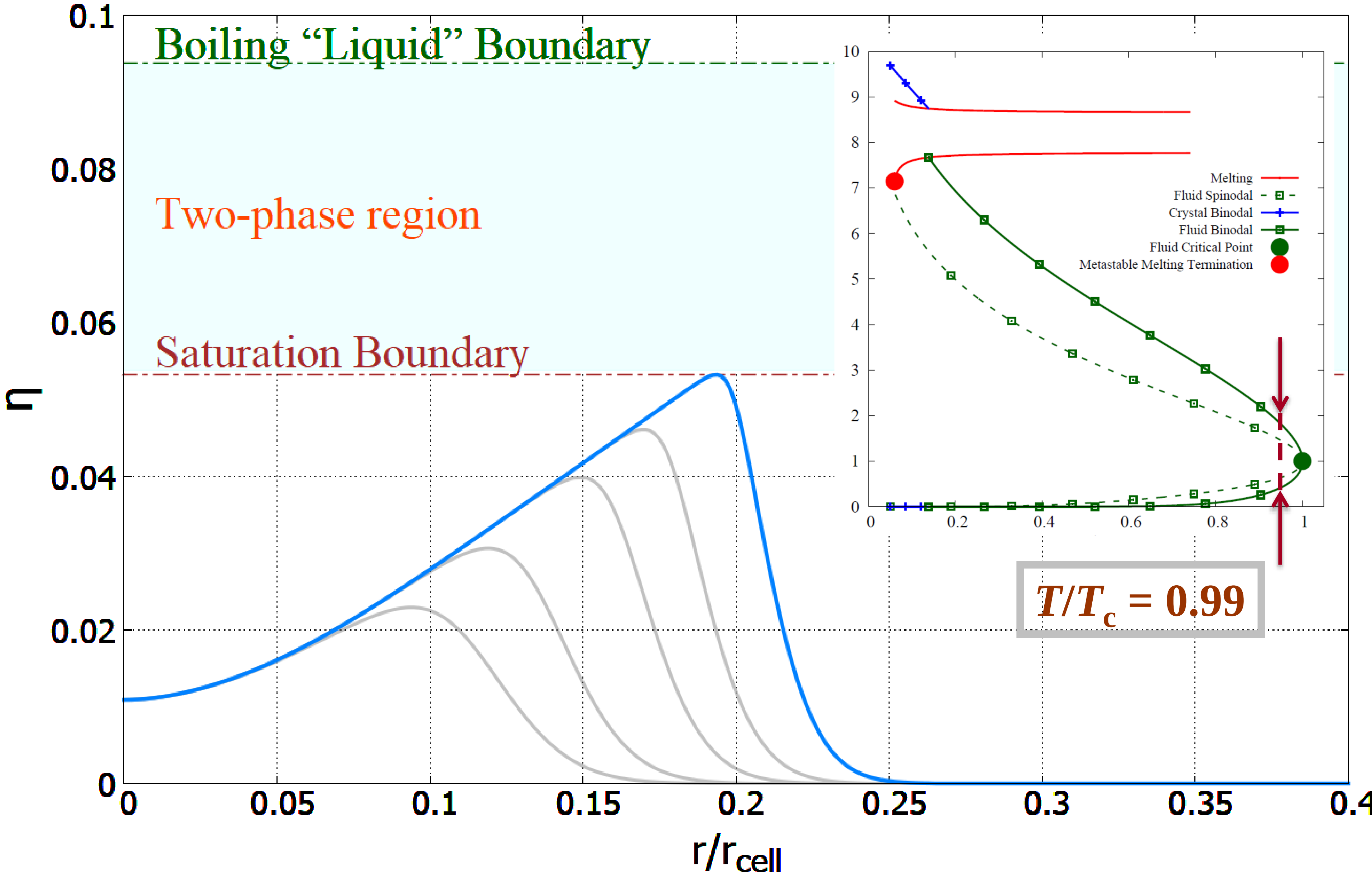
Toward the Mixed Phase Appearance ($Z < Z_1$)



Toward the Mixed Phase Appearance ($Z < Z_1$)



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.)

