Links to Thermodynamics and General (equilibrium) Physics

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Phase-transitions in conventional (grand-canonical) statistics in the thermodynamical limit:
Yang-Lee singularities. Why?
$\longrightarrow$Only homogeneous configuration $\longleftarrow$

Physical reason for phase transitions:
$\longrightarrow$Internal surfaces, inhomogeneities $\longleftarrow$

What is the difference between

Solid	Liquid	Gas
have internal surfaces		no surface
condensate volume less than external volume		fills any volume
surface has edges, is hard, fixed	surface has no edges, flexible, adjusts to container	

Effect of surfaces on entropy:

Boltzmann-Planck :

$$\boxed{\boxed{\mathrm{S{=}k^*lnW(E)}}}$$

$$S(E) \simeq N s_{volume}(e) - N^{2/3} s_{surface}(e) + \cdots$$

concave $\Updownarrow$

$$s_{surface}(e) \propto \frac{\sigma(e)}{T} \times \text{area/atom}$$

$\longrightarrow$convexity $\longleftarrow$

! No scaling !

No unique $T \Rightarrow E$

No canonical distribution, no T, no μ

The essence of first order phase transitions:

$\longrightarrow$Phase separation $\longleftarrow$

bimodality

The essence of difference between states of aggregation

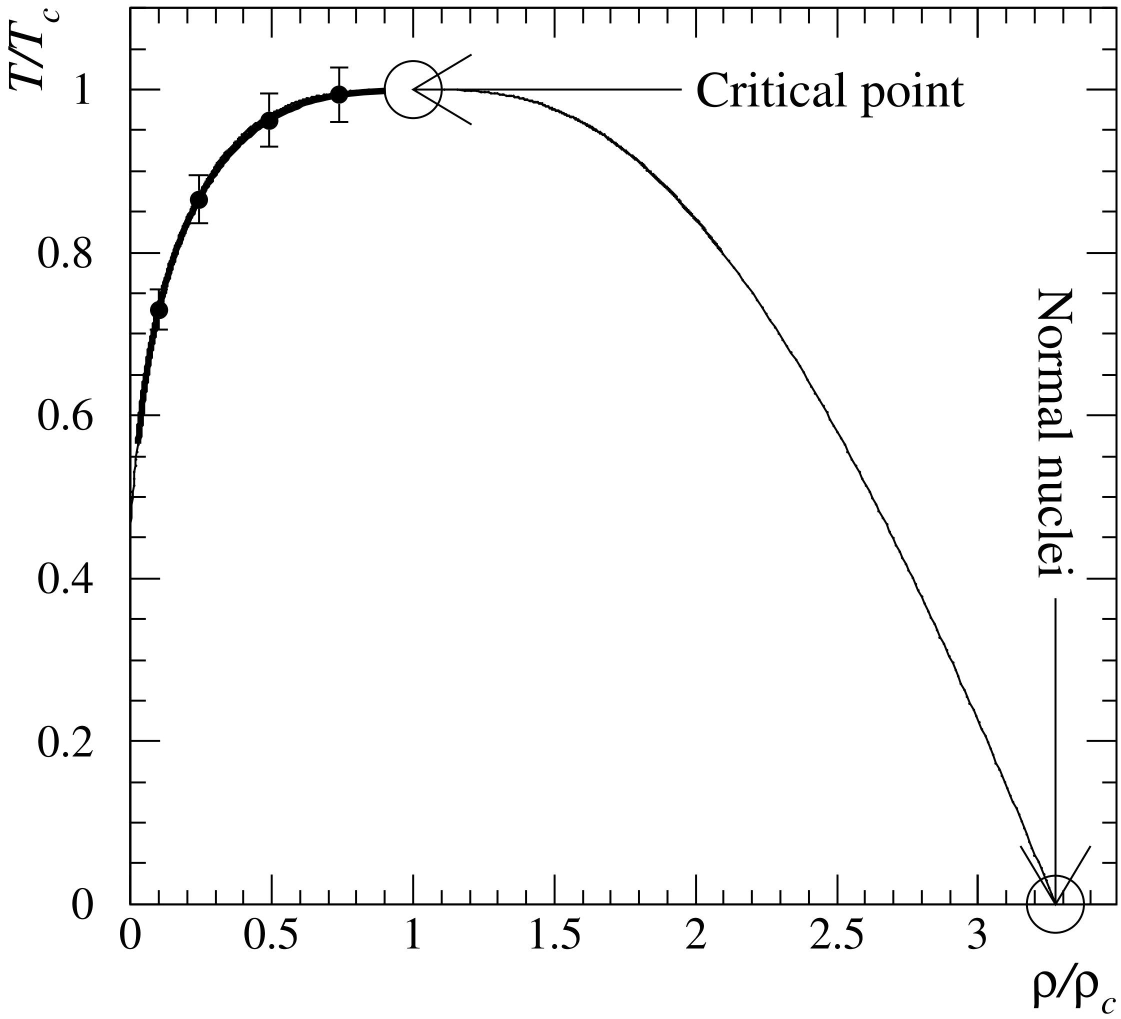
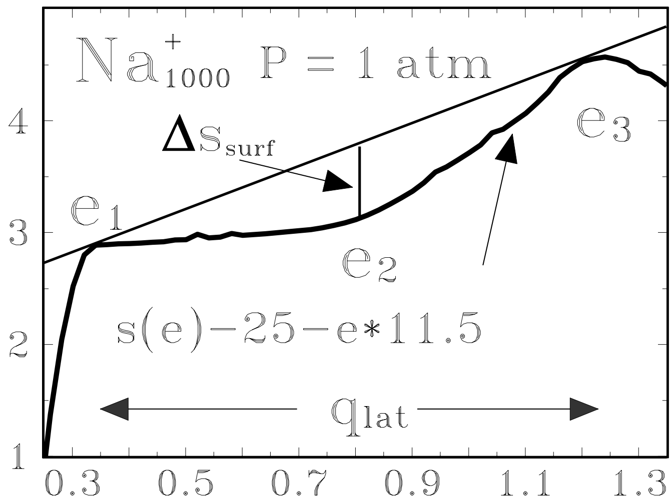


