

# Phase transition in finite systems

Francesca GULMINELLI and Philippe CHOMAZ

## ■ Finite systems

- ◆ Zeroes of the partition sum
- ◆ Bimodal event distributions
- ◆ Negative heat capacity
- ◆ Abnormal fluctuations

## ■ Experimental results

- ◆ Melting of Na clusters
- ◆ Superfluidity in atomic nuclei
- ◆ Fragmentation of nuclei
- ◆ Fragmentation of H-clusters



- I -

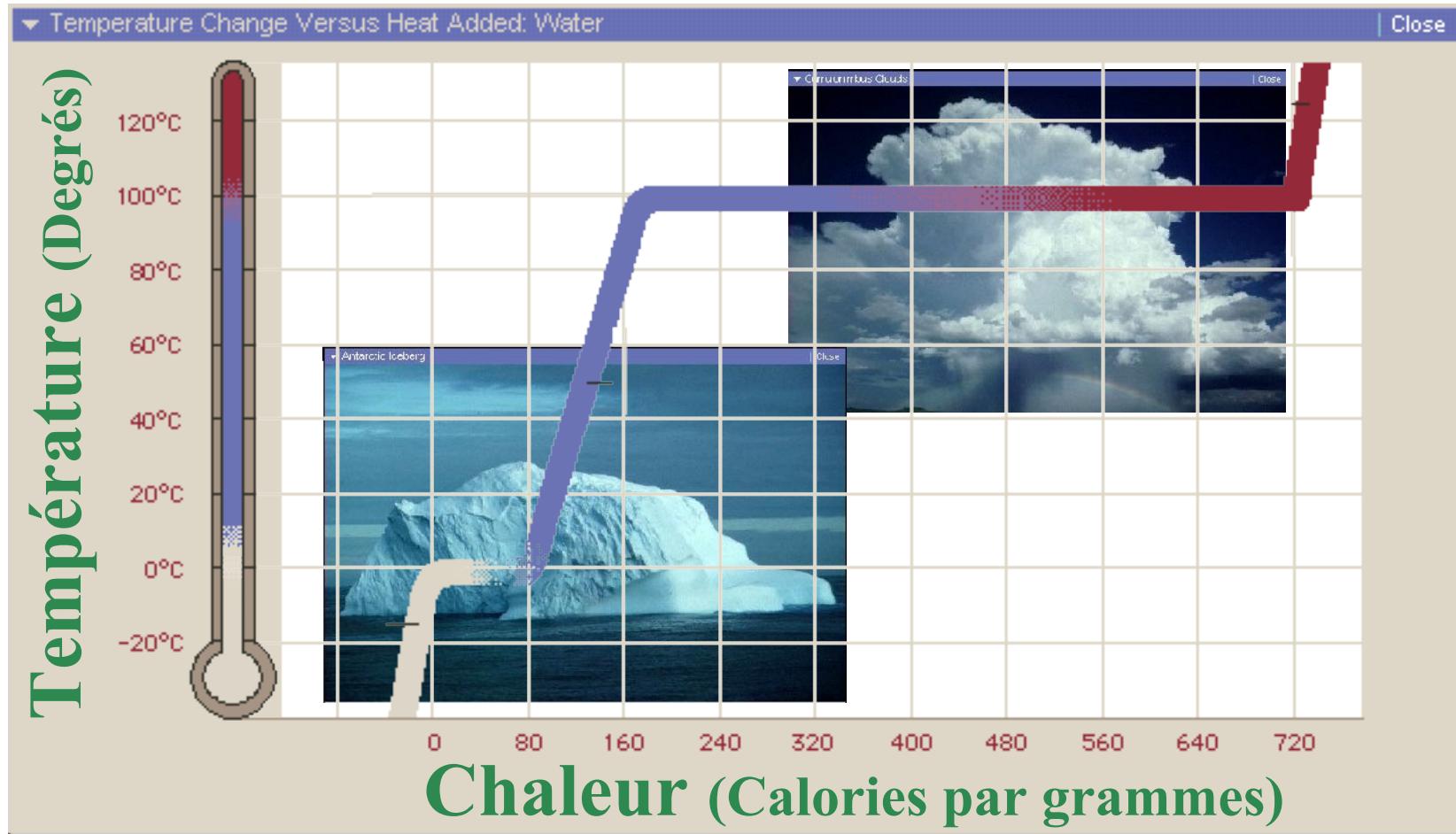
# Introduction

## Phase transition

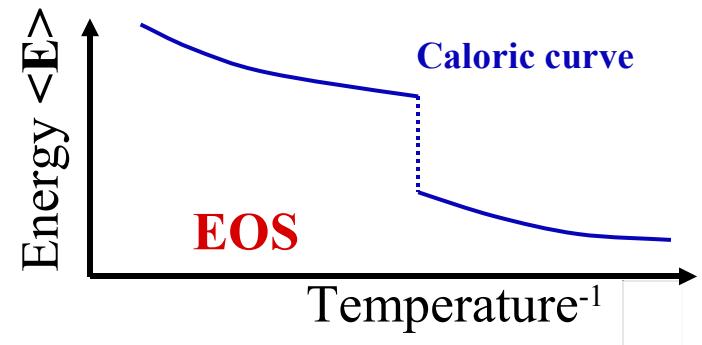
### Anomaly in thermo



# Transition de Phase



# Phase transition in infinite systems



- Ex: first order:  
discontinuous EOS:

# Phase transition in infinite systems

- Thermodynamical potentials: e.g.  $F = -T \log Z$   
non analytical at

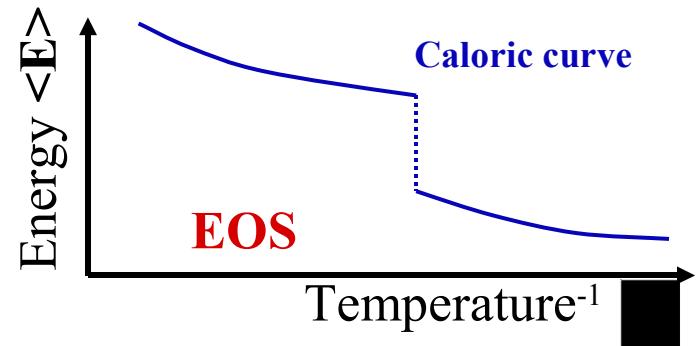
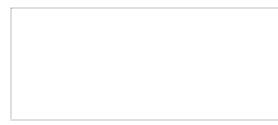
*L.E. Reichl, Texas Press (1980)*



$$\boxed{\text{?}} = \sum_{(n)} e^{-bE^{(n)}} \boxed{\text{?}}$$

- Order n:  
discontinuity in

*Ehrenfest's definition*



- Ex: first order:  
discontinuous EOS:

*R. Balian, Springer (1982)*



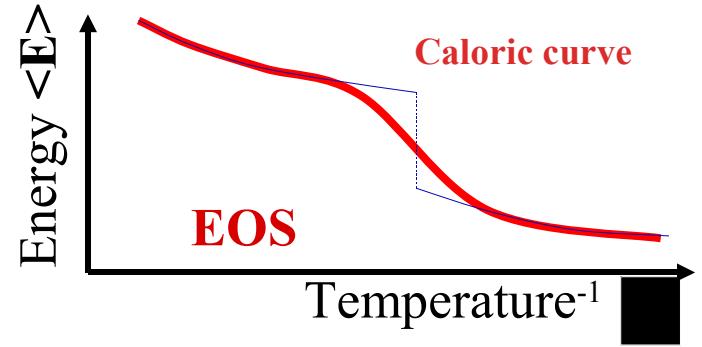
# Phase transition in finite systems

- Thermodynamical potentials:  $e.g. F = -T \log Z$   
 $Z$  analytical  $\varepsilon > 0$ ,  $\mathcal{T}$

$$\langle \dots \rangle = \frac{1}{Z} e^{-\beta E^{(n)}}$$

- No phase transition  
continuous

*Ehrenfest's definition*



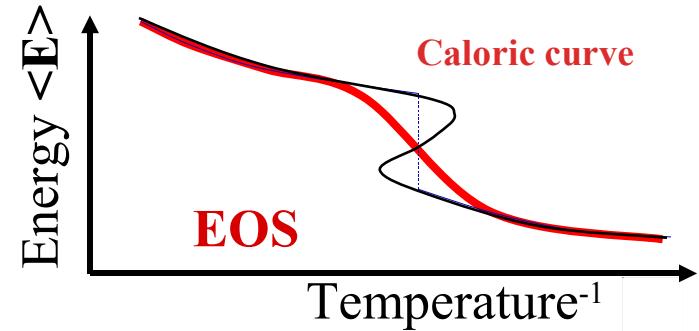
- Ex:  
Continuous EOS:

# Phase transition in finite systems

- Thermodynamical potentials:  $e.g. F = -T \log Z$
- $Z$  analytical  $\varepsilon > 0$ ,  $\mathcal{T}$

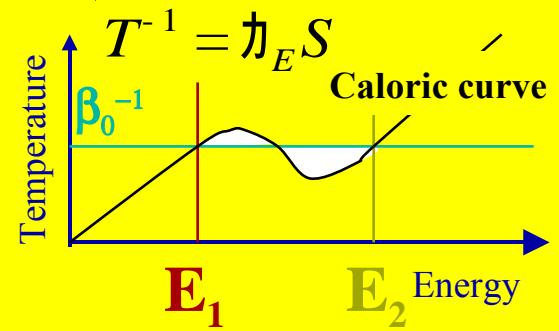
$$\langle \dots \rangle = \langle \dots \rangle_{(n)} e^{-bE^{(n)}} \langle \dots \rangle_{(n)}$$

- No phase transition  
continuous
- Ehrenfest's definition*



- But anomaly in the entropy  
Ex: negative heat capacity

*K. Binder, D.P. Landau Phys Rev B30 (1984) 1477;  
Lynden-Bell, D. & Wood, R. 1968, Mon. Not. R. Astr. Soc. 138, 495.;  
W. Thirring, Z. Phys. 235, 339 (1970),  
D.H.E. Gross, Rep. Prog. Phys. 53, 605 (1990),*



# 1st order in finite systems

PC & Gulminelli Phys A (2003)

## Free order param. (canonical)

- ◆ Zeroes of  $Z$  reach real axis

Yang & Lee Phys Rev 87(1952)404

- ◆ Bimodal distribution ( $P_\beta(E)$ )

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

## Fixed order para. (microcanonical)

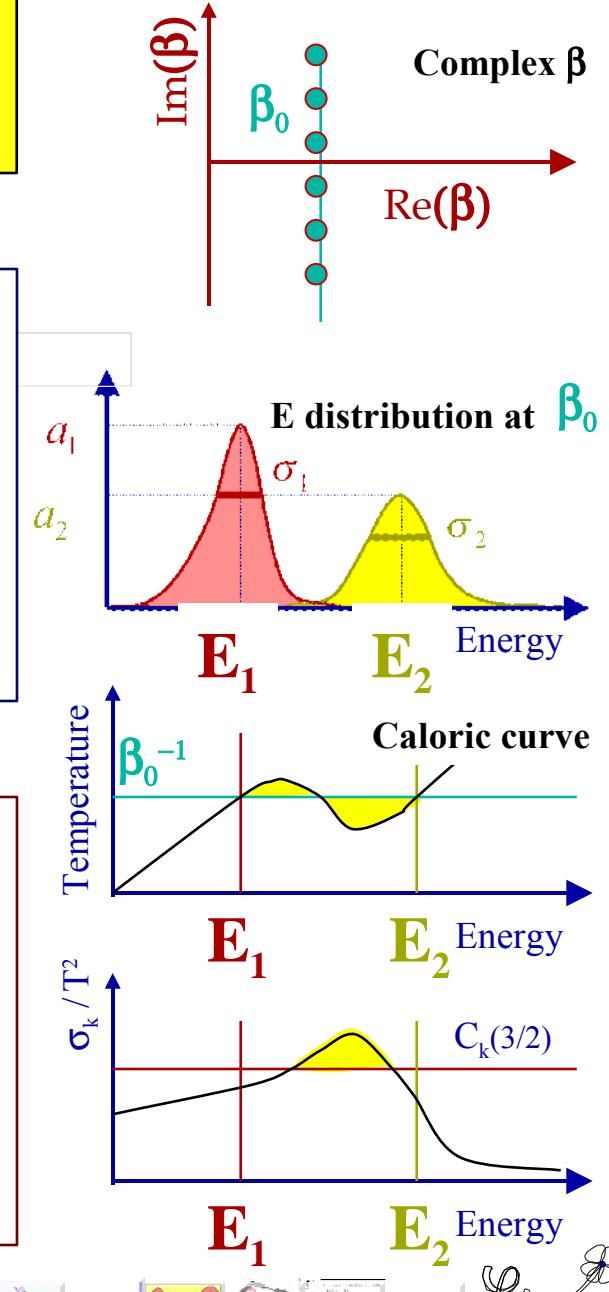
- ◆ Back Bending in EOS ( $T(E)$ )

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

Lynden-Bell, D. & Wood, R. 1968, Mon. Not. R. Astr. Soc. 138, 495.

- ◆ Abnormal fluctuation ( $\sigma_k(E)$ )

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



## - II -

# Origin of singularities

# Zeroes of Z ( $\beta$ )

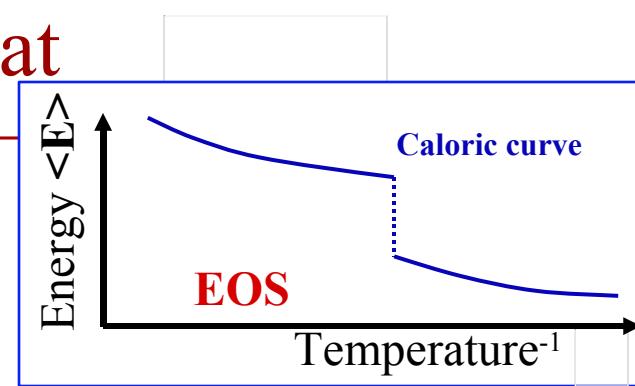
# Bimodal P(E)



Thermodynamical potentials: e.g.  $F = -T \log Z$   
non analytical at

L.E. Reichl, Texas Press (1980)

$$\boxed{\text{?} = (n) e^{-bE^{(n)}}}$$

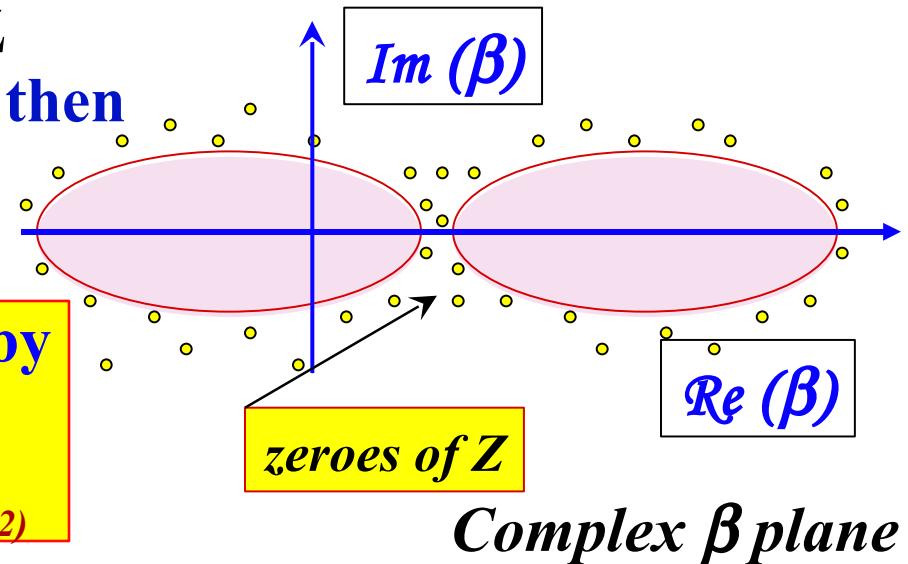


# Discontinuities from zeroes of Z

- If, when , no zeroes of Z converge on the *Real*  $\beta$  axis , then logZ remains analytical  
 $\Rightarrow$  No phase transition

- Phase transitions are defined by the asymptotic distribution of zeroes of the partition sum Z

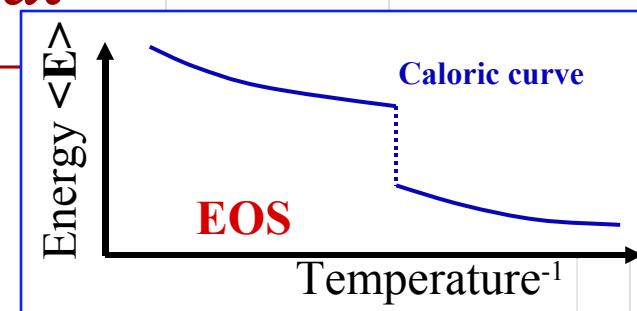
(C.N.Yang T.D.Lee 1952)



Complex  $\beta$  plane

- Thermodynamical potentials: e.g.  $F = -T \log Z$   
non analytical at

L.E. Reichl, Texas Press (1980)



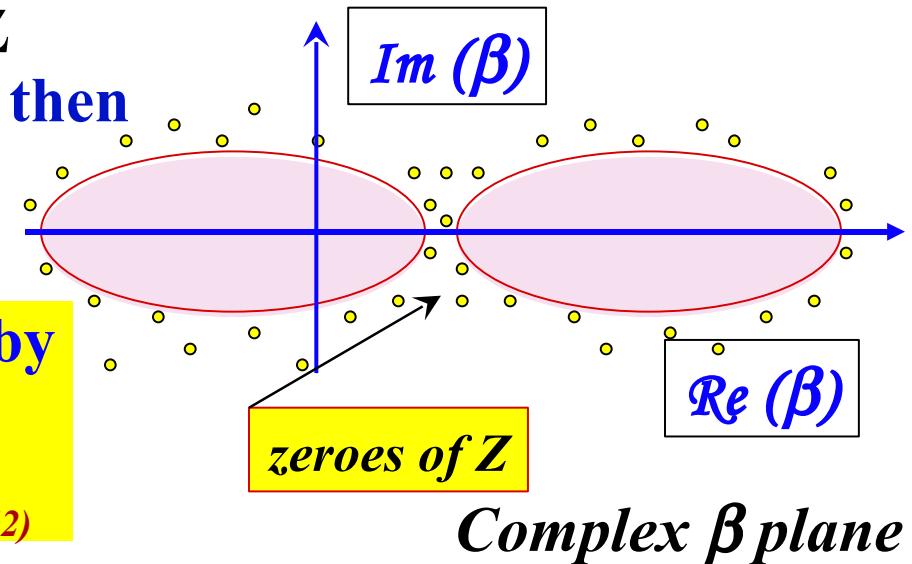
$$\boxed{\frac{d}{d\beta}} = \sum_{(n)} e^{-bE^{(n)}} \boxed{\frac{d}{d\beta}}$$

# Discontinuities from zeroes of Z

- If, when  $\beta \rightarrow \infty$ , no zeroes of Z converge on the Real  $\beta$  axis , then logZ remains analytical  
 $\Rightarrow$  No phase transition

- Phase transitions are defined by the asymptotic distribution of zeroes of the partition sum Z

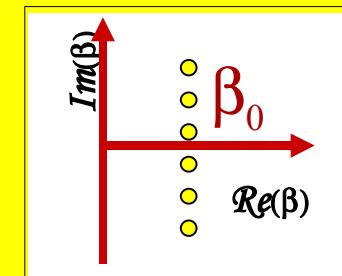
(C.N.Yang T.D.Lee 1952)



Complex  $\beta$  plane

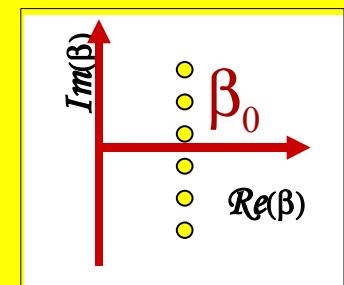
- First order phase transitions  
A uniform density of zero's on a line crossing the real  $\beta$  axis perpendicularly at  $\beta_0$

Yang - Lee theorem



■ First order phase transitions  
A uniform density of zero's on a line crossing  
the real  $\beta$  axis perpendicularly at  $\beta_0$

*Yang - Lee theorem*



## ■ A theoretical definition

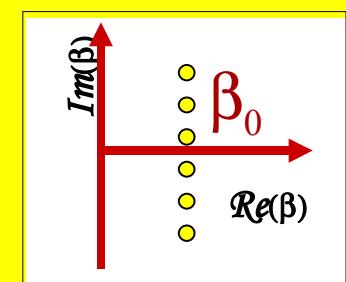
- ◆ Only valid asymptotically:  $V = \infty$
- ◆ How to extend it,  $V \neq \infty$  ?

## ■ How to use it experimentally ?

### ■ First order phase transitions

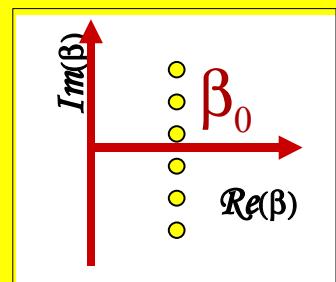
A uniform density of zero's on a line crossing the real  $\beta$  axis perpendicularly at  $\beta_0$

*Yang - Lee theorem*

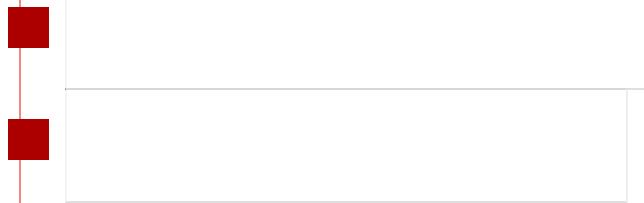


■ First order phase transitions  
A uniform density of zero's on a line crossing  
the real  $\beta$  axis perpendicularly at  $\beta_0$

*Yang - Lee theorem*



# Link with energy distribution P(E)

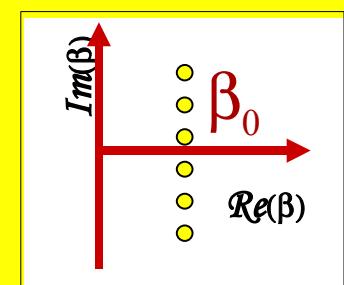


## Z Laplace transform of P:



Ph. Ch., F. Gulminelli, Physica A 2003

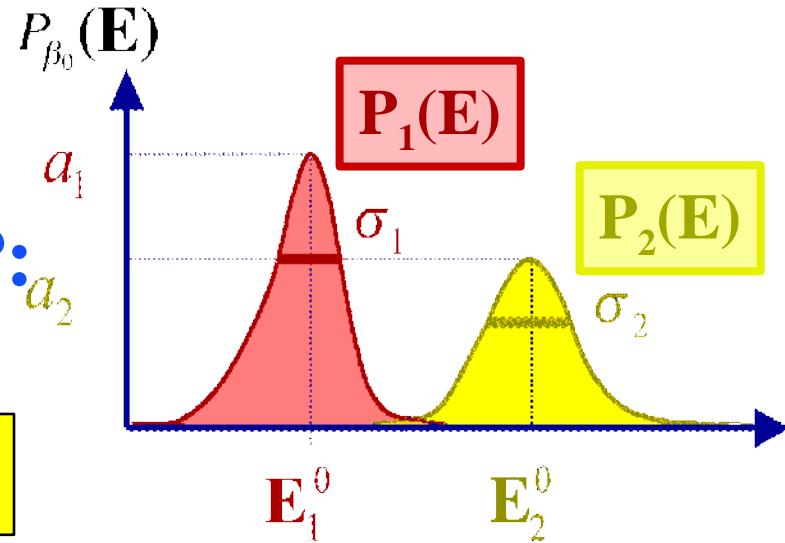
- First order phase transitions  
A uniform density of zero's on a line crossing the real  $\beta$  axis perpendicularly at  $\beta_0$



# Link with energy distribution $P(E)$

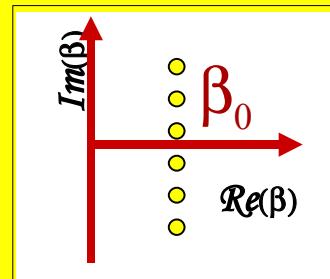
Z Laplace transform of  $P$ :

Bimodal  $P$  with  $\Delta E \propto N$

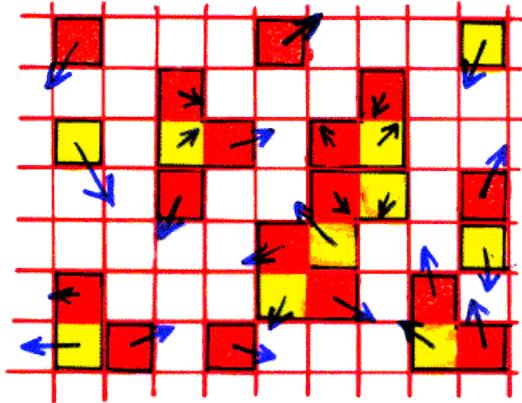


Ph. Ch., F. Gulminelli, Physica A 2003

First order phase transitions  
A uniform density of zero's on a line crossing  
the real  $\beta$  axis perpendicularly at  $\beta_0$

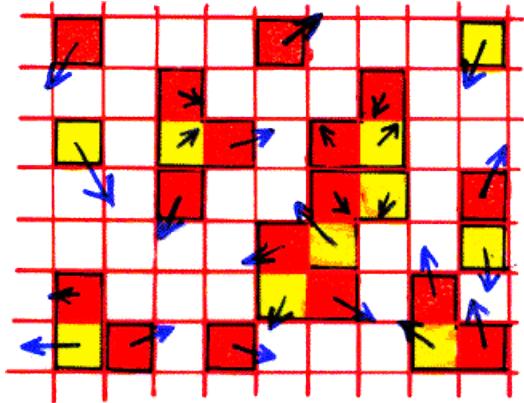


# Lattice gas model



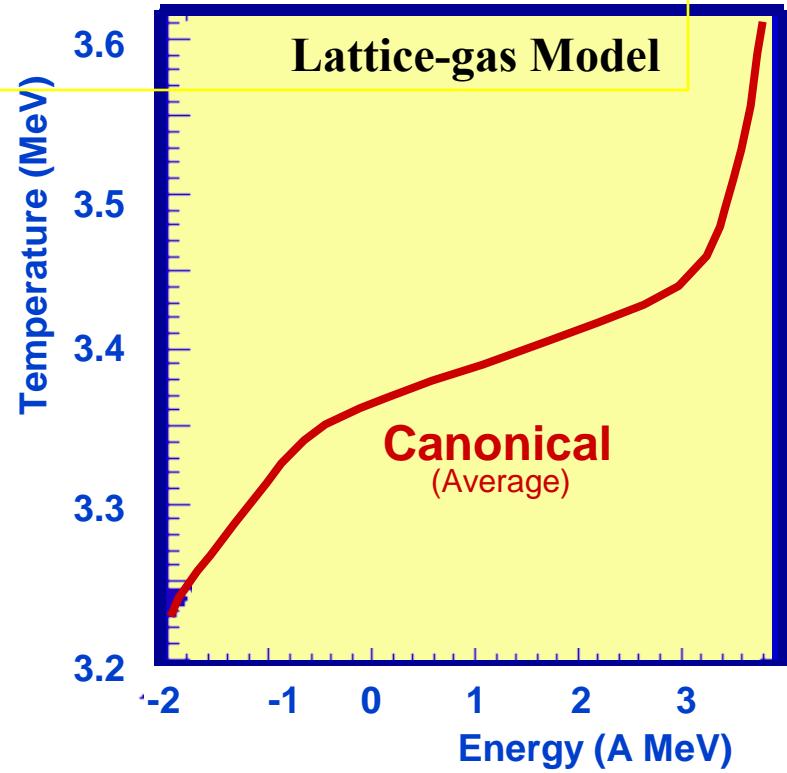
- Closest neighbors interaction
- Metropolis Boltzmann weight  $e^{-\beta E}$
- Average volume  $\langle V \rangle$  (pressure)

# Lattice gas model

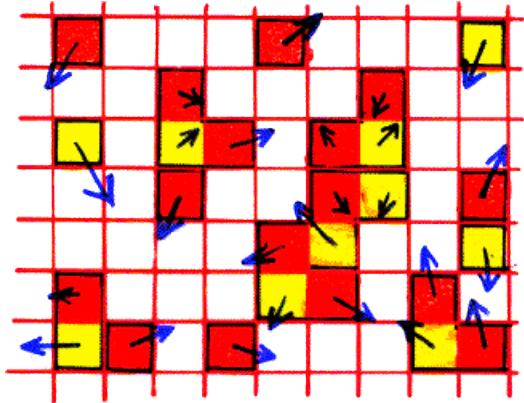


- $\langle E \rangle$  smooth fonction of  $\beta$   
(canonical caloric curve)

- Closest neighbors interaction
- Metropolis Boltzmann weight  $e^{-\beta E}$
- Average volume  $\langle V \rangle$  (pressure)

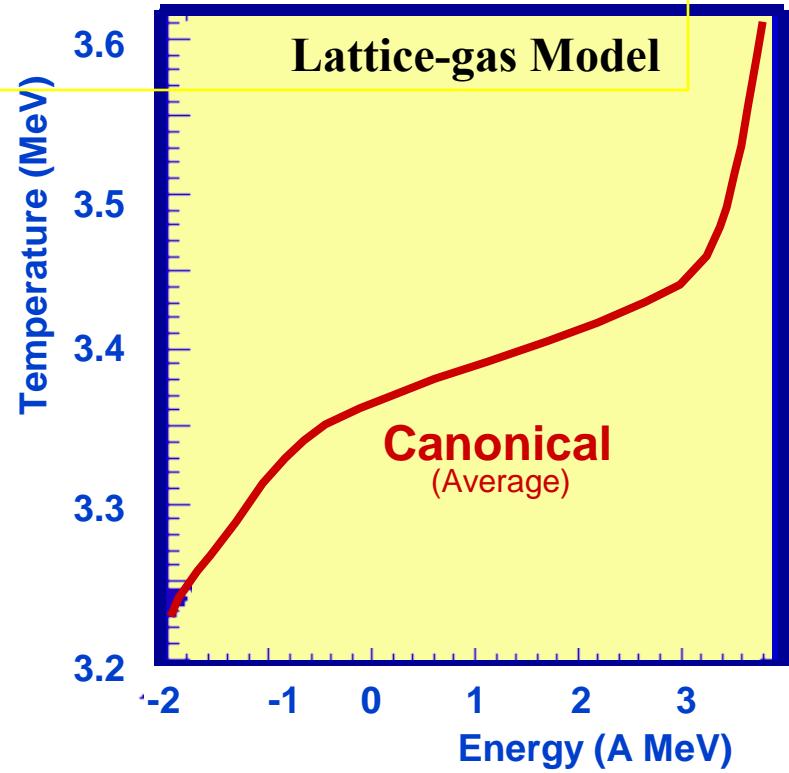


# Lattice gas model

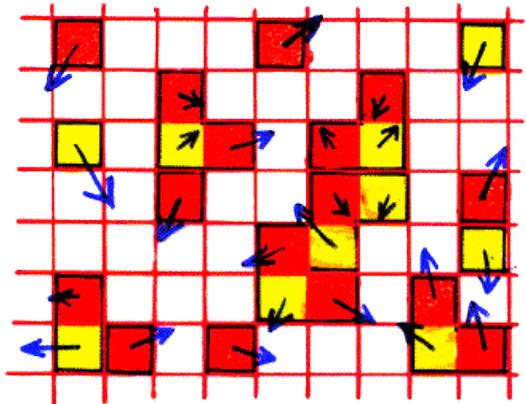


- $\langle E \rangle$  smooth function of  $\beta$   
(canonical caloric curve)

