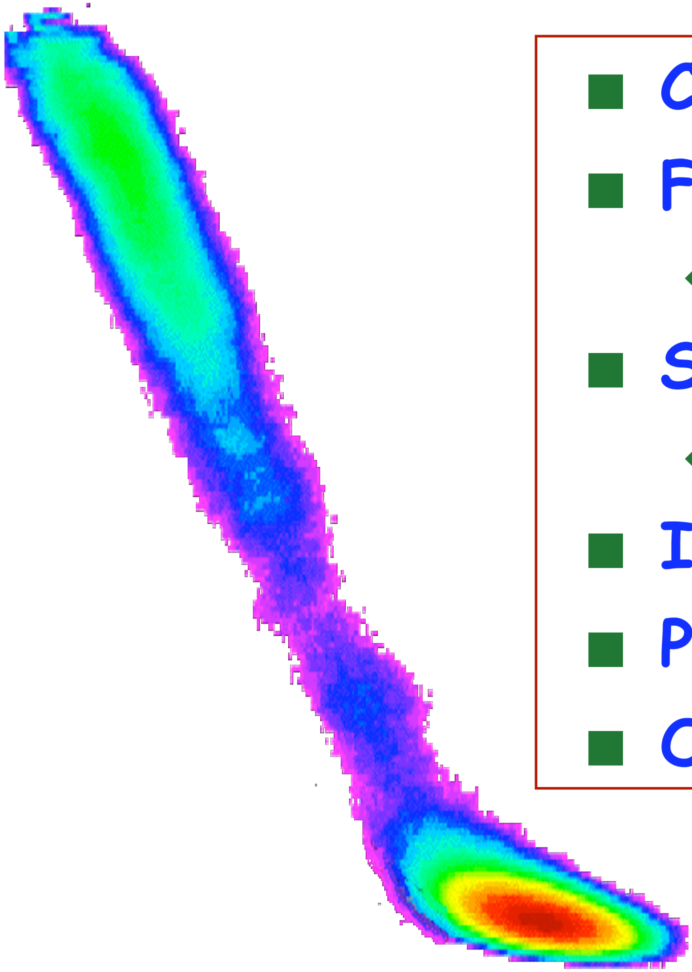
Challenges of finite systems stat. phys.

Ph. Chomaz, Caen France



- Connections to other chapters
- Finite systems
  - Boundary condition problem
- Statistical descriptions
  - Gibbs ensembles - Ergodicity
- Inequivalence, thermo limit
- Phase transitions
- Open, transient

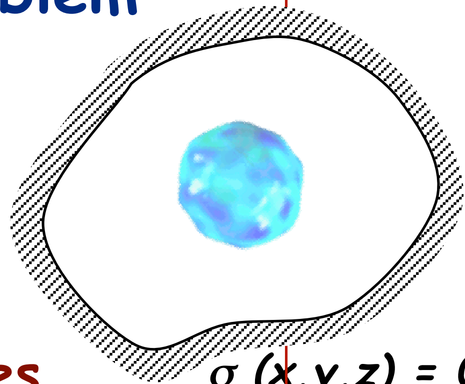
1) Connections to other chapters

- Non saturating infinite systems
  Dieter's chapter
- Clusters (evaporative ensemble)
  Eric's chapter
- Dynamics and equilibrium
  Many chapters
- Non extensive dynamics (Tsallis)
  Few discussions

2) Finite systems

- Finite number of particles in interaction

- Boundary conditions / continuum problem
  - Bound states OK
  - Trapped particles OK
  - Model cases OK



σ *(x,y,z) = 0*

  - In general, *H* undefined without boundaries

    => System & Thermodynamics undefined

    - => Ex: Entropy *S(E)*=log *W(E)* undefined

  - Boundaries, σ *(x,y,z) = 0* : infinite information

    => Use of information theory mandatory

    - => Use of constraints on volume and shape (eg $\langle r^2 \rangle$)

3) Statistical physics

R. Balian « Statistical mechanics »

- **Macroscopic**
  - One realization (event) <u>can</u> be an equilibrium
  - One ∞ system = ∞ ensemble of ∞ sub-systems