<u>See e.g.</u>

Ravenhall D., Pethick C. & Wilson J. // *Phys. Rev. Lett.* **50,** 2066 (1983)

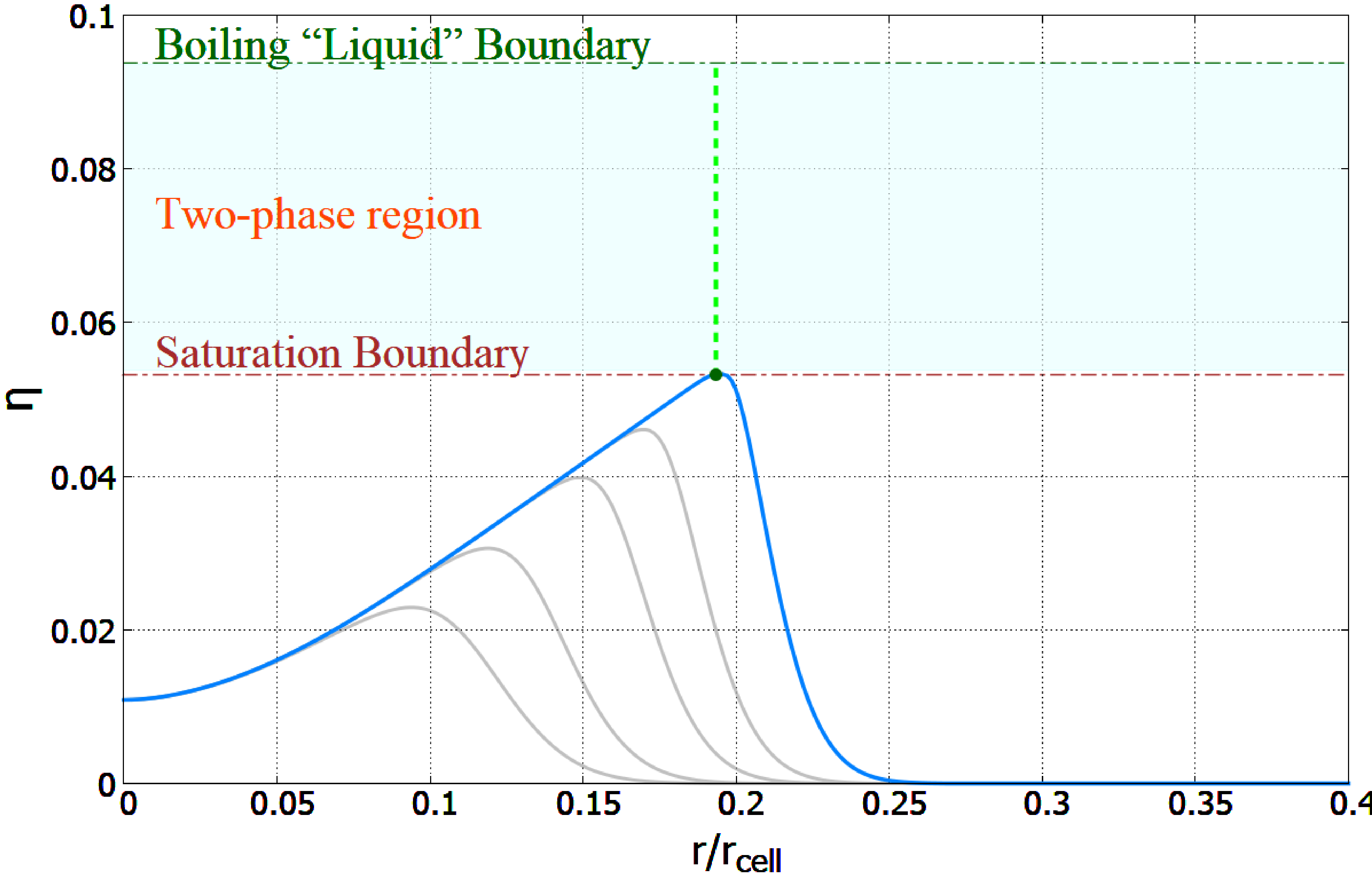
Maruyama T., Tatsumi T., Voskresenskiy D., Tanigava T., *Phys. Rev.* C **72,** (2005)

Iosilevskiy I., *Acta Physica Polonica B (Proc. Suppl.)* **3,** 589-600 (2010)