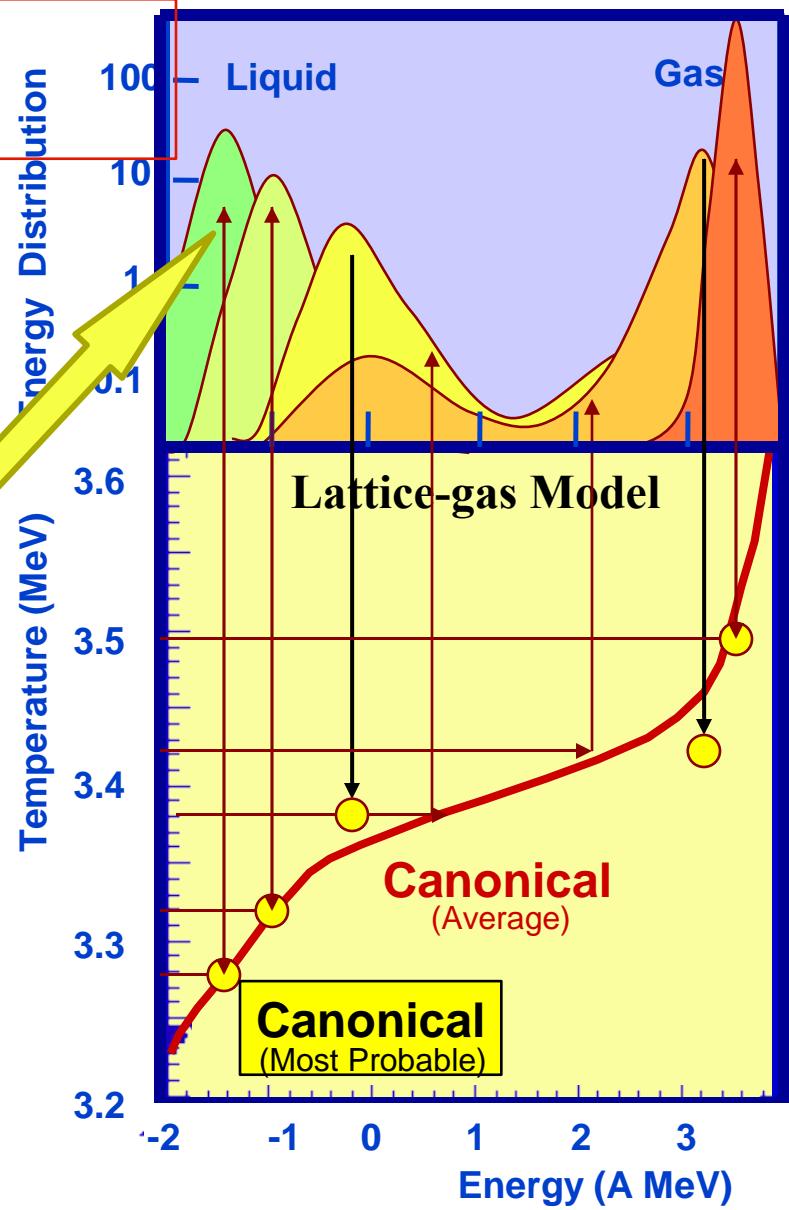
- Closest neighbors interaction
- Metropolis Boltzmann weight  $e^{-\beta E}$
- Average volume  $\langle V \rangle$  (pressure)



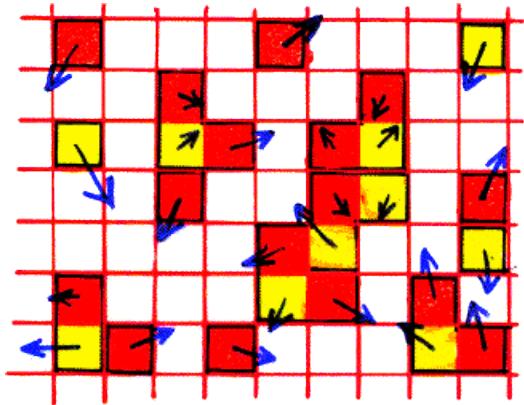
# Lattice gas model



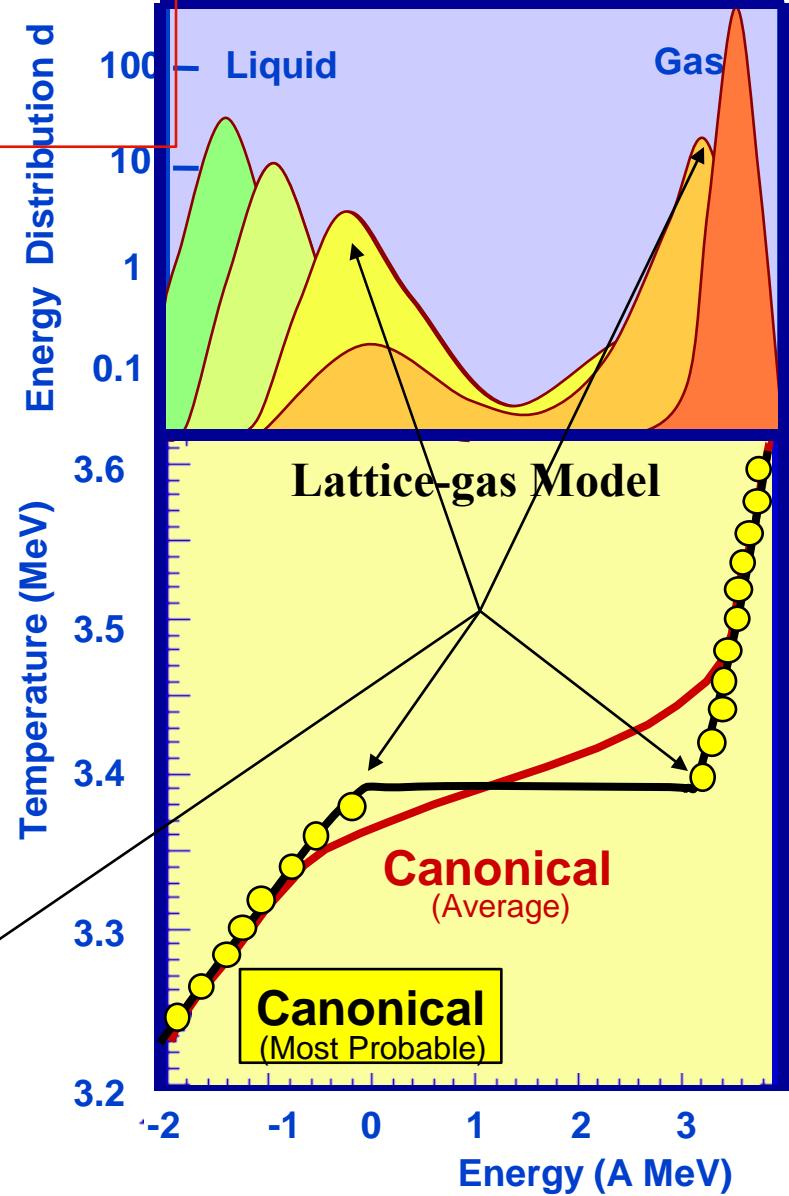
- Energy distribution at a fix temperature



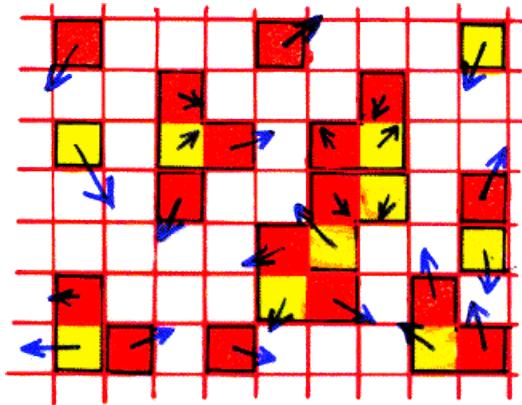
# Lattice-gas model



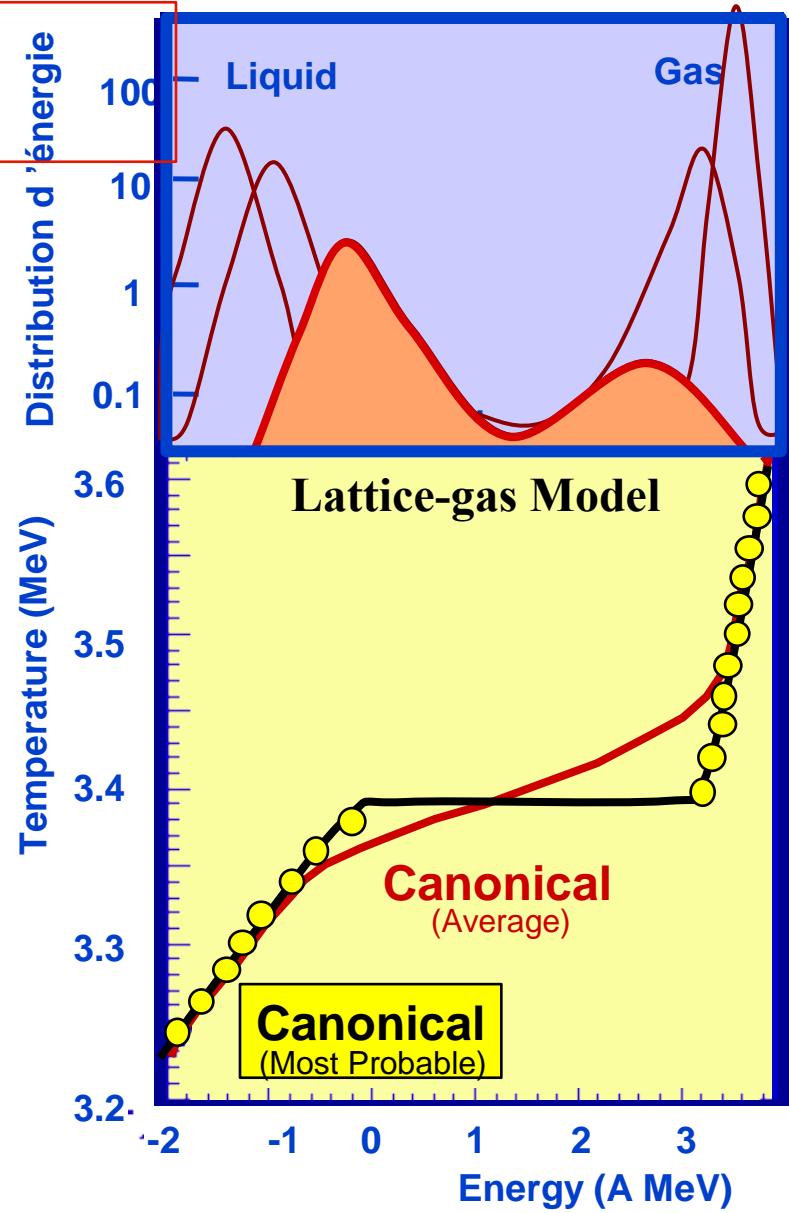
- Energy distribution at a fixed temperature
- Discontinuity of the probable



# Lattice-gas model



- Energy distribution at a fixed temperature
- Bimodal distribution
- Discontinuity of the probable



# A first order phase transition in finite systems



A bimodal (event) distribution of energy

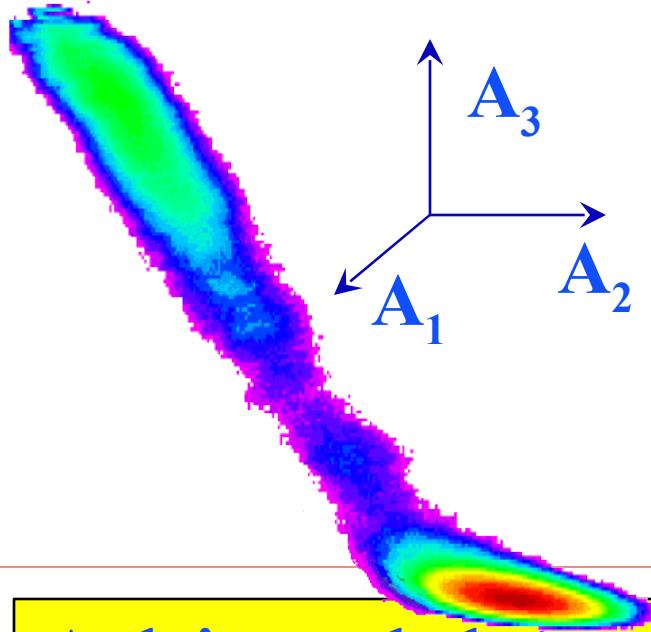
If the energy is free to fluctuate  
(canonical - energy reservoir)

# A first order phase transition in finite systems



A bimodal (event) distribution of an observable (order parameter)

If this observable is free to fluctuate (intensive ensemble)



- Access to order parameters
  - ◆ Nature of order parameter:
    - ♦ Is it collective?
  - ◆ Scaling of the jump with N:
    - ♦ What happen at the thermo limit ( $N = \infty$ ) ?
    - ♦ Is it a macro. phase transition?

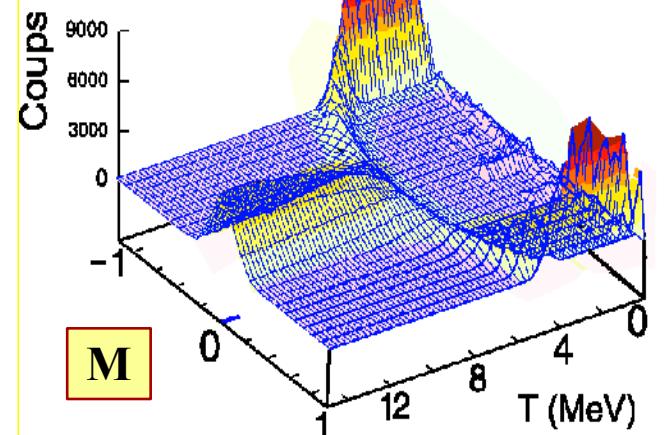
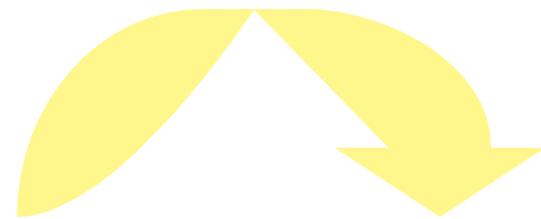
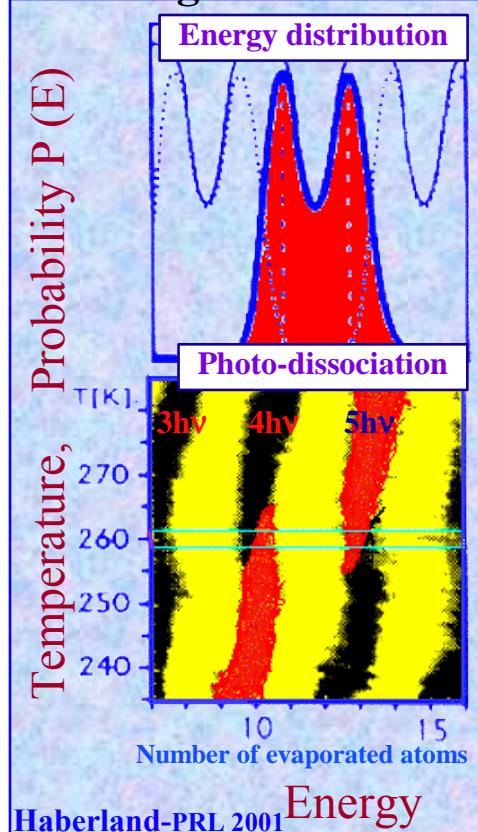
A bimodal (event) distribution of an observable (order parameter)

If this observable is free to fluctuate (intensive ensemble)

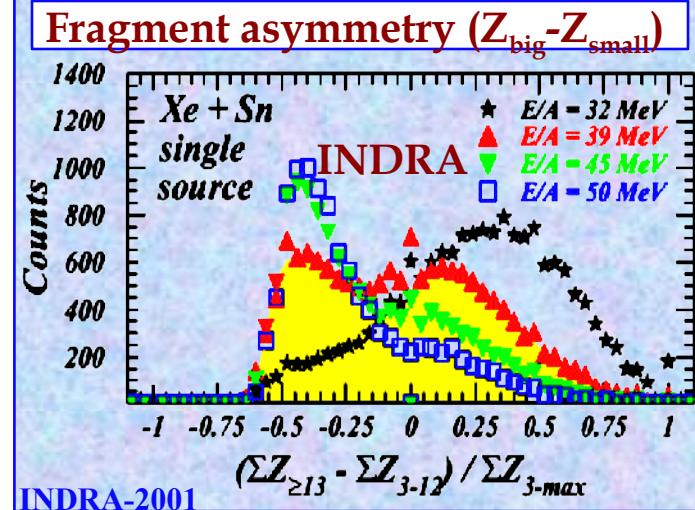
Ising model

# Bimodal distributions

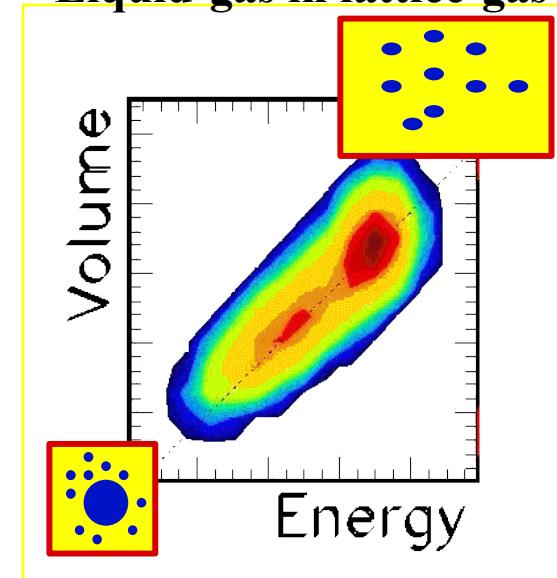
## Melting of Na Cluster



## Multifragmentation of nuclei

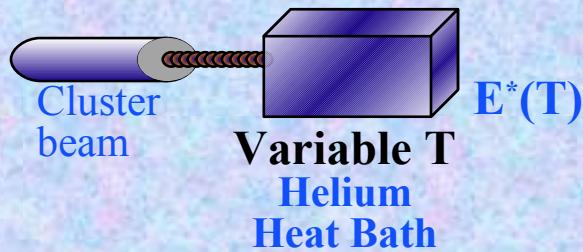
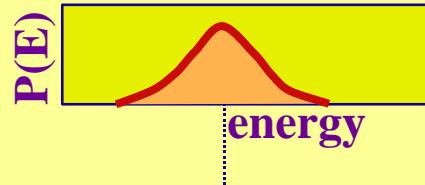


## Liquid-gas in lattice-gas



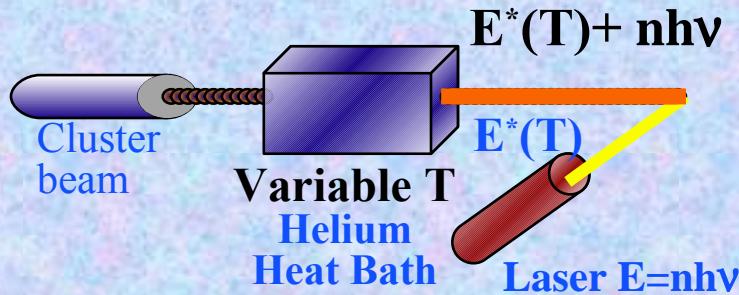
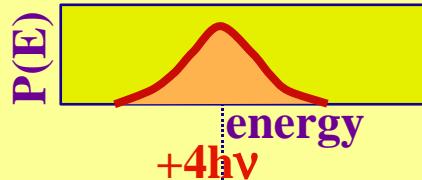
# Melting of $\text{Na}_{147}^+$

.



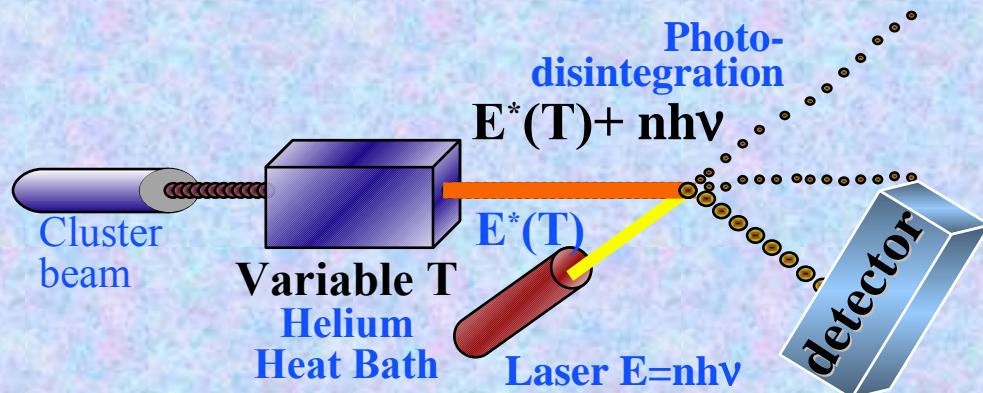
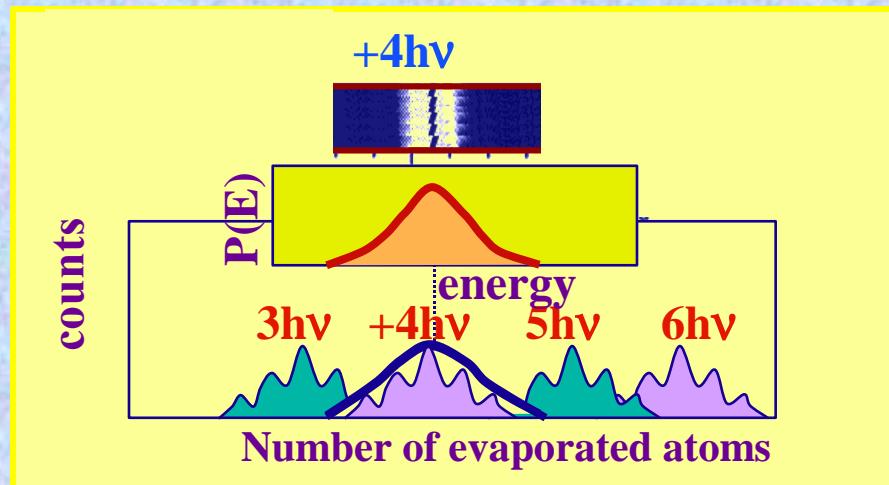
# Melting of $\text{Na}_{147}^+$

.



# Melting of $\text{Na}_{147}^+$

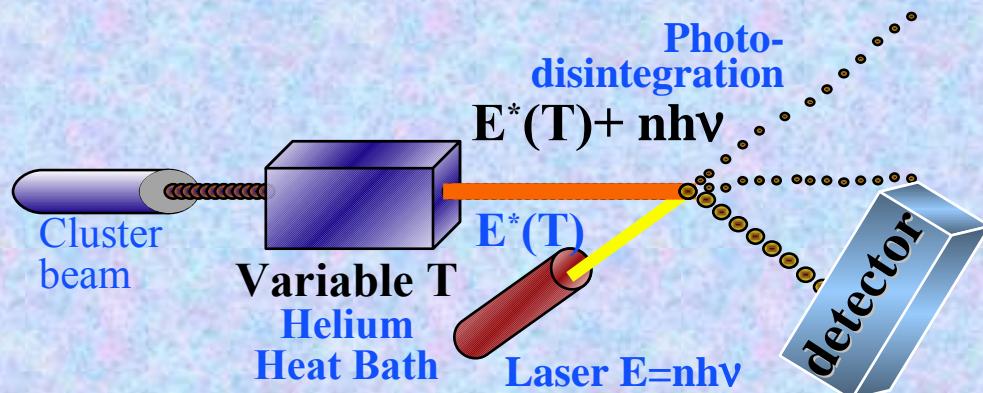
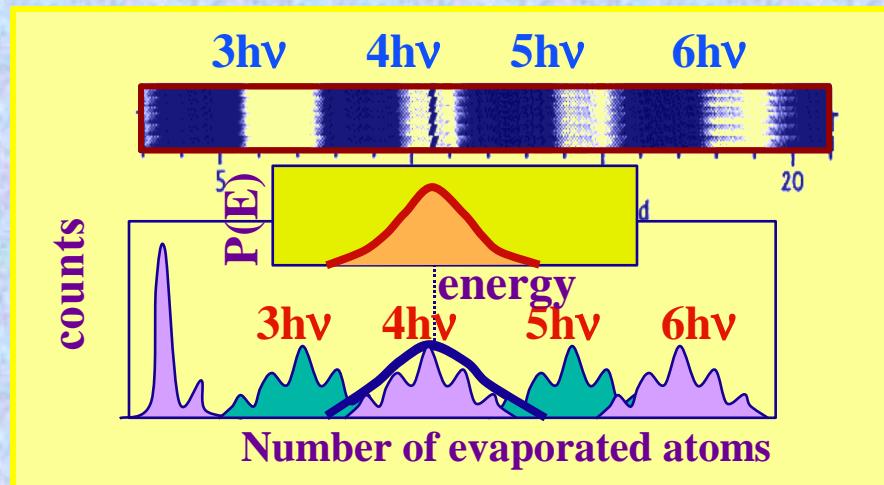
.



M.Schmidt et al, Nature 1999, PRL 2001

# Melting of $\text{Na}_{147}^+$

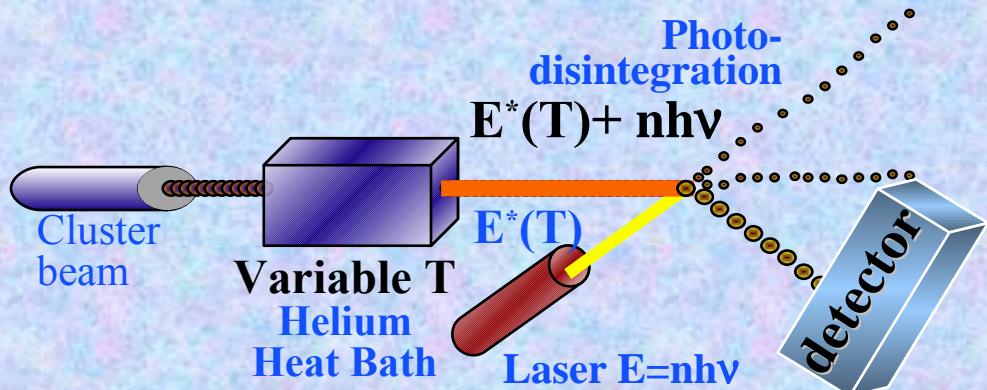
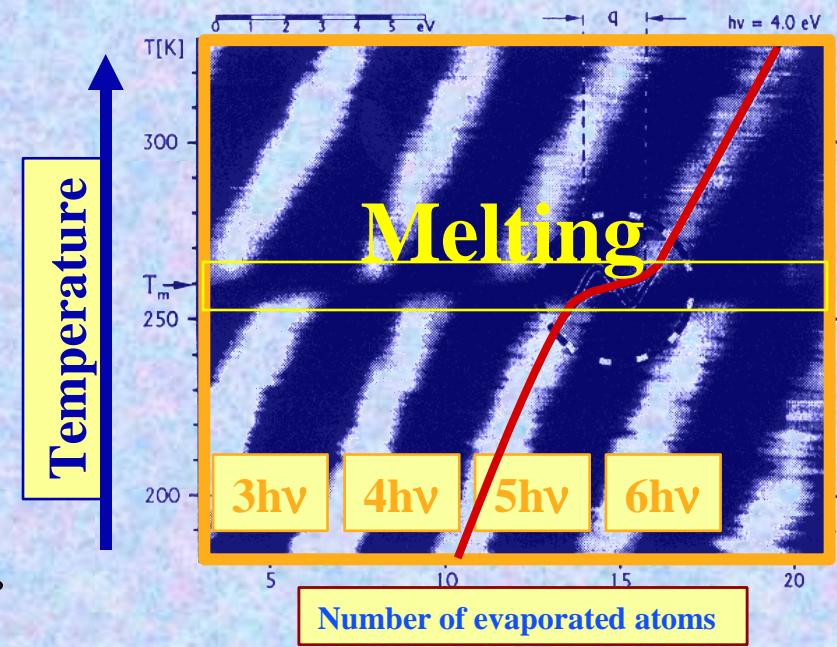
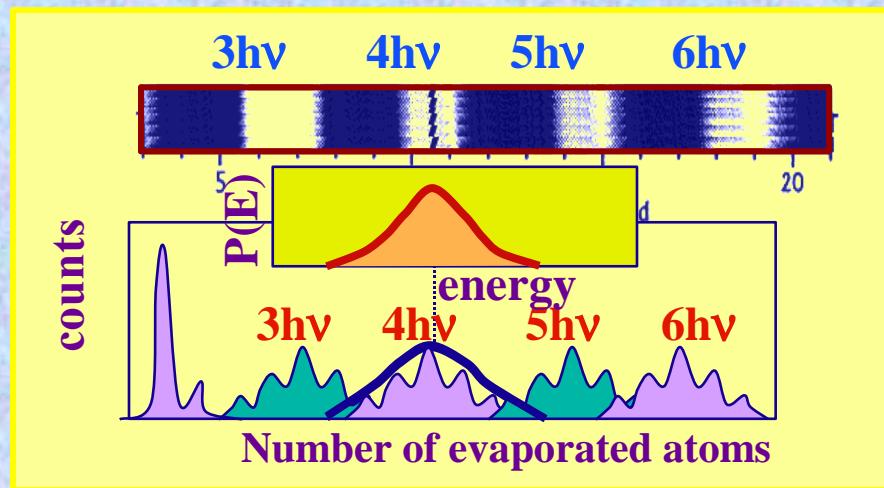
.



M.Schmidt et al, Nature 1999, PRL 2001

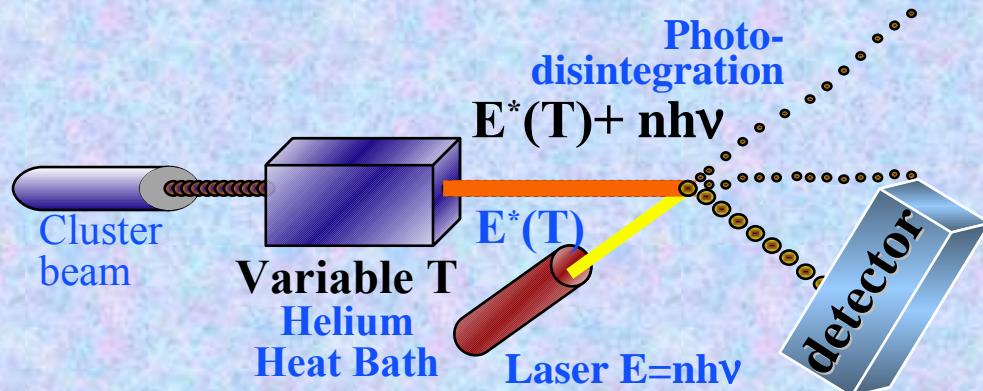
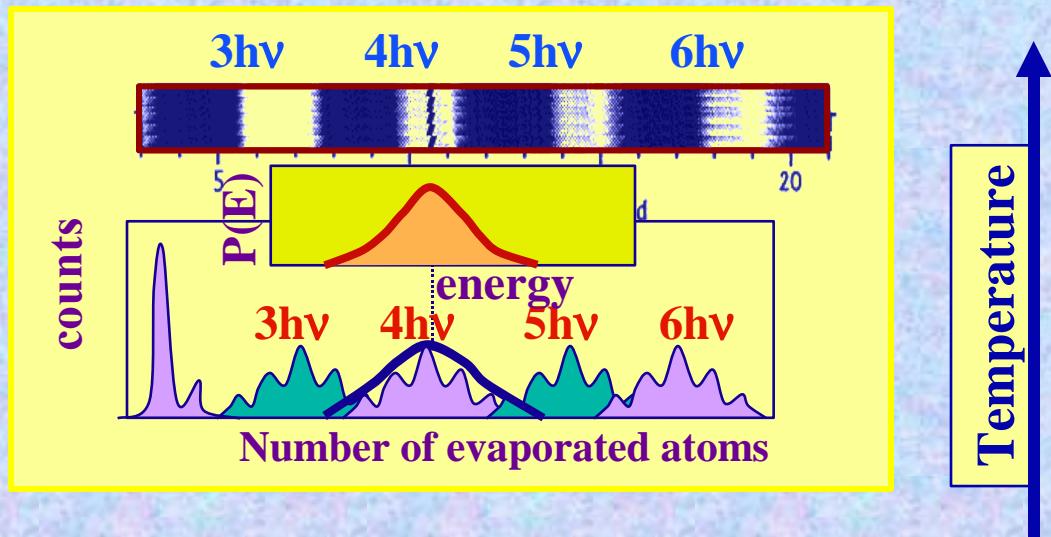
# Melting of $\text{Na}_{147}^+$

•



# Melting of $\text{Na}_{147}^+$

.