- **Microscopic**
  - <u>Ensemble of replicas</u> needed
  - One realization (event) <u>cannot</u> be an equilibrium

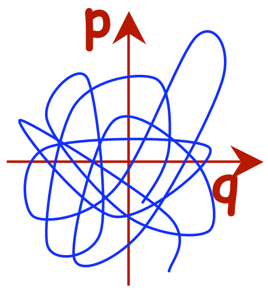
  - <u>Gibbs:</u> Equilibrium = maximum entropy
    - Average over time — if ergodic
    - Average over events — if chaotic/stochastic
    - Average over replicas — if minimum info

  ⚠ "Ergodic" some times used instead of "uniform population of phase space"

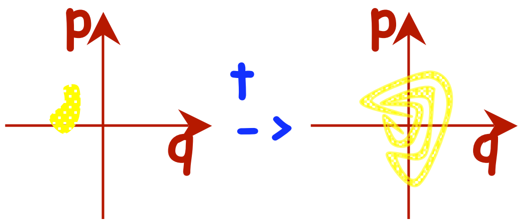
3) Statistical physics

R. Balian « Statistical mechanics »

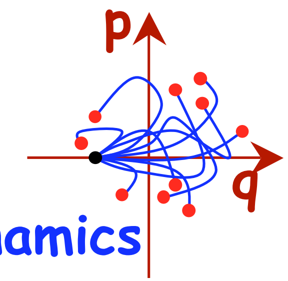
- **Ergodic** (Bound systems only) ⚠
  - ∞ time average = phase space average
  - Ergodic => <≠ statistics
  - Only conserved quantities (E, J, P …) ⚠



- **Mixing**

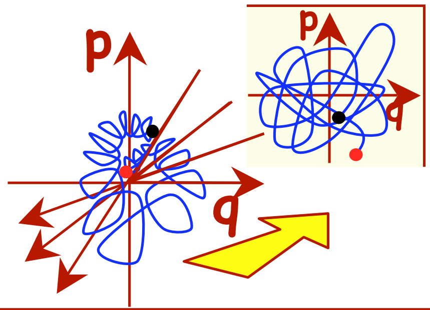


- **Stochastic**



  - Unknown initial conditions
  - Unknown dynamics
    - Not only conserved statistical variables

- **Complex / min info**
  - Few relevant observations $\langle A_l \rangle$
    => state variables (not only conserved)
  - Many irrelevant degree of freedom



Validity conditions

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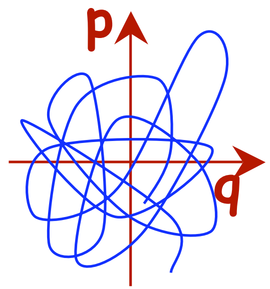
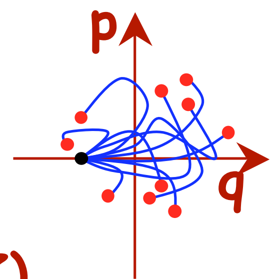
- **Ergodic**
  - Bound systems only
  - For time averages only
  - Should be demonstrated (difficult)
  - Only conserved quantities (E, J, P …)



- **Mixing**
- **Stochastic**
- **Complex / min info**
  - For ensemble of events
  - Should be demonstrated (difficult)
  - Comparison with models
  - Consistency checks (e.g. $T_1=T_2$, $\sigma_A^2=-\partial_l \log Z$)
  - Independence upon history



- **How far are we from equilibrium?**

Information theory for finite system

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- Statistical ensemble: $\left\{\left((n), p^{(n)}\right)\right\}$
- Shannon information: $I = \sum_{(n)} p^{(n)} \log p^{(n)}$
- Information = observations: $\{< \hat{A}_\ell >= \sum_{(n)} p^{(n)} A_\ell^{(n)}\}$

Min. bias state: min I under constraints $\{< \hat{A}_\ell >\}$

- λ_ℓ Lagrange multipliers
- => Boltzman probability
- Z Partition sum
- Constraints = EOS

$$p^{(n)} = Z^{-1} e^{-\sum_\ell \lambda_\ell A_\ell^{(n)}}$$

$$Z(\boldsymbol{\lambda}) = \sum_{(n)} e^{-\sum_\ell \lambda_\ell A_\ell^{(n)}}$$