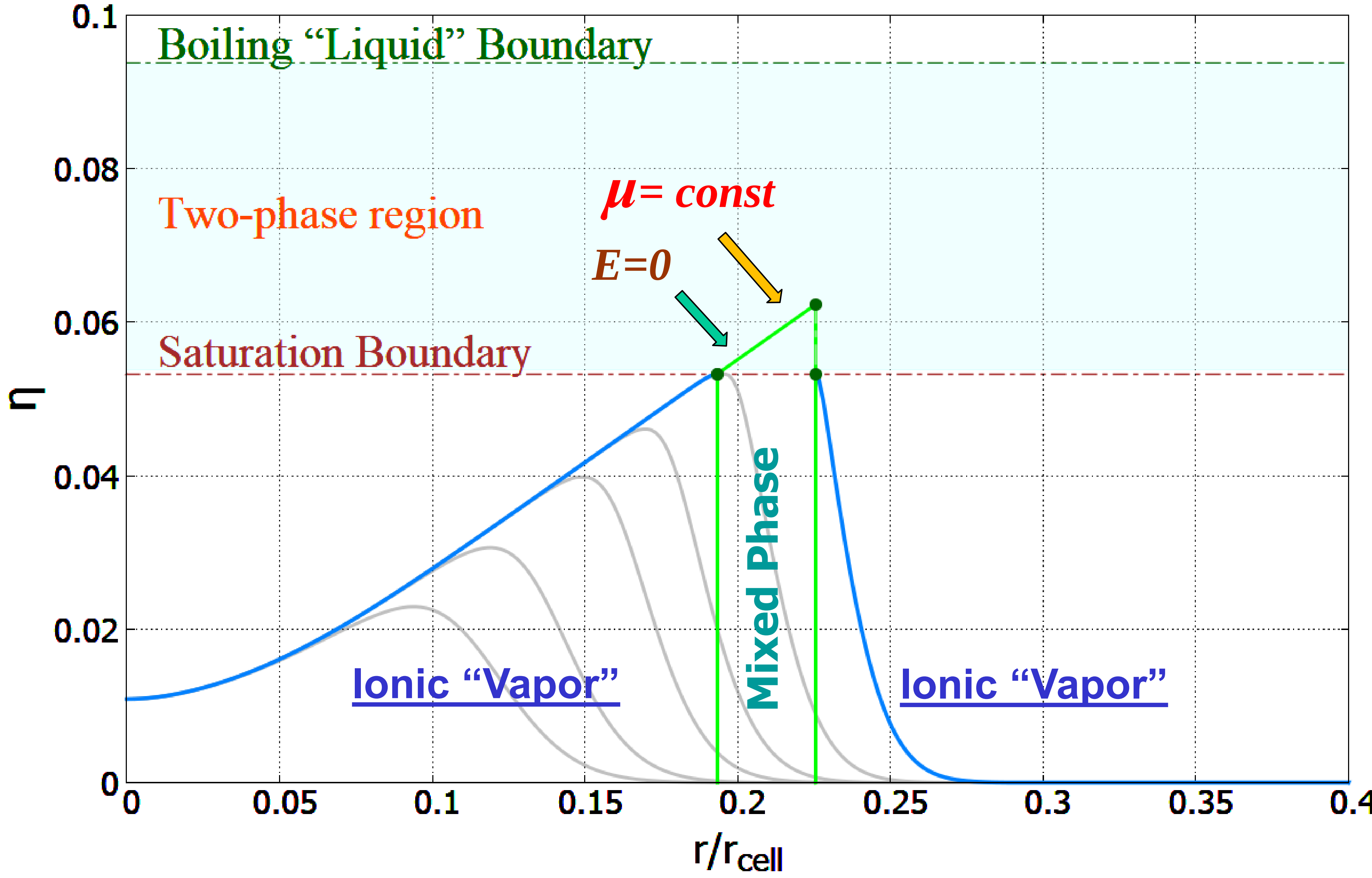
Hempel M., Dexheimer V., Schramm S. Iosilevskiy I., *Phys. Rev. C* **88**, (2013)