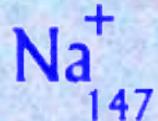
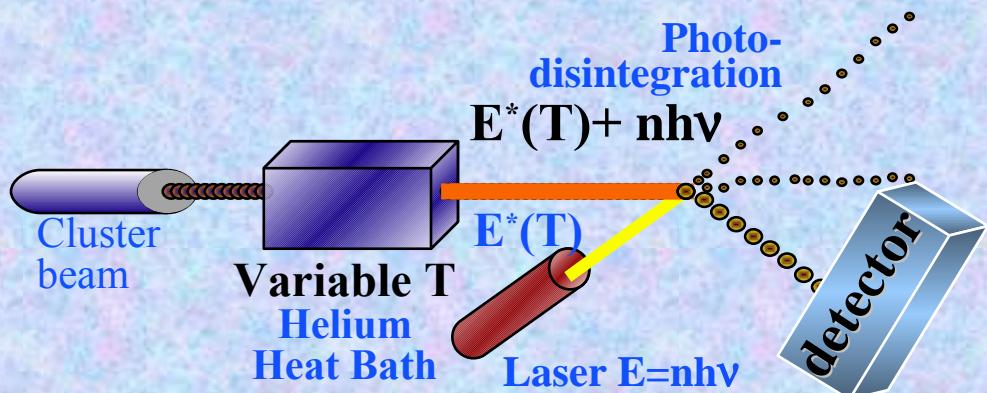
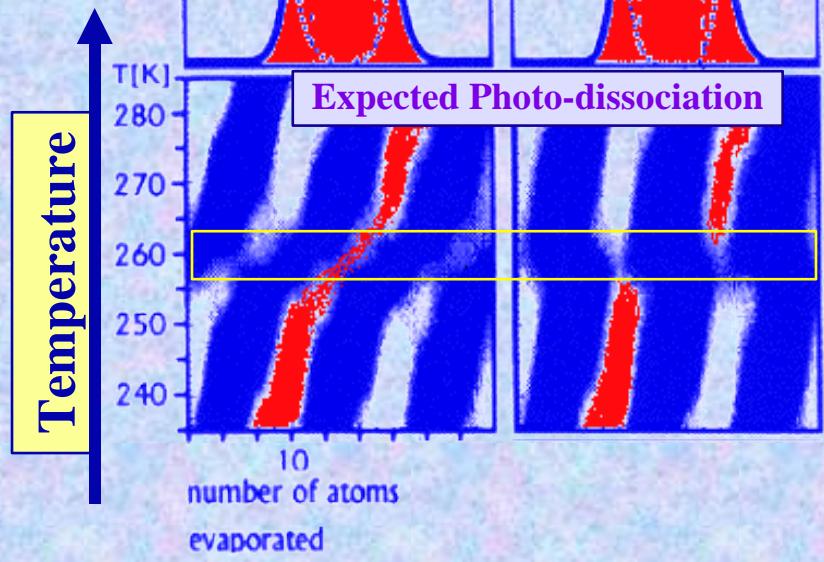
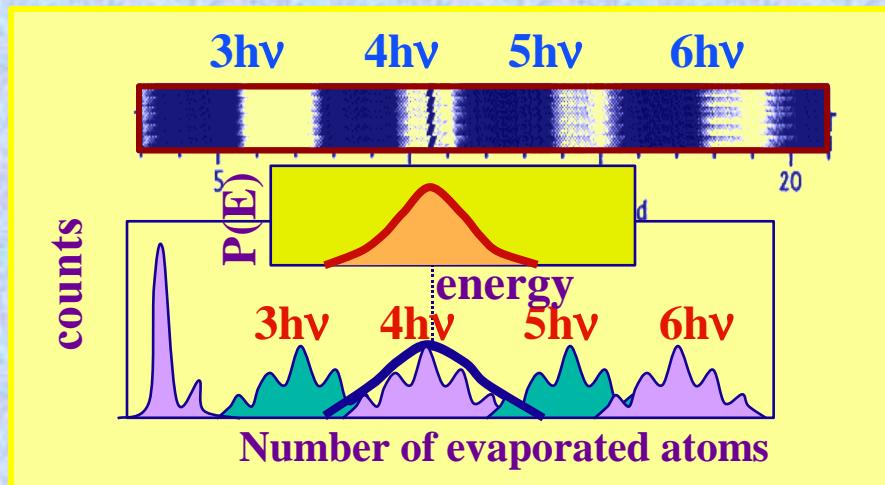


M.Schmidt et al, Nature 1999, PRL 2001

Number of evaporated atoms

# Melting of $\text{Na}_{147}^+$

.



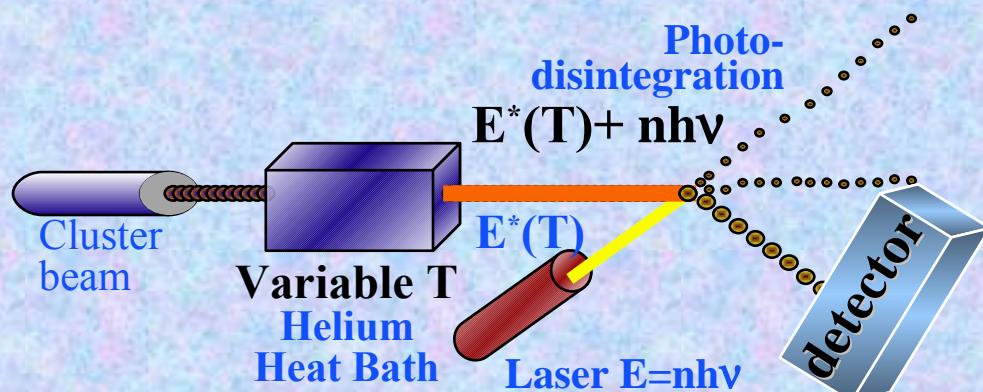
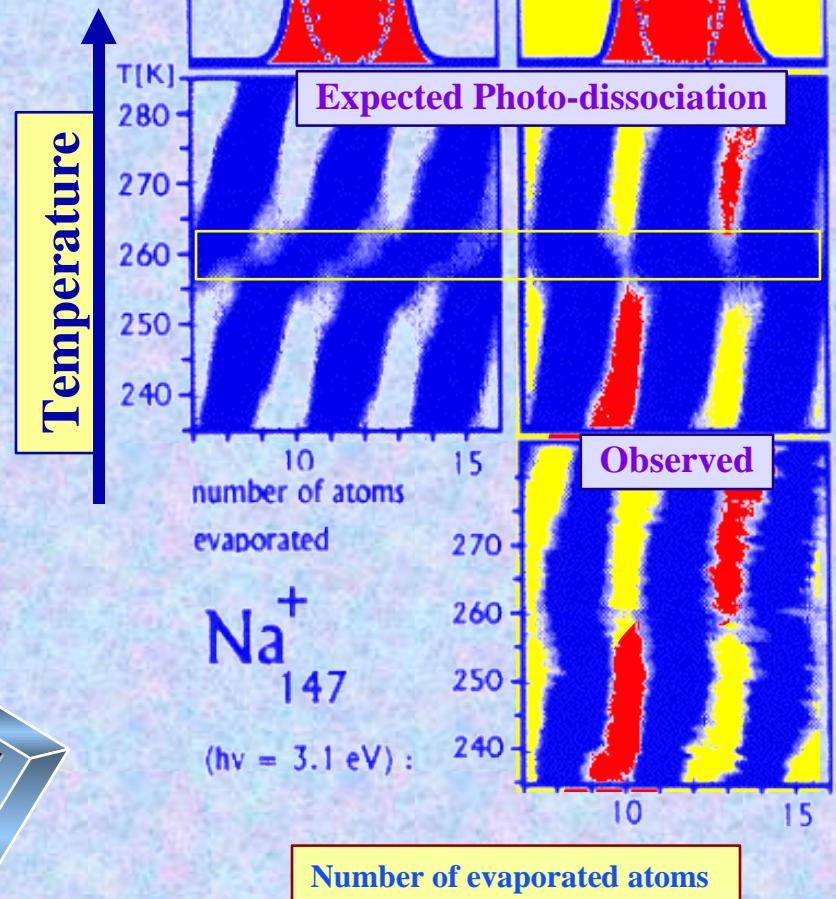
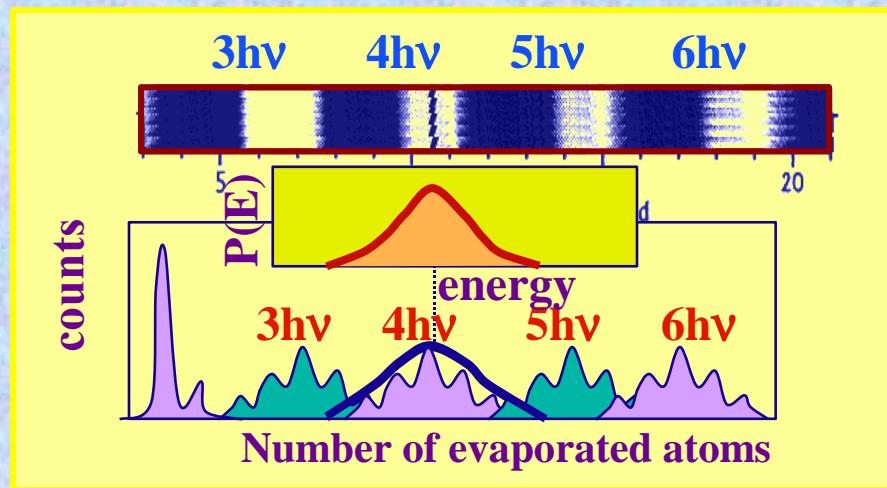
( $h\nu = 3.1 \text{ eV}$ ) :

Number of evaporated atoms

M.Schmidt et al, Nature 1999, PRL 2001

# Melting of $\text{Na}_{147}^+$

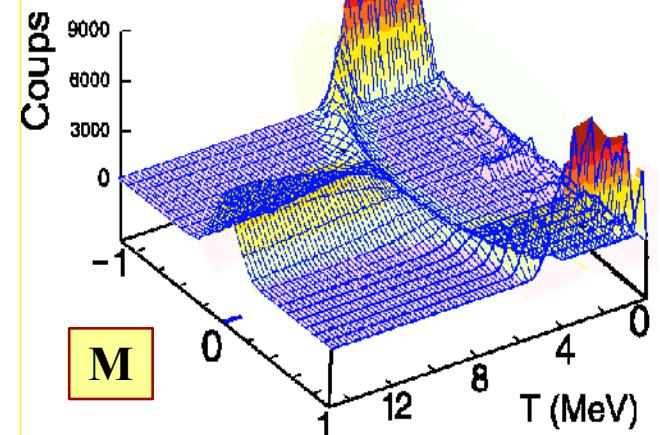
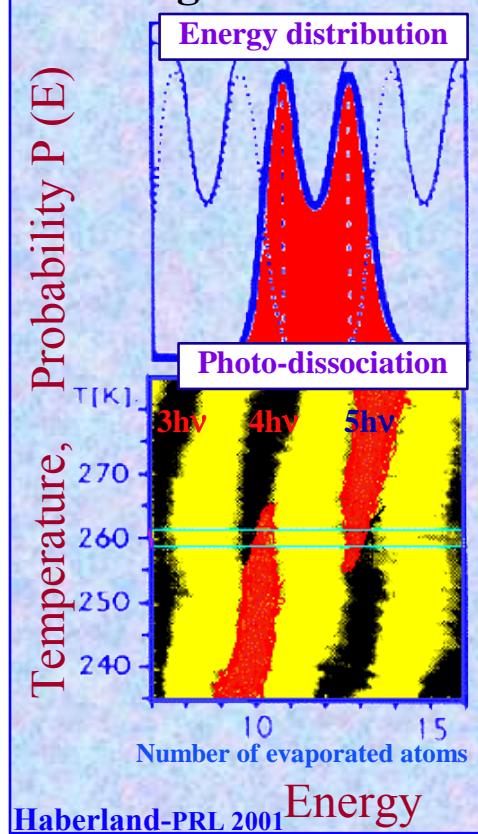
.



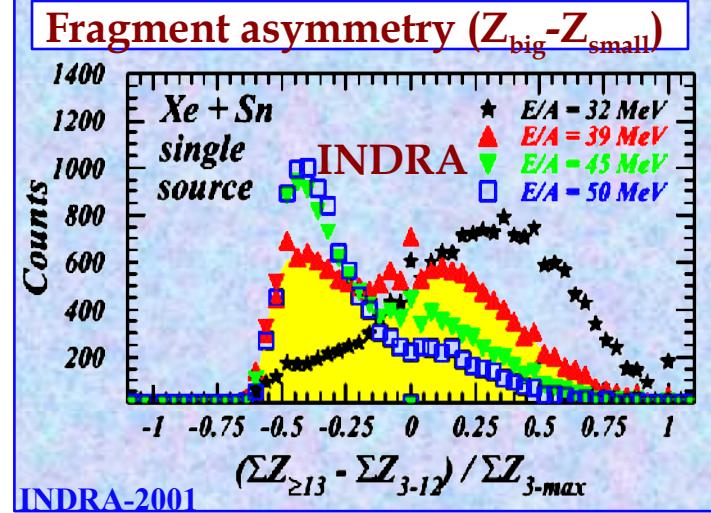
## Ising model

# Bimodal distributions

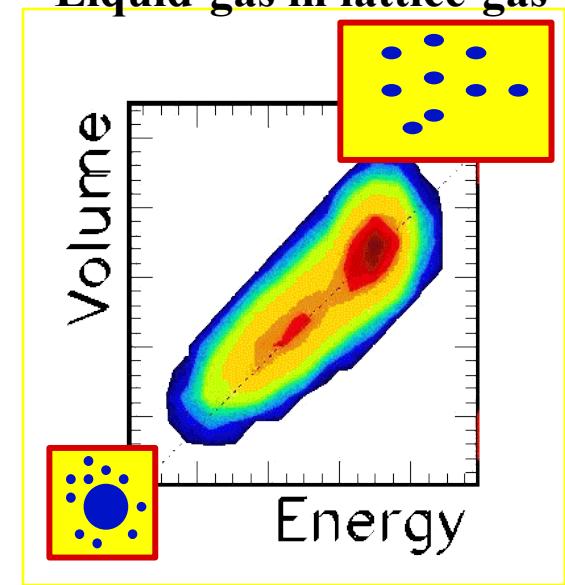
### Melting of Na Cluster



### Multifragmentation of nuclei



### Liquid-gas in lattice-gas



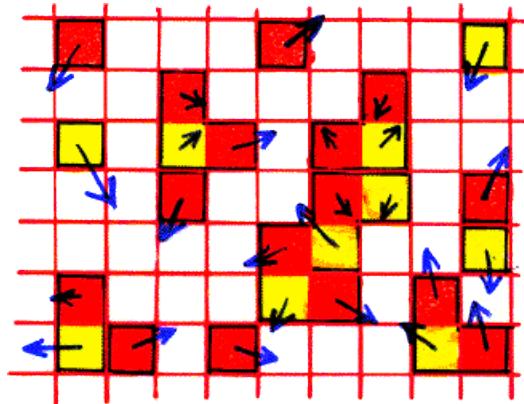
# - III -

# Convex S bending T

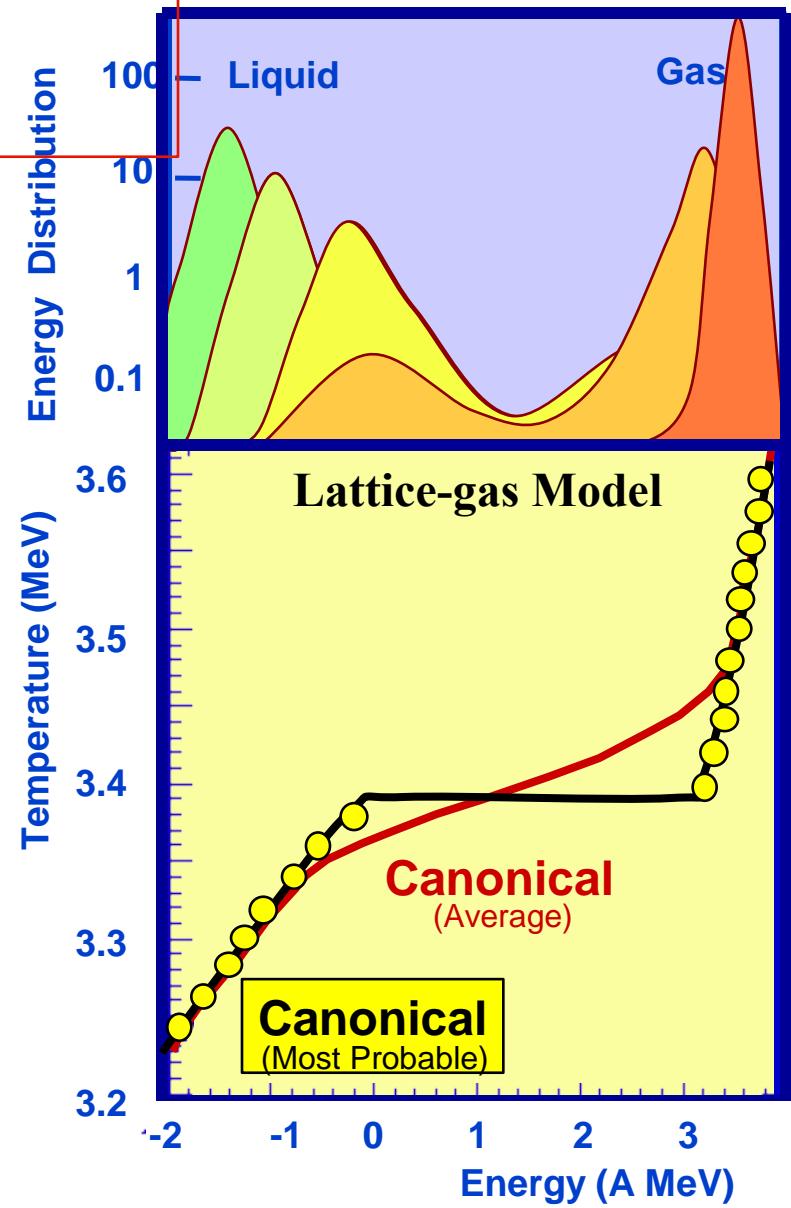
# Negative heat capacity



# Lattice-gas model



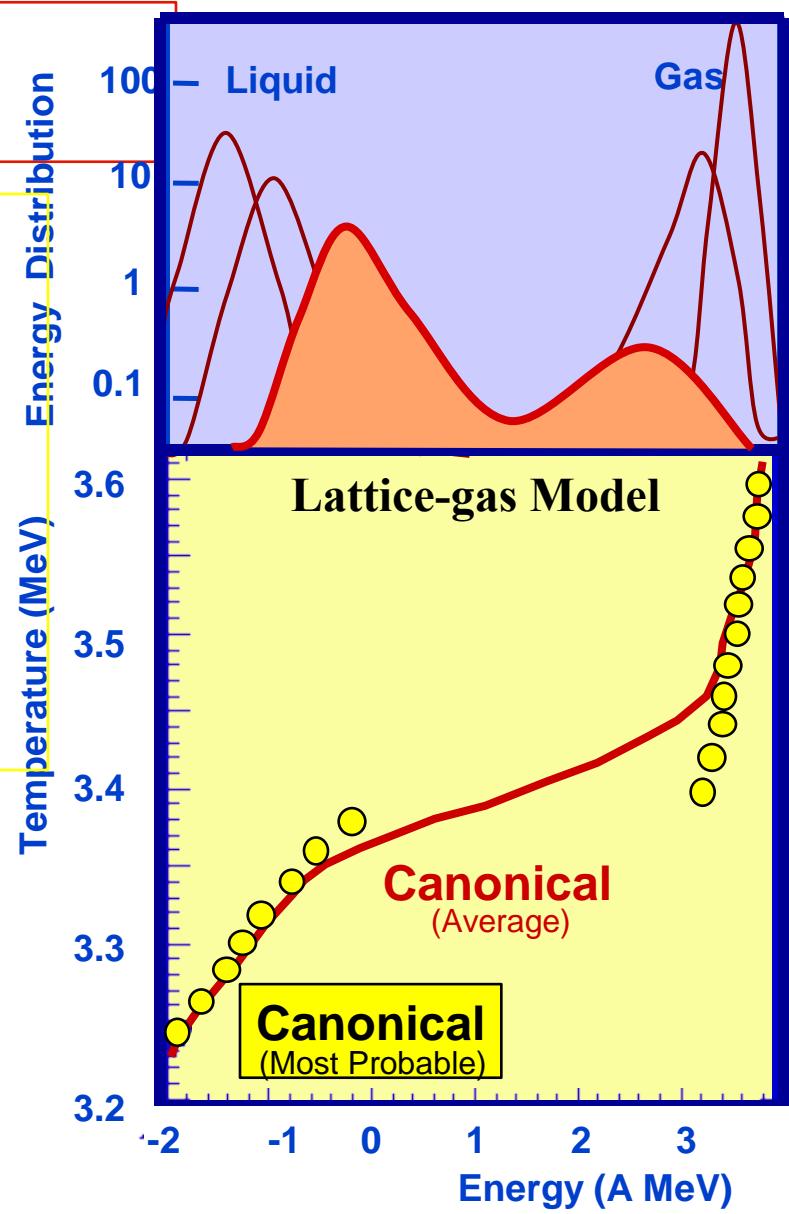
- Energy distribution at a fixed temperature
- Discontinuity of the probable



# Lattice-gas model

## ■ E distribution

$$\diamond P_\beta(E) = W(E) e^{-\beta E} / Z_\beta$$



# Lattice-gas model

■ Microcanonic:  $S = \log W$

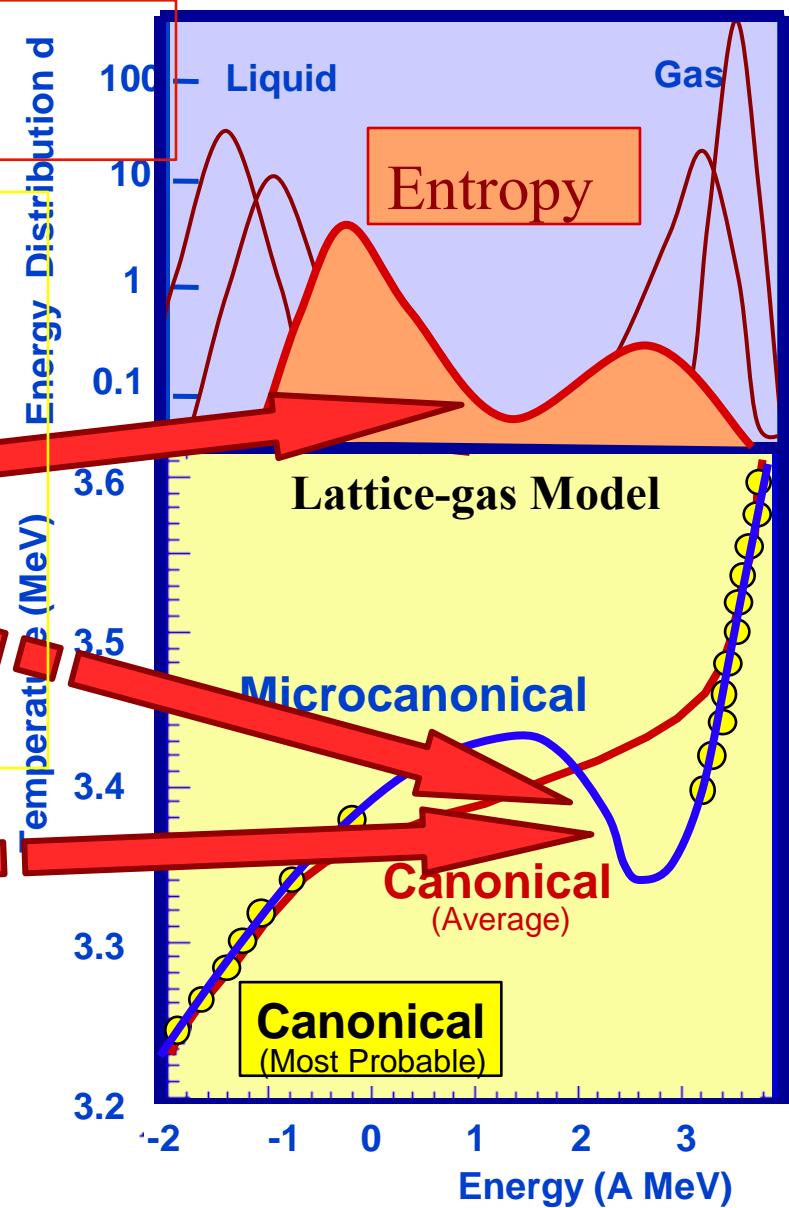
$$\diamond \log Z_\beta P_\beta(E) = S(E) - \beta E$$

■ Convex Entropy

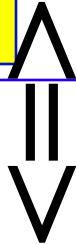
■ Decreasing T:  $T^{-1} = d_E S$

$$\diamond T^{-1} = \beta - d_E(\log P_\beta)$$

■ Negative Heat Capacity



# A first order phase transition in finite systems

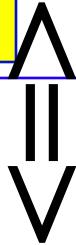


A negative heat capacity

If the energy is fixed  
(microcanonical)



# A first order phase transition in finite systems

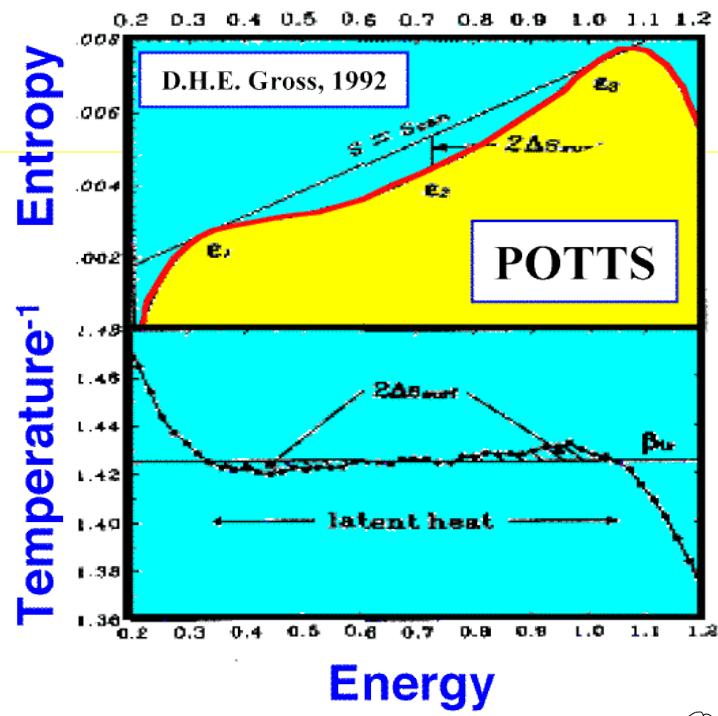
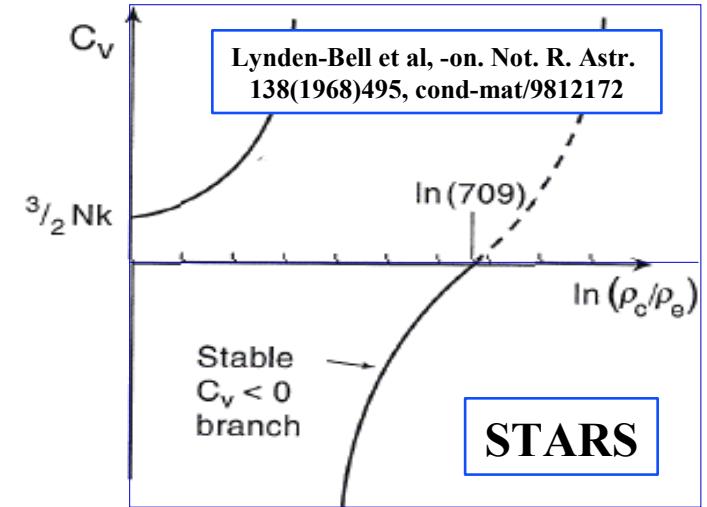
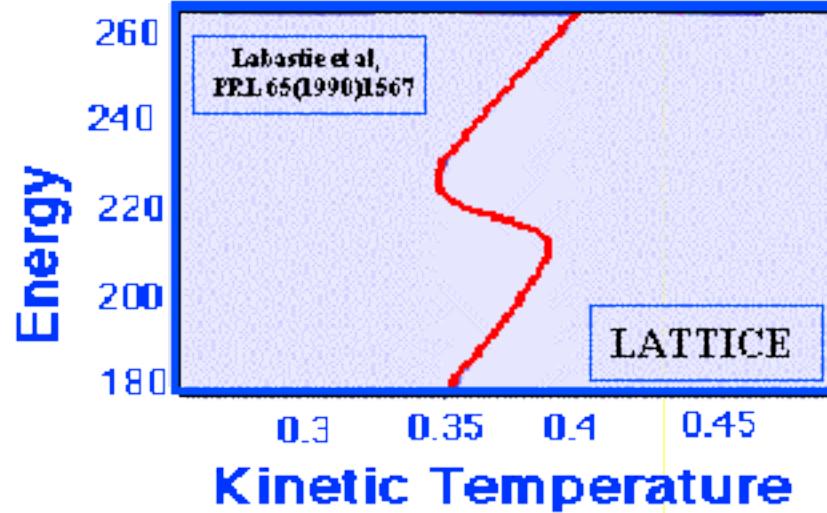


A inverted curvature of the thermodynamical potential

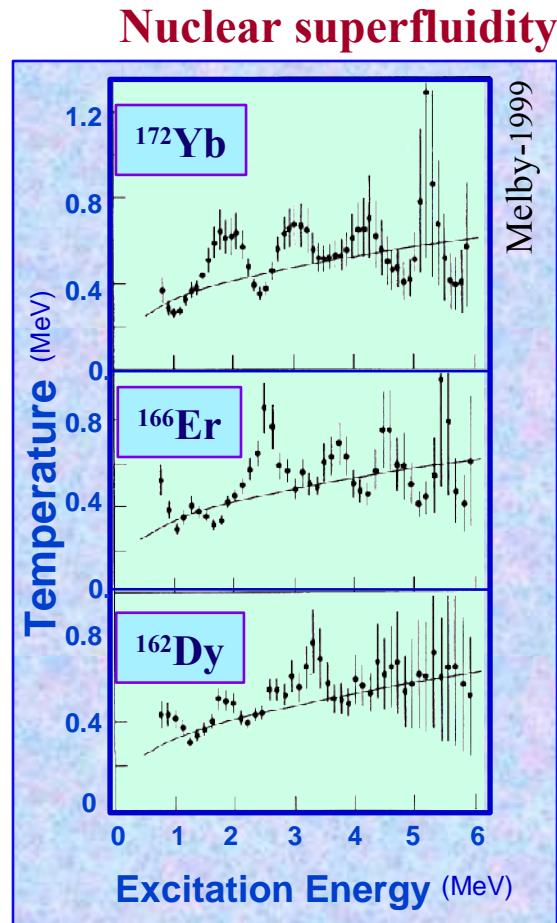
If the observables (order param.)  
are fixed (intensive ensemble)

# Negative Heat Capacity

## First Order Phase Transition in Finite Systems

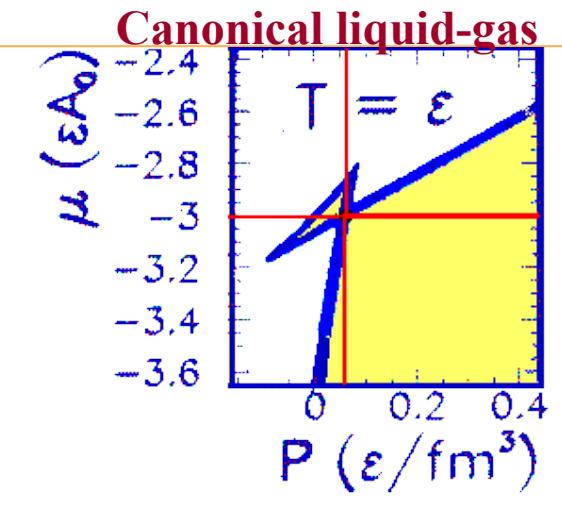
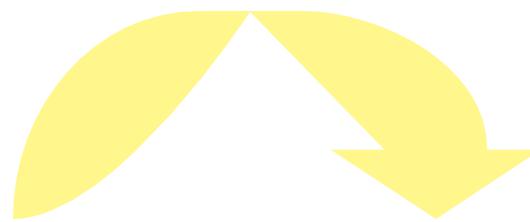


