Капли Ван-дер-Ваальса, балансирующие между жикостью и газом

INFINUM25

Фазовая диаграмма
Область высоких температур
Методы исслеований

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van der Waals droplets balancing between liquid and vapor

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van der Waals EoS -> Phase diagram

Hot region -- Analytical tools

V.N.Kondratyev

BLTP, JINR

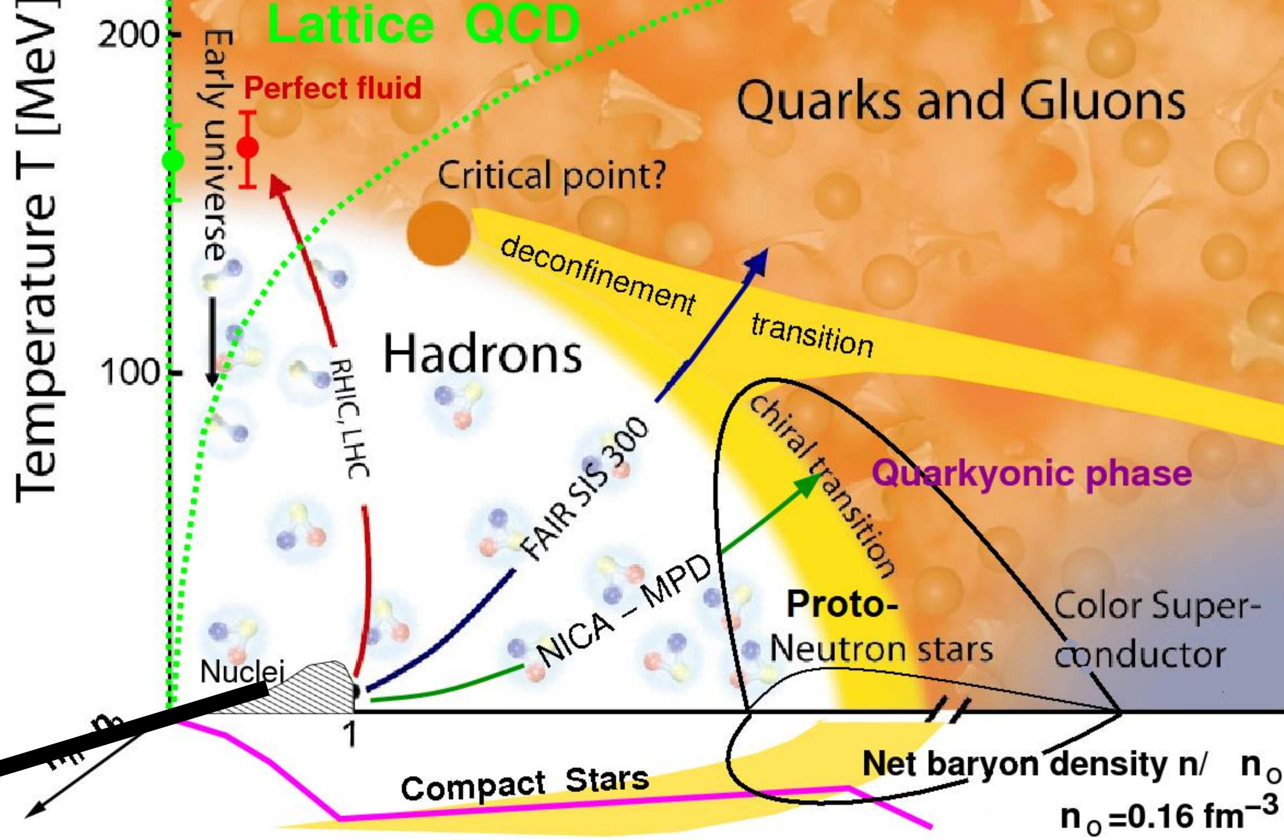
Liquid van der Waals State Equation

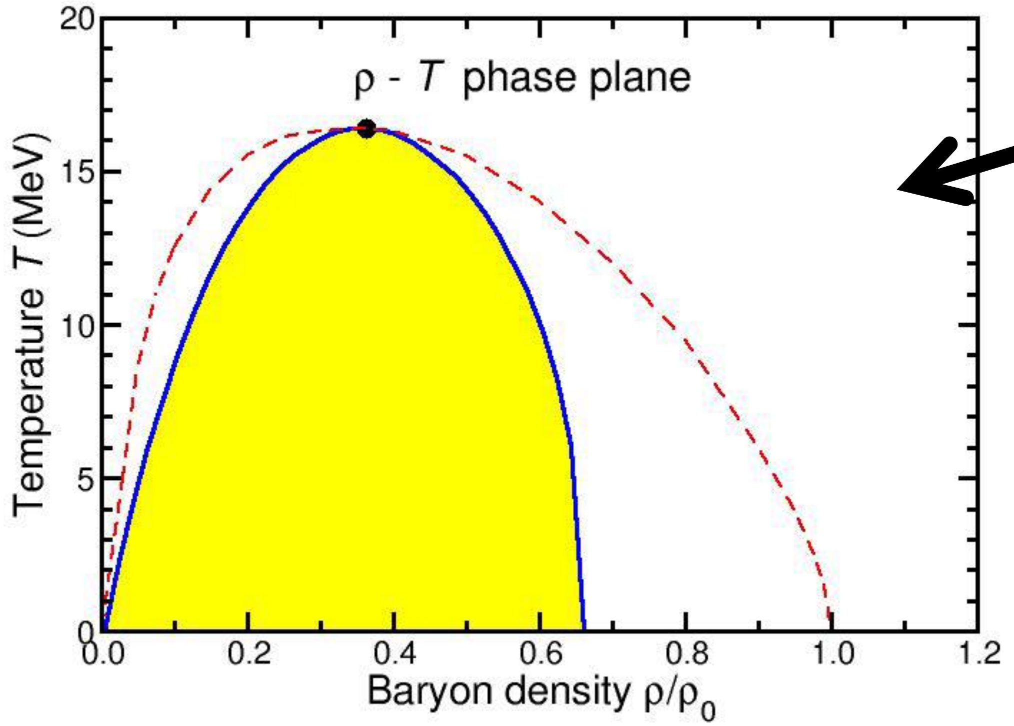
↘⬉

Droplet properties

- …
- FEMTO`-`Nuclear Matter State Equation
- NANO   – Device Thermal Stability
- …