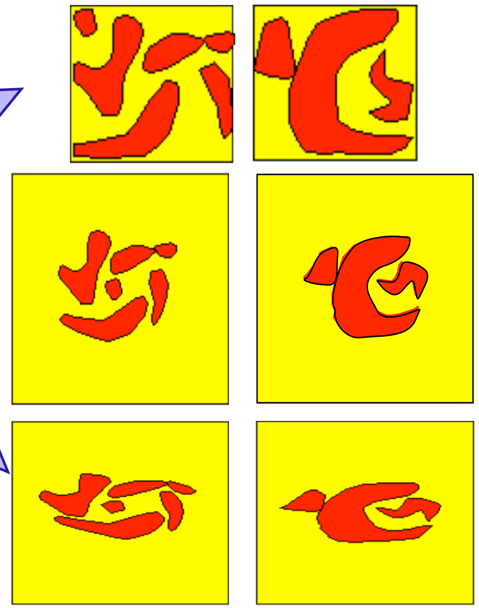
$$< \hat{A}_\ell >= -\partial_{\lambda_\ell} \log Z(\boldsymbol{\lambda})$$

Many different ensembles

- Constraints
- Conserved quantities
- Sorting
- Boundaries

⚠ Boundary = ∞ information
Microcanonical undefined

E	Microcanonical
⟨E⟩	Canonical
V	Isochore
$\langle r^3 \rangle$	Isobare
$\langle Q_2 \rangle$	Deformed
⟨p.r⟩	Expanding
⟨A⟩	Grand
⟨L⟩	Rotating
…	Others



- **Boundaries = spatial constraints**, ex: $\langle V \rangle = \langle r^3 \rangle$
  - => $p_{\beta\lambda}^{(n)} = Z^{-1} \exp - \beta E^{(n)} - \lambda_0 V^{(n)}$ => isobar ensemble

- Valid also for open systems (extension $\langle r^2 \rangle$)

4) Finite systems => ensemble inequivalence

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Géneral ref.:

- Thirring W 1970 Z. Phys. 235 339
- Huller A 1994 Z. Phys. B 93 401
- Ellis R S, Haven K and Turkington B 2000 J. Stat. Phys. 101 999
- Dauxois T , Holdsworth P and Ruffo S 2000 Eur. Phys. J. B 16 659
- Gross D H E 2001 Microcanonical Thermodynamics: Phase Transitions in Small Systems (Lecture Notes in Physic 66) (World Scientific)
- Barré J, Mukamel D and Ruffo S 2001 Phys. Rev. Lett. 87 030601 Cond-mat/0209357
- Ispolatov I and Cohen E G D 2001 Physica A 295 475
- Gulminelli F and Chomaz Ph. 2002 Phys. Rev. E 66 046108

Phase trans.:

- Kastner M, Promberger M and Huller A 2000 J. Stat. Phys. 99 1251
- Gross D H E and Votyakov E V 2000 Eur. Phys. J. B 15 115
- Huller A and Pleimling M 2002 Int. J. Mod. Phys. C 13 947
- Pleimling M, Behringer H and Hüller A 2004 Phys. Lett. A 328 432
- P. Chomaz and F. Gulminelli , in T. Dauxois et al, Lecture Notes in Physics Vol. 602, Springer (2002),
- J. Barré, D. Mukamel & S. Ruffo Cond-mat/0209357
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- Kastner M, J. Stat. Phys. 107 (2002) 133
- I. Ispolatov & E.G.D. Cohen, Physica A 295 (2001) 475

4) Finite systems => ensemble inequivalence

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- **Microcanonical ensemble:** $p^{(n)} = \delta(E - E^{(n)}) / W(E)$
  - Shannon = Boltzmann: $S(E) = \log W(E)$
  - Temperature (EOS): $T^{-1} = \partial_E S(E)$