etc

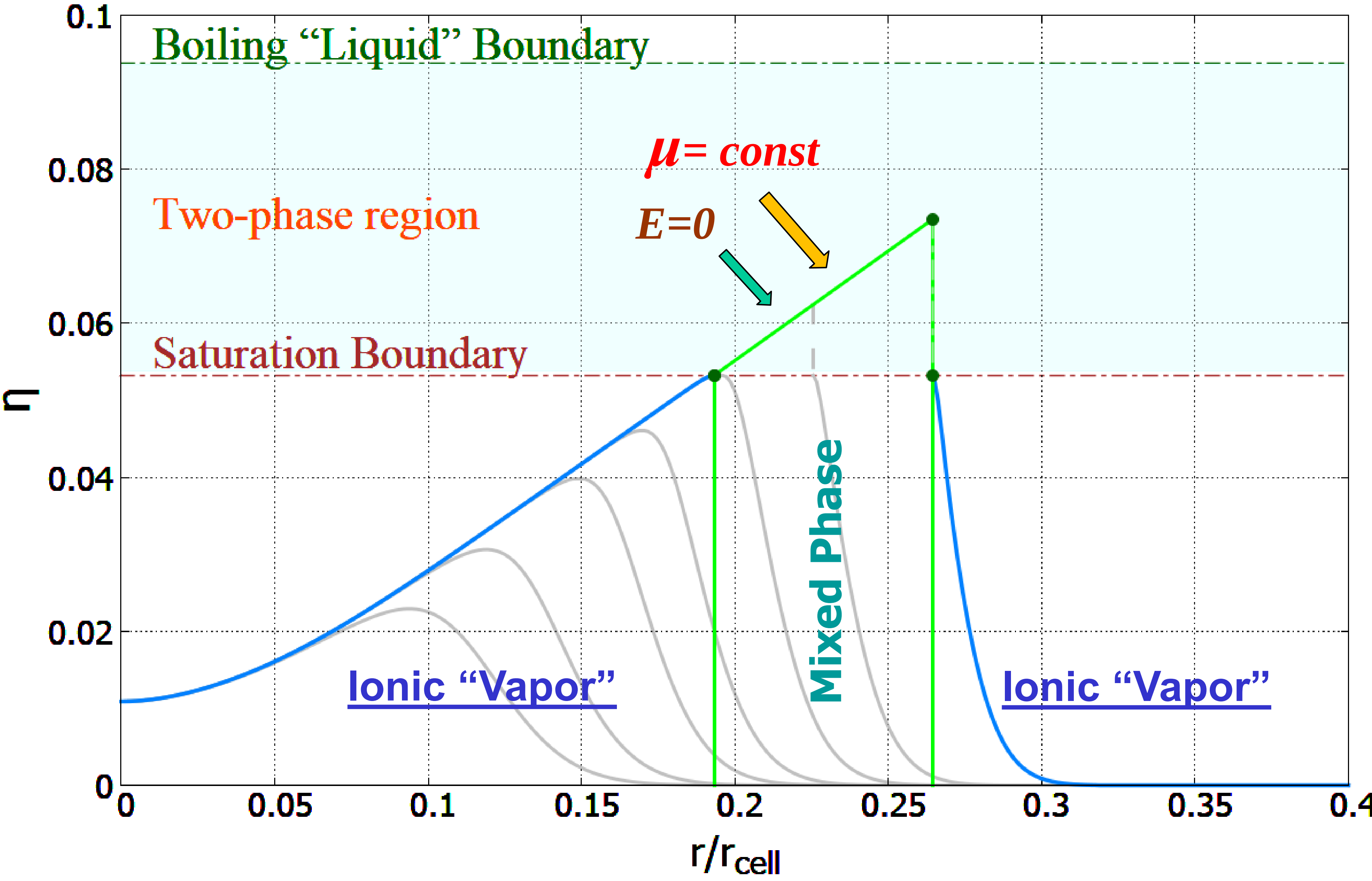
Ionic “Vapor” Saturation Moment ($Z = Z_1$)