Hot region Phase diagram
Liquid Gas phase transition

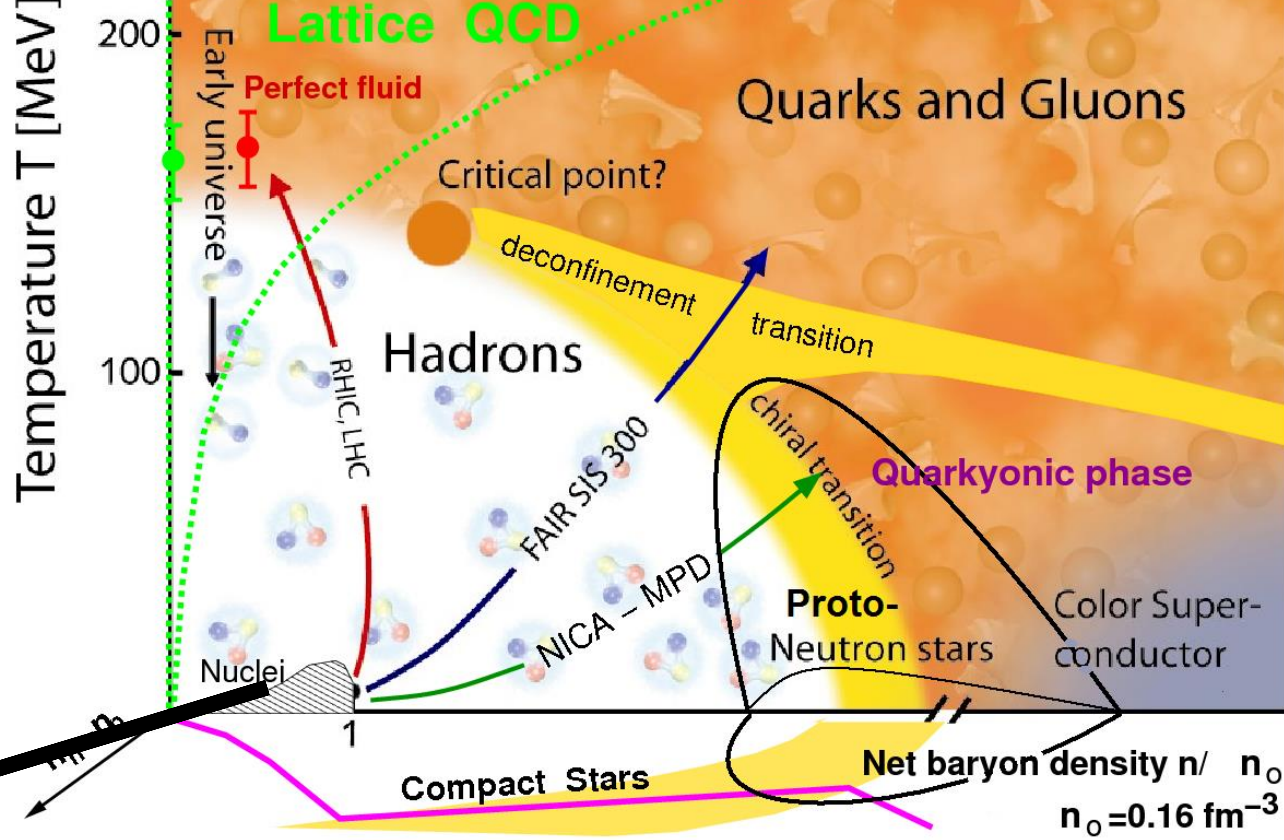


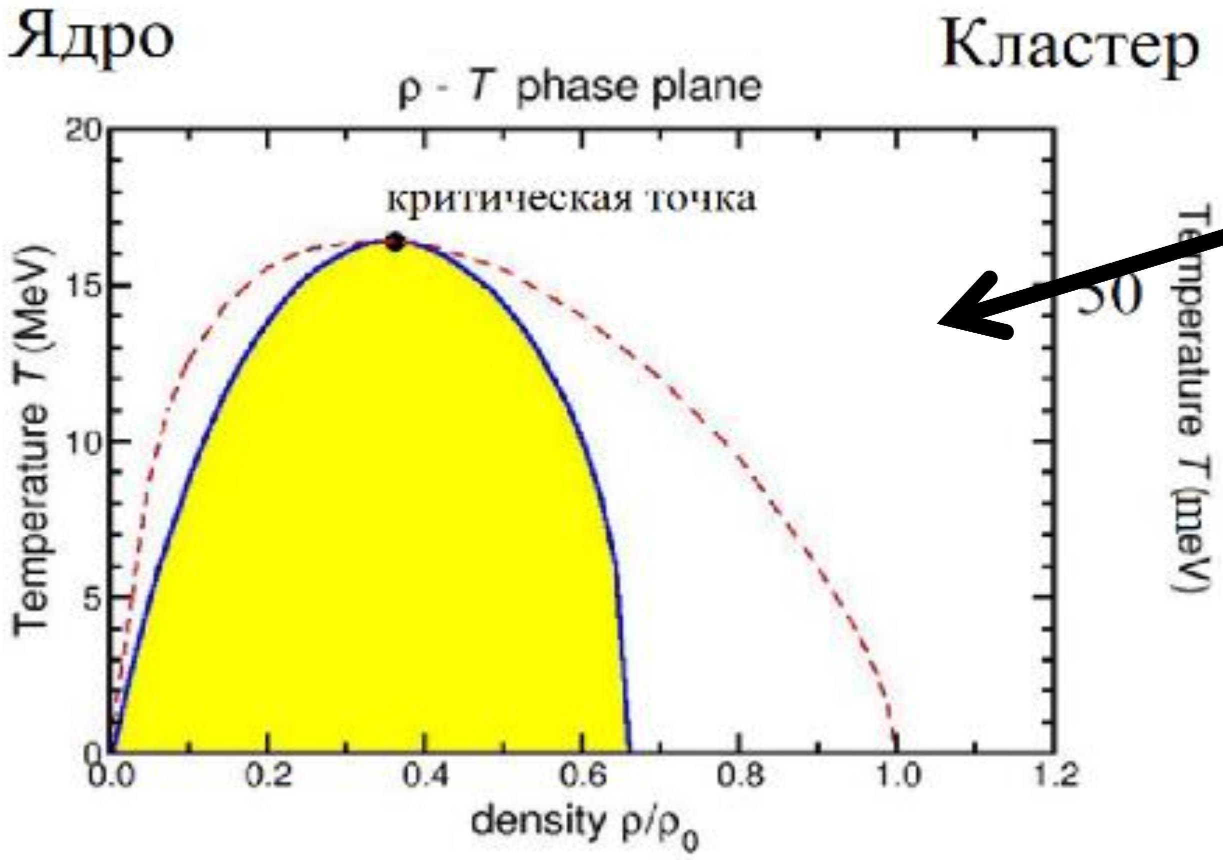


$$p = \frac{T}{v-b} - \frac{a}{v^2}$$

van der Waals EoS

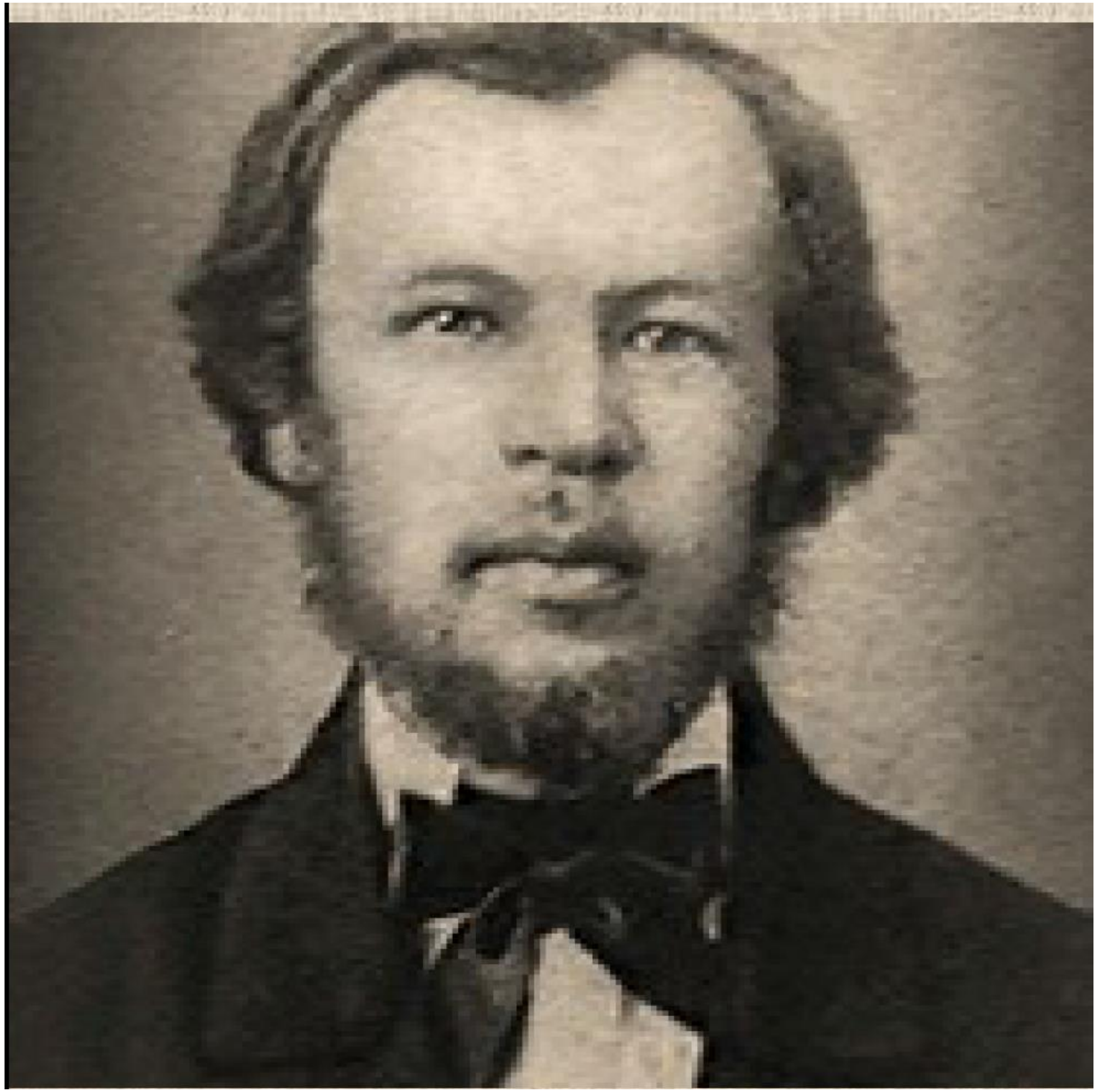
Hot region Phase diagram
Liquid Gas phase transition





$$p = \frac{T}{v-b} - \frac{a}{v^2}$$

van der Waals EoS

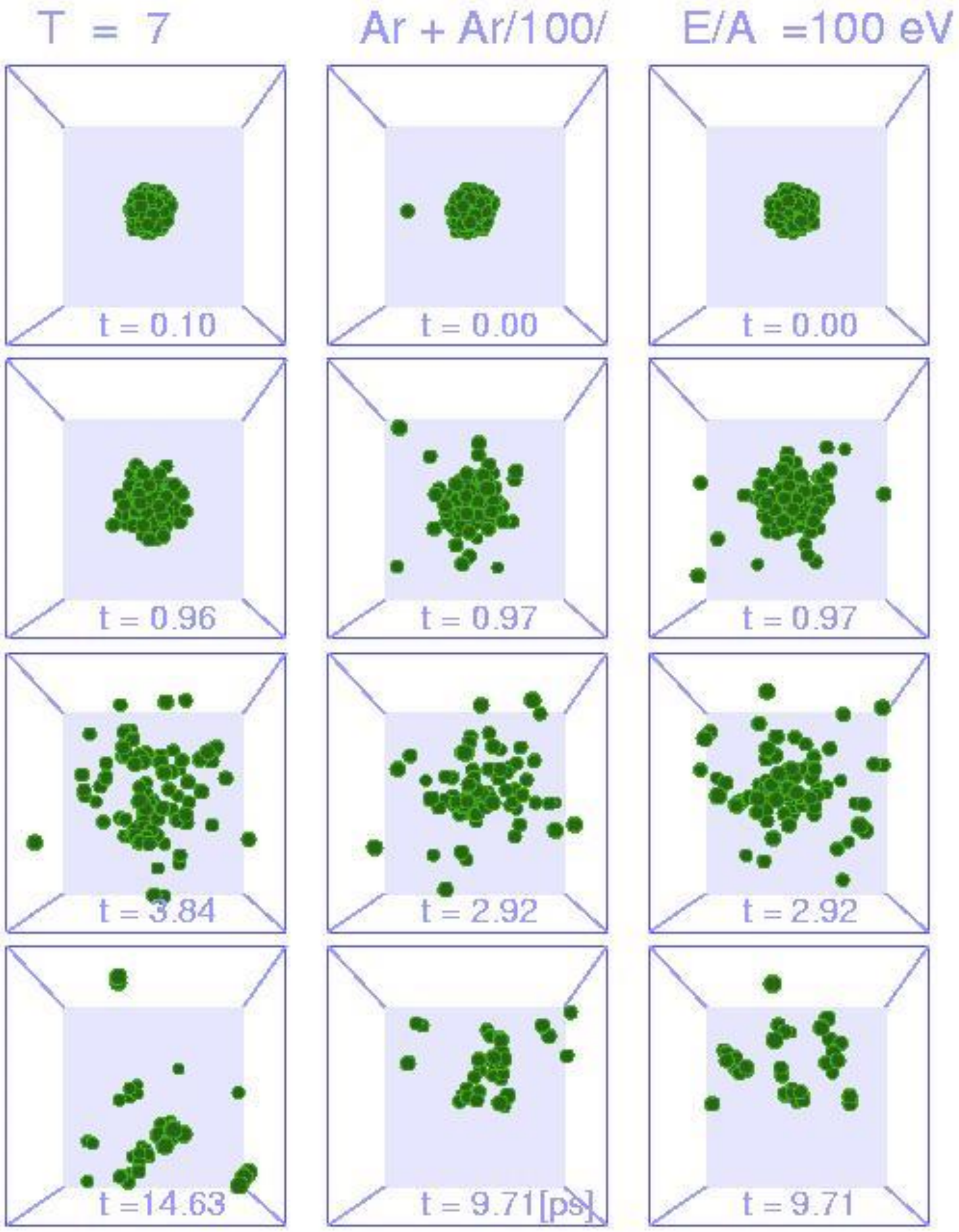


- Д.И. Менделеев: открыл критическую температуру Tc для фазового перехода жидкость-газ (1860)
-