# Abnormal curvatures

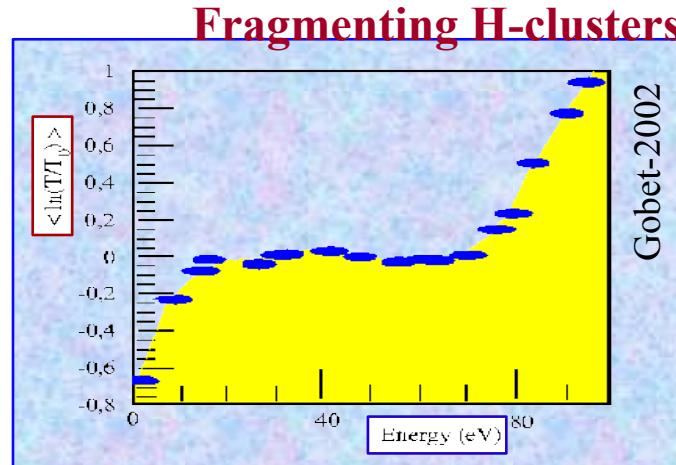


**Convex entropy**

Japan 2006



**Compressibility  $< 0$**   
**Susceptibility  $< 0$**

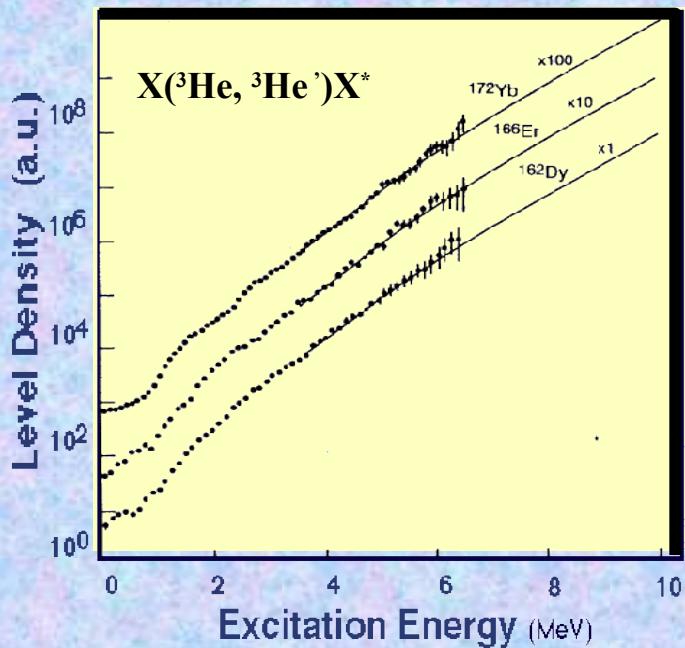


**T decreasing with E**

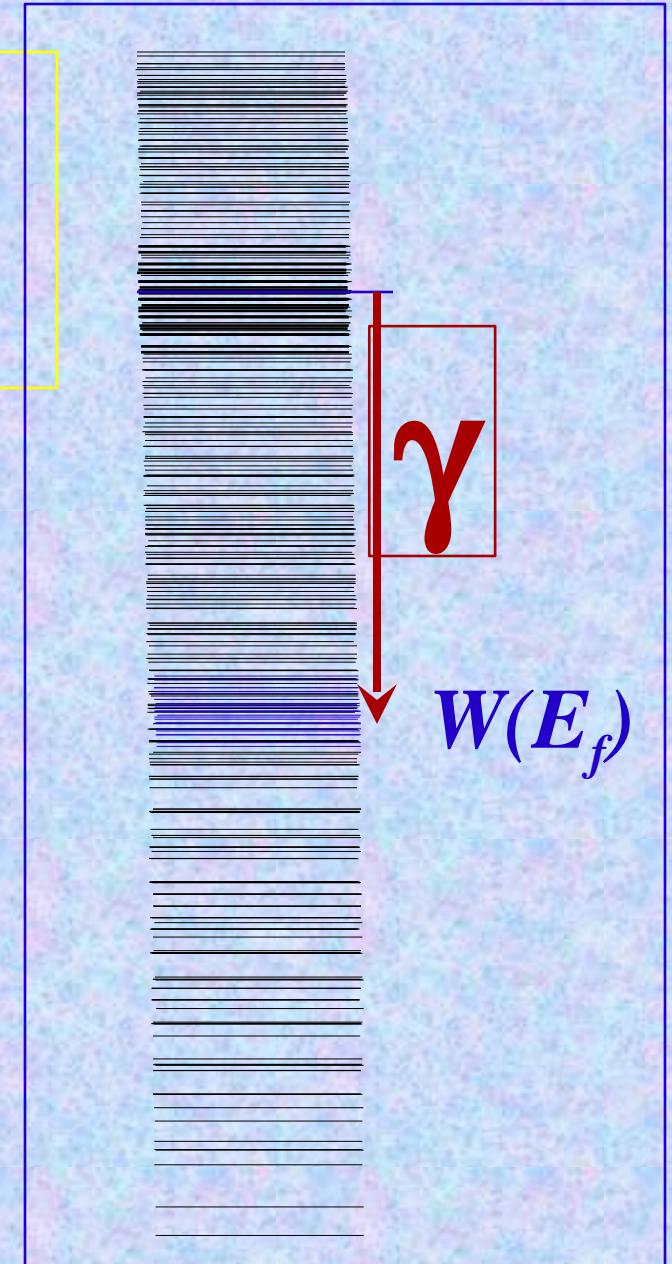


F. Gulminelli, Ph. Ch. PRL(1998)

# At low energy $\gamma$ Decay: level density



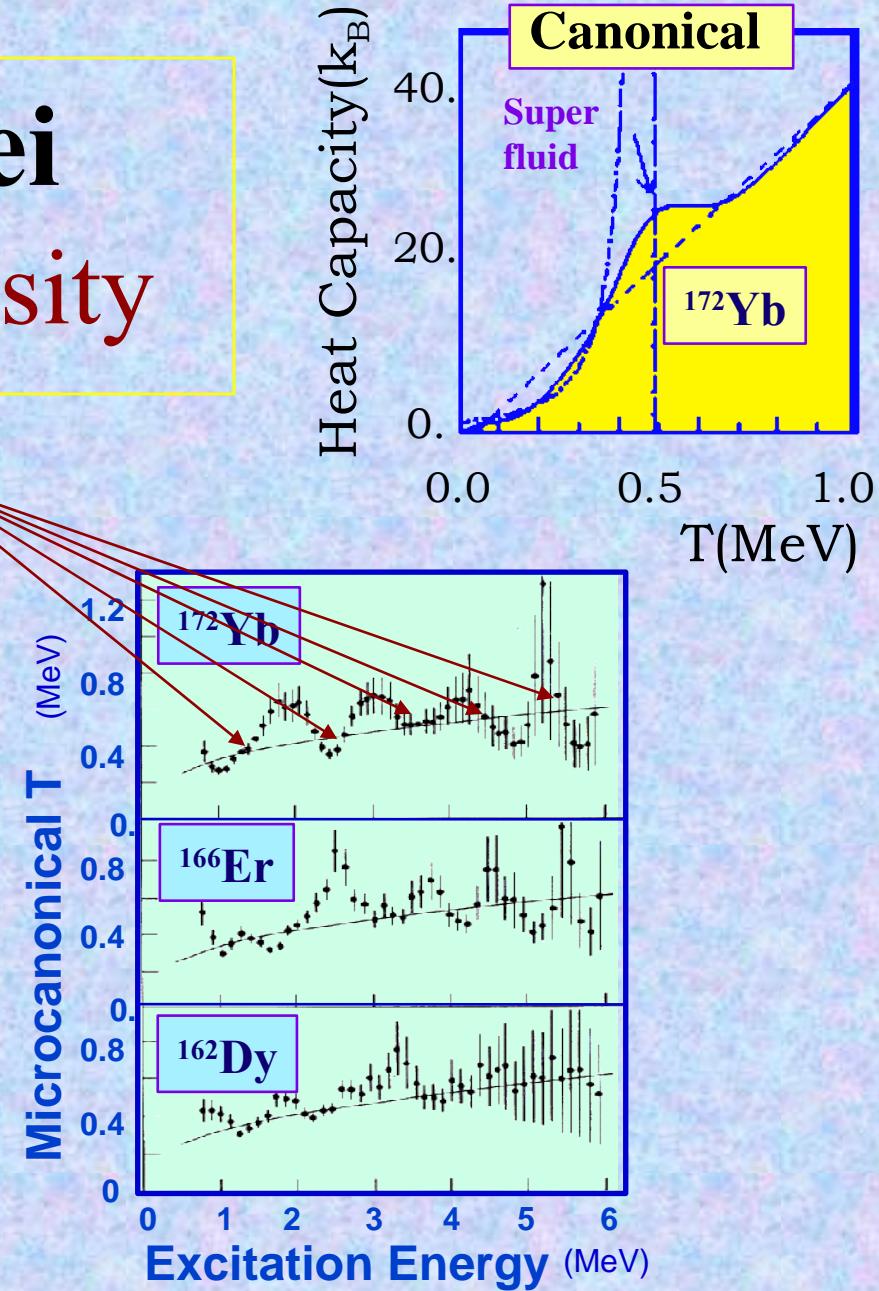
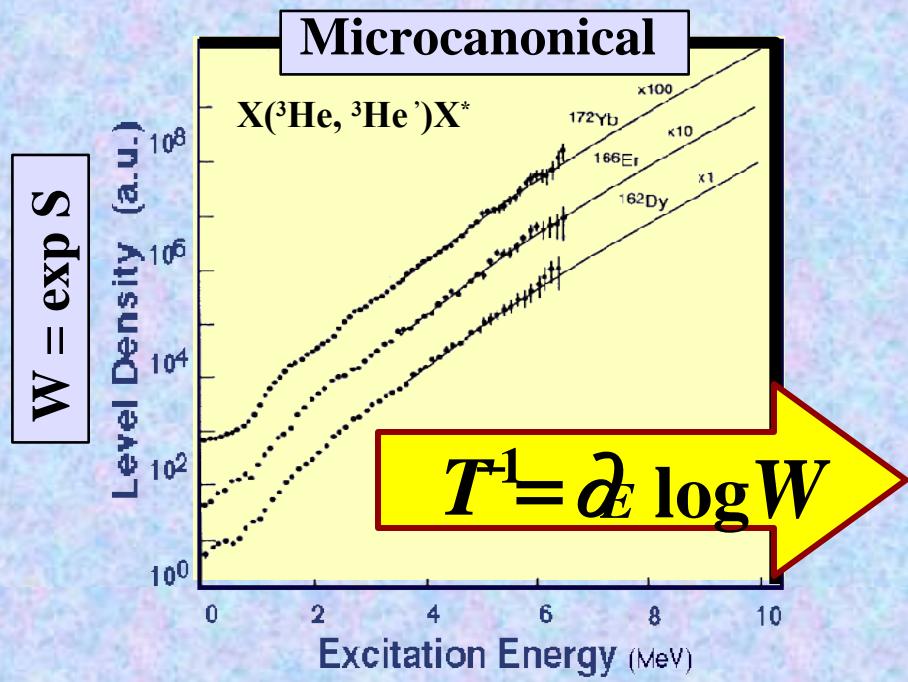
Melby et al, PRL 83(1999)3150



# Superfluid Nuclei

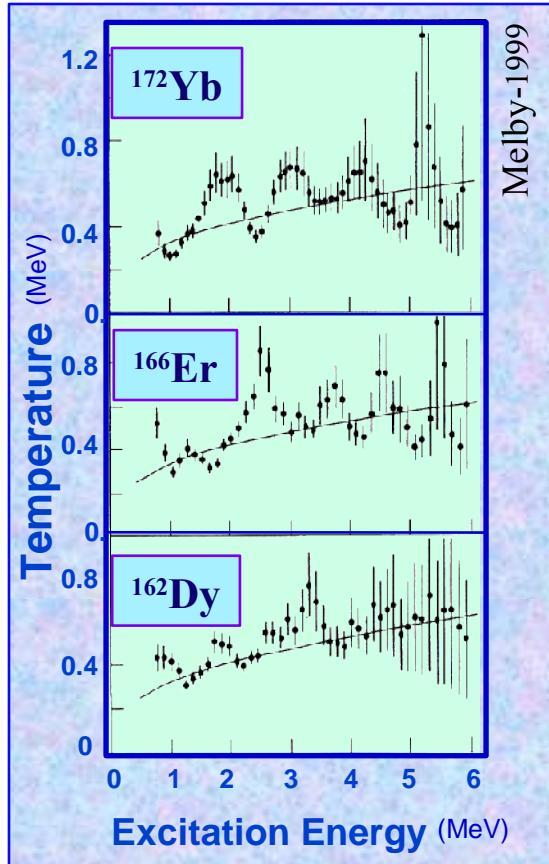
## $\gamma$ Decay: level density

### ■ Breaking of pairs



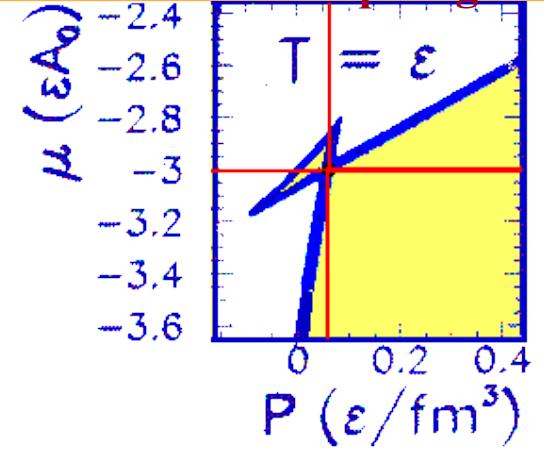
# Abnormal curvatures

Nuclear superfluidity



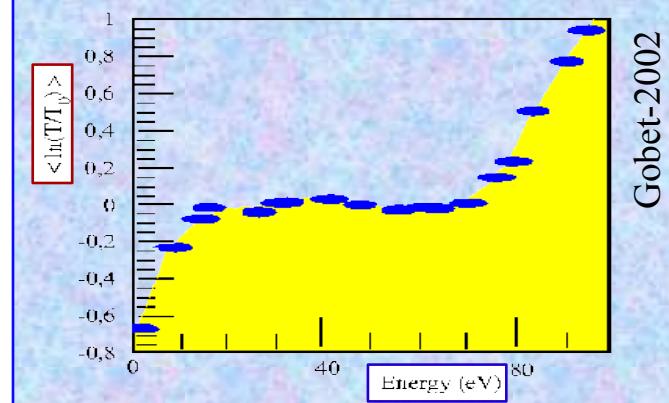
Convex entropy

Canonical liquid-gas



Compressibility  $< 0$   
Susceptibility  $< 0$

Fragmenting H-clusters



T decreasing with E

- IV -

# Negative heat capacities

## Abnormal energy fluctuations

## Multifragmentation



# Heat capacity from energy fluctuation

■ Canonical: fluct.  $E_{\text{tot}}$

$$Z_{\text{tot}} = Z_k Z_p$$

$$\sigma_E^2 = \sigma_k^2 + \sigma_p^2$$

$$\partial_\beta^2 \log Z_i = C_i / \beta^2 = \sigma_i^2$$

■ Microcanonical:  
fluct. partial energy

$$W_{\text{tot}} = W_k \otimes W_p$$

$$\sigma_E^2 = 0, \quad \sigma_k^2 = \sigma_p^2$$

$$\partial_\beta^2 \log W_{\text{tot}} = -1/CT^2 = f(\sigma_k^2)$$



PC, Gulminelli NPA(1999)

# Heat capacity from energy fluctuation

## ■ Canonical: fluct. $E_{\text{tot}}$

$$Z_{\text{tot}} = Z_k Z_p$$

$$\sigma_E^2 = \sigma_k^2 + \sigma_p^2$$

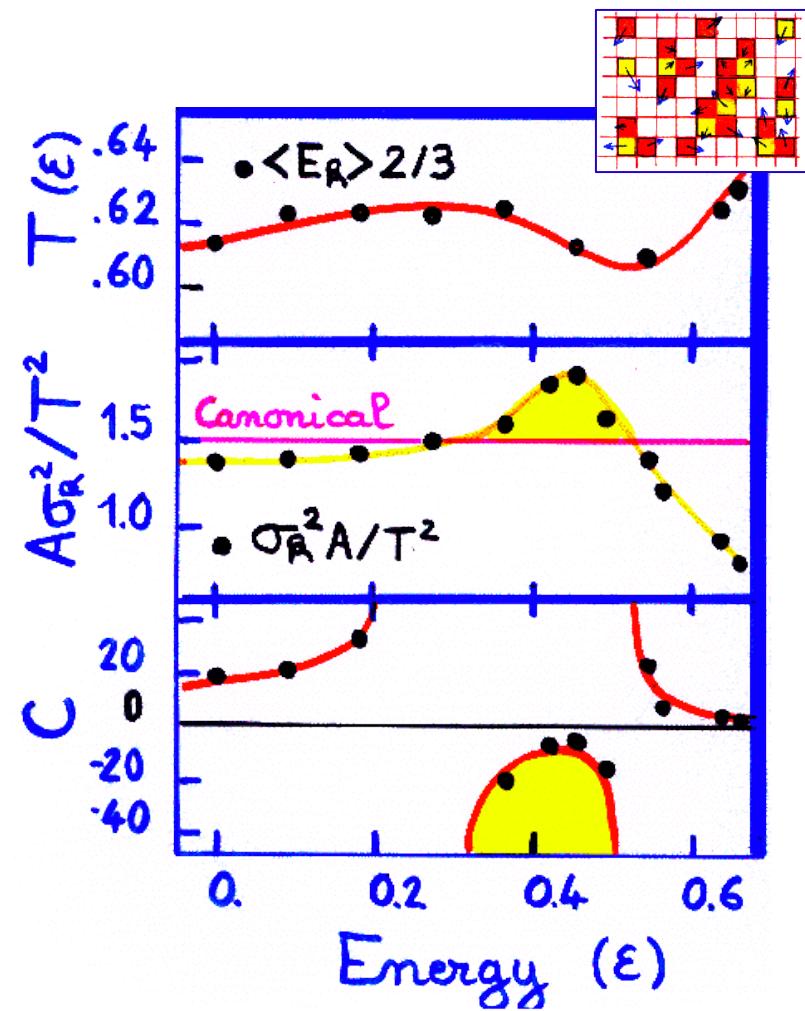
$$\partial_\beta^2 \log Z_i = C_i / \beta^2 = \sigma_i^2$$

## ■ Microcanonical: fluct. partial energy

$$W_{\text{tot}} = W_k \otimes W_p$$

$$\sigma_E^2 = 0, \quad \sigma_k^2 = \sigma_p^2$$

$$\partial_\beta^2 \log W_{\text{tot}} = -1/CT^2 = f(\sigma_k^2)$$



PC, Gulminelli NPA(1999)

# Heat capacity from energy fluctuation

## ■ Canonical: fluct. $E_{\text{tot}}$

$$Z_{\text{tot}} = Z_k Z_p$$

$$\sigma_E^2 = \sigma_k^2 + \sigma_p^2$$

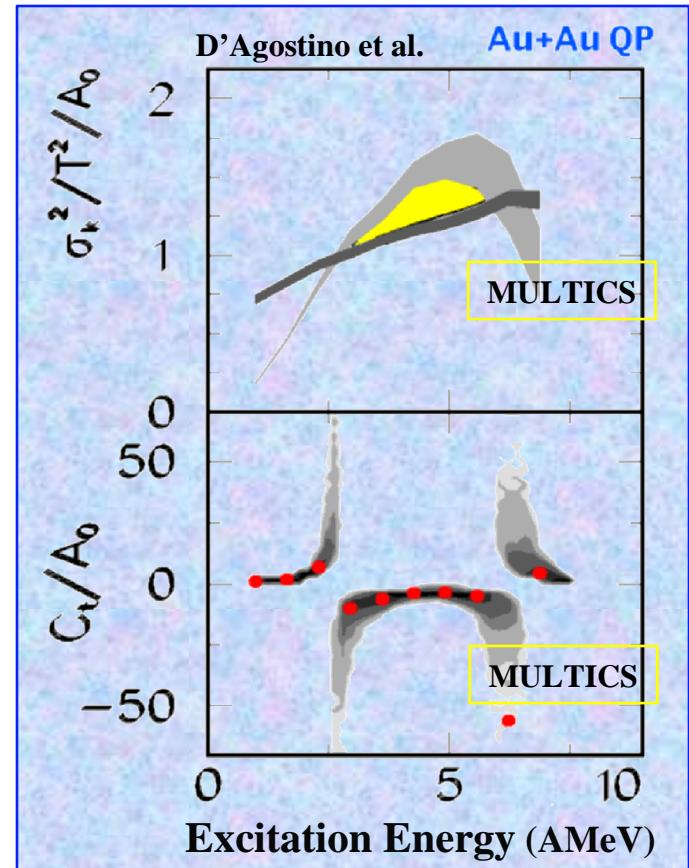
$$\partial_\beta^2 \log Z_i = C_i / \beta^2 = \sigma_i^2$$

## ■ Microcanonical: fluct. partial energy

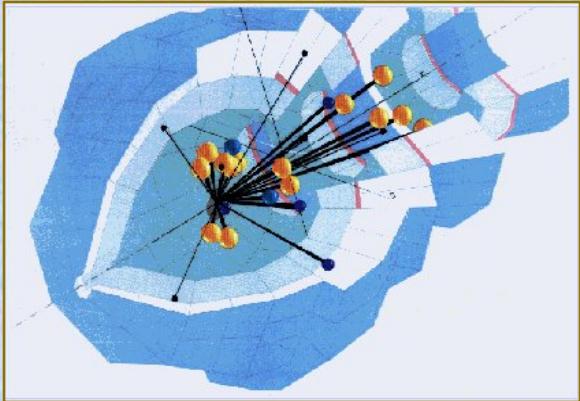
$$W_{\text{tot}} = W_k \otimes W_p$$

$$\sigma_E^2 = 0, \quad \sigma_k^2 = \sigma_p^2$$

$$\partial_\beta^2 \log W_{\text{tot}} = -1/CT^2 = f(\sigma_k^2)$$

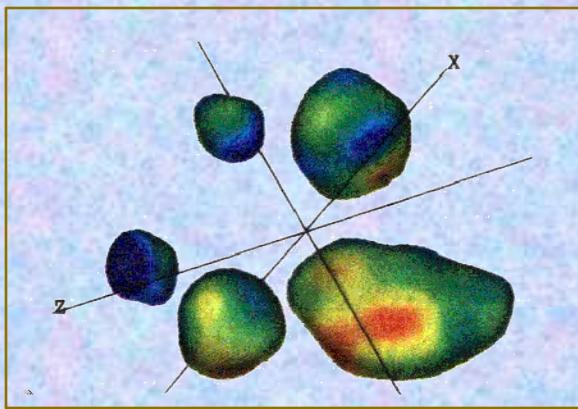
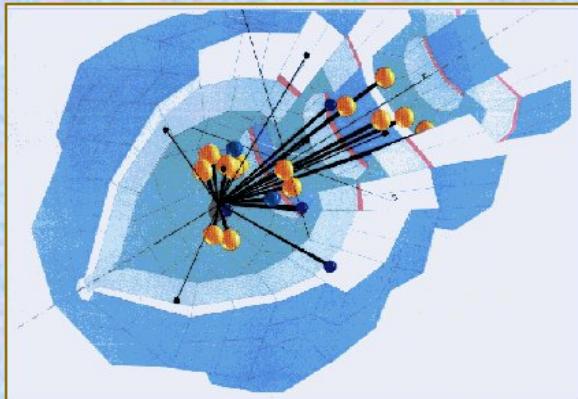


# Multifragmentation experiment



■ Sort events in  $E^*$  (Calorimetry)

# Multifragmentation experiment



- Sort events in  $E^*$  (Calorimetry)
- Reconstruct a freeze-out partition

1- Primary fragments:

$$m_i$$

2- Freeze-out volume:

$$E_{\text{coul}}$$

- $E_2 = \sum_i B_i + E_{\text{coul}}$
- $E_1 = E^* - E_2 \quad \Rightarrow \quad \langle E_1 \rangle, \sigma_1$

3- Kinetic EOS:

$$T, C_1, \sigma_{\text{can}}^2 = C_1 T^2$$

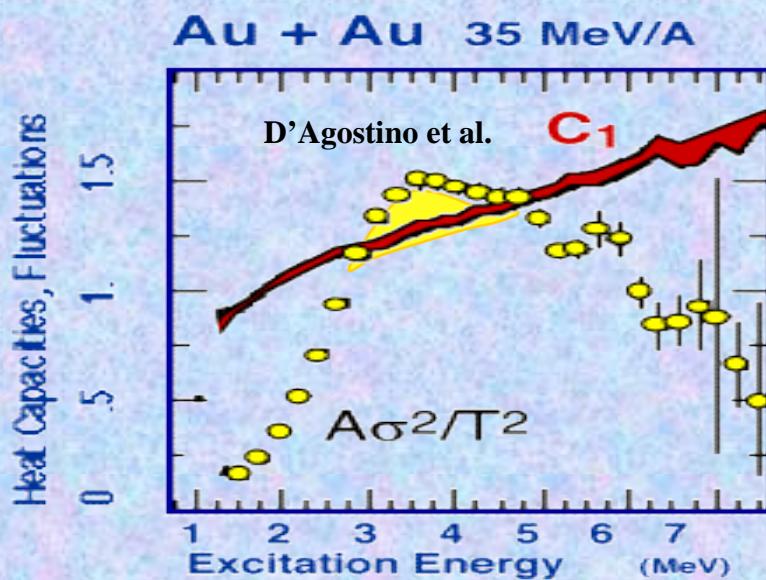
- $\langle E_1 \rangle = \langle \sum_i a_i \rangle T^2 + 3/2 \langle M-1 \rangle T$

■ Deduce C:

# Heat capacity from energy fluctuation

■ Large fluctuations

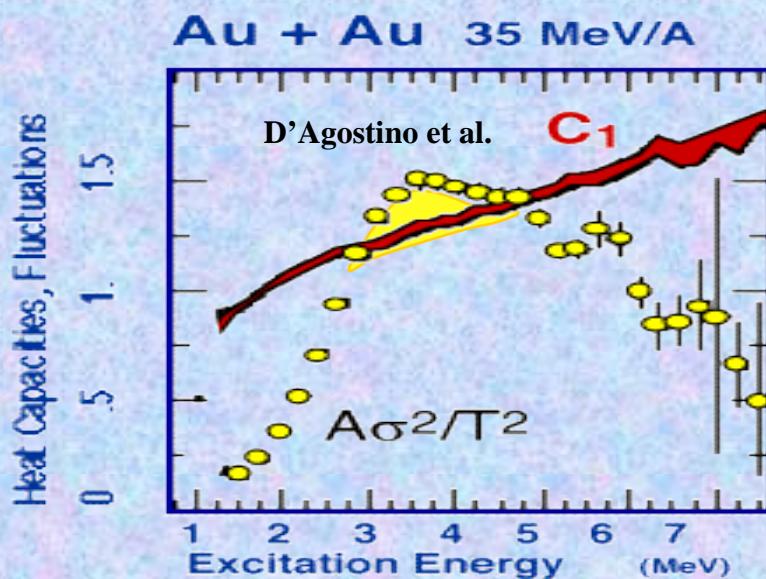
$$C = \frac{C_1^2}{C_1 - \sigma^2/T^2}$$



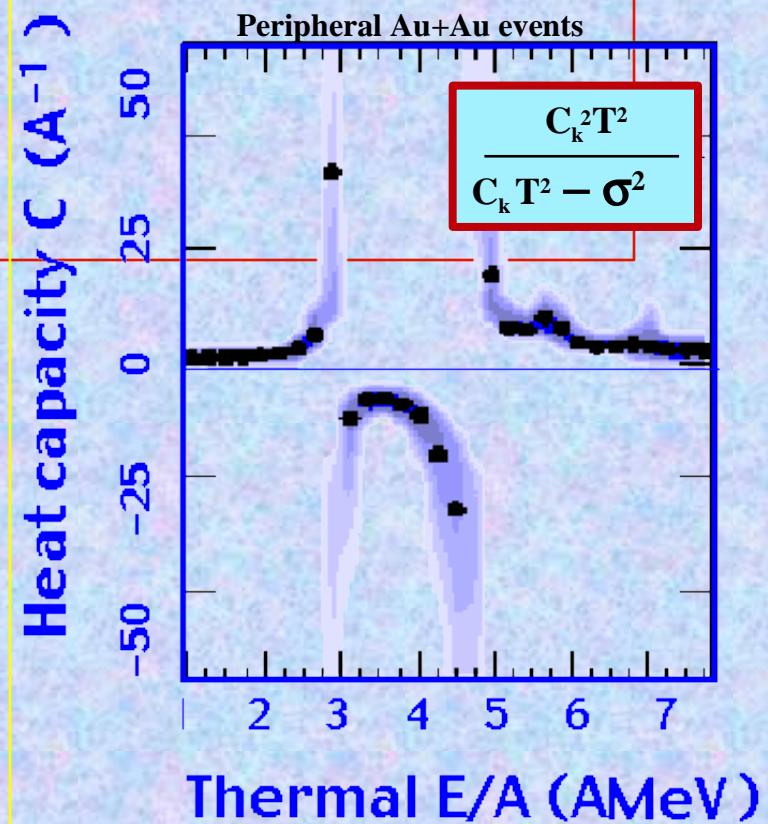
# Heat capacity from energy fluctuation

■ Large fluctuations

$$C = \frac{C_1^2}{C_1 - \sigma^2/T^2}$$

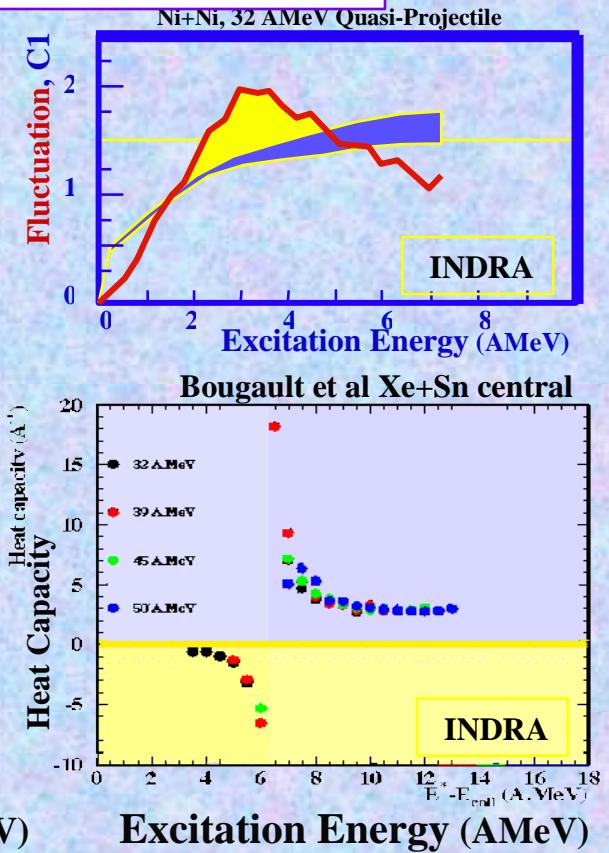
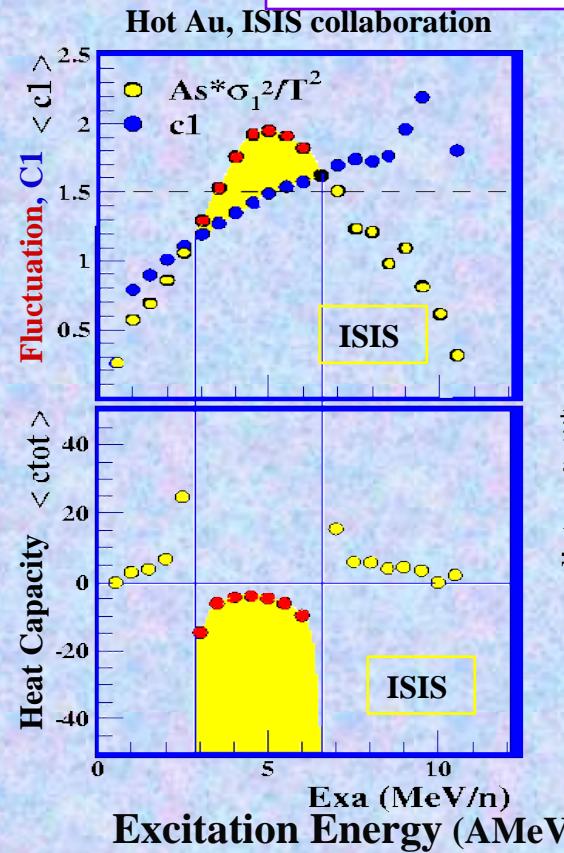
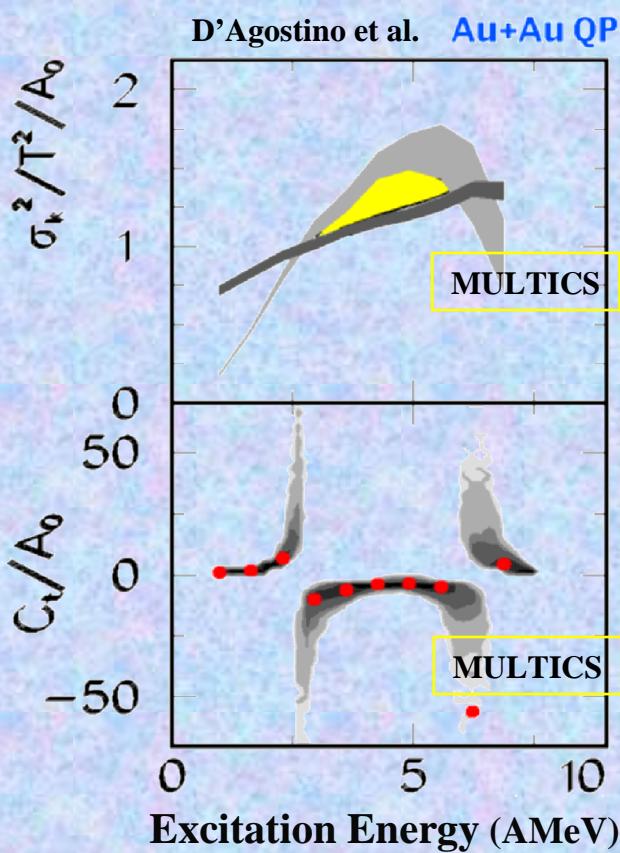