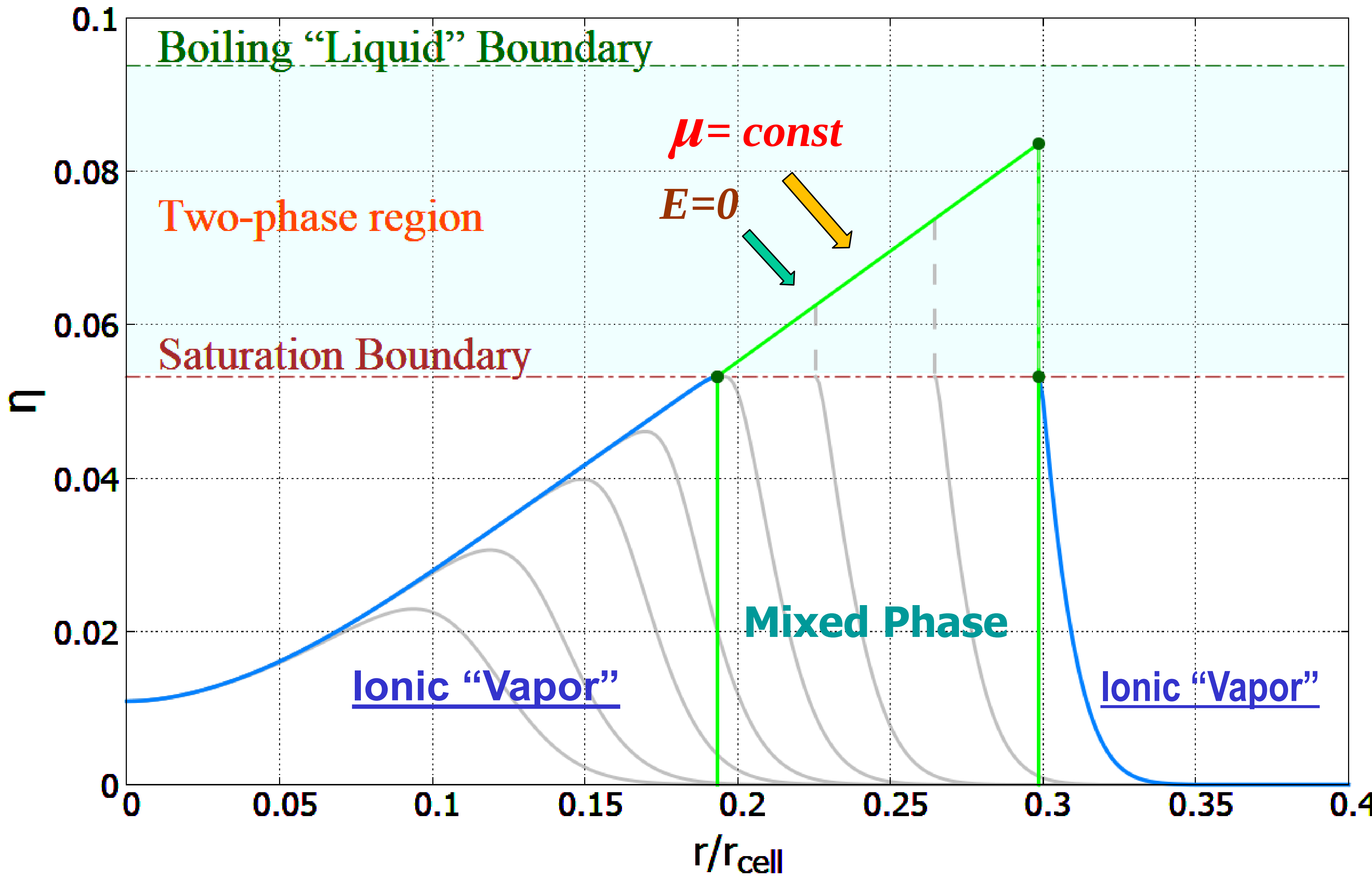
“Mixed Phase” Layer Appearance $(Z_1 < Z < Z_2)$



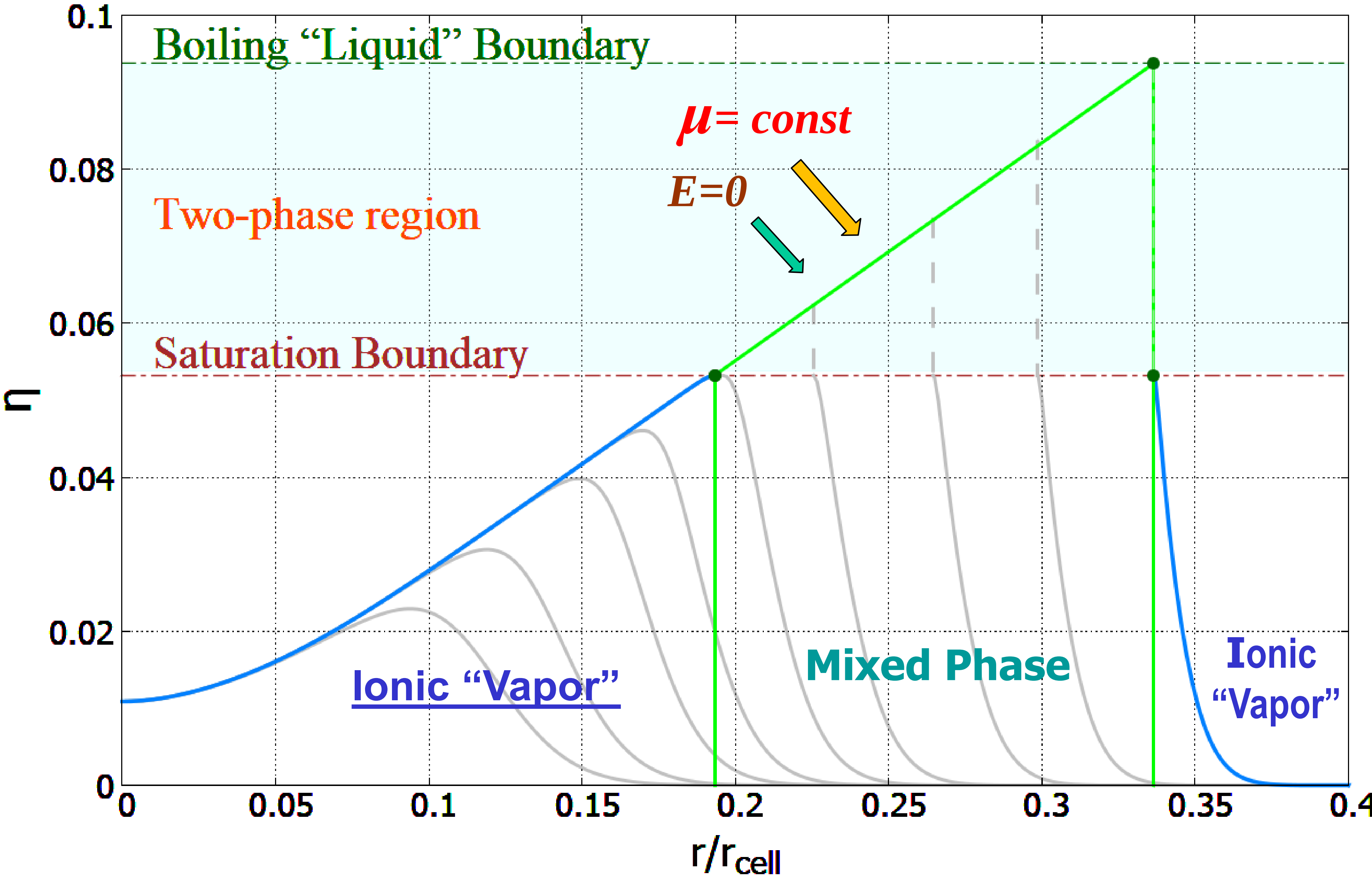
Mixed Phase Layer Growth ($Z_1 < Z < Z_2$)