вода: Tc =374 ^{o}C

спирт: Tc =243 ^{o}C

Collision *vs* Thermal expansion



classical molecular dynamics (CMD)

evolution of the system is described by of a set classical Hamilton's equations

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m}; \qquad \frac{d\mathbf{p}_i}{dt} = -\nabla_i \sum_{j \neq i} V(\mathbf{r_i} - \mathbf{r_j}).$$

combined two-body potential

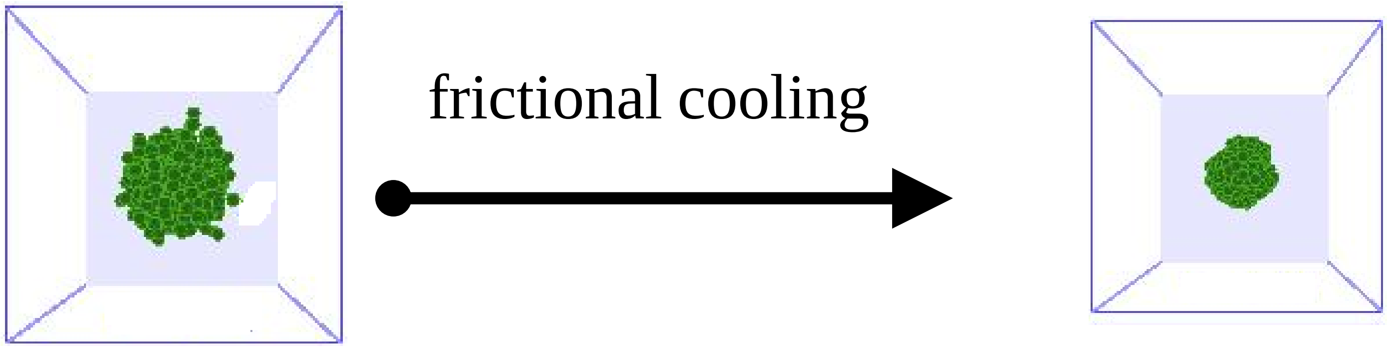
$$V(r) = \begin{cases} 0 & \text{for } r > r_c \\ \epsilon\left(\left(\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right) - \left(\left(\frac{r_0}{r_c}\right)^{12} - 2\left(\frac{r_0}{r_c}\right)^{6}\right)\right) & \text{for } r_c > r > r_1 \\ a_0 + a_1 r + a_2 r^2 + a_3 r^3 & \text{for } r_1 > r > r_2 \\ \Phi(r/a)\cdot Z_1 Z_2 e^2/r & \text{for } r < r_2 \end{cases}$$

6-12 Lennard-Jones potential

Ziegler, Biersack and Littmark (ZBL) screening

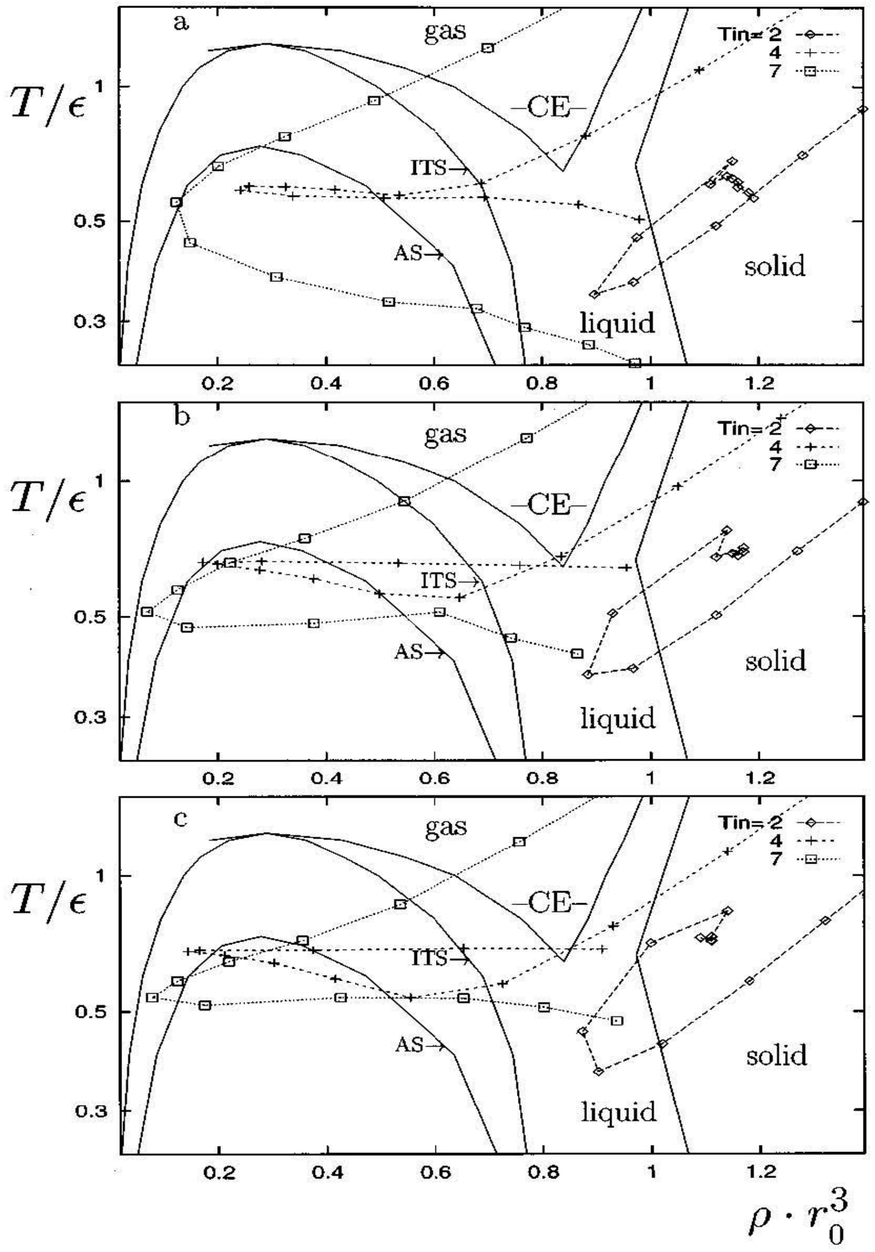
Initialization: microcanonical ensemble for the dynamical evolution

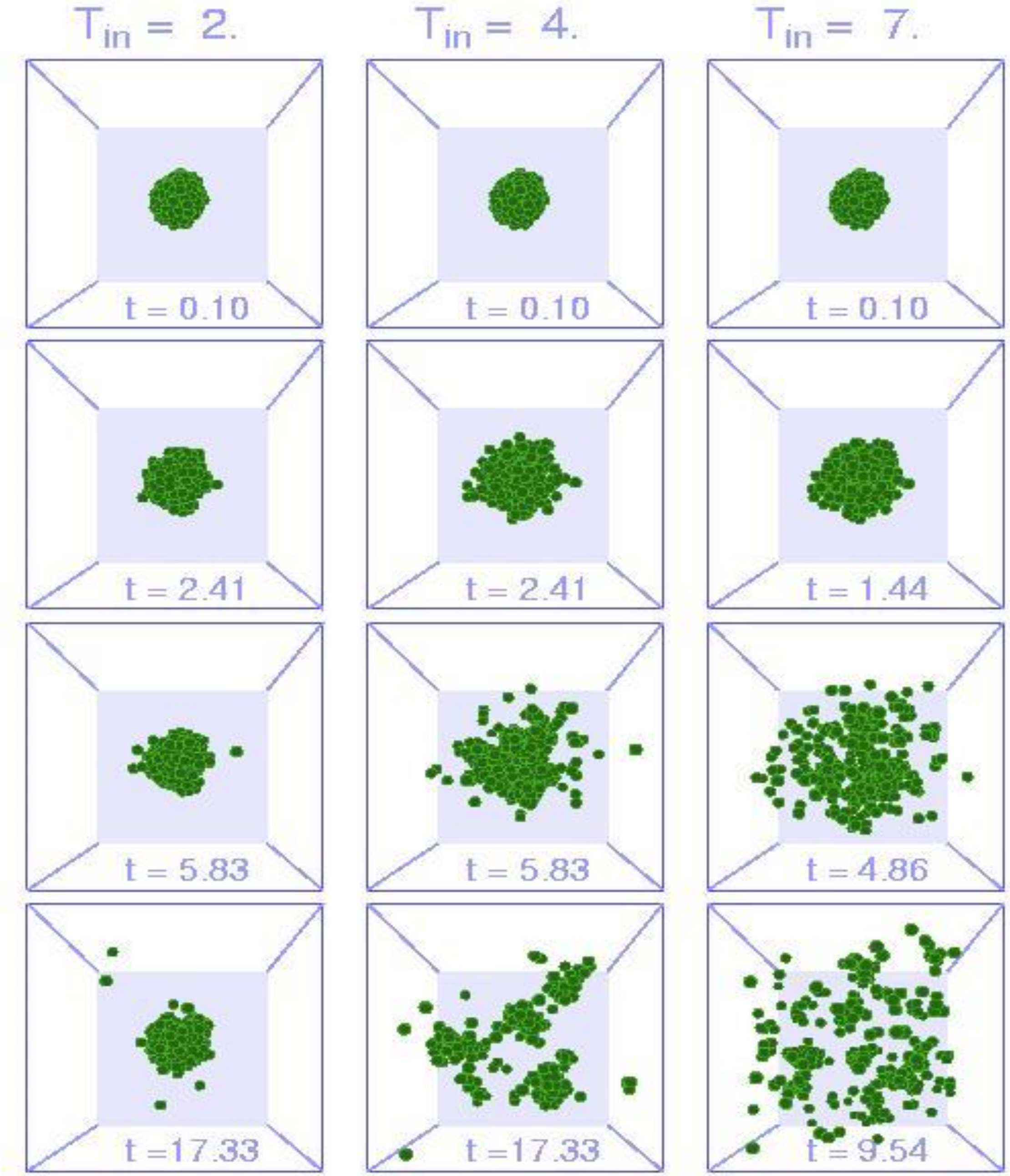
Particles are distributed randomly in a large sphere the initial density is about $0.75/r_0^3$ and propagated using the frictional cooling method to a local minimum of the total potential energy.