■ Negative C

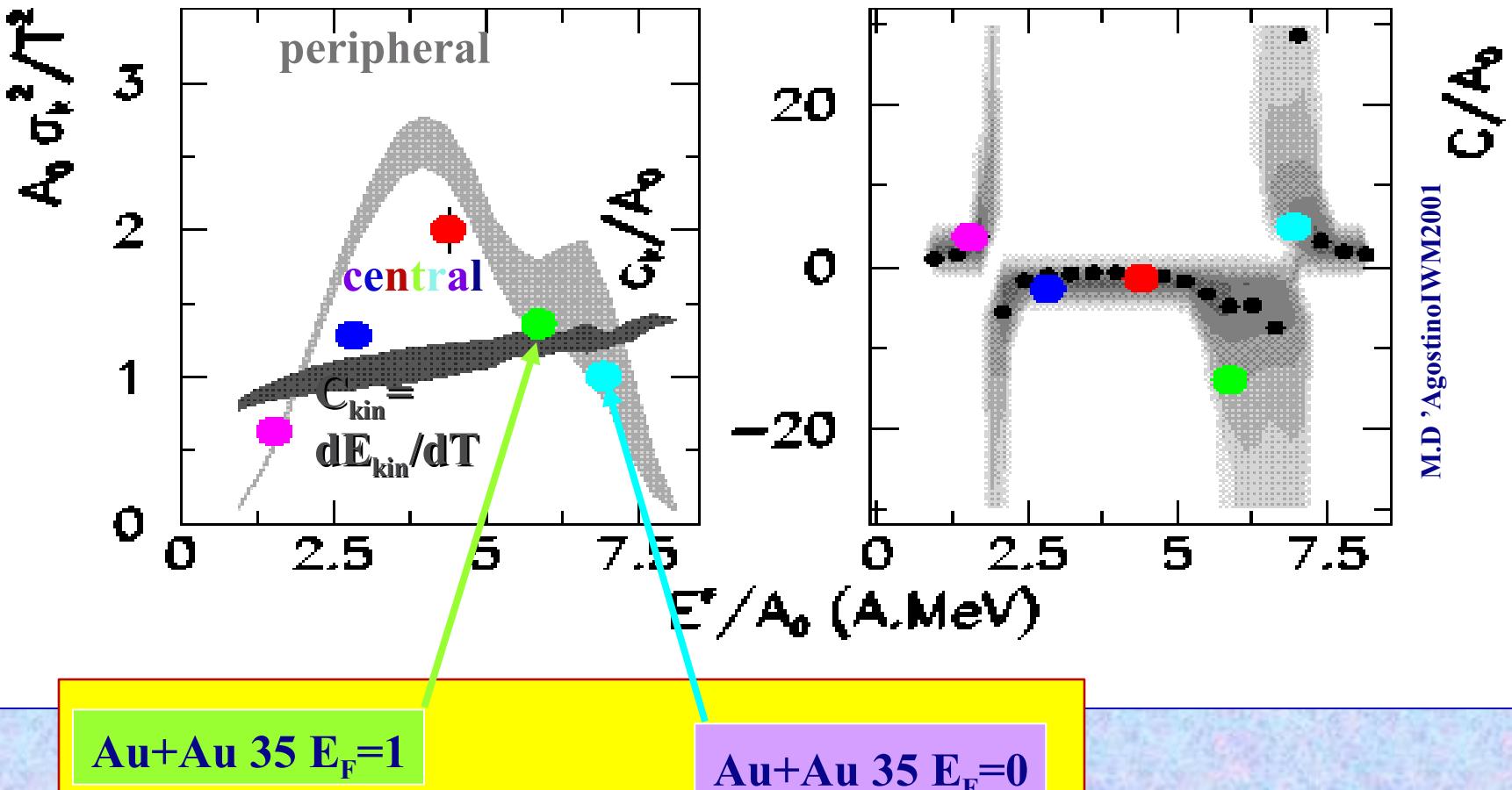


# Heat capacity from energy fluctuation

Multics  $E_1=2\pm0.3$   $E_2=6.5\pm0.7$   
Isis  $E_1=2.5$   $E_2=7.$   
Indra  $E_2=6.\pm0.5$



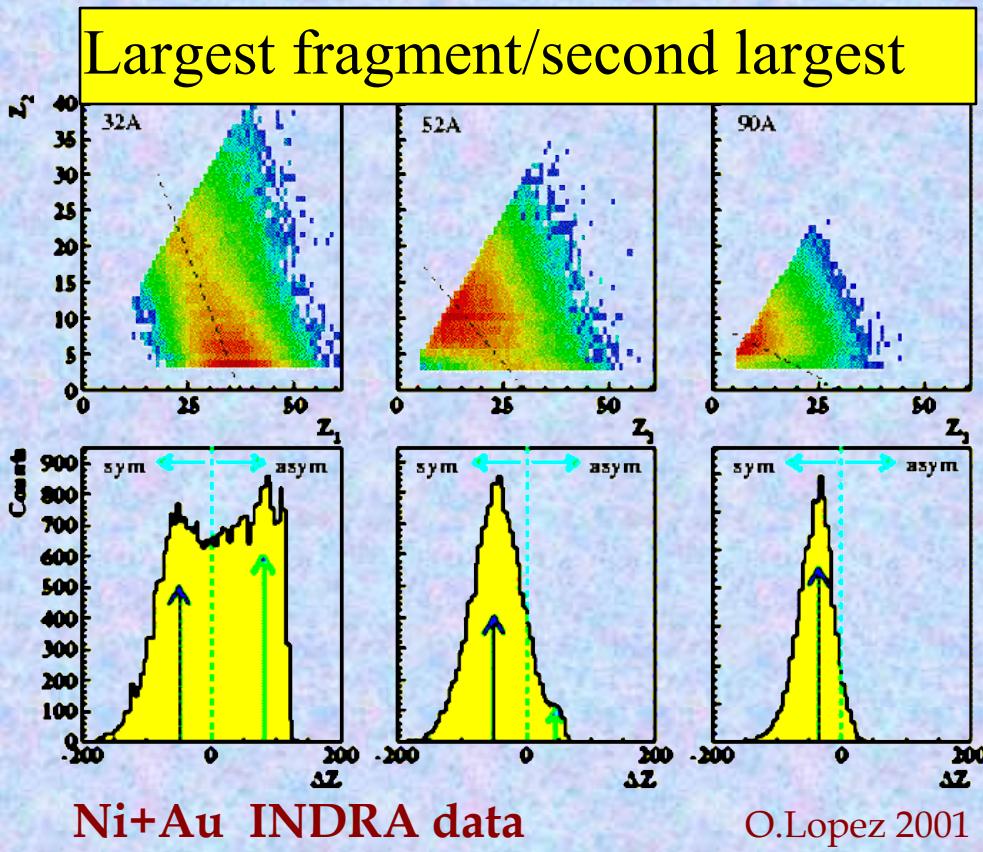
# Comparison central / peripheral



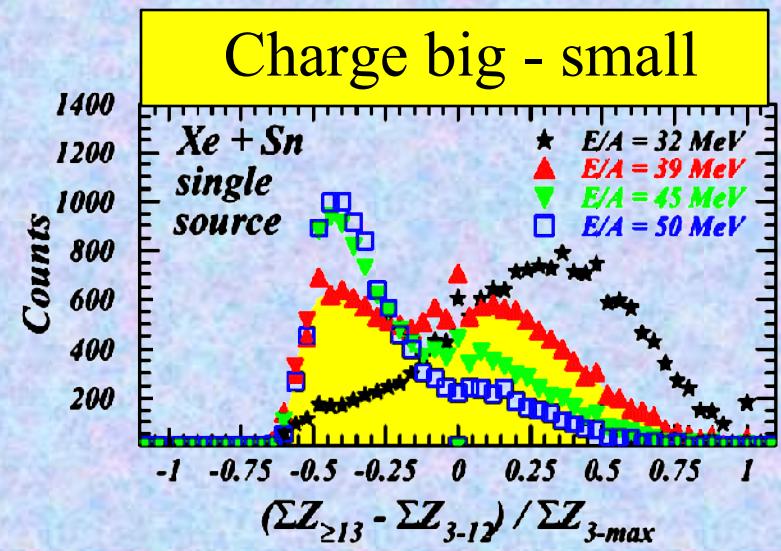
Up to  $\approx 35$  A.MeV the flow ambiguity  
is a small effect

# Multifragmentation of nuclei

## Bimodality in event distribution



Distribution  
of events.

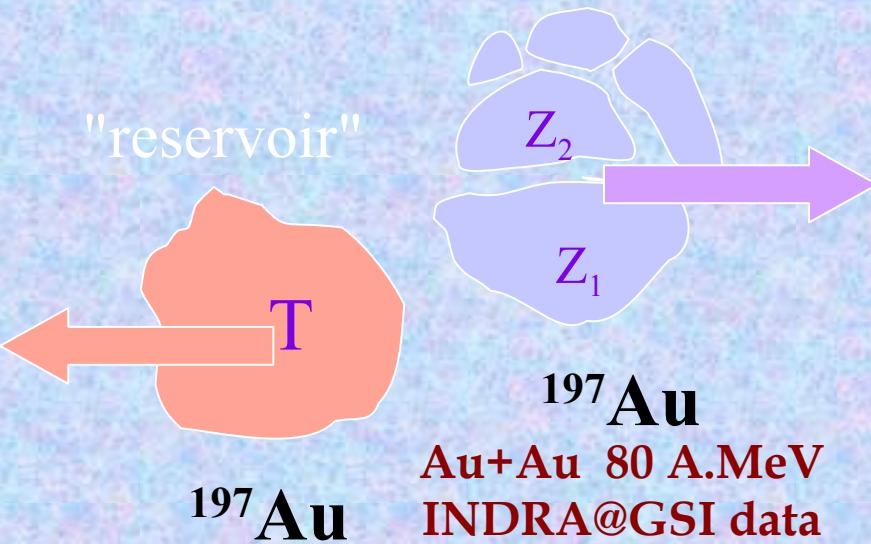


Xe+Sn INDRA data B. Borderie, 2001

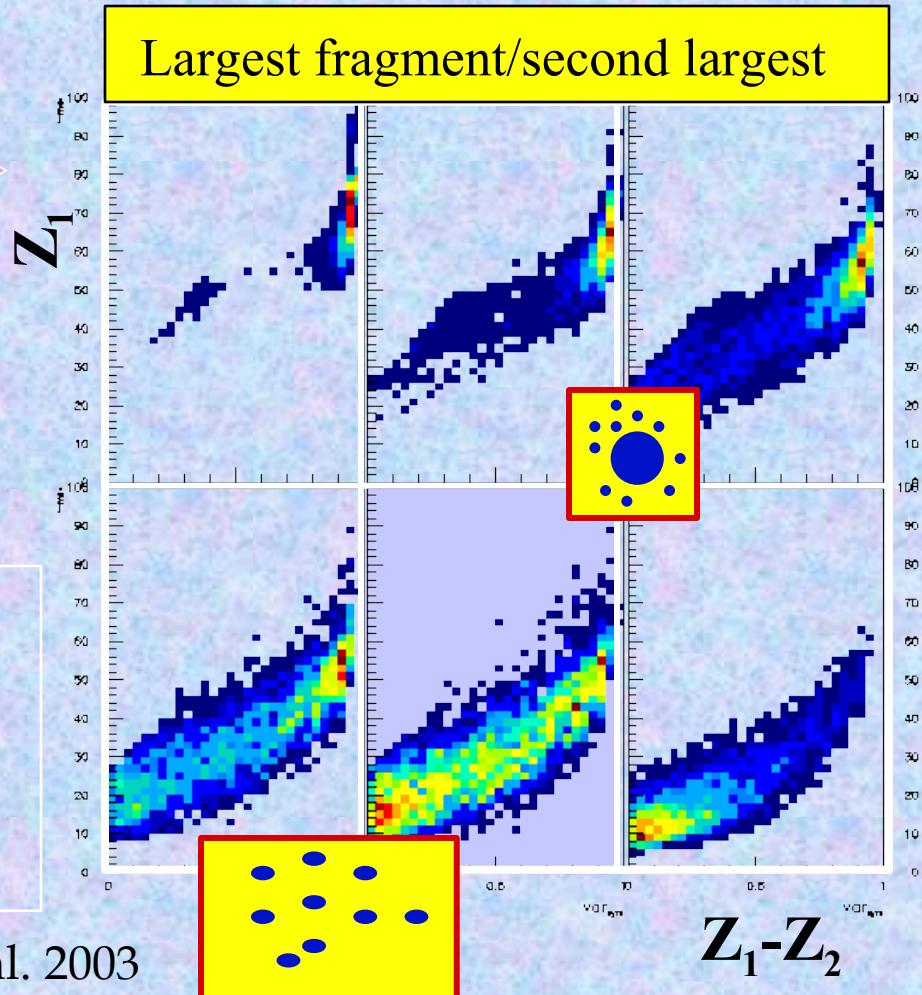
# Multifragmentation of nuclei

## Bimodality in event distribution

# Multifragmentation of nuclei Bimodality in event distribution



- Order parameter
  - ◆  $Z_1 - Z_2$  (big-small)
  - ◆ cf



- V -

# Conclusion

Negative heat capacities  
Bimodality, fluctuations



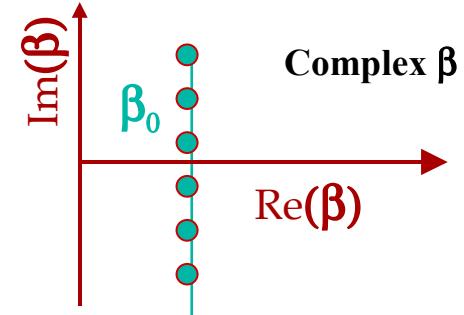
# 1st order in finite systems

PC & Gulminelli Phys A (2003)

## ■ Order param. free (canonical)

- ◆ Zeroes of Z reach real  $\beta$  axis

Yang & Lee Phys Rev 87(1952)404



# 1st order in finite systems

PC & Gulminelli Phys A (2003)

## ■ Order par. free (canonical)

- ◆ Zeroes of Z reach real axis

Yang & Lee Phys Rev 87(1952)404

- ◆ Bimodal E distribution ( $P_\beta(E)$ )

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

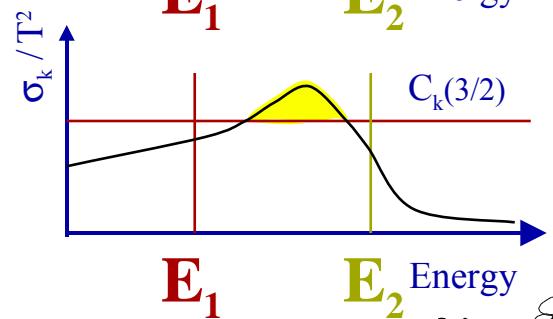
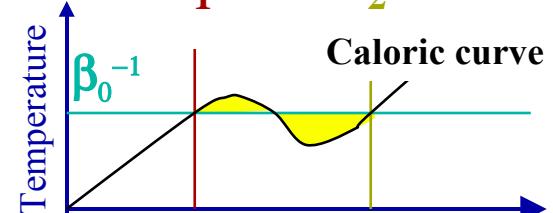
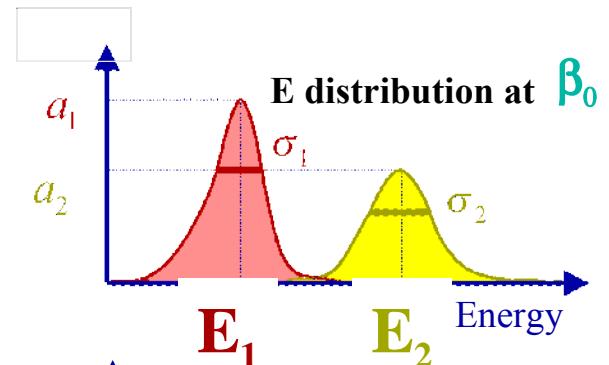
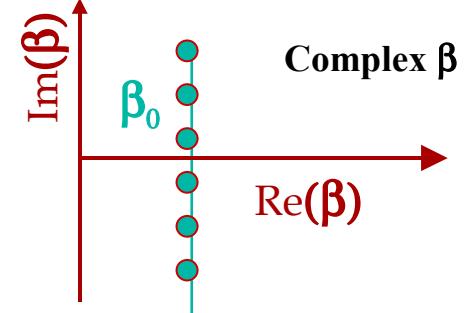
## ■ Order par. fixed (microcanonical)

- ◆ Back Bending in EOS ( $T(E)$ )

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

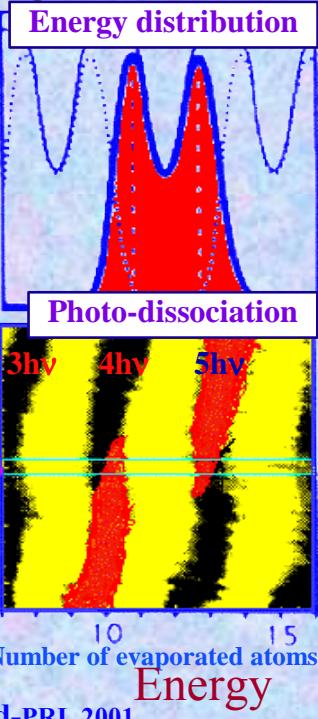
- ◆ Abnormal fluctuation ( $\sigma_k(E)$ )

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

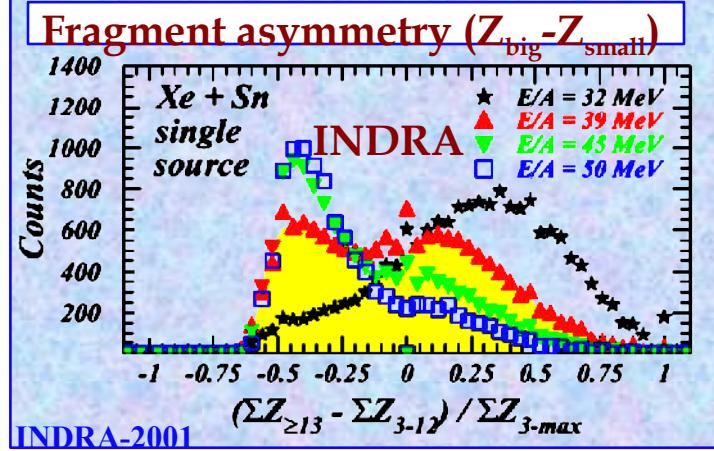


## Melting of Na Cluster

Temperature, Probability P (E)

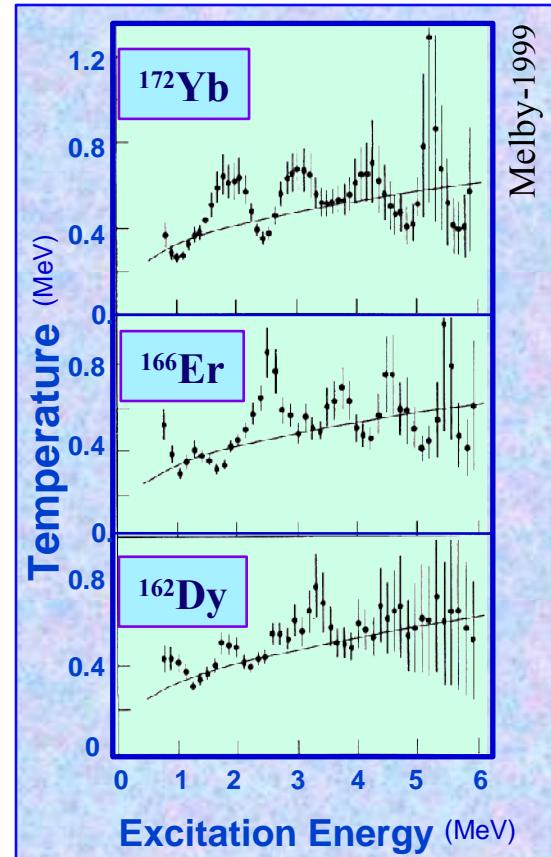


## Multifragmentation of nuclei

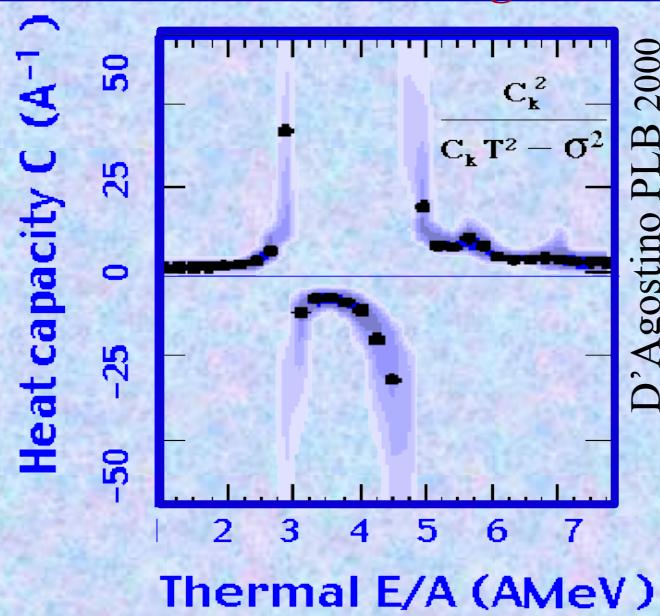
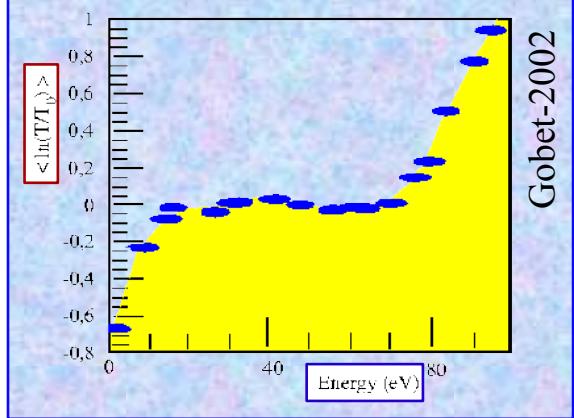


# Seen in experiments

## Nuclear superfluidity

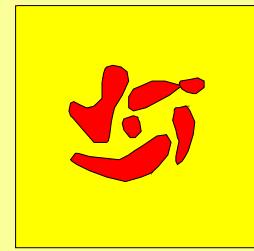


## Fragmenting H-clusters





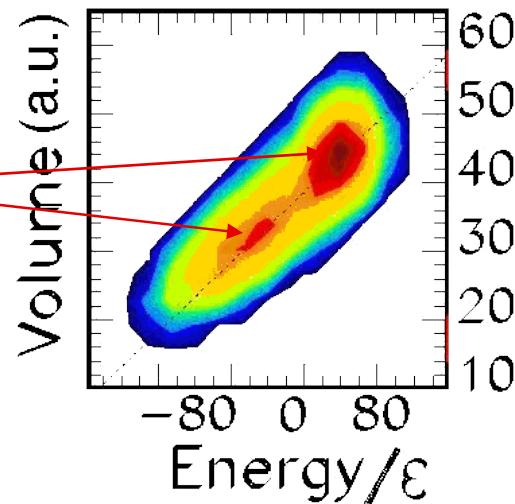
# Liquid-gas



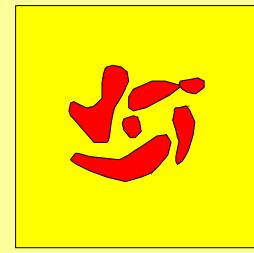
Isobare  
ensemble

$$P^{(i)} \propto \exp -\lambda V^{(i)}$$

- Phase transition and bimodality



# Liquid-gas

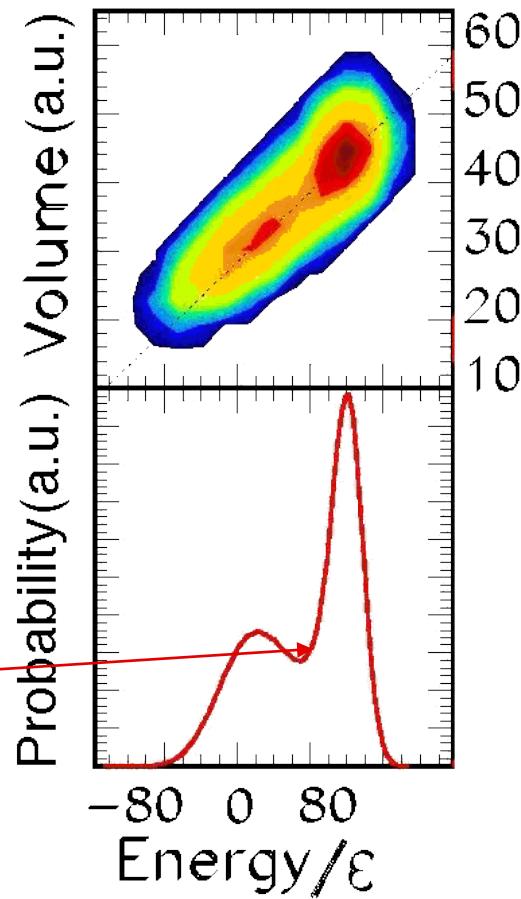


Isobare  
ensemble

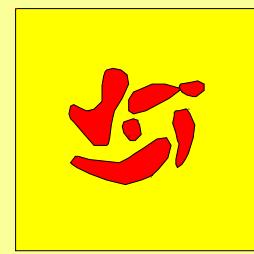
$$P^{(i)} \propto \exp -\lambda V^{(i)}$$

- Phase transition and bimodality

- Negative heat capacity



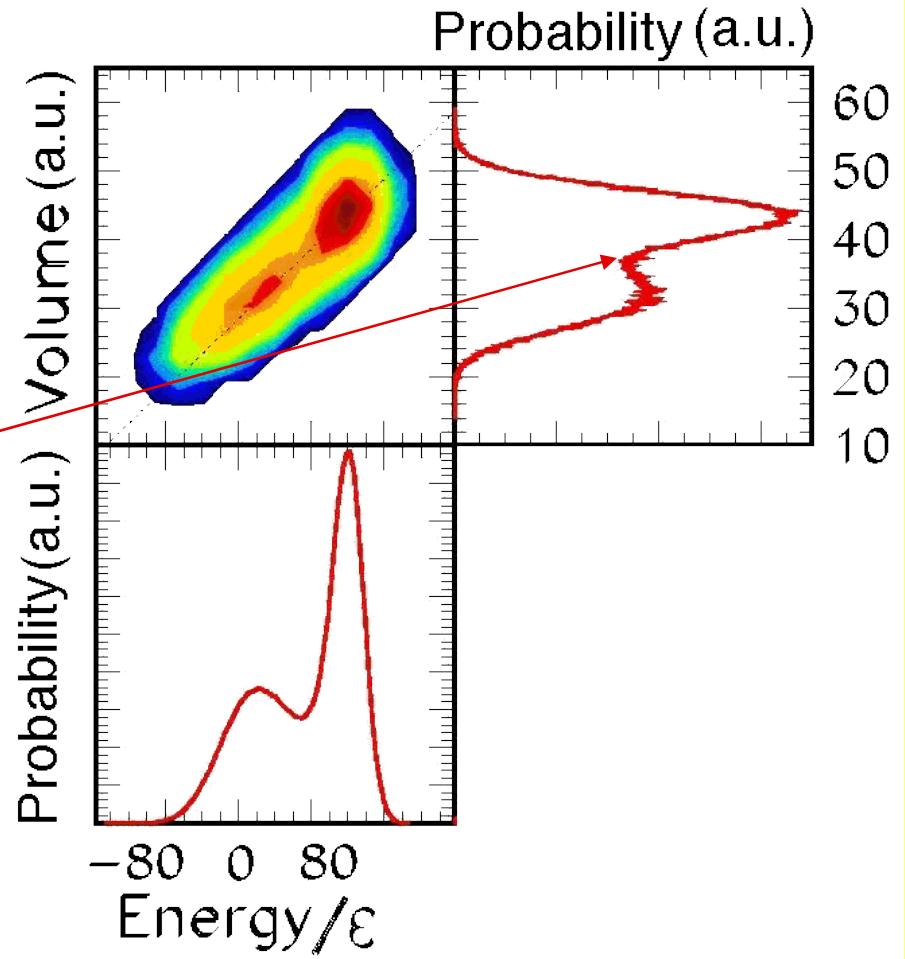
# Liquid-gas



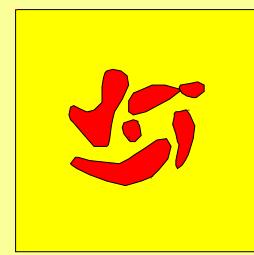
Isobare  
ensemble

$$P^{(i)} \propto \exp -\lambda V^{(i)}$$

- Phase transition And bimodality
- Negative compressibility
- Negative heat capacity



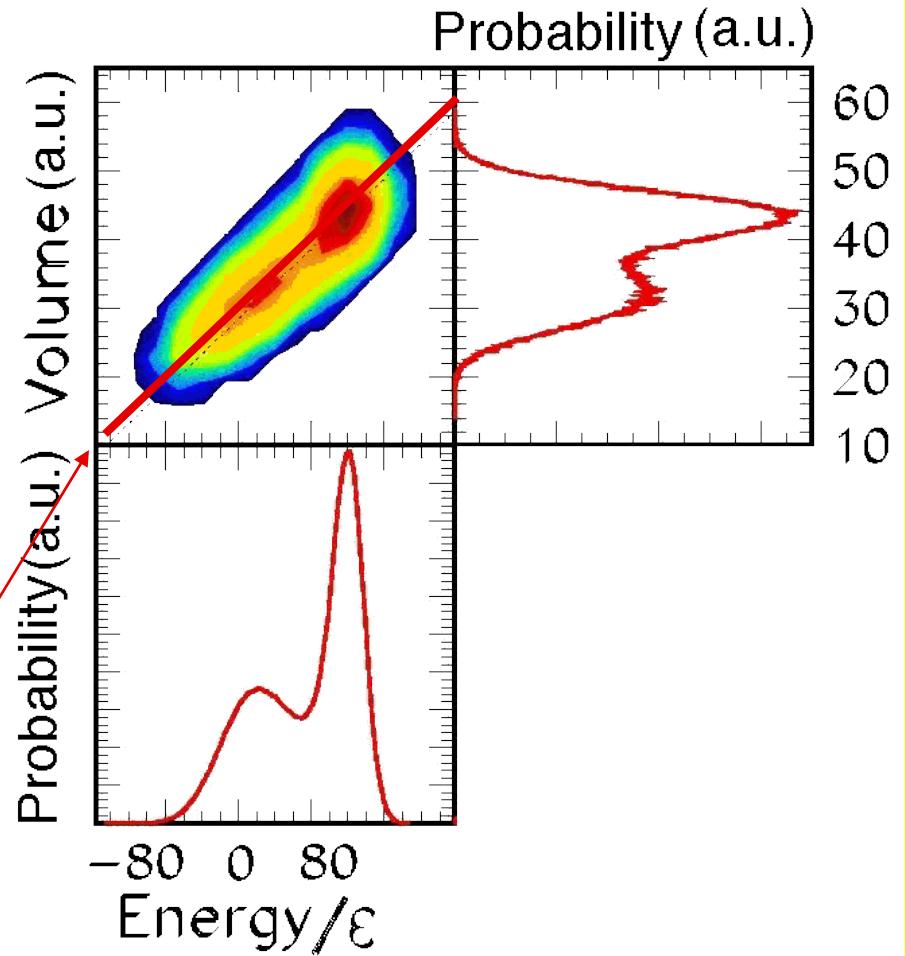
# Liquid-gas



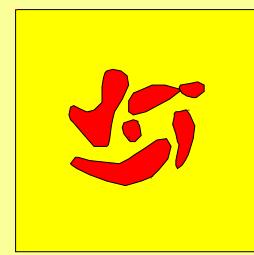
Isobare  
ensemble

$$P^{(i)} \propto \exp -\lambda V^{(i)}$$

- Phase transition And bimodality
- Negative compressibility
- Negative heat capacity
- Order parameter