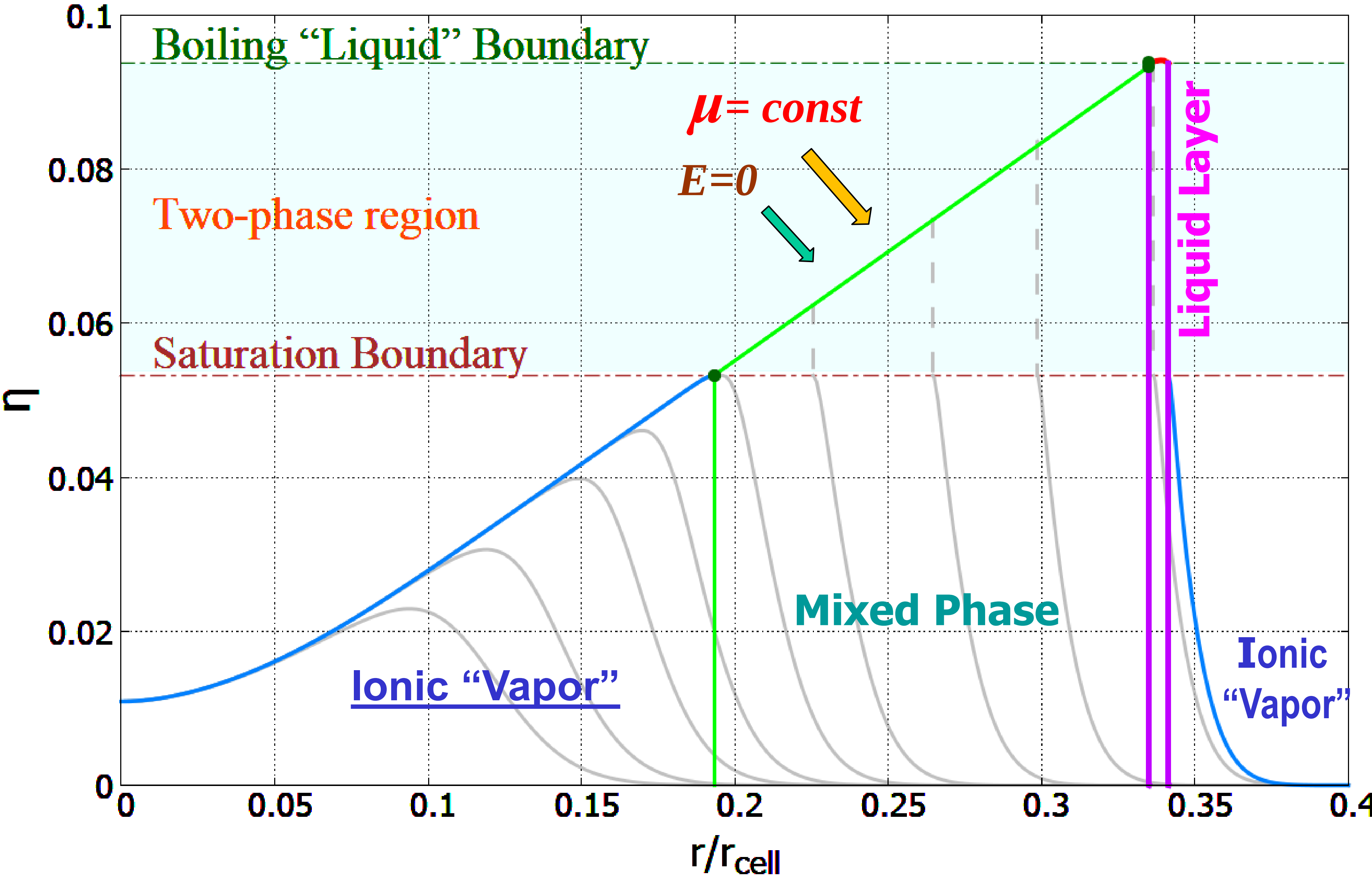
Mixed Phase Layer Growth ($Z_1 < Z < Z_2$)