FIG. 4. The reduced density-temperature phase diagram: the thick line is the calculated low density branch of the coexistence curve, the points are selected calculated errors, and the thin lines are a fit to and reflection of Guggenheim's equation.

Elliot et al.

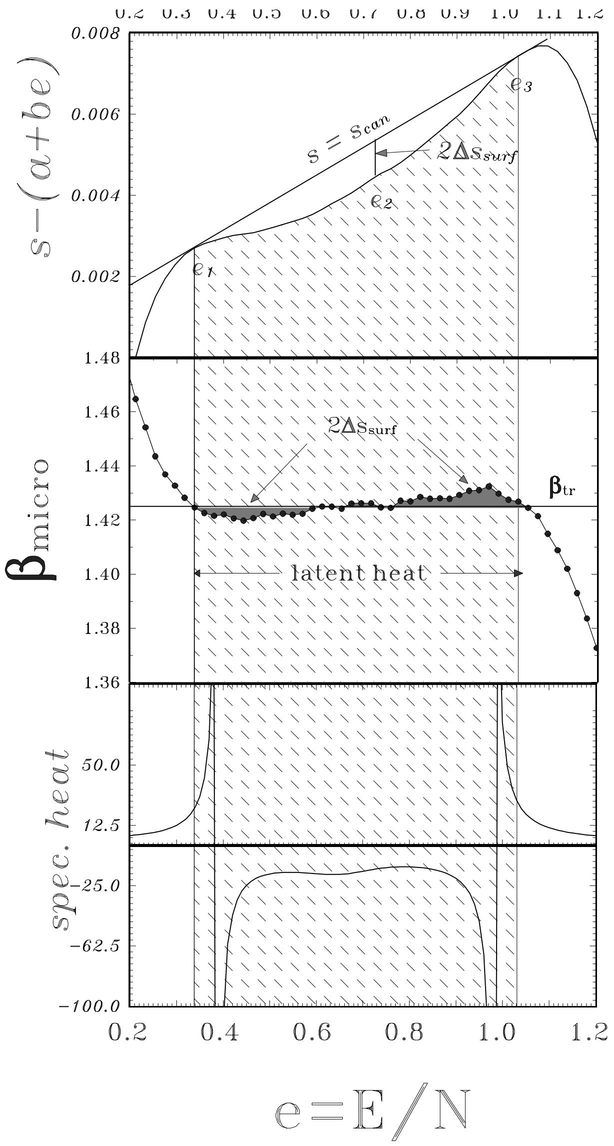
Here $S(E) - \beta E$ has at least two extremes. The two phases Example: Atomic clusters



	N_0	200	1000	3000	**bulk**
Na	T_{tr} $[K]$	940	990	1095	**1156**
	q_{lat} $[eV]$	0.82	0.91	0.94	**0.923**
	s_{boil}	10.1	10.7	9.9	**9.267**
	Δs_{surf}	0.55	0.56	0.44	
	N_{surf}	39.94	98.53	186.6	∞
	σ/T_{tr}	2.75	5.68	7.07	**7.41**

Convexity, negative heat capacity necessary signal for a phase transition of first order.