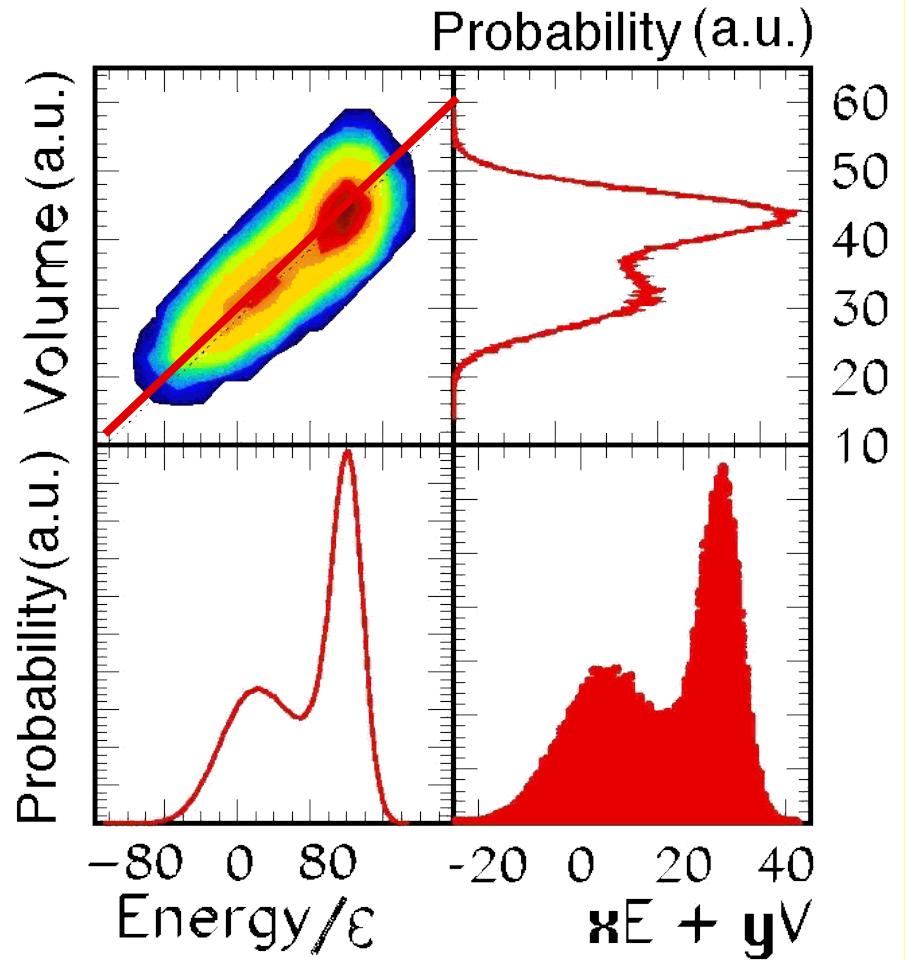
# Liquid-gas



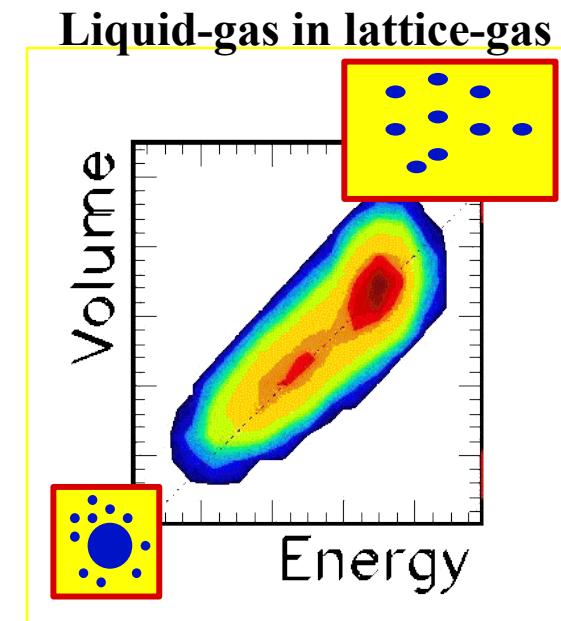
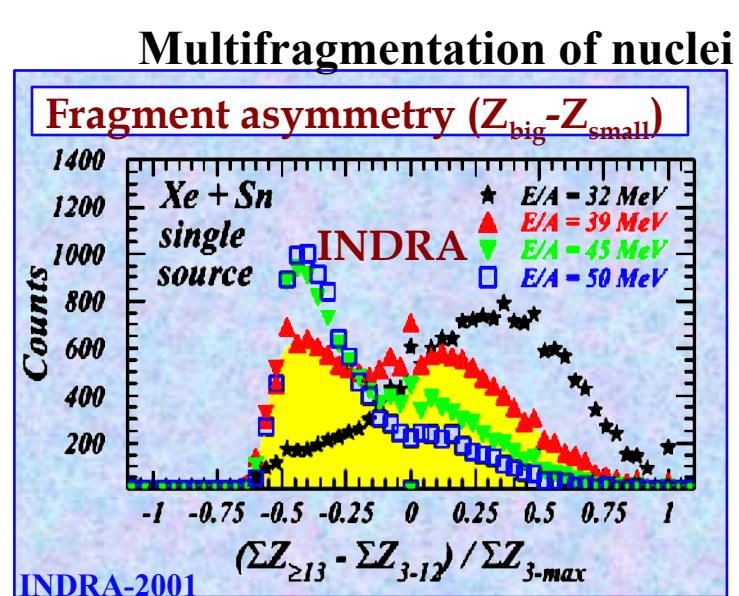
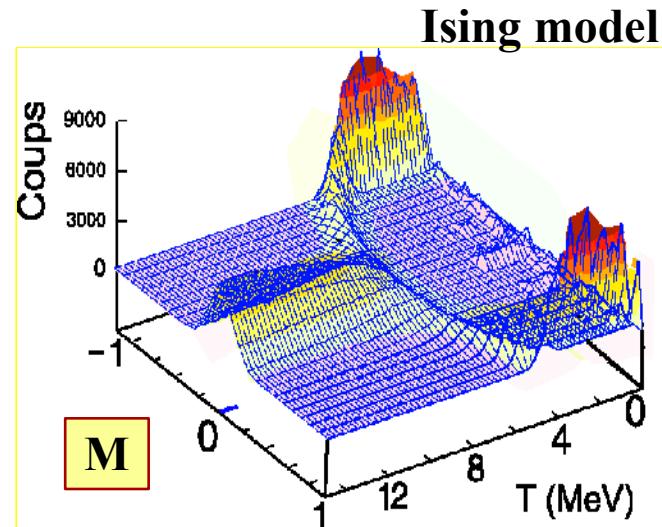
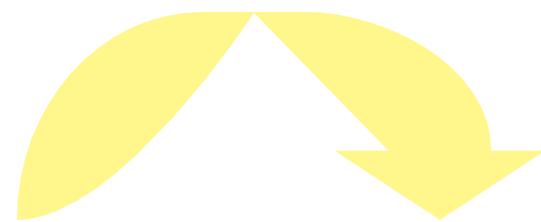
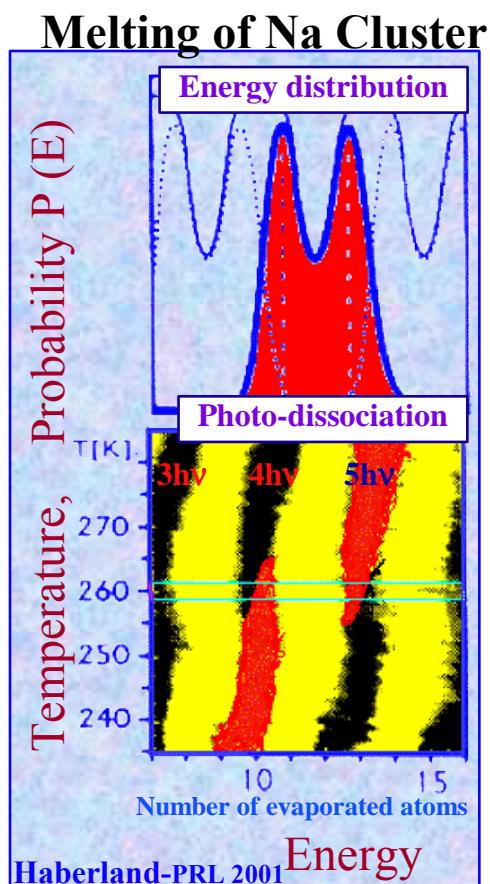
Isobare  
ensemble

$$P^{(i)} \propto \exp -\lambda V^{(i)}$$

- Phase transition And bimodality
- Negative compressibility
- Negative heat capacity
- Order parameter

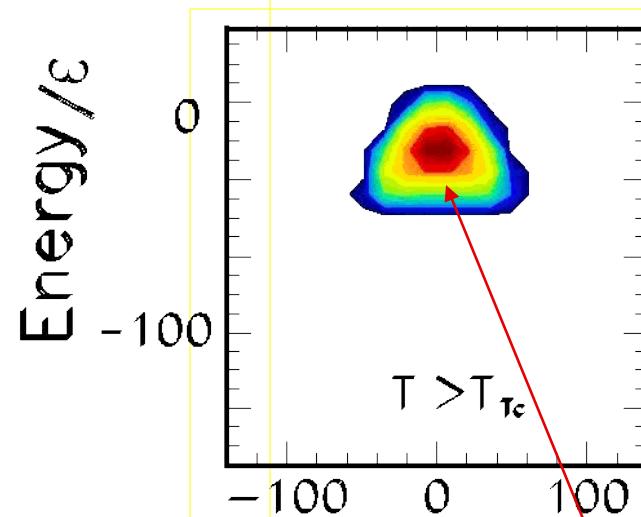


# Bimodal distributions





# Magnetization in Ising Model



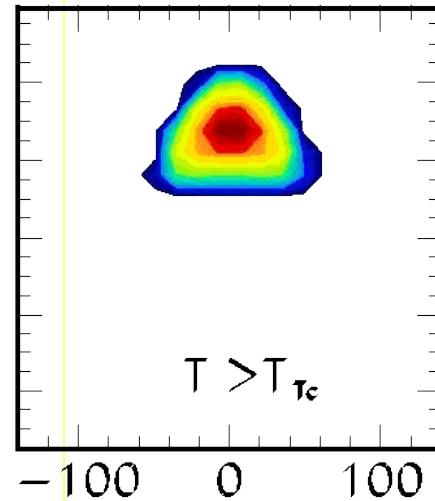
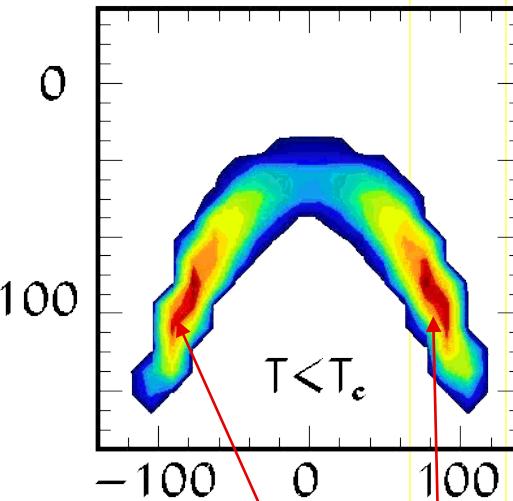
One Phase



Play

# Magnetization in Ising Model

Energy /  $\epsilon$

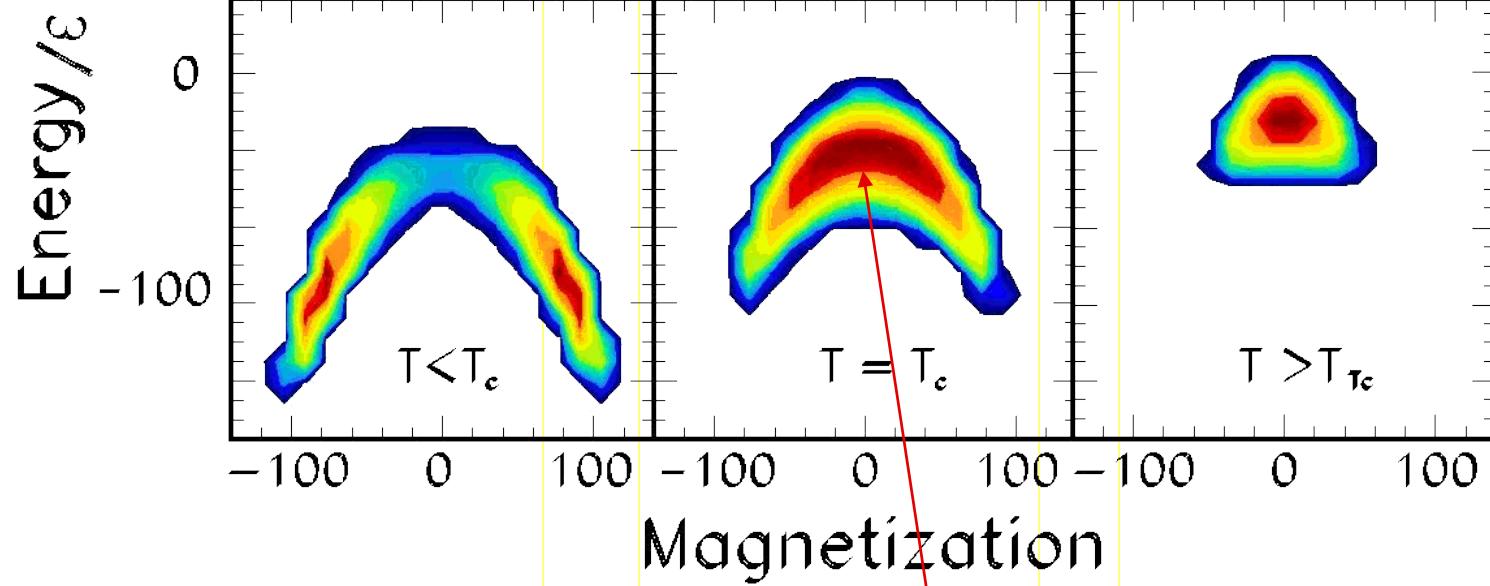


Magnetization

- **Bimodal  
Two Phases**

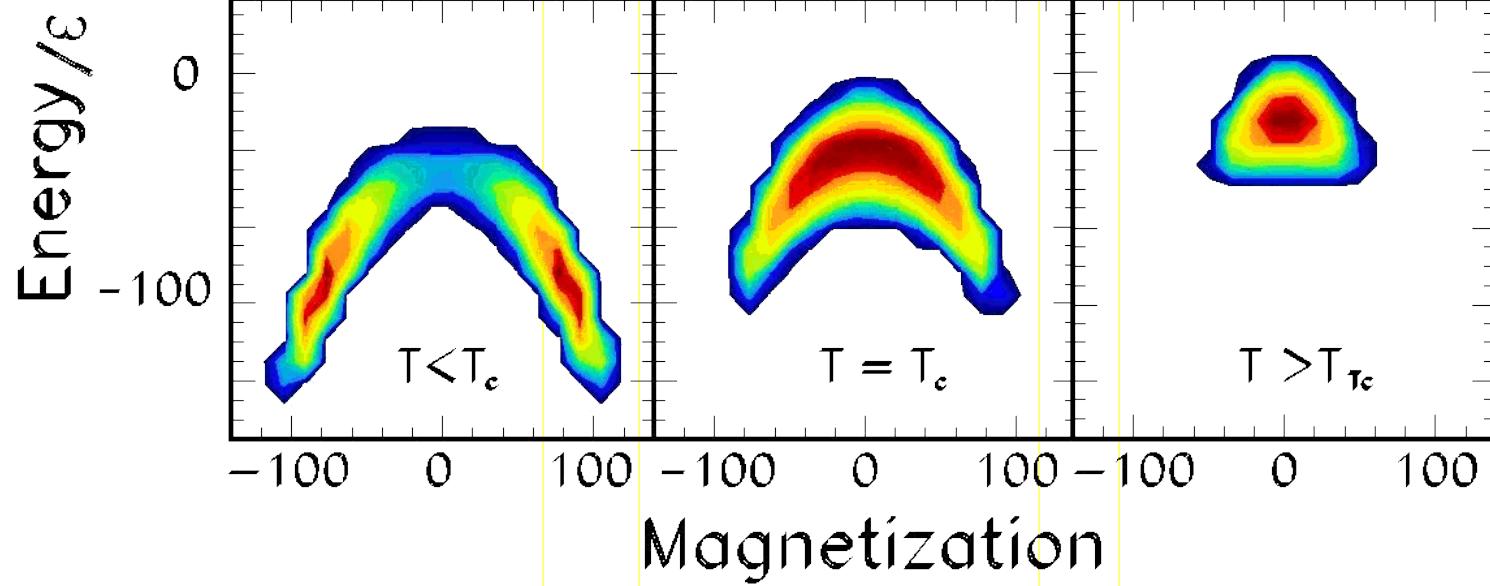
- **One Phase**

# Magnetization in Ising Model



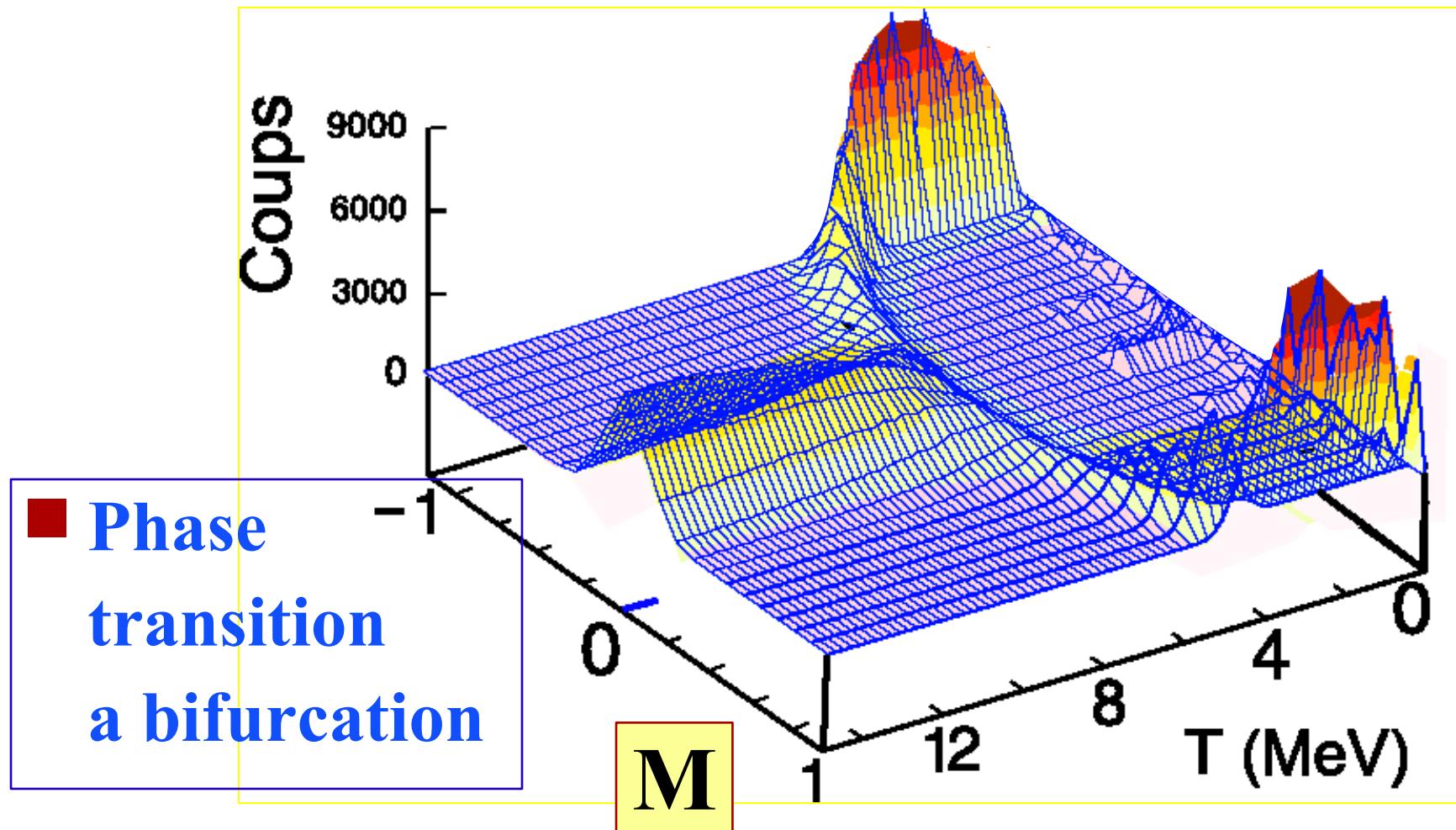
- Bimodal Two Phases
- Second Order
- One Phase

# Magnetization in Ising Model

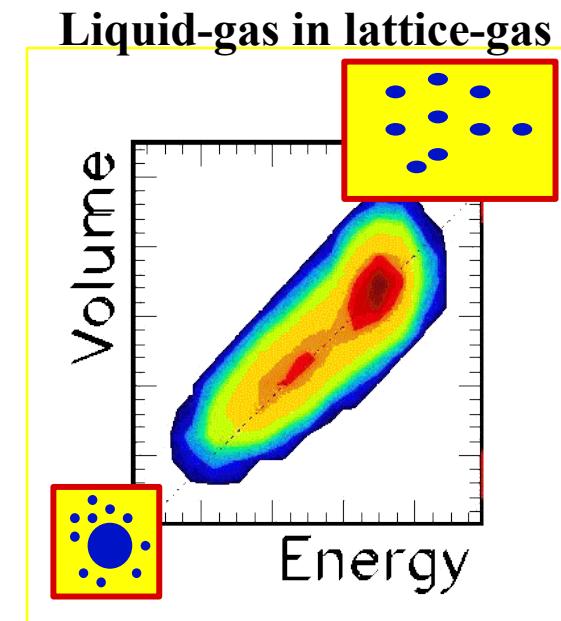
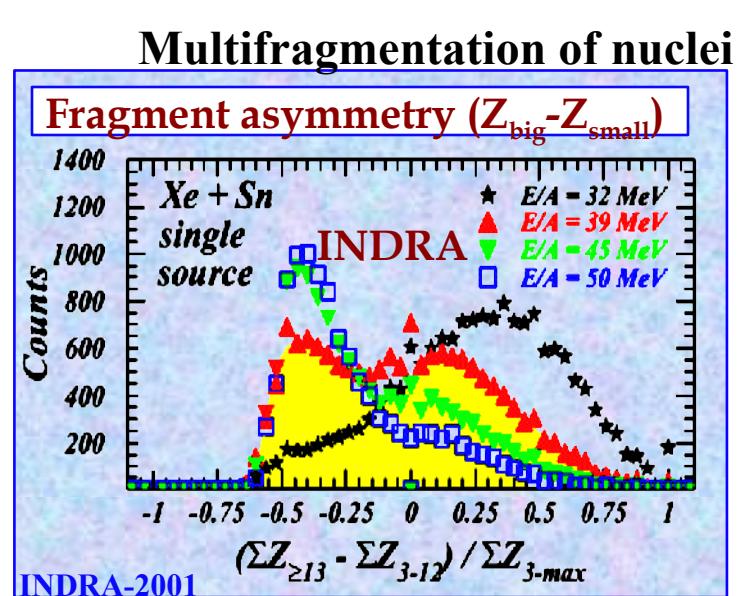
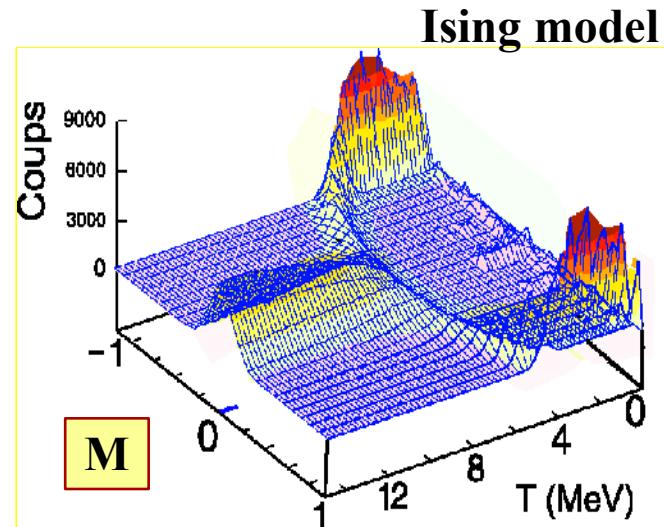
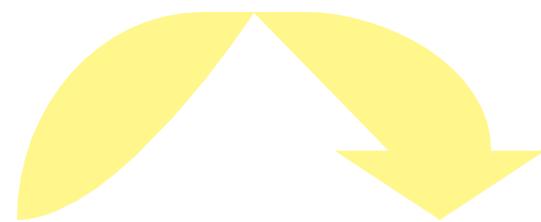
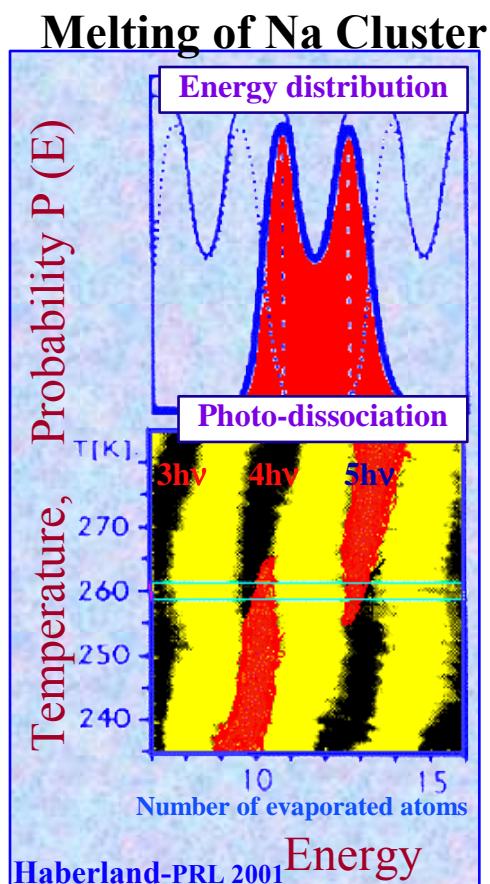


- Bimodal Two Phases
- Second Order
- One Phase

# Magnetization in Ising Model

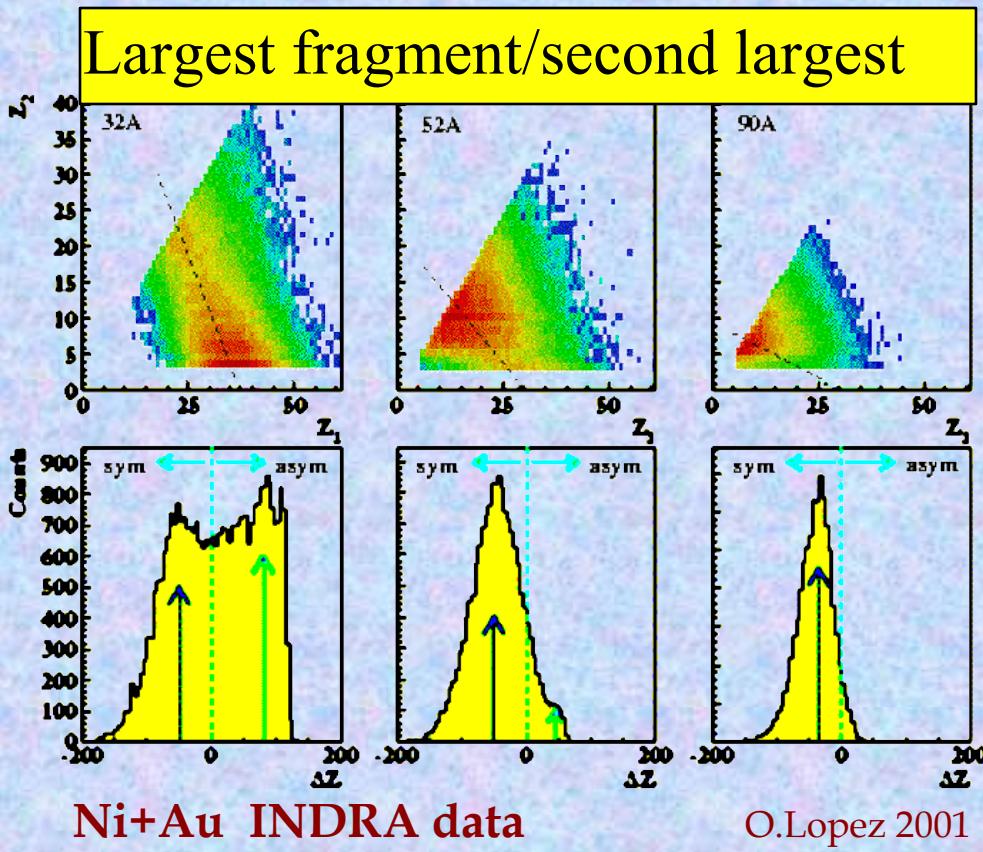


# Bimodal distributions

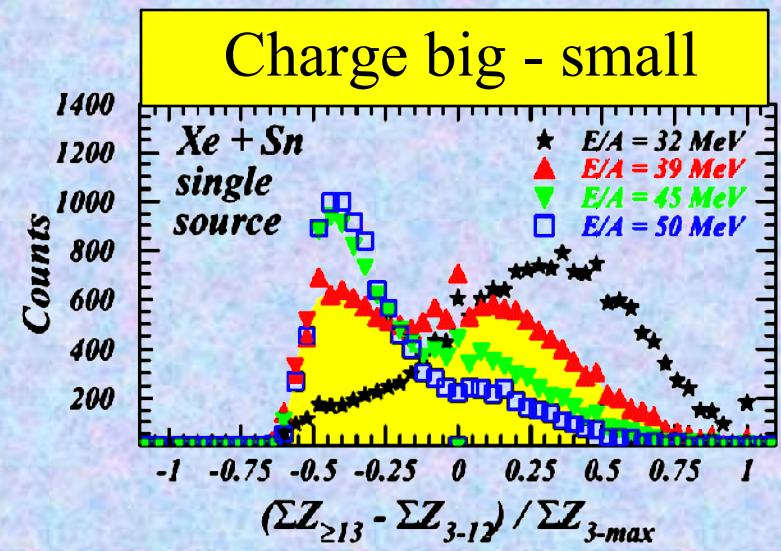


# Multifragmentation of nuclei

## Bimodality in event distribution



Distribution  
of events.