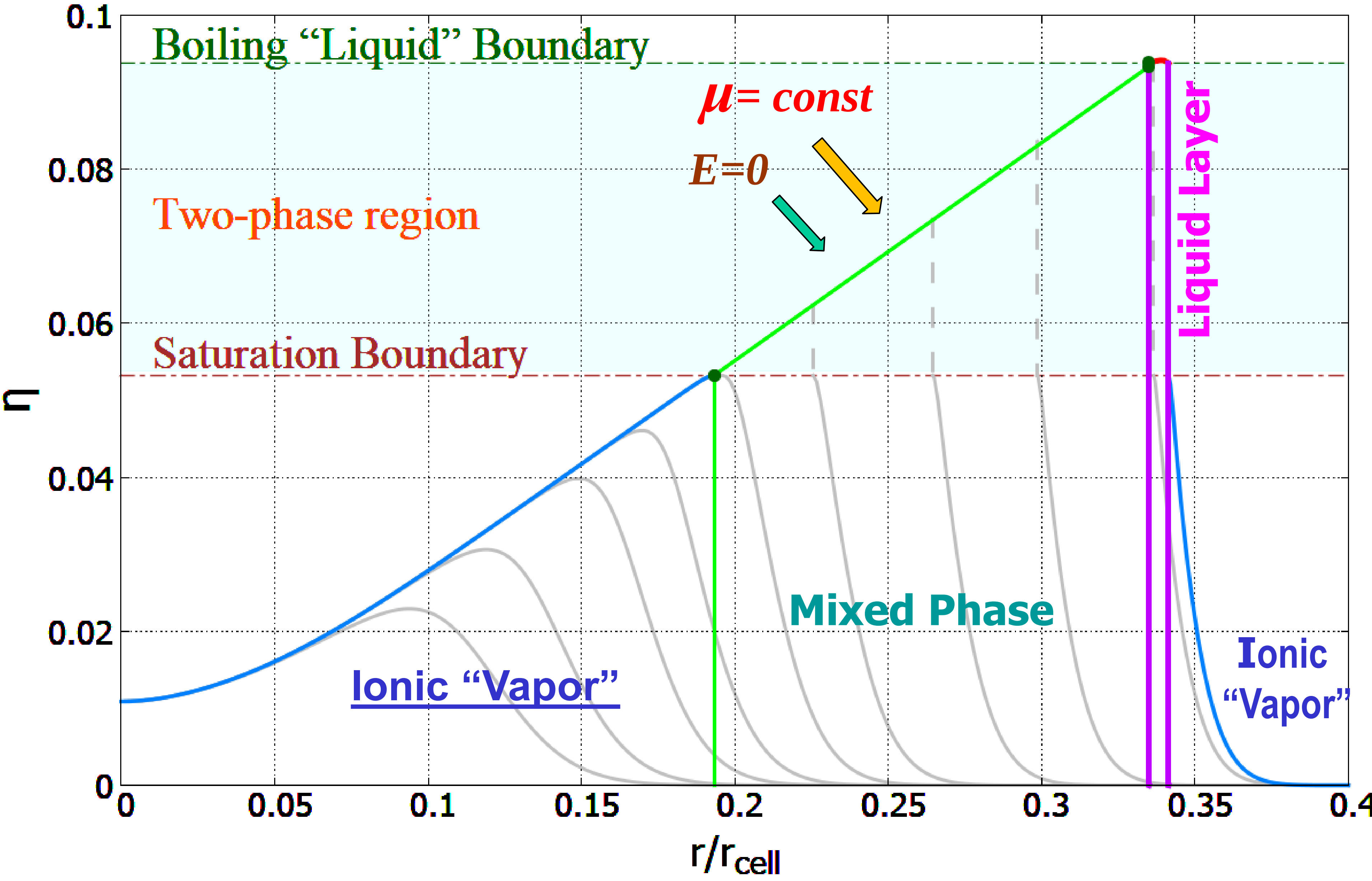
Liquid Layer Appearance ($Z = Z_2$)