Canonical statistics unable to describe phase-separations.



Heat flows from cold to hot!

No peculiarity of gravitating systems!

Here the most interesting Thermodynamics:
is hidden behind Yang-Lee "singularity":

Original task of Thermodynamics was the explanation of steam engines
Here boiling water experiences phase separation
and becomes inhomogeneous

Canonical, homogeneous description fails !
No intensive T,μ,P
No Boltzmann-Gibbs

⇒ THIS CAN BE LEARNED FROM NUCLEAR FRAGMENTATION⇐

Phase-separation in hot nuclei:
Evaporation$\mapsto$ Fission$\mapsto$
Multifragmentation$\mapsto$ Vaporization
This is all lost in conventional (canonical) statistics.

Facts that resolved meanwhile from experiments:

1. at $E^* \leq 5MeV * A$:
evaporation of light fragments
{e.g.Au*, Viola et al PRL 93.132701 (2004)}

2. above $E^* \geq 5MeV * A$:
source expands $\Rightarrow \rho/\rho_0 \sim 0.2$,
equilibrize and decays by multiple IMF's
I.e. sudden rise of entropy $S(E)$,
phase-space filling due to
multiple, sudden, production of interfaces
as predicted by statistical models

This is a beautiful laboratory to study phase transitions by creation of surfaces.

Other example:
Atomic cluster fragmentation give detailed insight into region of phase-separation, <u>here no Coulomb</u> ↦ most interesting physics