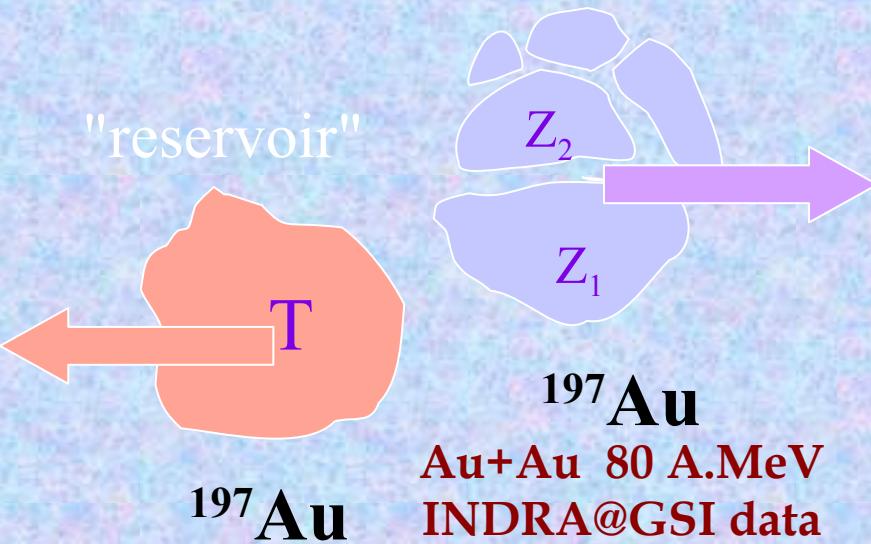


Xe+Sn INDRA data B. Borderie, 2001

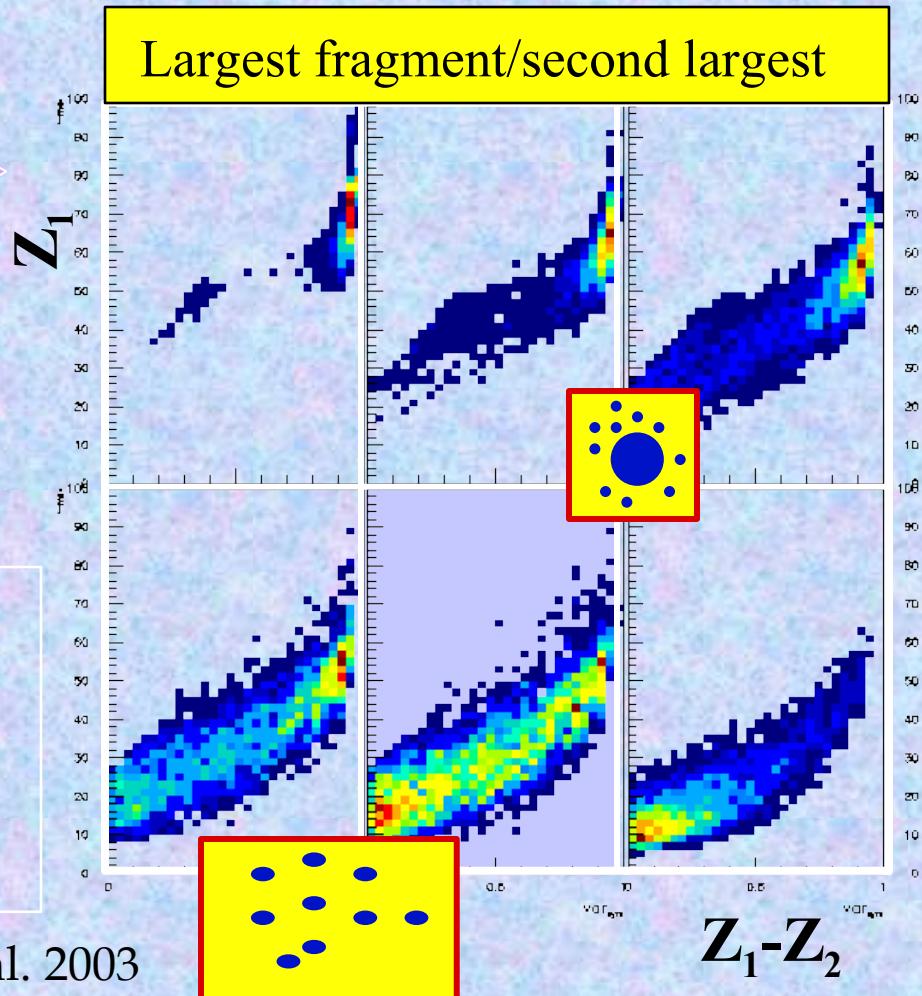
# Multifragmentation of nuclei

## Bimodality in event distribution

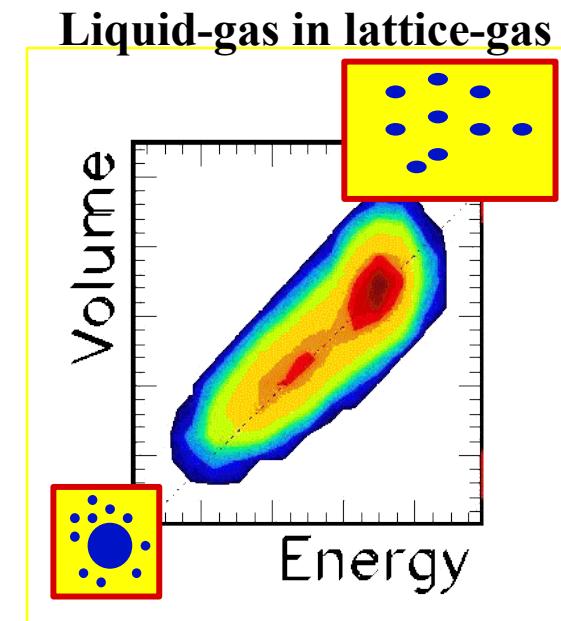
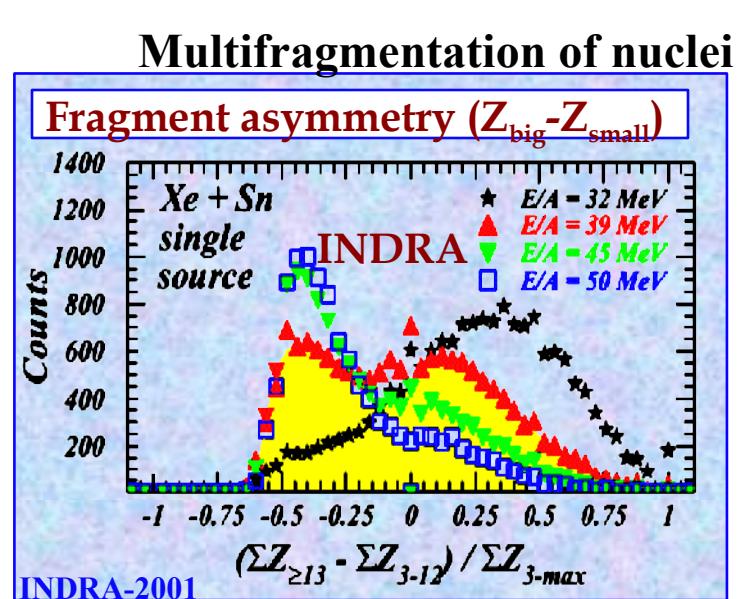
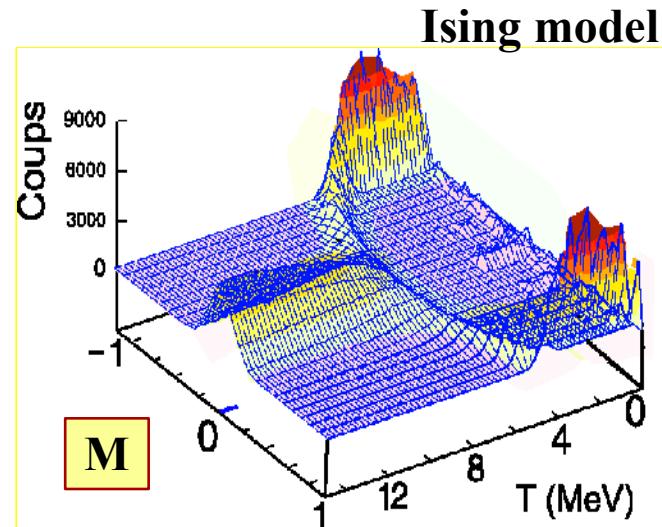
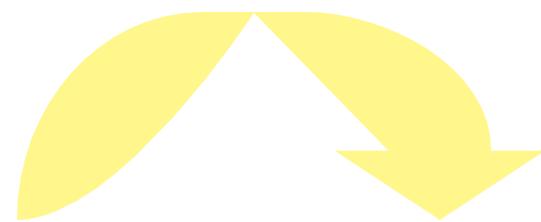
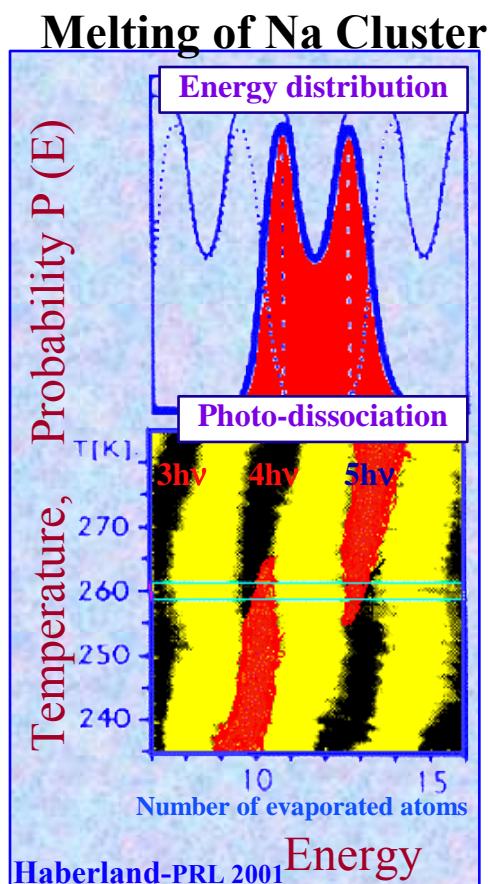
# Multifragmentation of nuclei Bimodality in event distribution



- Order parameter
  - ◆  $Z_1 - Z_2$  (big-small)
  - ◆ cf



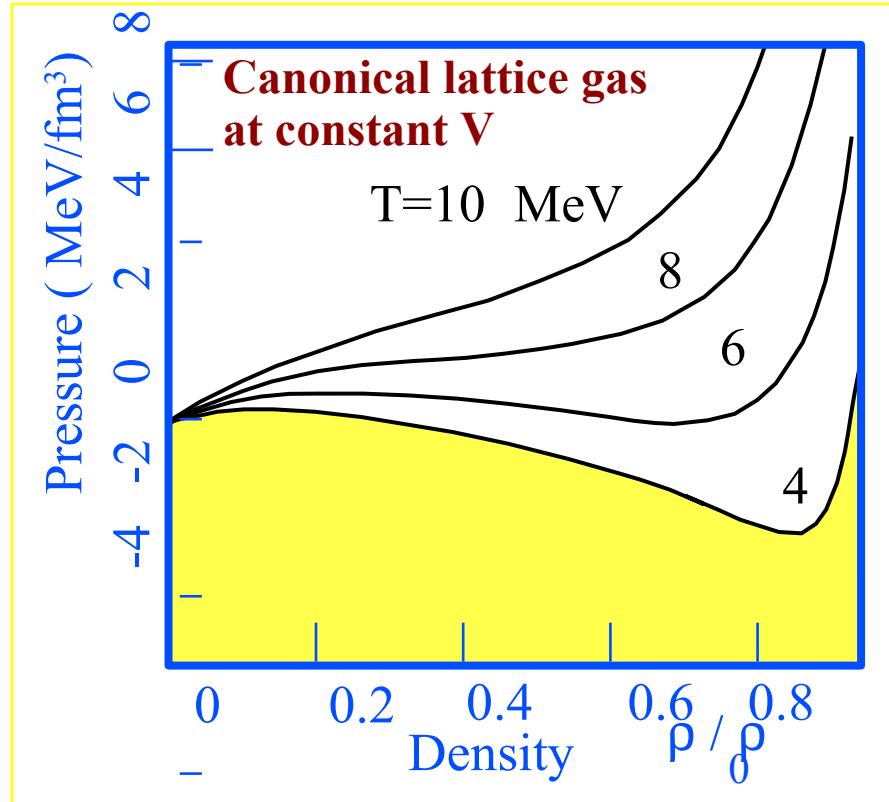
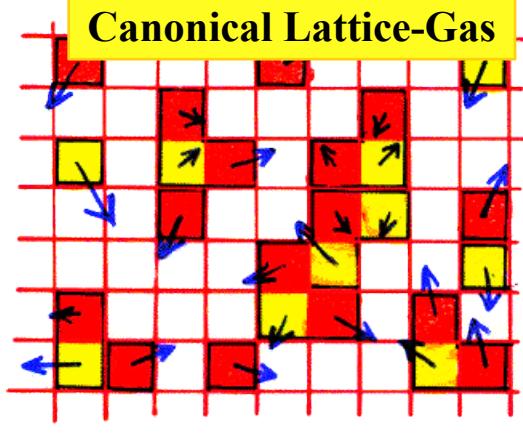
# Bimodal distributions



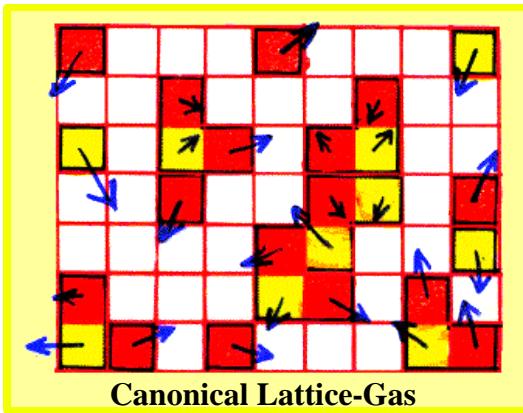


# Density: Order parameter:

- Usually  $V=cst$ 
  - ◆ (“box”)
  - ◆ Isochore ensemble
- Negative compressibility

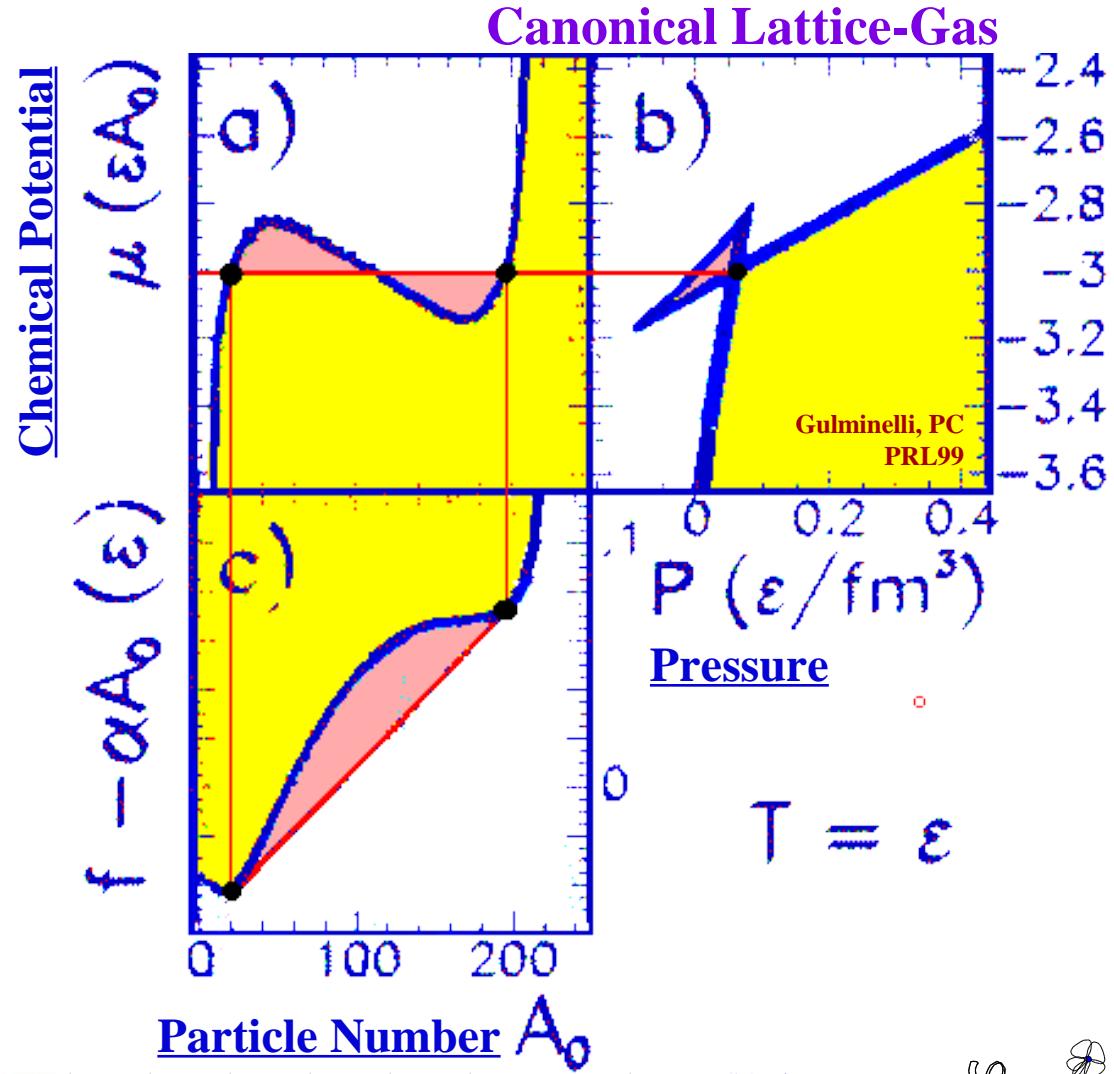


# Generalization: inverted curvatures

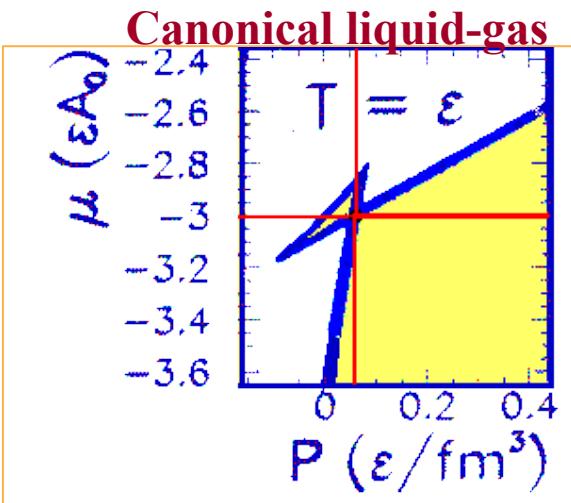
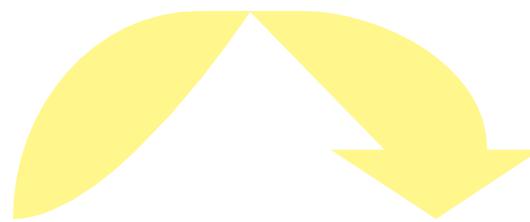
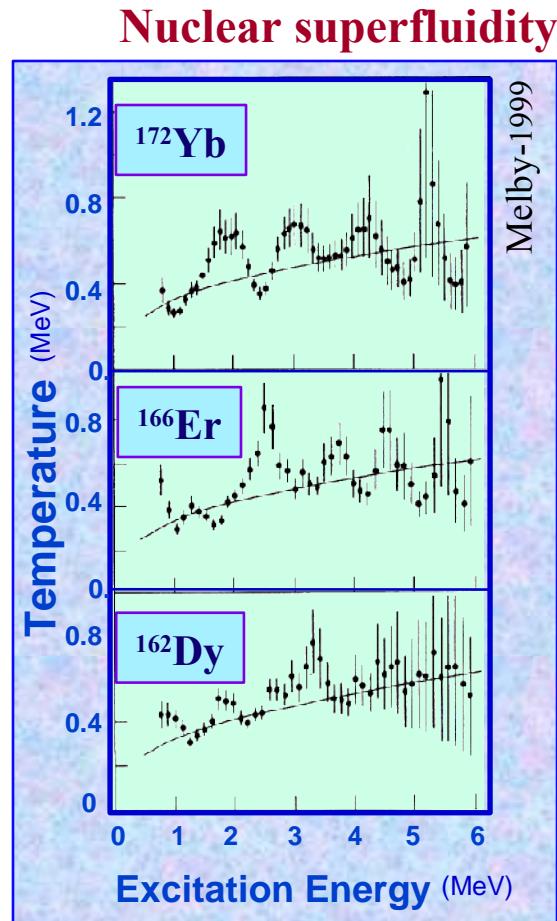


Canonical Lattice-Gas

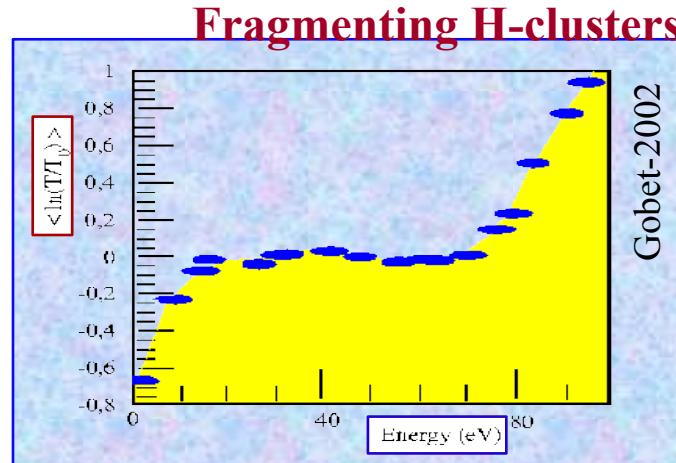
■ Negative Susceptibility and Compressibility



# Abnormal curvatures



Compressibility  $< 0$   
Susceptibility  $< 0$



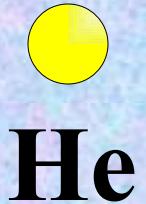
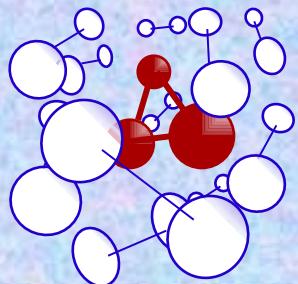
Convex entropy

T decreasing with E

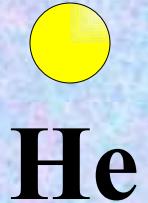
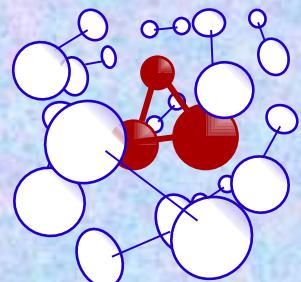


# Fragmentation of hydrogen clusters

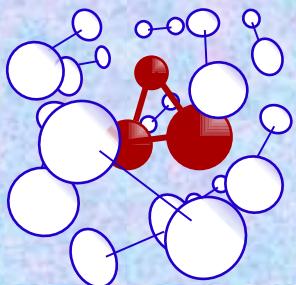
$H_3^+(H_2)_n$



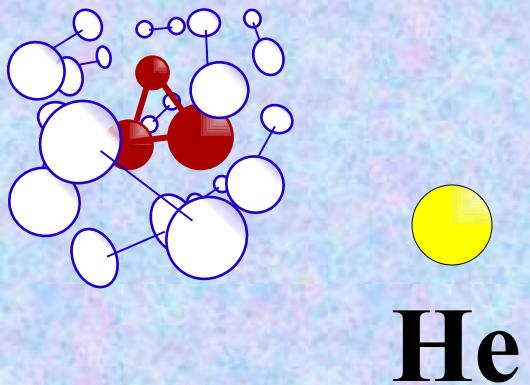
# Fragmentation of hydrogen clusters



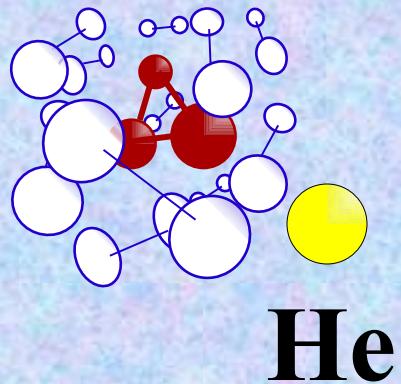
# Fragmentation of hydrogen clusters



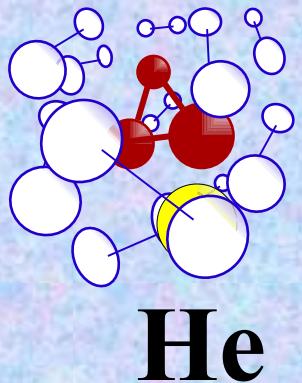
# Fragmentation of hydrogen clusters



# Fragmentation of hydrogen clusters

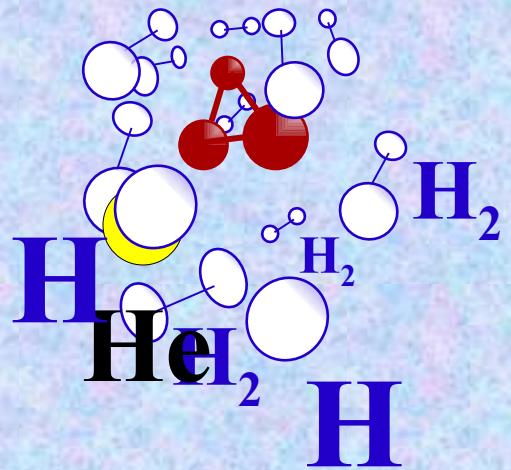


# Fragmentation of hydrogen clusters



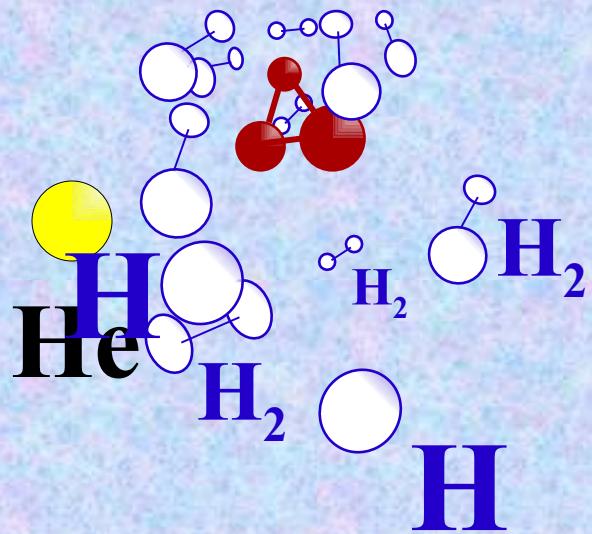
# Fragmentation of hydrogen clusters

$H_3^+(H_2)_n,$

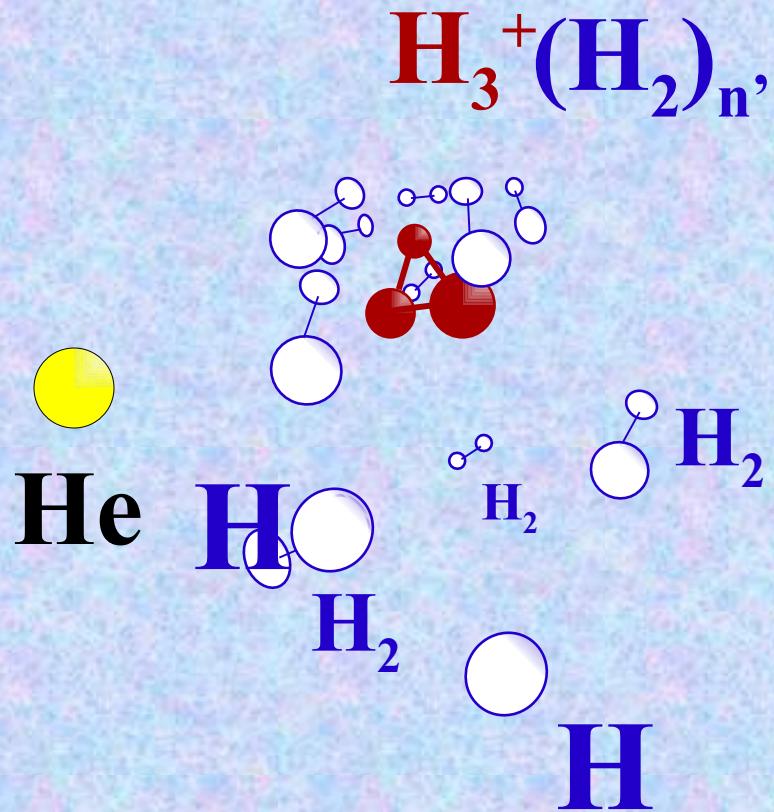


# Fragmentation of hydrogen clusters

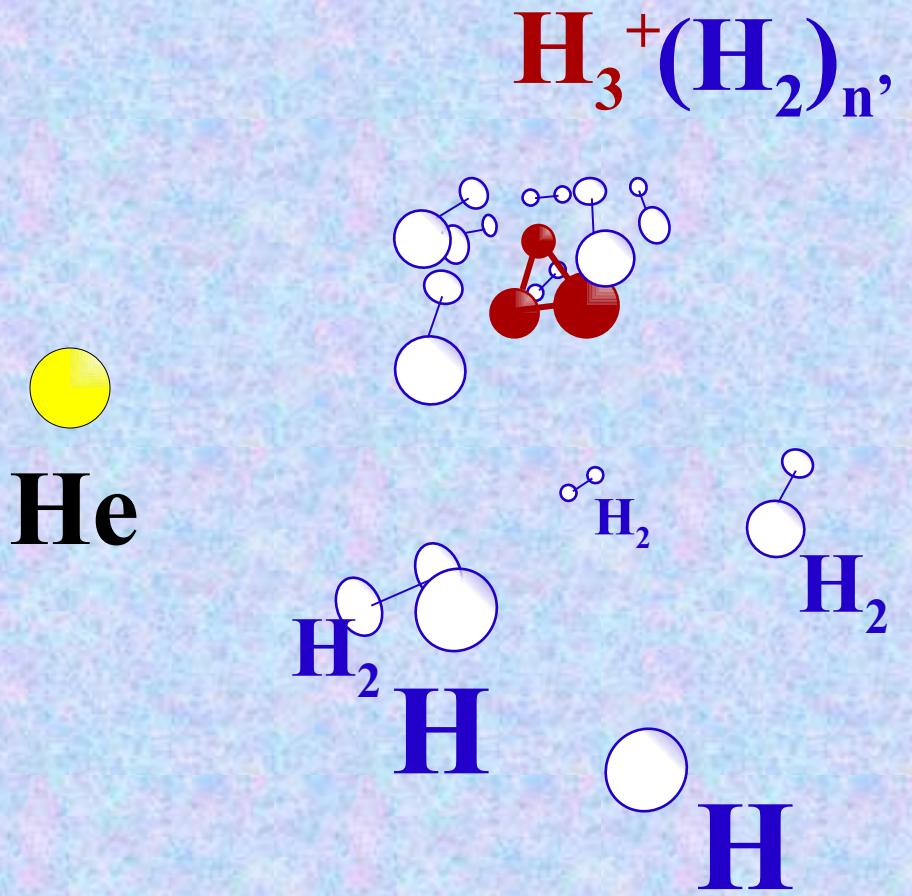
$\text{H}_3^+(\text{H}_2)_n,$



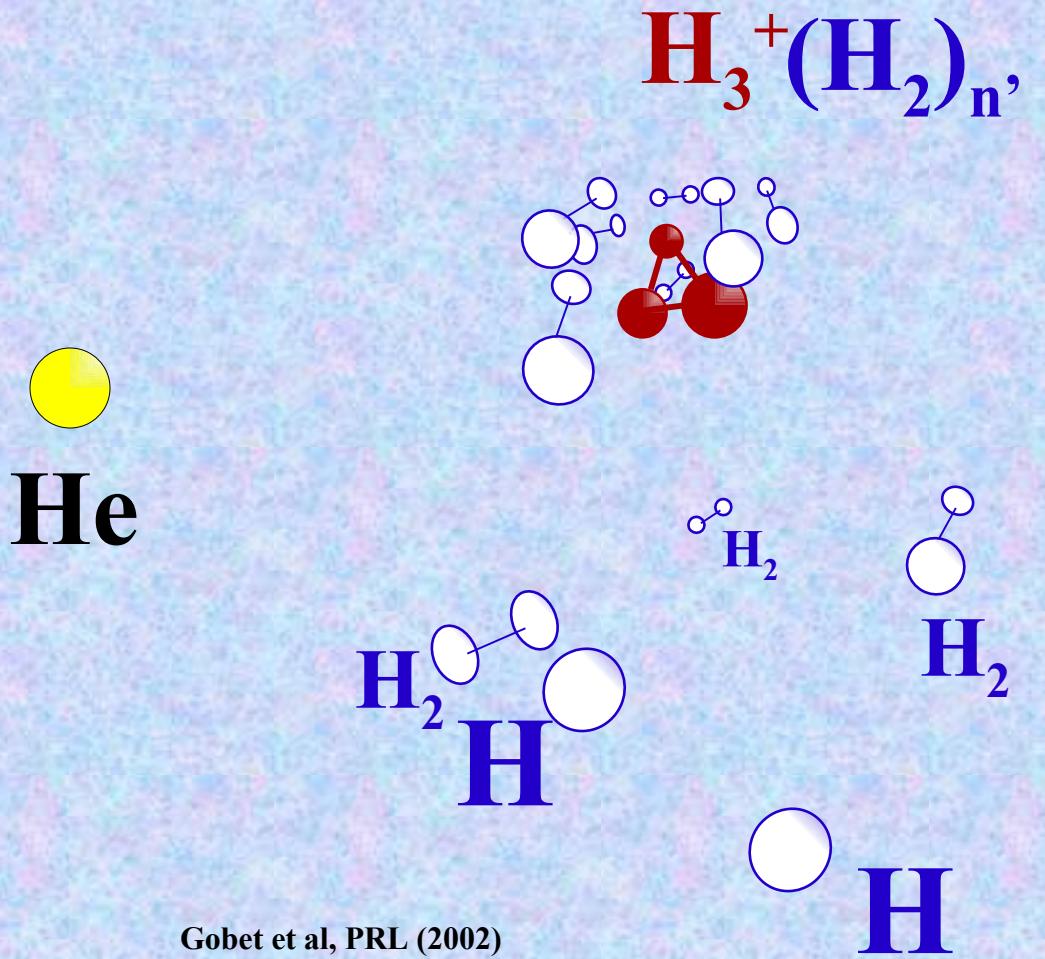
# Fragmentation of hydrogen clusters



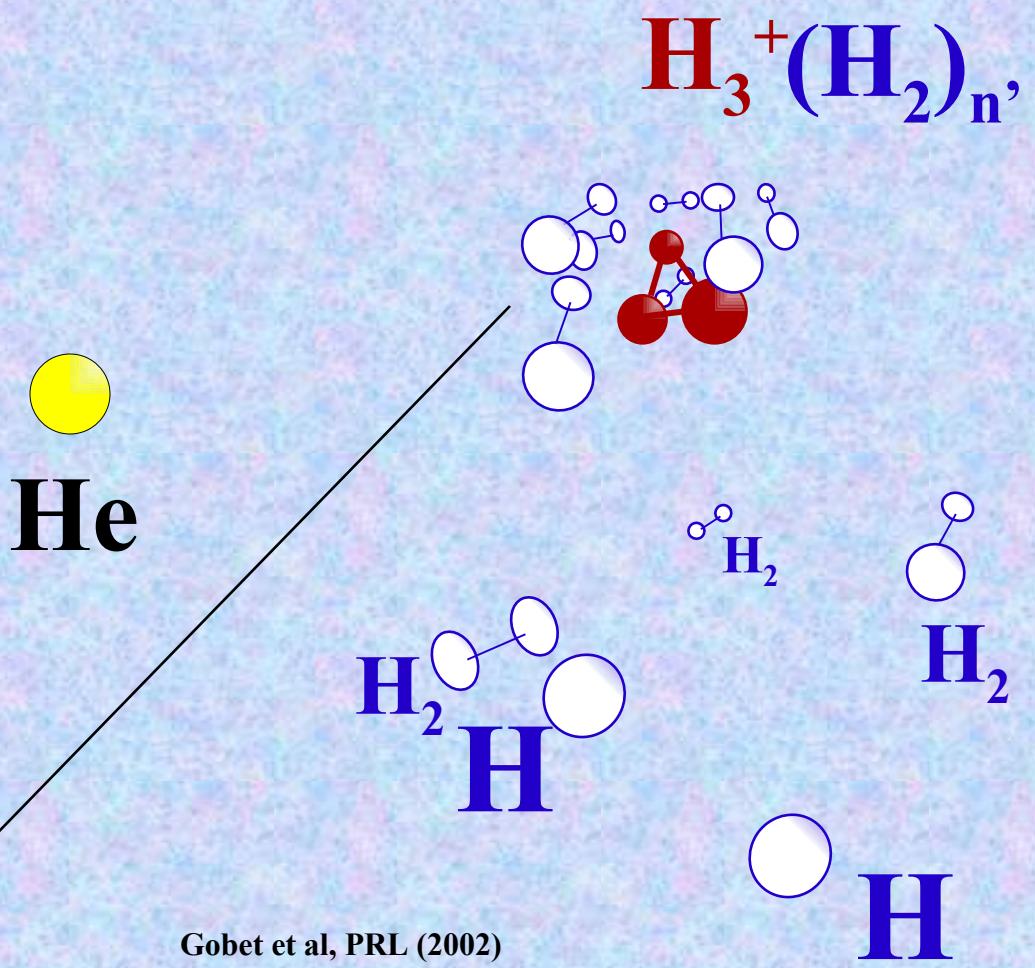
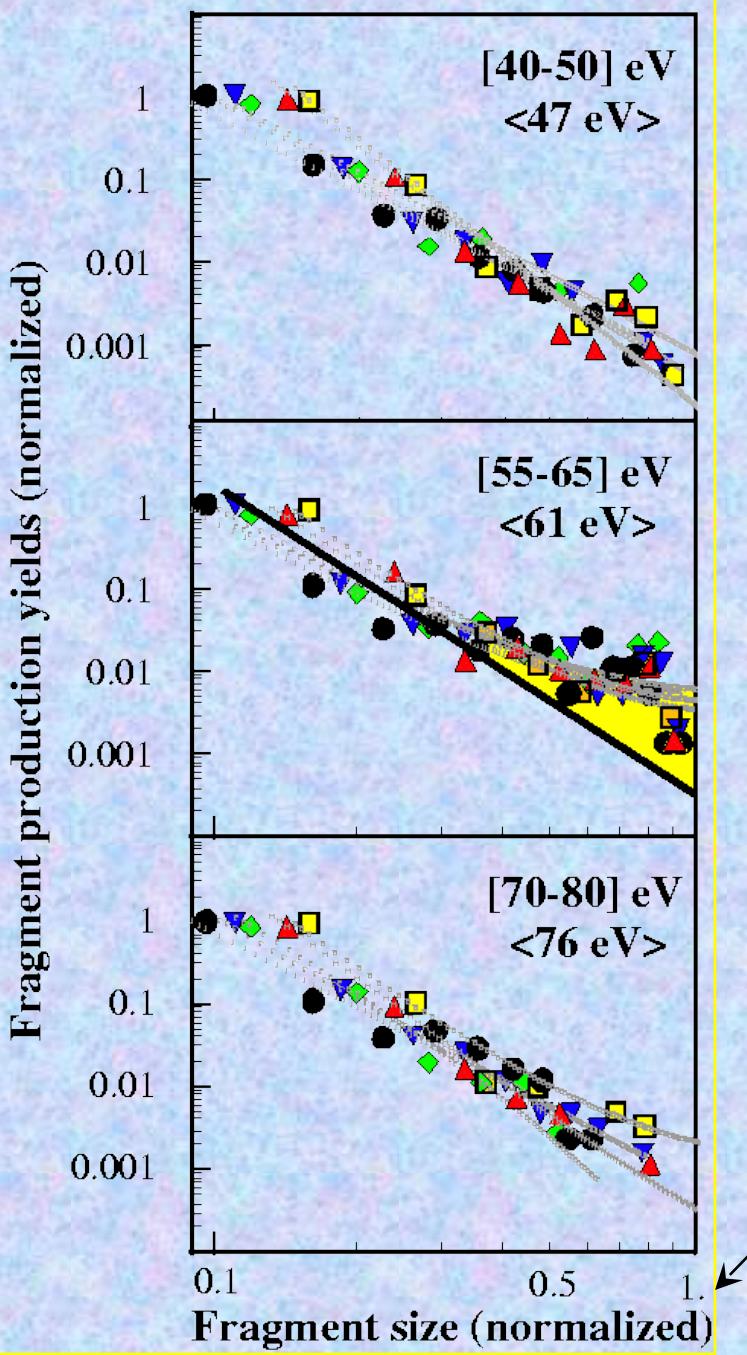
# Fragmentation of hydrogen clusters