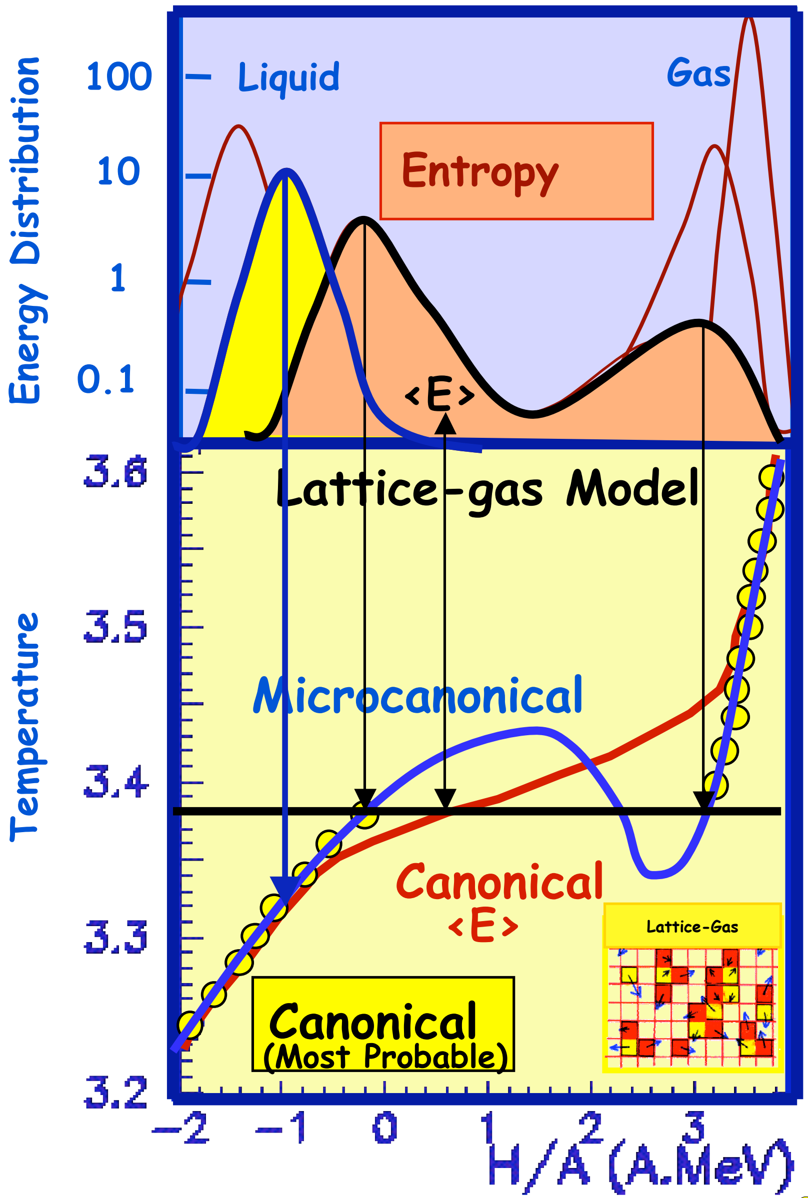
- **Canonical ensemble:** $p^{(n)} = e^{-\beta E^{(n)}} / Z(\beta)$
  - Partition sum = Laplace tr.: $Z(\beta) = \int dE\, e^{-\beta E}\, W(E)$
  - Caloric curve (EOS) $< E > = -\partial_\beta \log Z(\beta)$
  - Canonical S_c = Legendre tr.: $S_c(< E >) = \log Z(\beta) + \beta < E >$

- **But canonical $S_c(<E>) \neq$ microcanonical $S(E)$**
  - => Canonical EOS ≠ microcanonical EOS

Inequivalence

- **Canonical Energy dist.**
  - $P_\beta(E) = e^{S(E)-\beta E} / Z(\beta)$
    Exact link microcan. entropy
- **Monomodal $\overline{E}$**
  - Most probable: $\partial_E S(\overline{E}) = \beta$
  - Average: $<E>_\beta \approx \overline{E}_{T=\beta^{-1}}$
  - Canonical EOS ≈ microcan.
- **Bimodal: ensembles inequivalent**
  - $< E >_\beta \approx p^{(1)} \overline{E}^{(1)}_{T=\beta^{-1}} + p^{(2)} \overline{E}^{(2)}_{T=\beta^{-1}}$
  - Canonical interpolates 2 stable microcan. solutions