Maxwell-Boltzmann distribution

Maxwell-Boltzmann distribution





CMD *vs* mean field treaqtment

One-body distribution function $f_1(\mathbf{r},\mathbf{p},t)$

$$f_1(\mathbf{r},\mathbf{p},t)=\sum_{i=1}^{A_{\mathrm{tot}}} \delta(\mathbf{r}-\mathbf{r}_i)\,\delta(\mathbf{p}-\mathbf{p}_i),$$

$$\partial_t f_1 + \frac{\mathbf{p}}{m}\,\partial_{\mathbf{r}} f_1 = \int \partial_{\mathbf{r}} V(\mathbf{r},\mathbf{r}_2)\,\partial_{\mathbf{p}} f_2\, d\mathbf{r}_2\; d\mathbf{p}_2$$

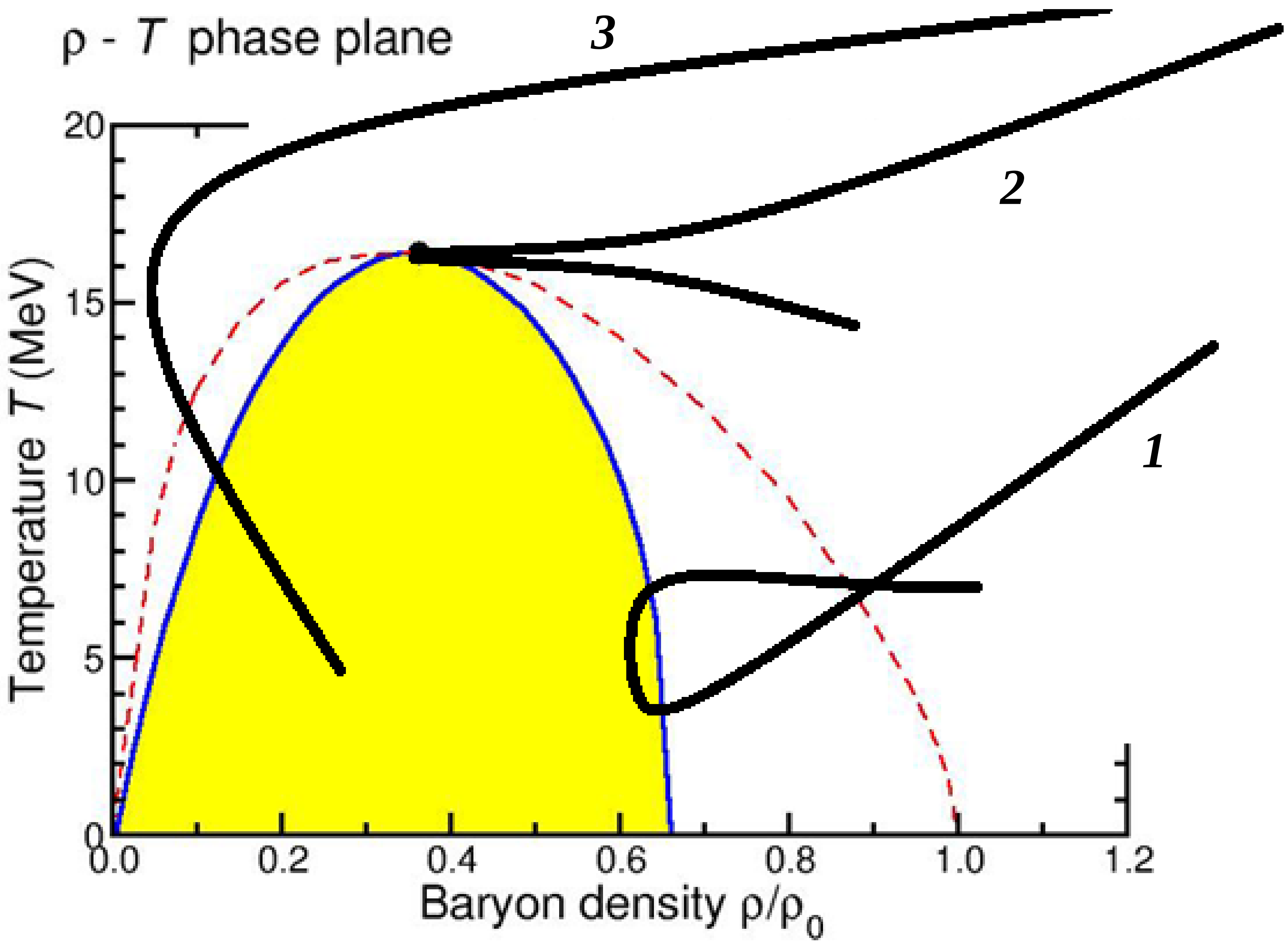
$$f_2(\mathbf{r},\mathbf{r}_2,\mathbf{p},\mathbf{p}_2,t)=\sum_{i\neq j} \delta(\mathbf{r}-\mathbf{r}_i)\,\delta(\mathbf{p}-\mathbf{p}_i)\,\delta(\mathbf{r}_2-\mathbf{r}_j)\,\delta(\mathbf{p}_2-\mathbf{p}_j)$$

$$f_1=\overline{f_1}+\delta f_1; \qquad U=\overline{U}+\delta U$$

$$\partial_t \overline{f_1} + \frac{\mathbf{p}}{m}\,\partial_{\mathbf{r}} \overline{f_1} - \partial_{\mathbf{r}} \overline{U}\,\partial_{\mathbf{p}}\,\overline{f_1} = \langle \partial_{\mathbf{r}} \delta U\, \partial_{\mathbf{p}} \delta f_1 \rangle .$$

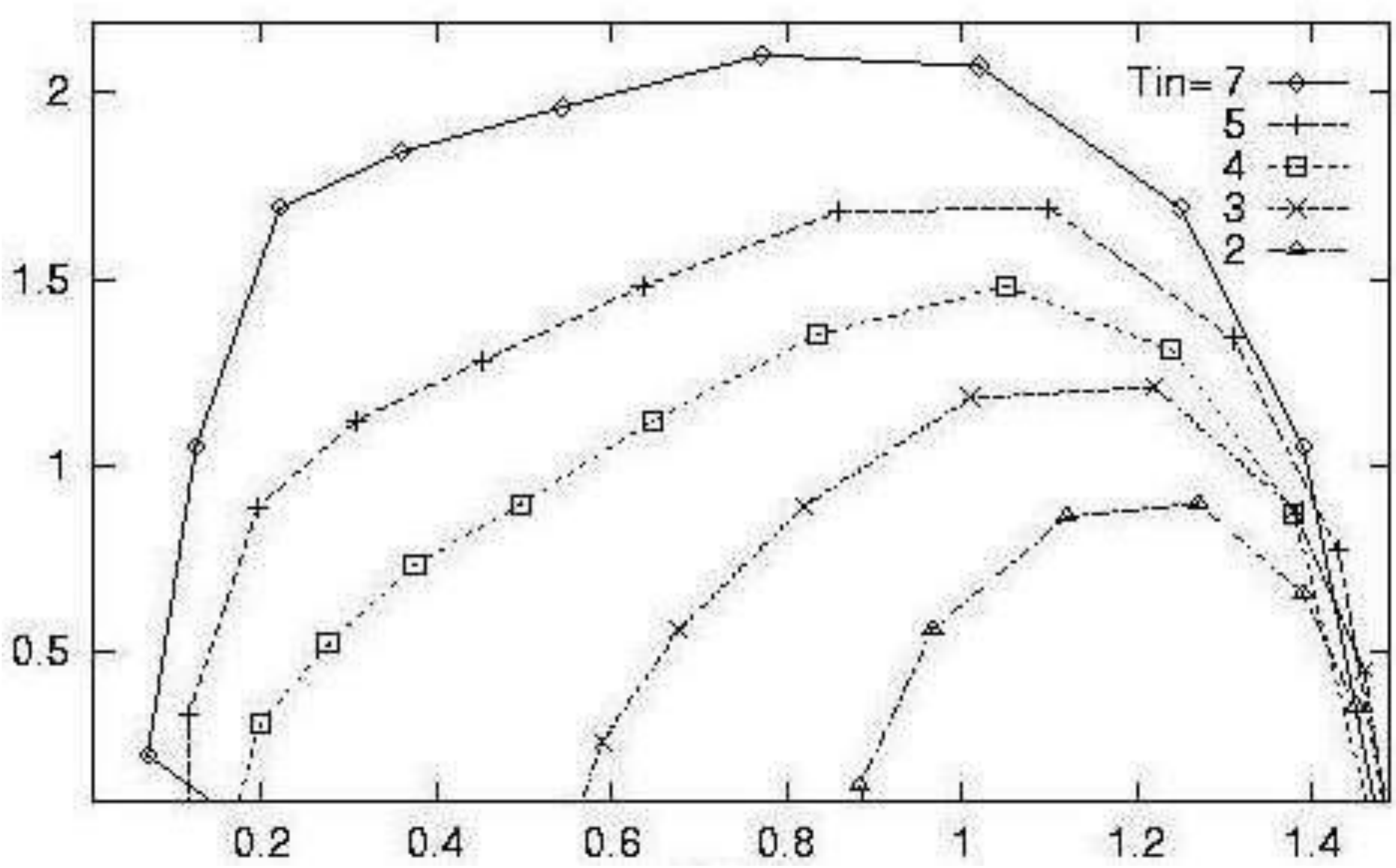
Vlasov, mean field

Collision term


ρ - T phase plane
3
2
1
Temperature T (MeV)
0
5
10
15
20
0.0
0.2
0.4
0.6
0.8
1.0
1.2
Baryon density ρ/ρ0