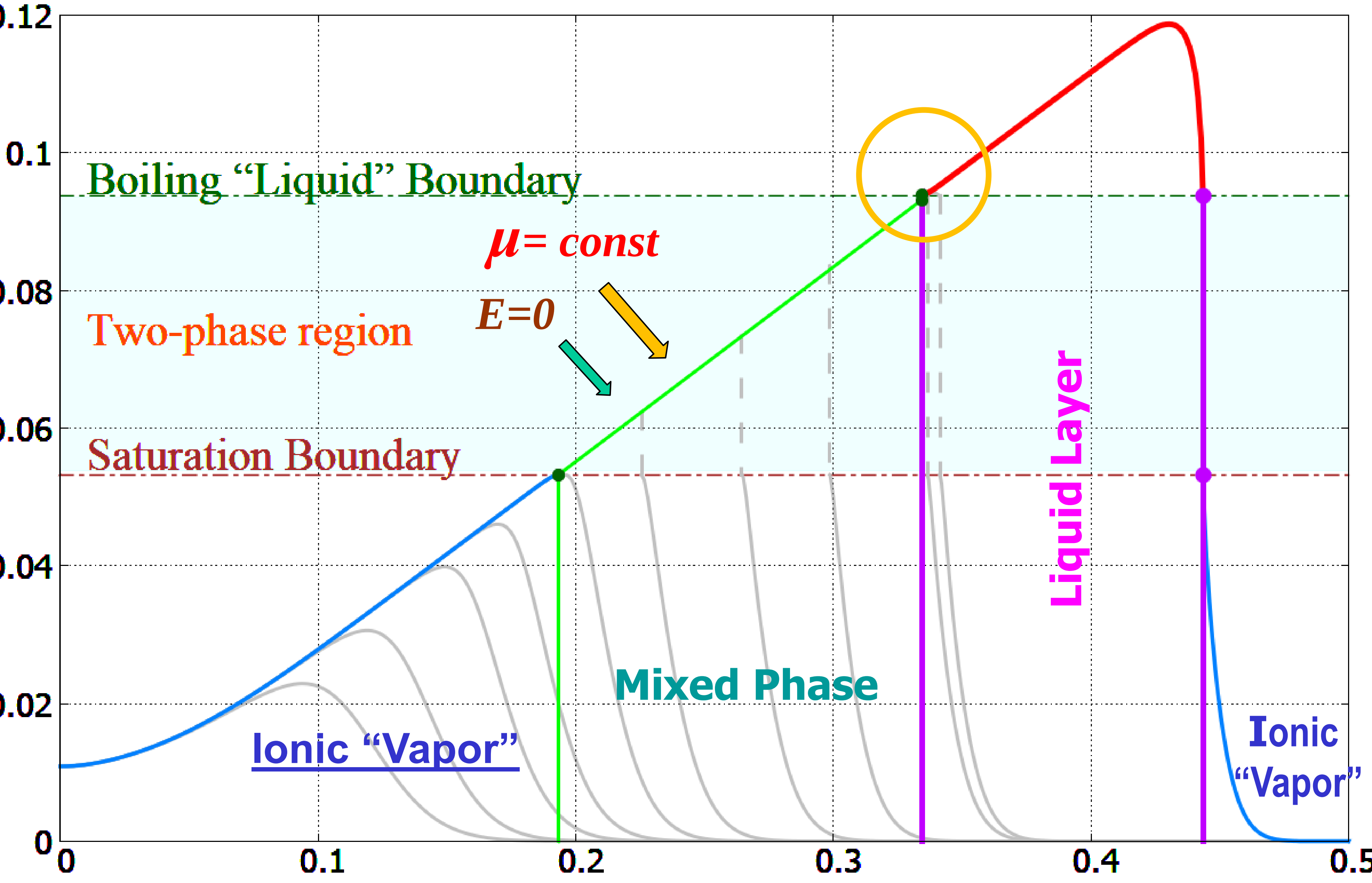
Liquid Layer Growth ($Z > Z_2$)



Liquid Layer Growth ($Z > Z_2$)



Liquid Layer Growth ($Z > Z_2$)



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 Γ) 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(~)), which EOS replaces ideal gas Equation of State in Local Density Functional when we take into account correlations of charged particles.