F. Gulminelli & Ph. Ch., PRE 66 (2002) 46108



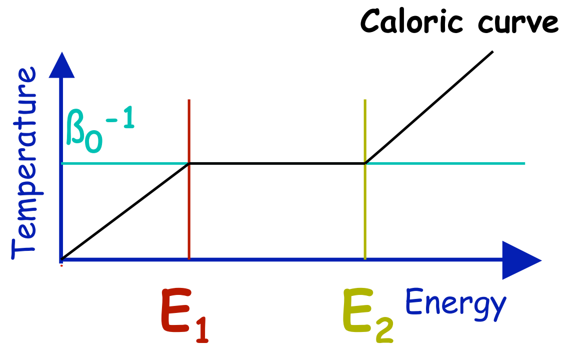
Finite systems => ensemble inequivalence

- **Many different ensembles:**
  - Constraints and boundaries
  - Boundaries = ∞ information incompatible with max S
- **Various ensembles are related:**
  - Laplace transform: $Z(\beta) = \int dE\, e^{-\beta E}\, W(E)$
  - Probabilities (sorting): $P_\beta(E) = W(E) e^{-\beta E} / Z(\beta)$
- **But are not equivalent:**
  - Small corrections far from phase transitions
  - Strong deviations associated with phase transitions
  - Disappears at thermo limit,

5) Phase transition in infinite systems

- **Thermodynamical potentials** $F = -T \log Z$
  non analytical at $N \rightarrow \infty$ $\left(Z = \sum_{(n)} e^{-\beta E^{(n)}}\right)$
  L.E. Reichl, Texas Press (1980)

- **Order of transition:**
  discontinuity in $\partial_\beta^n \log Z$
  Ehrenfest's definition



- **Ex: first order:**
  discontinuous EOS: $<E> = -\partial_\beta \log Z$
  R. Balian, Springer (1982)

1st order in finite systems

PC & Gulminelli Phys A 330(2003)451

⇕

Free order param. (canonical)

- Zeroes of Z reach real axis

Yang & Lee Phys Rev 87(1952)404

⇕

- Bimodal distribution (P_b (E))

K.C. Lee Phys Rev E 53 (1996) 6558

⇕

Fixed order para. (microcanonical)

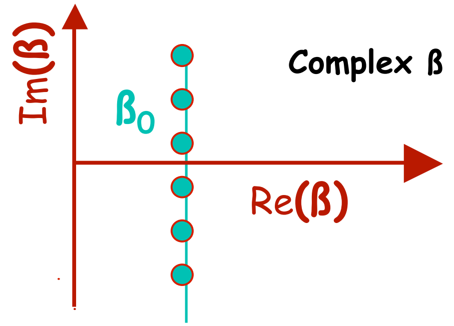
- Back Bending in EOS (T(E))

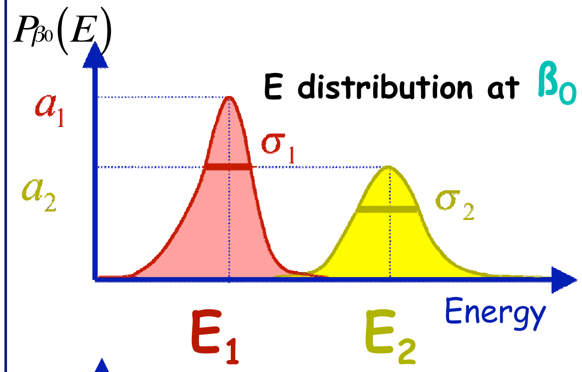
K. Binder, D.P. Landau Phys Rev B30 (1984) 1477