Flow velocity

v
e
l
o
c
it
y



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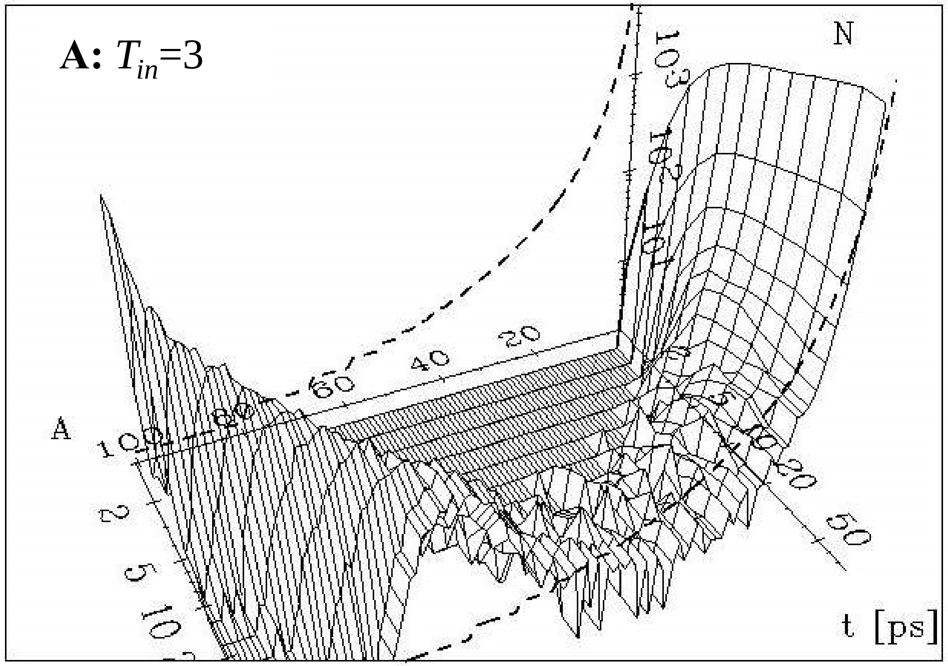
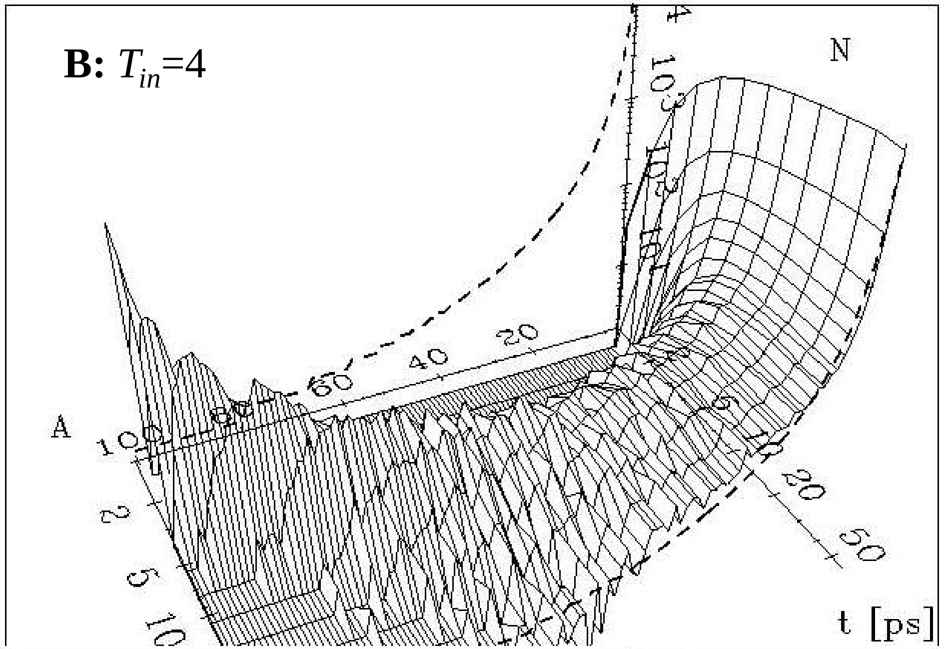
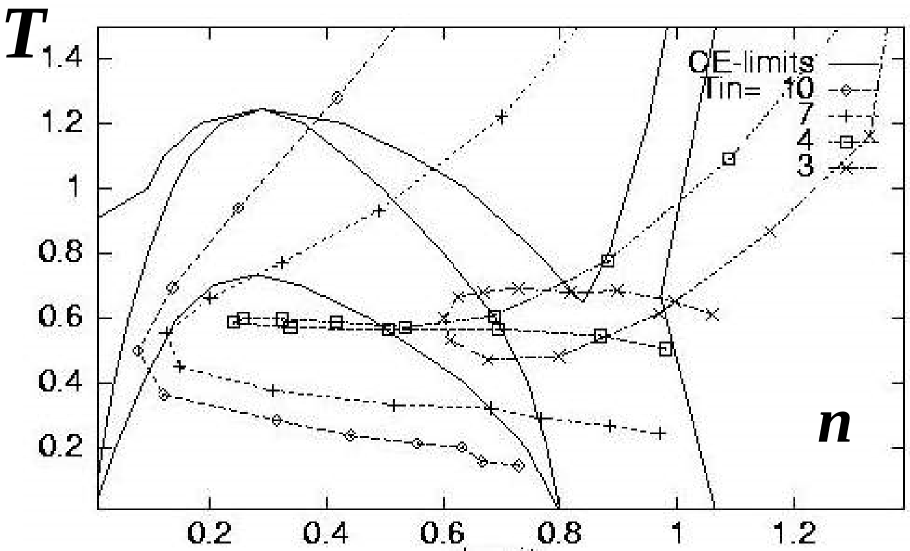
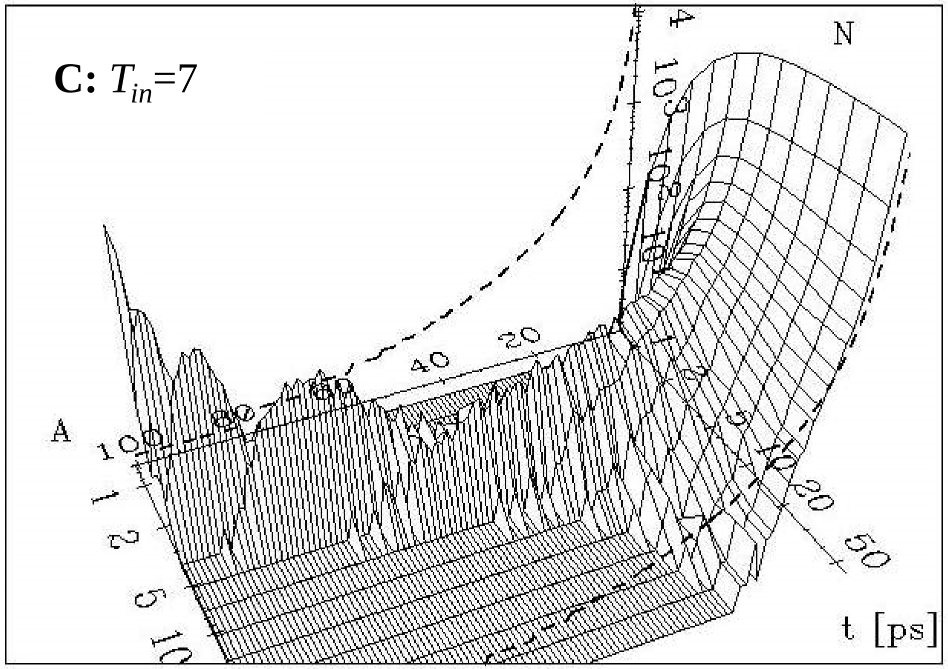
STATISTICAL PROPERTIES OF INCLUSIVE SIZE DISTRIBUTIONS



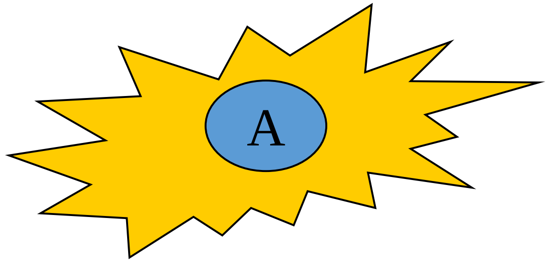






FISHER'S DROPLET MODEL

$$G_{\text{no drop}} = \mu_g (A + B)$$



$$G_{\text{with drop}} = \mu_l A + \mu_g B + 4\pi R^2 \sigma + k_B T \tau \ln A$$

the fragment mass distribution ~ exp{-$\Delta G/\kappa T$}

$$N(A) = \left[Y_0 \exp\left(\frac{\Delta\mu}{k_B T} A - \frac{4\pi r_0^2 \sigma}{k_B T} A^{2/3} - \tau \ln A \right) \right]$$

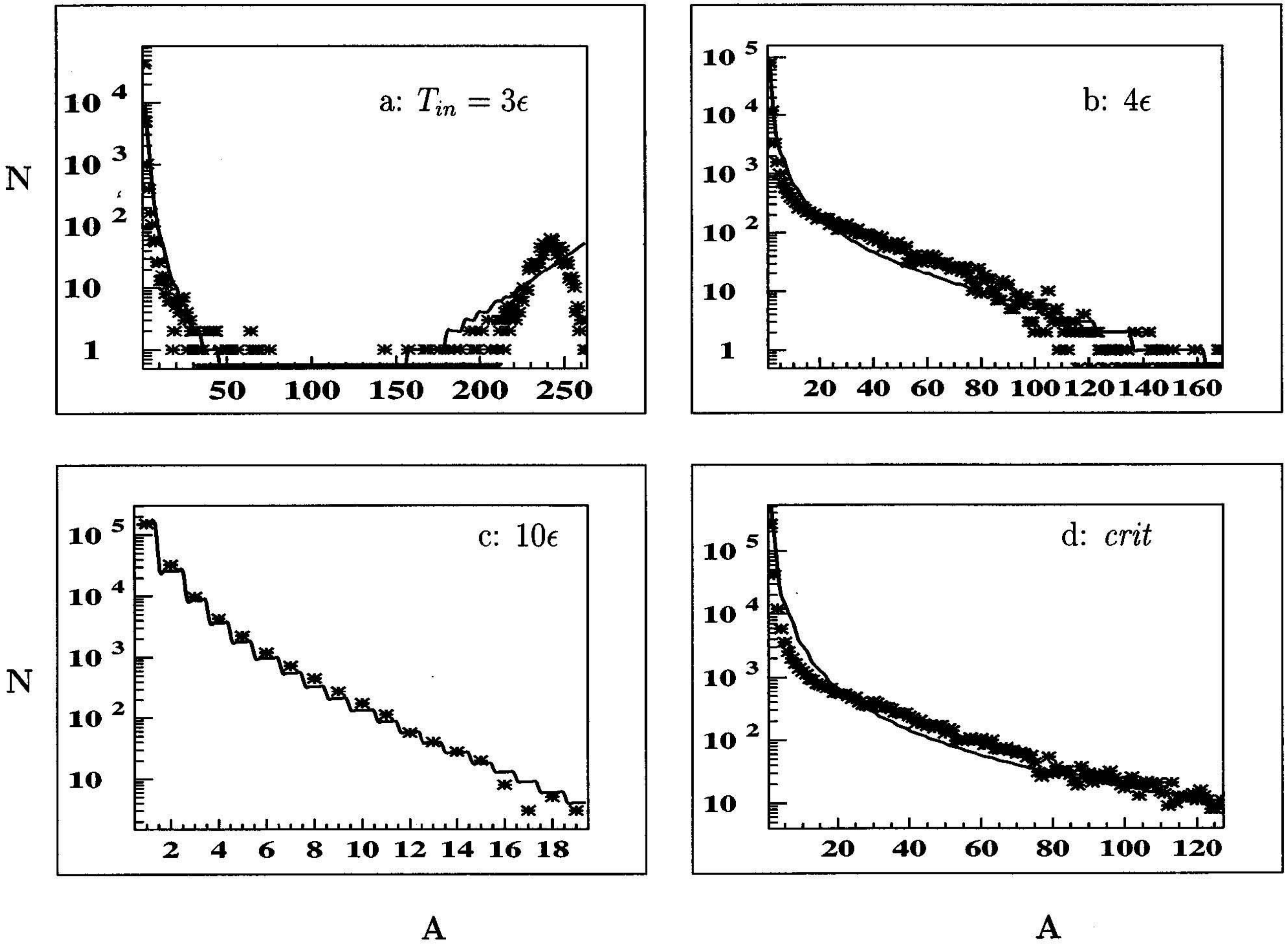
difference in the gas and liquid chemical potentials