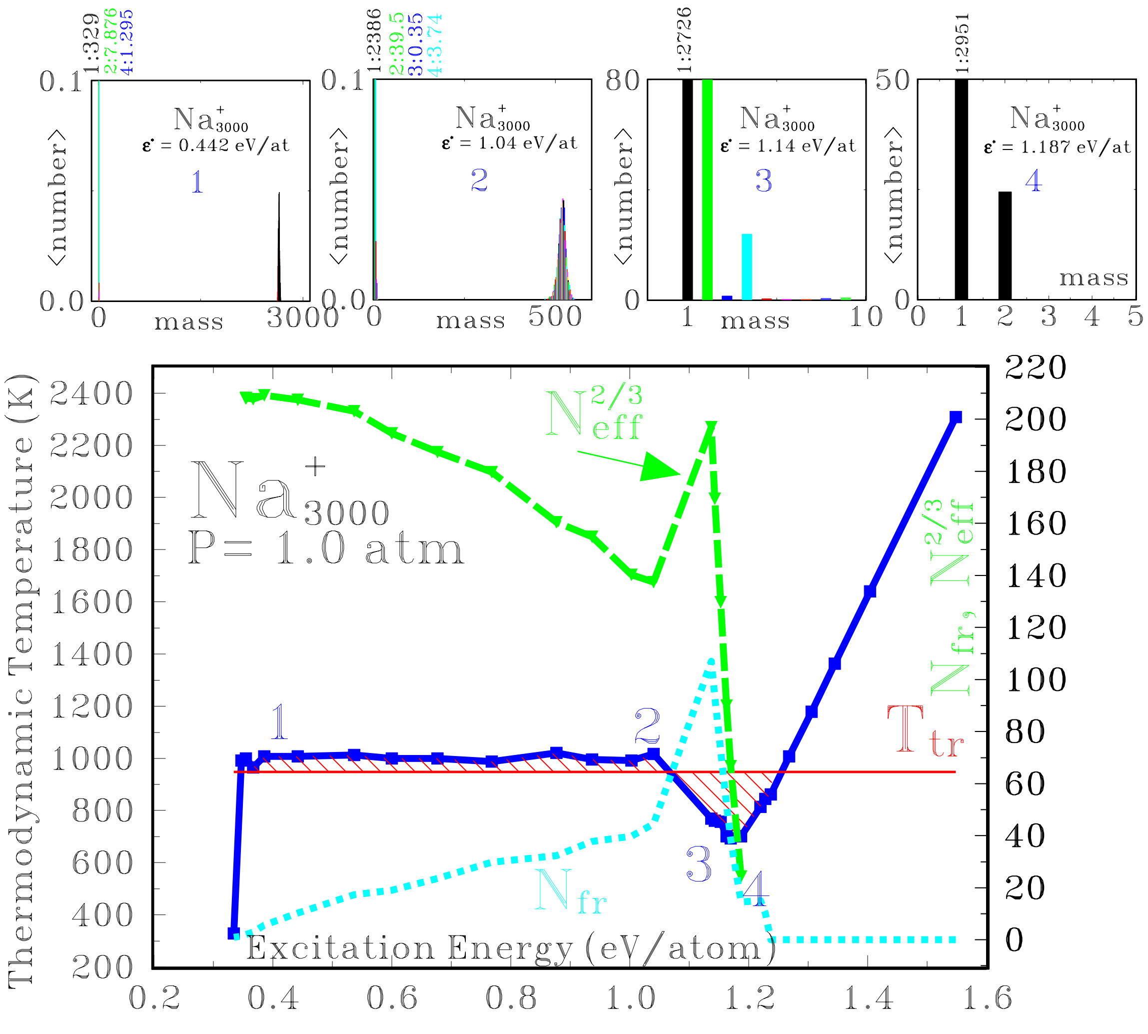


FIG. 3. Same as 1 but for Na^{+}_{3000}. The four small figures at the top show the mass distribut of fragments at four different excitation energies which are indicated in the main figure by tl number. The small vertical numbers on top of the mass-distributions give the real number fragments e.g.: 2:7.876 means there are 7.876 dimers on average at $\varepsilon = 0.442\text{eV/atom}$.

Stars and galaxies

Cover page of
Phys.Rev.Lett. vol 89, (July 2002)

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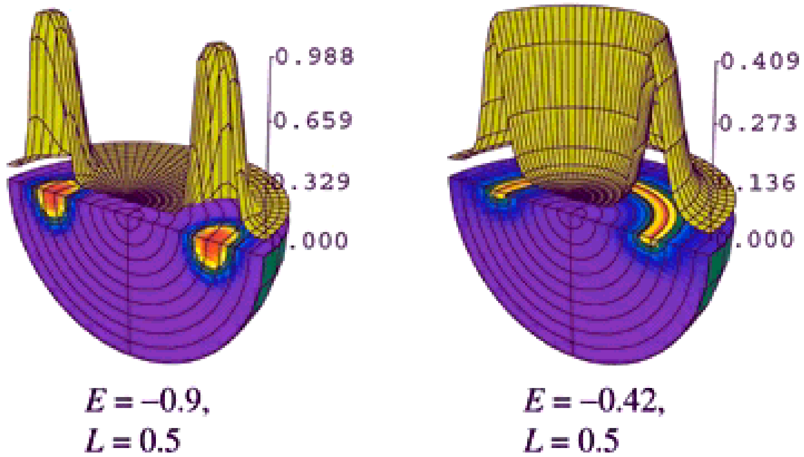


Contour plots and density profiles of a rotating, self-gravitating *N*-body system showing the formation of a stable double cluster (left) and an unstable ring (right) at different energies. The double-cluster structure illustrates the spontaneous breaking of rotational symmetry at intermediate energy and high angular momentum.