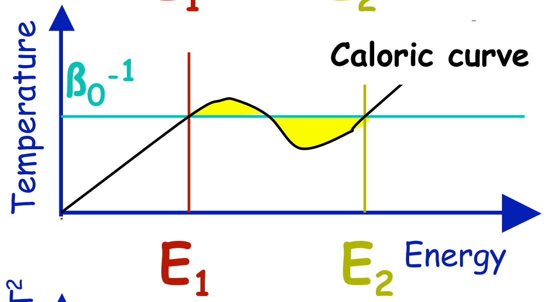
⇕

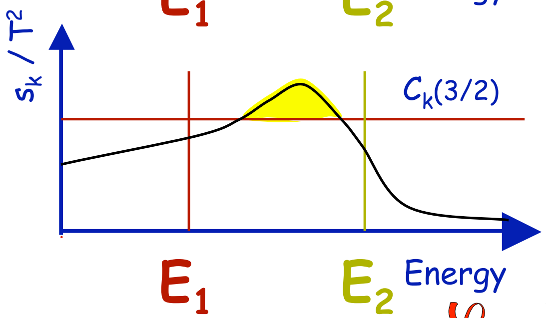
- Abnormal fluctuation (σ_k(E))

J.L. Lebowitz (1967), PC & Gulminelli, NPA 647(1999)153









Curvature of S should not be confused with variations of variables along transformations

Microcanonical specific heat ($C<0$) & bimodalities:

- **Astro:**
  - V.A. Antonov Len. Univ. 7,135 (1962); IAU Symp.113, 525 (1995).
  - D. Lynden-Bell & R. Wood, Mon. Not. R. Astron. Soc. 138, 495 (1968); D. Lynden-Bell, Physica A 263, 293 (1999).
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  - F. Bouchet & J. Barré, Cond-mat/0303307
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  - J. Barré, D. Mukamel & S. Ruffo Cond-mat/0209357
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  - M. Antoni, S. Ruffo, A. Torcini, Cond-mat/0401177
- **Clusters:**
  - R.M. Lynden-Bell, Mol. Phys. 86 (1995) 1353
  - P. Labastie et al,PRL 65(1990)1567
- **DNA:**
  - A. Wynveen, D.J. Lee & A.A. Kornyshev, Physics/0408063
- **Scaling:**
  - H. Behringer, M. Pleimling & A. Hüller, Cond-mat/0411153&0311211
  - M. Kastner & M Promberger, J. Stat. Phys. 53 (1988) 795

Topologie Σ_E:
- R. Franzosi, M. Pettini & L. Spinelli, Math-Ph0305032

Entropy:
- J. Naudts, Cond-mat/0412683

6) Statistical description evolving systems

- **Time dependent statistical ensemble**
  - Max *S* at *t* with constraint *<A>* from $t_0 = t - Dt$,
  - Heisemberg picture: $$\hat{A} \rightarrow e^{-i\Delta t\hat{H}}\hat{A}e^{i\Delta t\hat{H}} = \hat{A} - i\Delta t[\hat{H},\hat{A}] + \dots$$
  - => time odd observables $$\hat{B} = -i[\hat{H},\hat{A}]$$

- **Ex: unconfined finite <r²> system and radial flow**
  - Finite <r²> system at t_0: $$p^{(n)} \propto \exp-\beta(E^{(n)} - \lambda_0^{'}\hat{r}^{2^{(n)}})$$
  - <=> External potential <=> equilibrium in a trap $\lambda_0 r^2$
  - State at time *t*:
  - <=> Radial flow $$\hat{B} = -i[\hat{H},\hat{r}^2] = (\hat{r}\cdot\hat{p} + \hat{r}\cdot\hat{p})/m$$
  - Ex: Ideal gas: $$p^{(n)}(t) \propto \exp-\beta(t)\frac{(\mathbf{p}^{(n)} - h(t)\mathbf{r}^{(n)})^2}{2m} - \lambda(t)r^{(n)^2}$$

Balian, Al-Hassid & Reinhardt, An. Phys. (1987); PC & Gulminelli & Juillet (2004)

7) Conclusions: Challenges

- Statistical description of non extensive systems
  - Conceptual justification
  - Inequivalence
- Phase transition in finite systems
  - Abnormal thermodynamics
  - Negative curvature
- Phase transition in Nuclei
  - EOS
  - Phase diagram