$$N(A) = \left[Y_0 \exp\left(\frac{\Delta\mu}{k_B T} A - \tau \ln A \right) \right]; \quad T \geq T_c$$

$$N(A) = [Y_0 A^{-\tau}]; \quad T = T_c$$

Fragment size distributions fit

T=2.23



conditional moments

$$M_k^{(j)} = \sum_A A^k n^{(j)}(A)$$

At critical point

$$N(A) = [Y_0 A^{-\tau}]; \quad T = T_c$$

$$M_k \sim \int_1^{Infinity} A^{(\kappa-\tau)}\, dA \sim$$

$$\sim A^{(\kappa+1-\tau)} \Big|_1^{Infinity}$$

~Const at k= 0,1

~ Infinity at k> 1

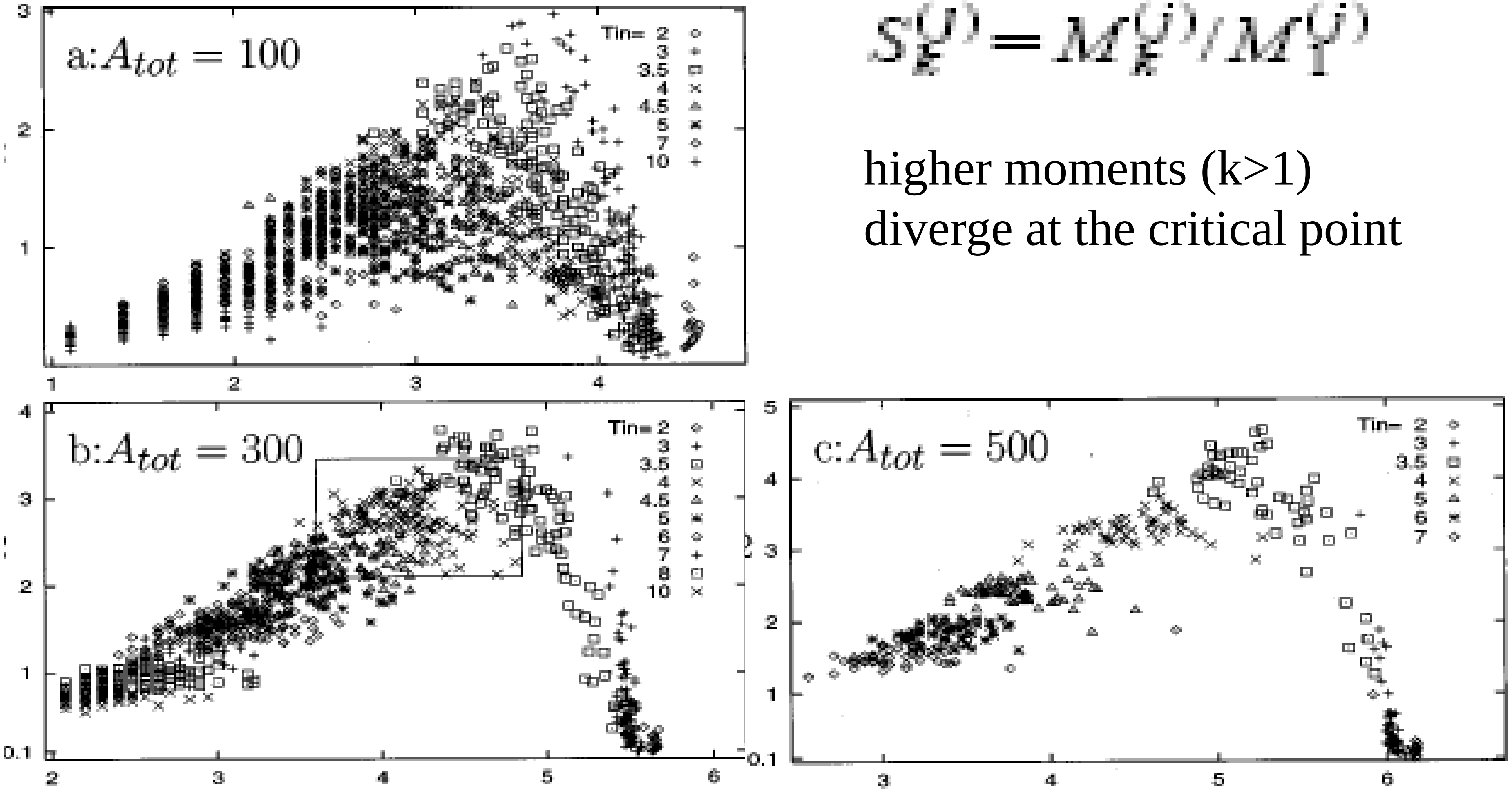
Campi scatter plot

conditional moments $M_k^{(j)} = \sum_A A^k n^{(j)}(A)$

$S_k^{(j)} = M_k^{(j)} / M_1^{(j)}$

higher moments (k>1)
diverge at the critical point

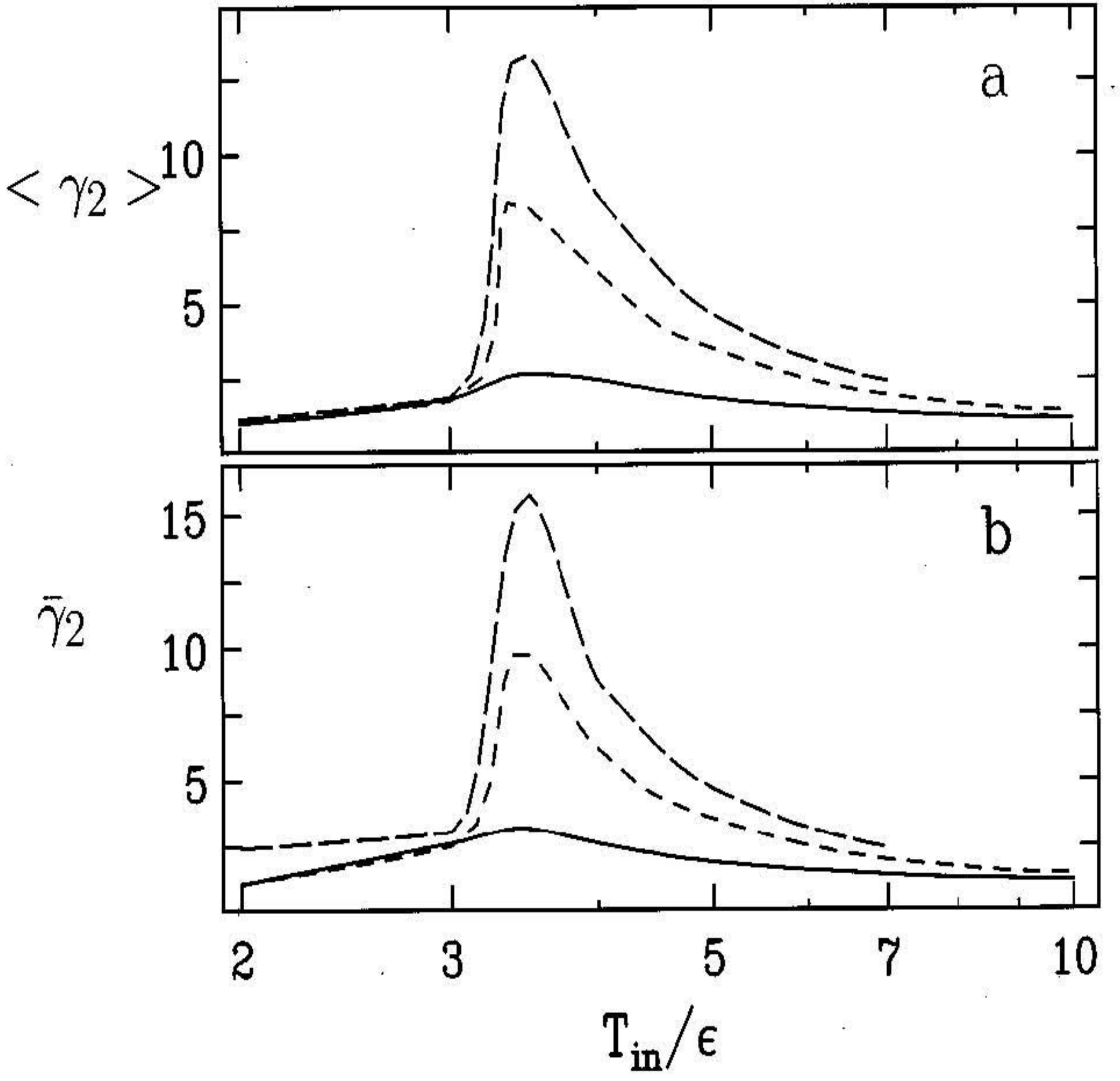