Read the Article

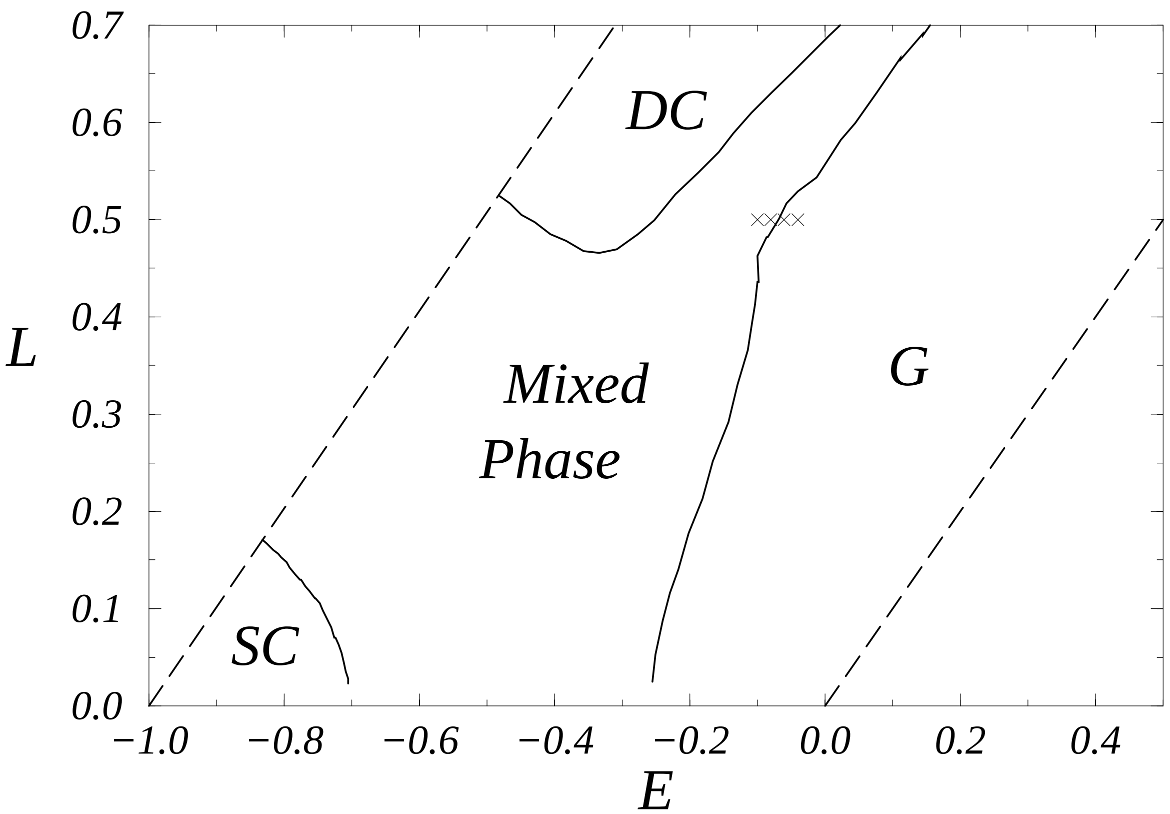
Back

E.V. Votyakov et al.

Phase diagram of self-gravitating and rotating system

$$intensive\ \Omega : E_{random} = E - \frac{\Theta\Omega^2}{2} - E_{pot}$$

$$extensive\ L : E_{random} = E - \frac{L^2}{2\Theta} - E_{pot}.$$



Microcanonical Entropy

$$W(E,N,\mathcal{V}) =$$

$$\frac{1}{N!(2\pi\hbar)^{3N}}\int_{\mathcal{V}^N} d^{3N}\,\vec{r}_i \int d^{3N}\,\vec{p}_i\;\delta[E-\sum_i^N \frac{\vec{p}_i^{\,2}}{2m_i} - V^{int}\{\vec{r}_i\}] =$$

$$\frac{\mathcal{V}^N (E-E_0)^{(3N-2)/2}\prod_1^N m_i^{3/2}}{N!\Gamma(3N/2)(2\pi\hbar^2)^{3N/2}}\int_{\mathcal{V}^N}\frac{d^{3N}r_i}{\mathcal{V}^N}\left(1-\frac{V^{int}\{\vec{r}_i\}-E_0}{E-E_0}\right)^{(3N-2)/2}$$

$$= W^{id-gas}(E-E_0,N,\mathcal{V}) \times W^{config}(E-E_0,N,\mathcal{V})$$

$$= e^{[S^{id-gas}+S^{config}]}$$

Rigorous split into ideal gas and configuration entropy

$$W^{config}(E-E_0,N,\mathcal{V}) = \left[\frac{\mathcal{V}(E)}{\mathcal{V}}\right]^N \le 1$$

$$[\mathcal{V}(E)]^N \stackrel{\text{def}}{=} \int_{\mathcal{V}^N} d^{3N}r_i\left(1-\frac{V^{int}\{\vec{r}_i\}-E_0}{E-E_0}\right)^{(3N-2)/2}$$

$$S^{config}(E-E_0,N,\mathcal{V}) = N\ln\left[\frac{\mathcal{V}(E)}{\mathcal{V}}\right] \le 0$$

$$S^{config}(E-E_0) \to \begin{cases} 0 & E \gg V^{int} \\ ln\left\{\left[\frac{\mathcal{V}_0}{\mathcal{V}}\right]^{N-1}\right\} < 0 & E \to E_0 \end{cases}$$

All interesting phenomena of Thermodynamics are encrypted in S^{config}

Statistical Mechanics of inhomogeneities, no scaling, phase transitions≡ the physics of interfaces (also multifragmentation) :

Solid	Liquid	Gas
have internal surfaces		no surface
condensate volume less than external volume		fills any volume
surface has edges, is hard, fixed	surface has no edges, flexible, adjusts to container	

Research is not to think what everybody else has thought, but to see what everybody else has seen.
≇ Albert Szent-Gyorgi(1893- 1986)

Moral:
Conserved quantities
⇒ only microcanonical⇐

If the mechanism mixes different constraints (e.g. volumes) then its physics determines the weights $p(V)$ not any arbitrary Lagrange parameter (or belief !)