ln S_2



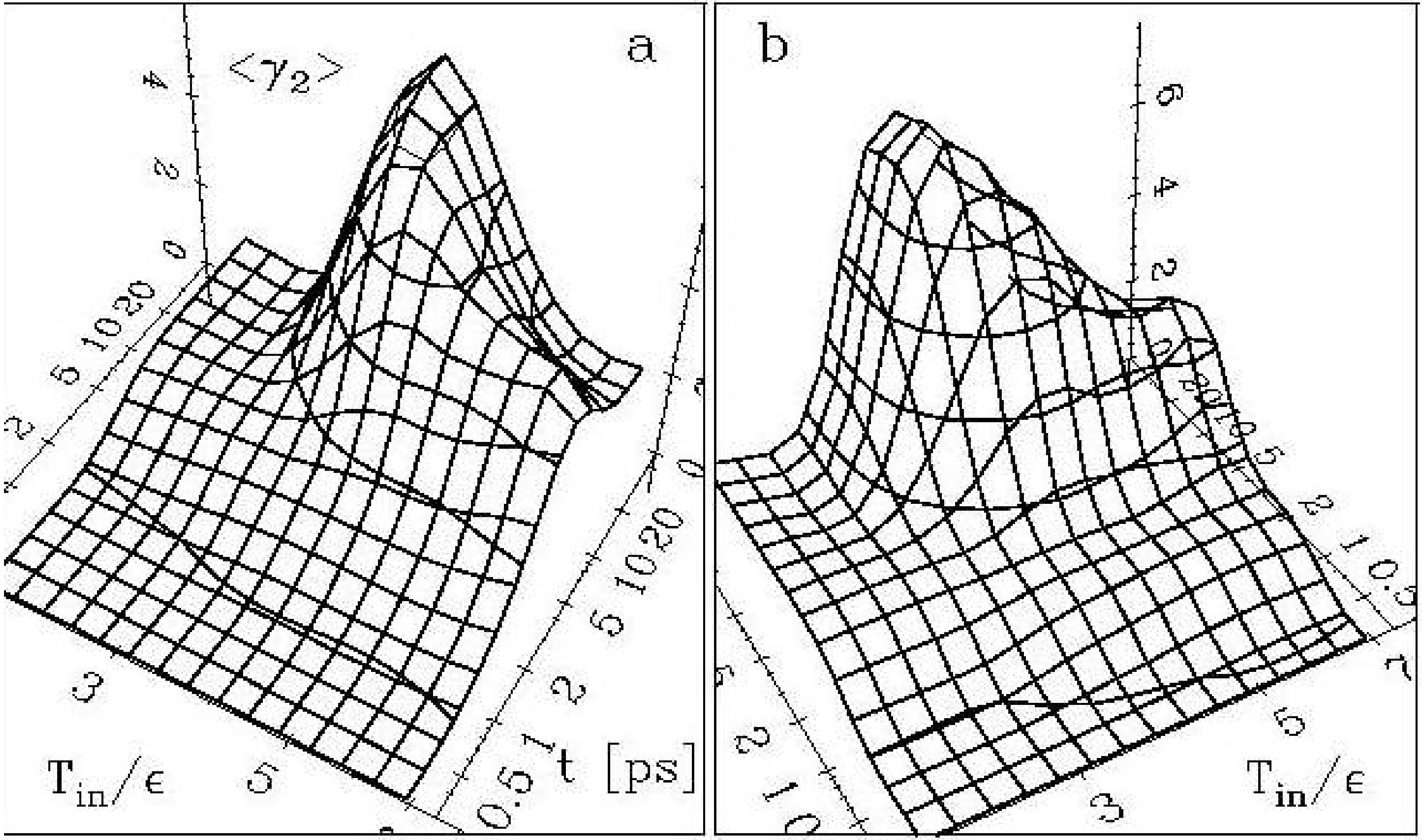
ln A_b *ln* A_b

Reduced variance

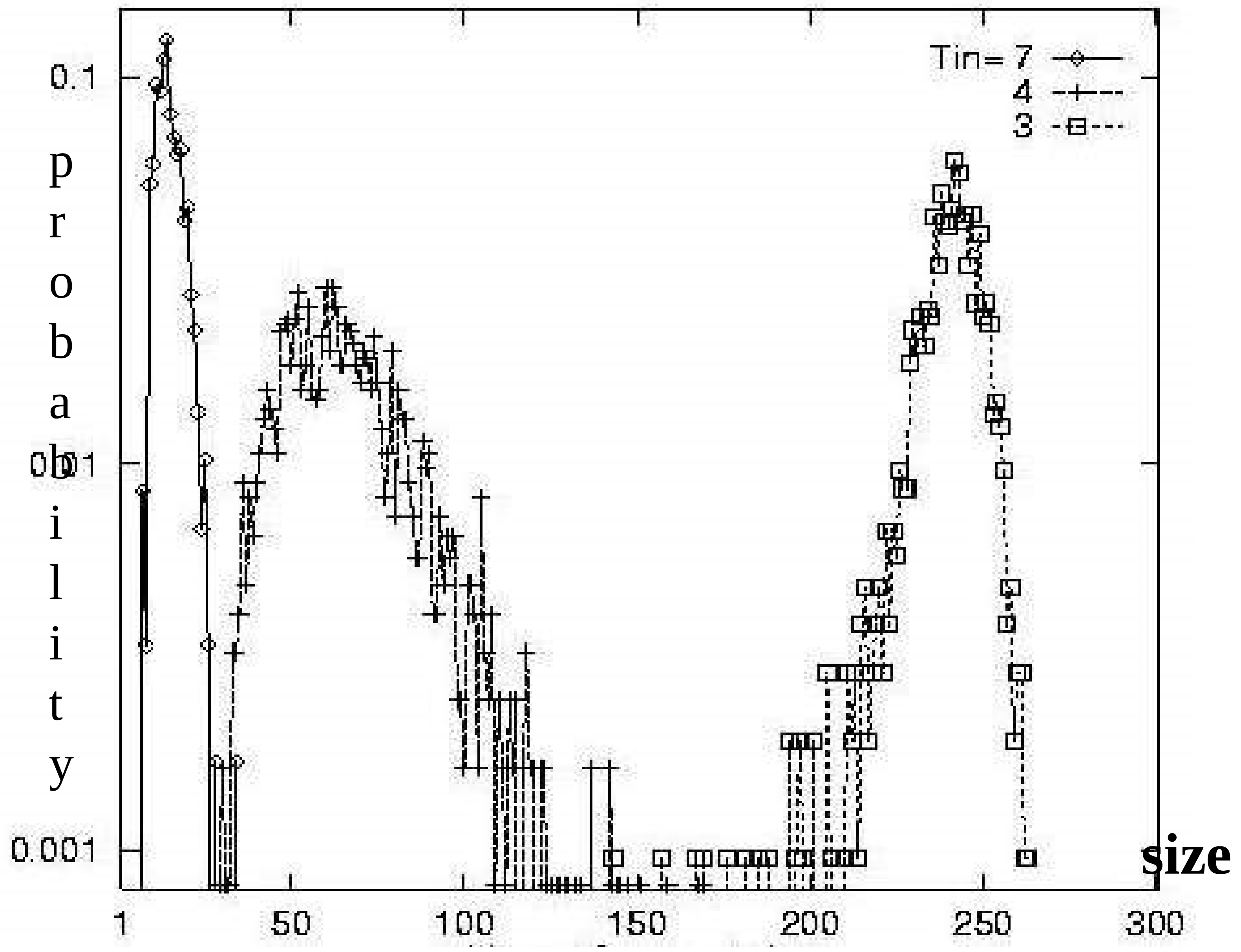
$$\gamma_2 = \frac{M_2 M_0}{M_1^2}$$



Reduced variance *vs* time



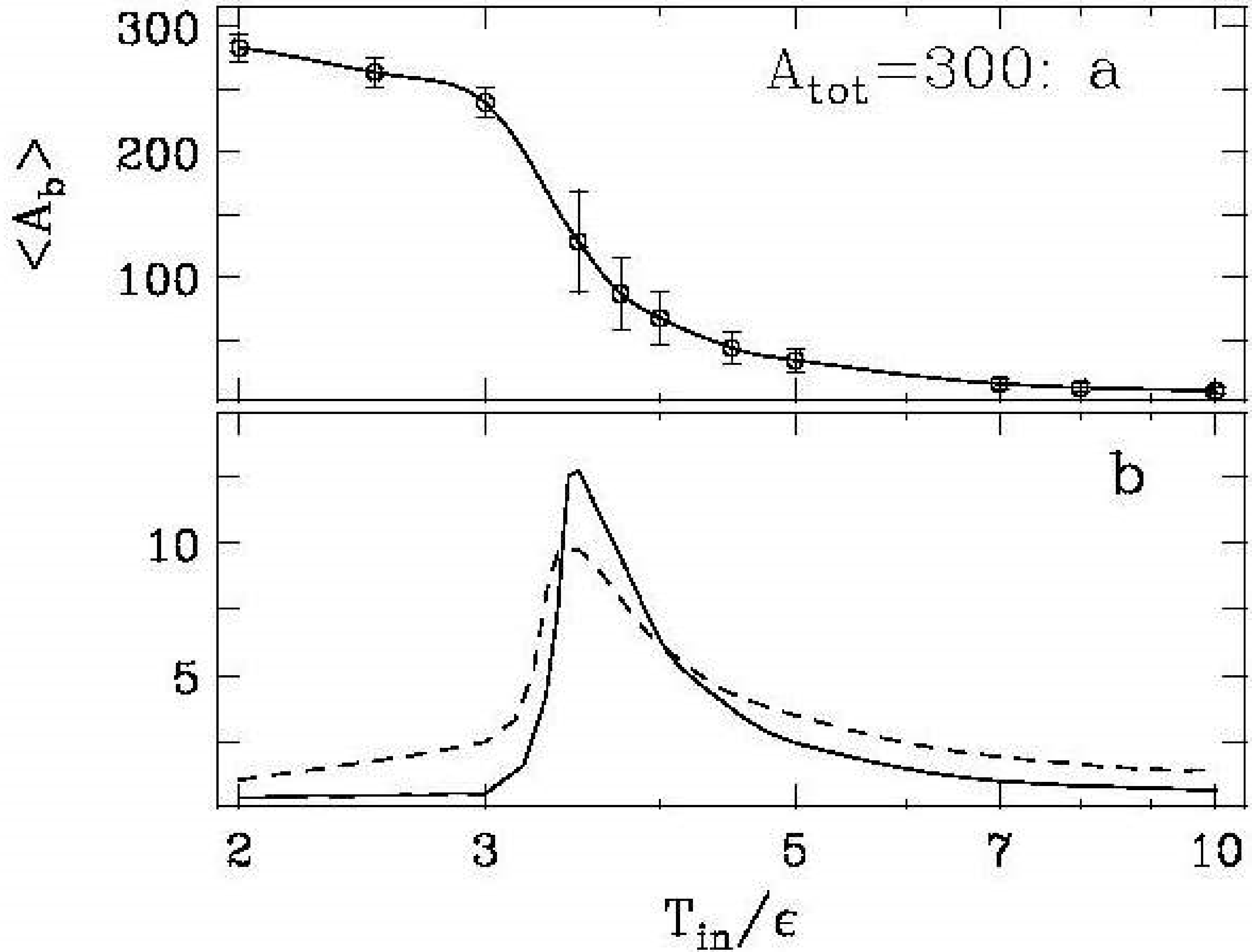
Biggest fragment



normalized variance of the size of the biggest fragment, NVB

$$\Delta^2_{A_b} = \langle A_b^2 \rangle - \langle A_b \rangle^2.$$

$$\gamma_{NVB} = \frac{\Delta^2_{A_b}}{\langle A_b \rangle}$$



Summary

- **Critical evolution of hot van der Waals droplets**
- Regimes
  - isentropic expansion
    - Fragmentation (4 - 6 units)
      - Cooling of fragments
- Critical behavior become visible by the use of different analytical tools

statistics, correlations, fluctuations

- droplet thermal stability changes sharply at critical point

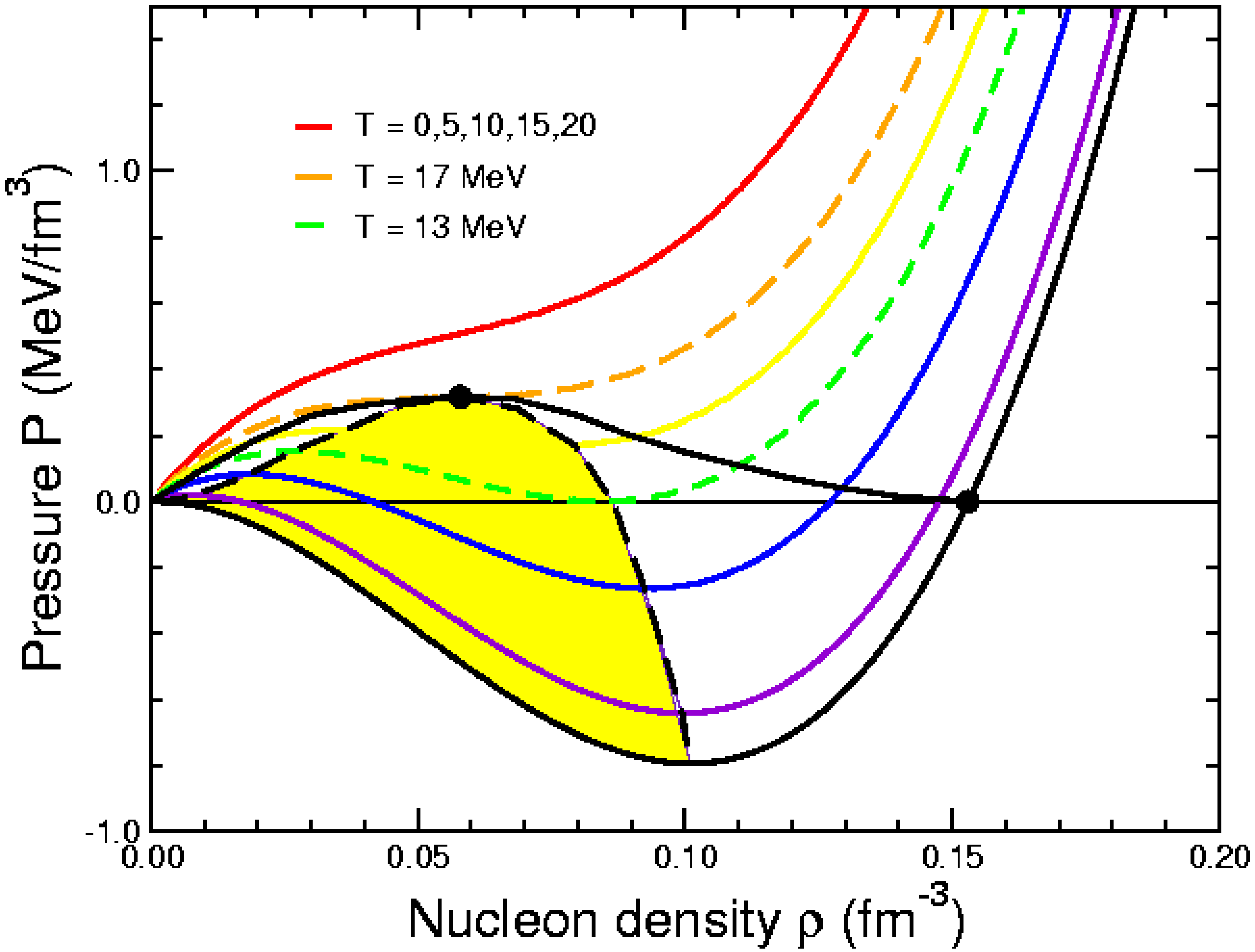
Thank you

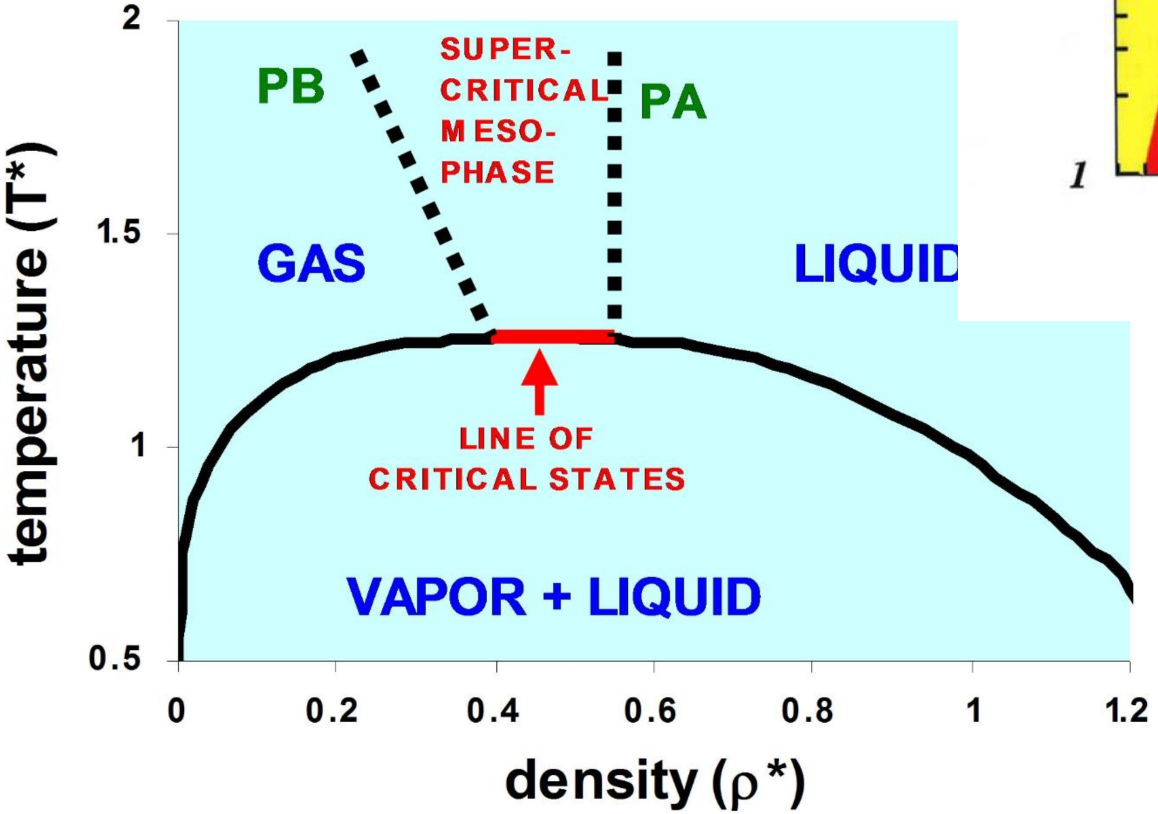
Magnetic field B

$$\boldsymbol{p} = \frac{\boldsymbol{T}}{\boldsymbol{v}-\boldsymbol{b}} - \frac{\boldsymbol{a}}{\boldsymbol{v}^2} + \frac{\boldsymbol{h}}{\boldsymbol{v}^{2/3}}$$

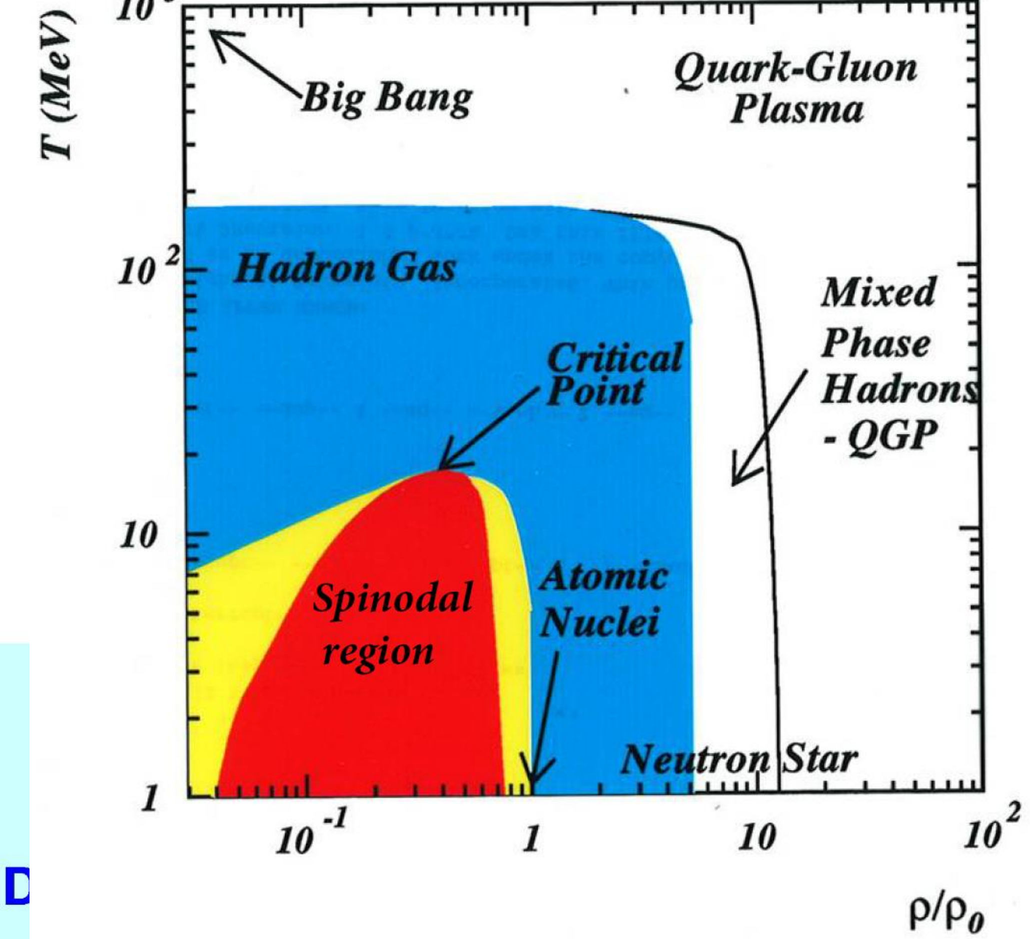
$$\boldsymbol{h} = \frac{\boldsymbol{B}^2}{2\mu} = \mathbf{15}\mathrm{keV}\frac{\boldsymbol{B}^2}{\mathrm{TT}^2}$$

matter: *Equation of state: pT(ρ)*





temperature (T*)
density (ρ*)
2
1.5
1
0.5
0
0.2
0.4
0.6
0.8
1
1.2
PB
SUPER-
CRITICAL
MESO-
PHASE
PA
GAS
LIQUID
LINE OF
CRITICAL STATES
VAPOR + LIQUID



T (MeV)
Big Bang
Quark-Gluon
Plasma
Hadron Gas
Mixed
Phase
Hadrons
- QGP
Critical
Point
Spinodal
region
Atomic
Nuclei
Neutron Star
10
1
10 -1
1
10
10 2
ρ/ρ0