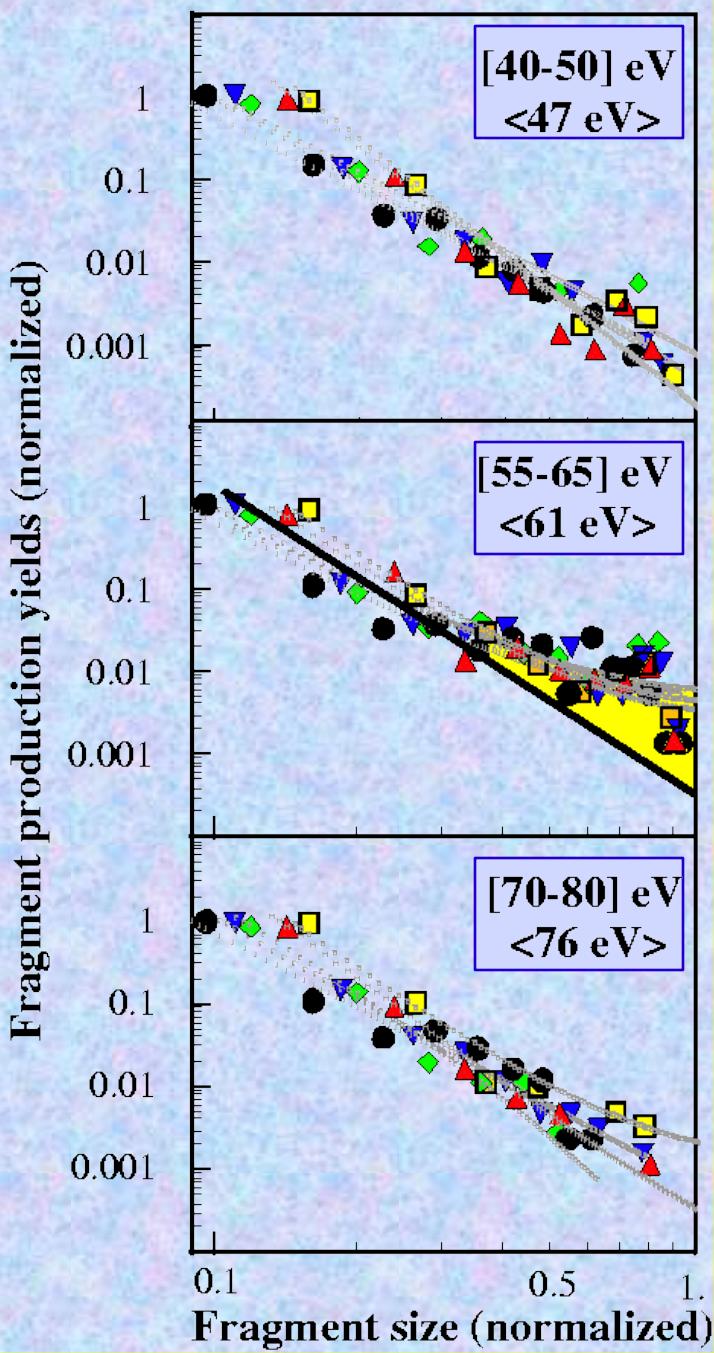
# Fragmentation of hydrogen clusters



# Fragmentation of hydrogen clusters

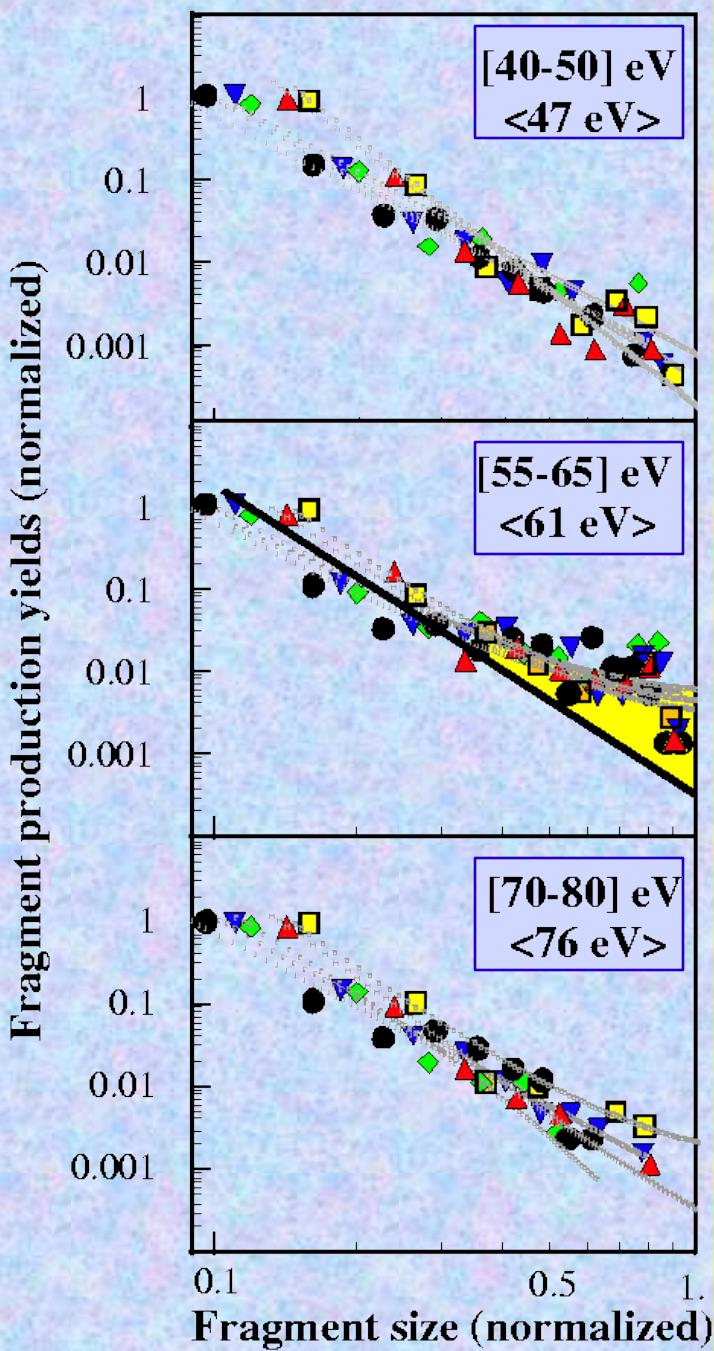


Gobet et al, PRL (2002)



# Fragmentation of hydrogen clusters

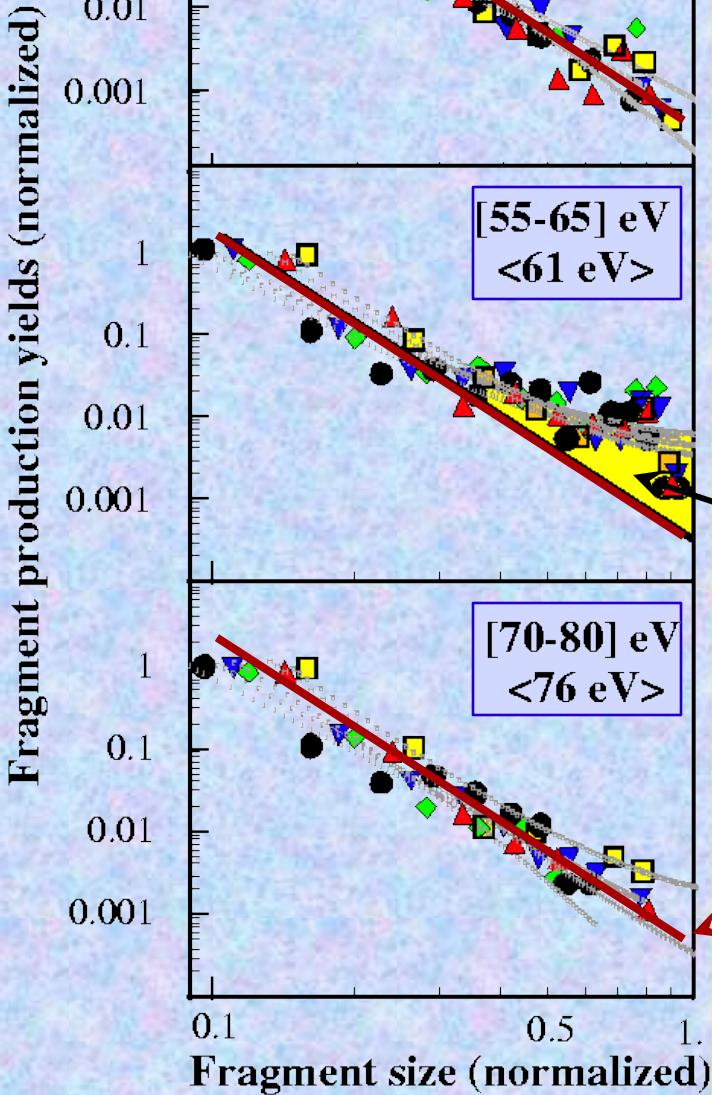
■ Partition => energy



# Fragmentation of hydrogen clusters

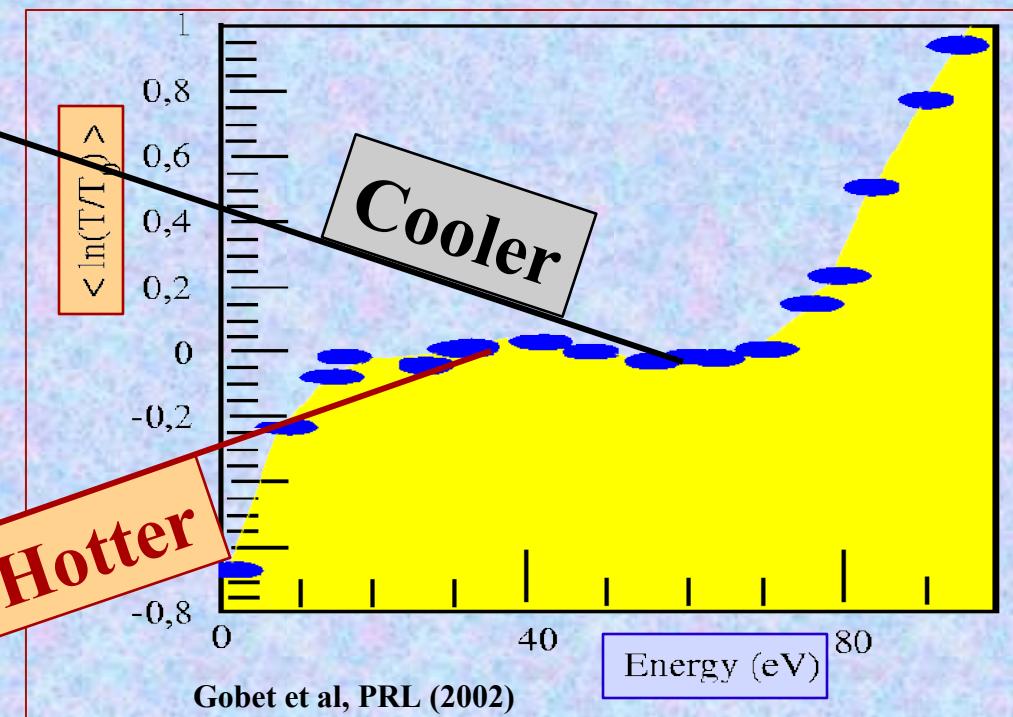
- Partition => energy
- Largest => Temperature

# Fragmentation of hydrogen clusters

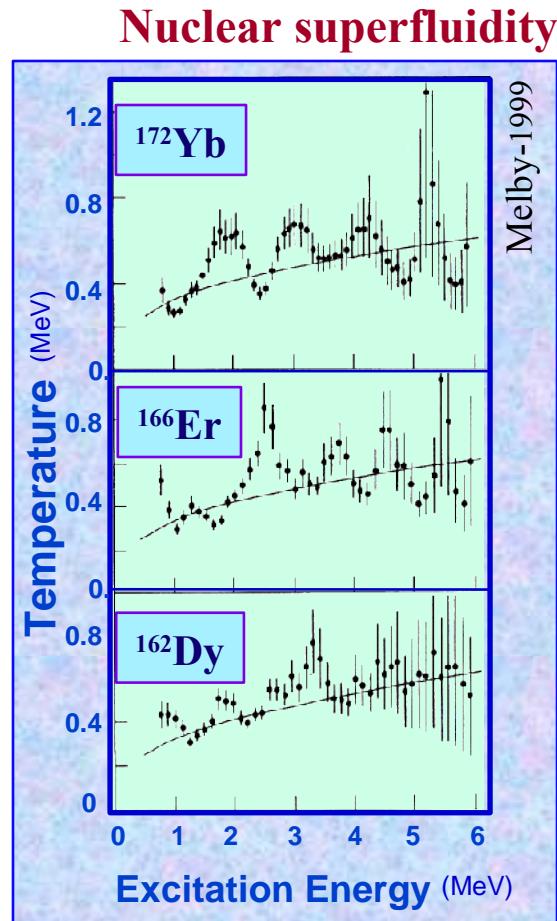


■ Partition => energy

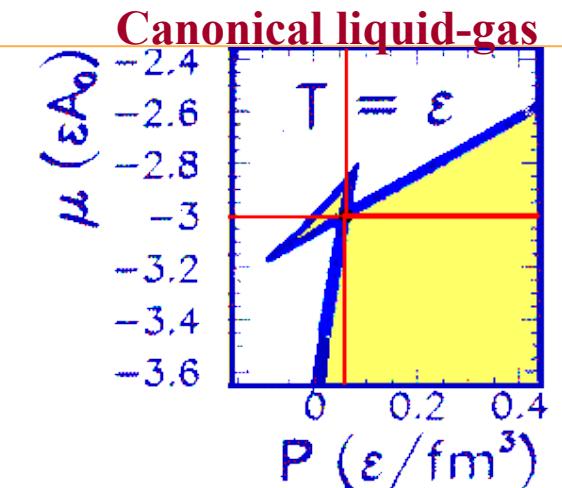
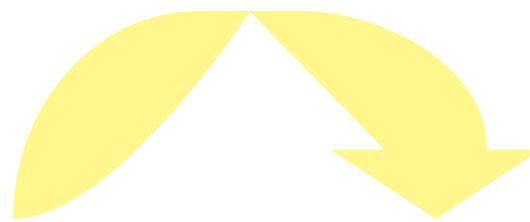
■ Largest => Temperature



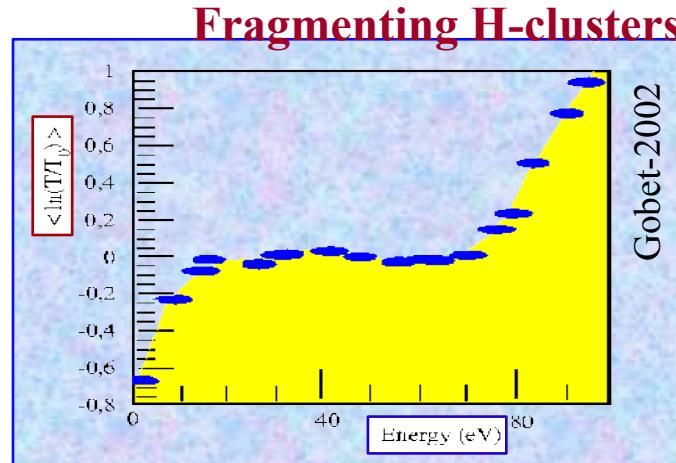
# Abnormal curvatures



Convex entropy



Compressibility  $< 0$   
Susceptibility  $< 0$



T decreasing with E

# -Appendix - I -

## Phase transition under flows

### ■ Exact theory for radial flow

- ◆ Isobar ensemble required
- ◆ Phase transition not affected

### ■ Example of oriented flow (transparency)

- ◆ Exact thermodynamics
- ◆ Effects on partitions



# Radial flow at “equilibrium”



- Equilibrium = Max S under constrains
- Additional constrains: radial flow  $\langle p_r(r) \rangle$

◆ Additional Lagrange multiplier  $\gamma(r)$

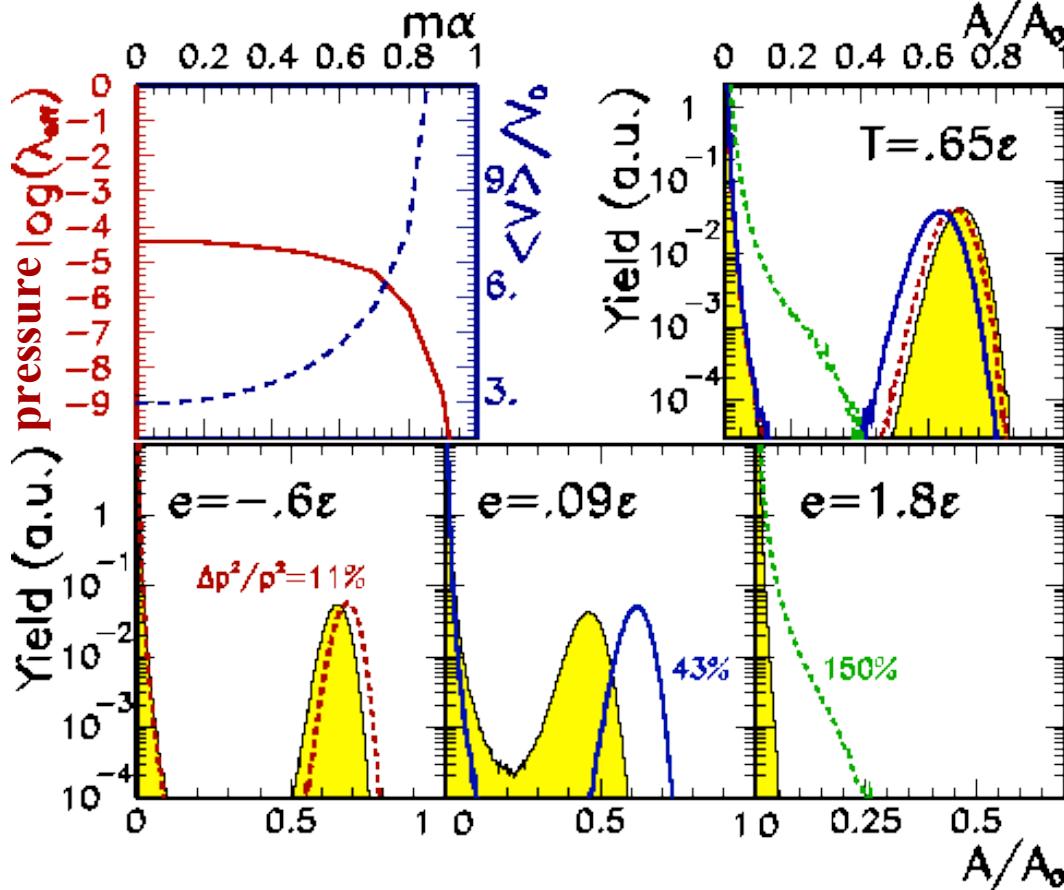
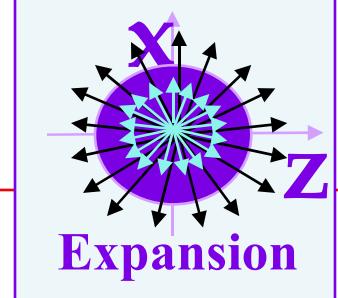
◆ Self similar expansion  $\langle p_r(r) \rangle = m \propto r \Rightarrow \gamma(r) = \beta \propto r$

Thermal distribution in the moving frame

Negative pressure Isobar ensemble

- Does not affect thermo is flow subtracted

# Radial flow at “equilibrium”

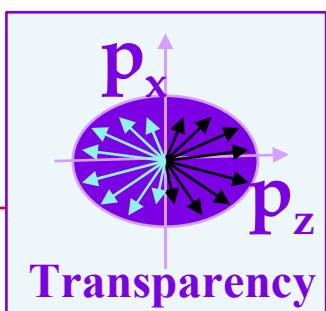


- ◆ Does not affect  $r$  partitioning
- ◆ Only reduces the pressure
- ◆ Shifts  $p$  distribution
- ◆ Changes fragment distribution:  
fragmentation less effective

■ **Does not affect thermo is flow subtracted**

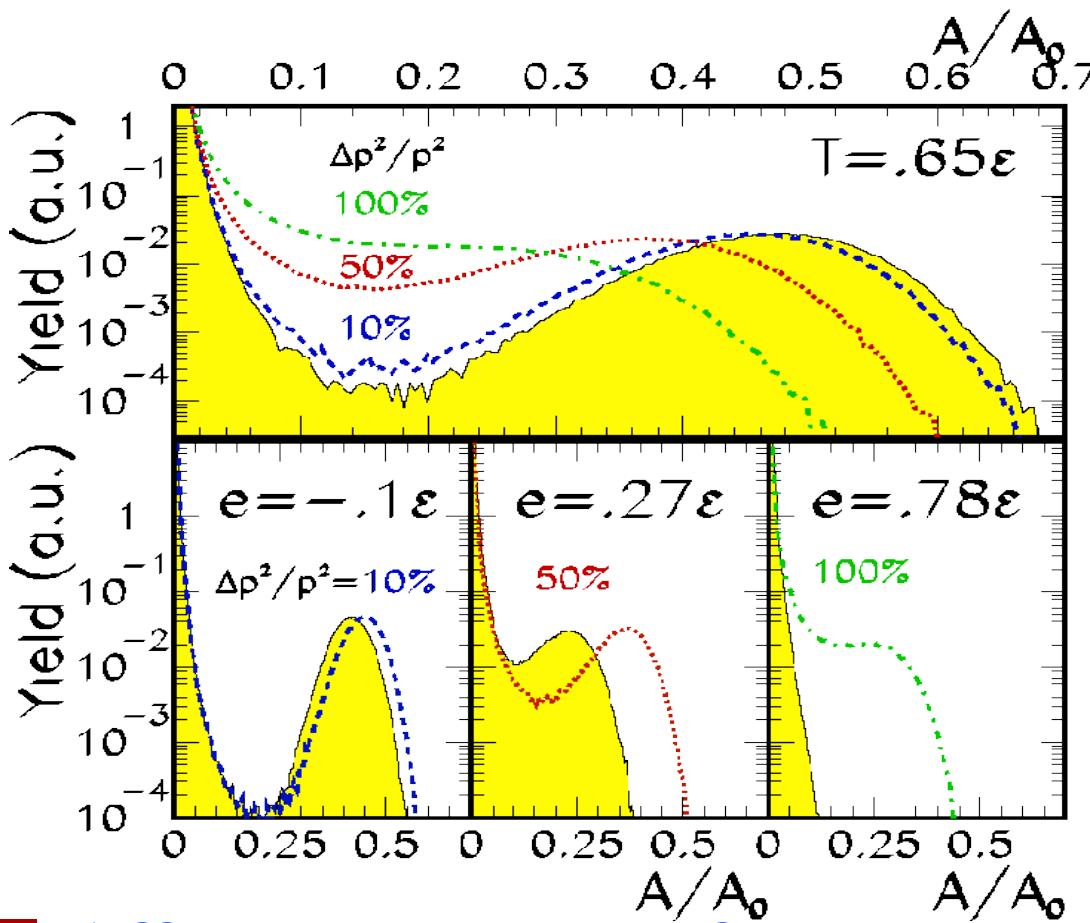
# Transparency at “equilibrium”

- Equilibrium = Max S under constrains
- Additional constrains: memory flow  $\langle \tau p_z \rangle$  { $\tau = -1$  target  
 $\tau = 1$  projectile
  - ◆ Additional Lagrange multiplier  $\alpha$
  - ◆ EOS leads to  $\langle \tau p_z \rangle = Ap_0$  with
- Affects p space and fragments,
- Does not affect the thermo if  $E_{flow}$  subtracted



Thermal distribution  
in moving frame

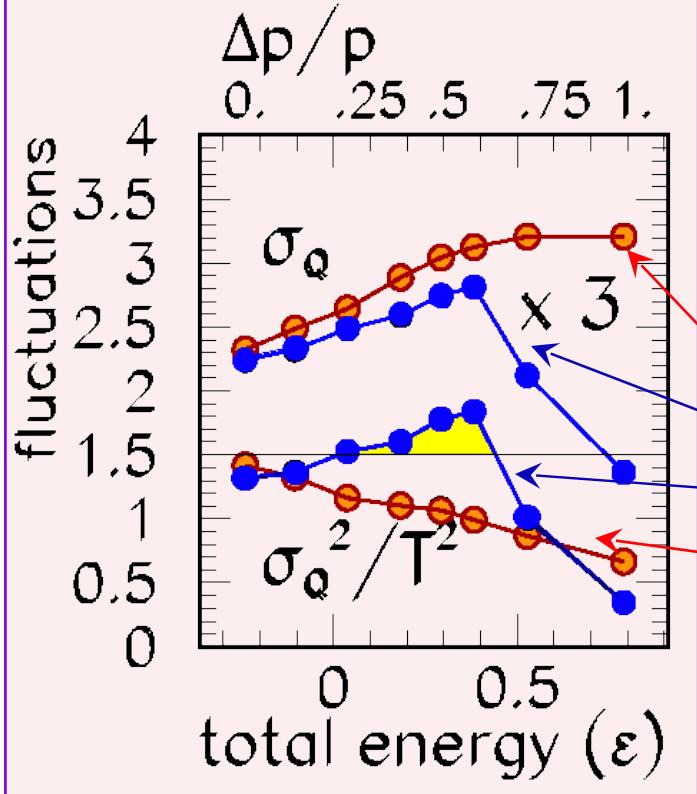
# Transparency at “equilibrium”



- ◆ Does not affect  $r$  partitioning
- ◆ Shifts  $p$  distribution
- ◆ Changes fragment distribution:  
fragmentation less effective

■ Affects  $p$  space and fragments

# Transparency at “equilibrium”



- Fragmentation less effective
- If  $E_{\text{flow}}$  not subtracted
  - ◆ Affect  $\langle E \rangle$
  - ◆ Affect  $T$  from  $\langle E_k \rangle$
  - ◆ Ex: Fluctuations of  $Q$  values
    - ◆ All thermal (from  $E = -2\varepsilon$ )
    - ◆ All relative motion
- Up to 10-15% no effect

- Affects  $p$  space and fragments



# - Appendix -II-

## Thermo with Coulomb

- Coulomb reduces coexistence and  $C < 0$  region
- Statistical treatment of Coulomb
  - ◆  $(E_N, V_C)$  a common phase diagram for charged and uncharged systems



# Coulomb reduces L-G transition

- Reduces coexistence

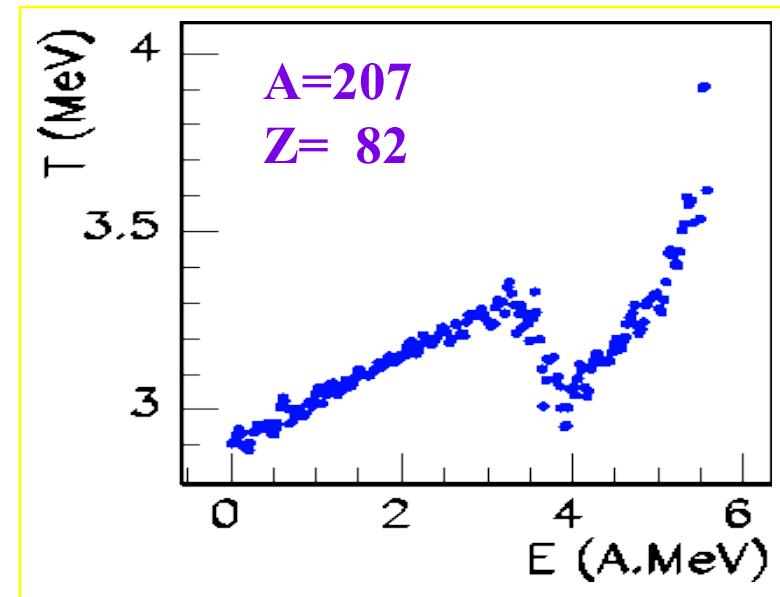
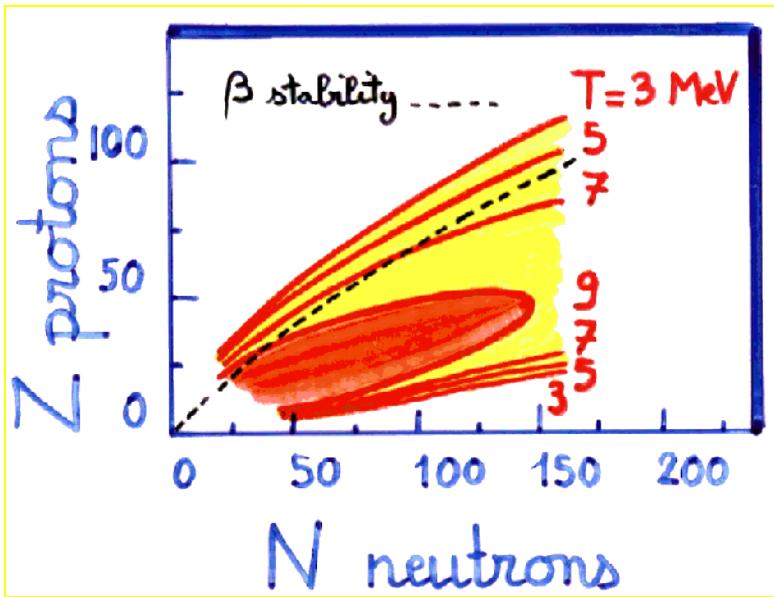
- ◆ Bonche-Levit-Vautherin

*Nucl. Phys. A427 (1984) 278*

- Reduces  $C < 0$

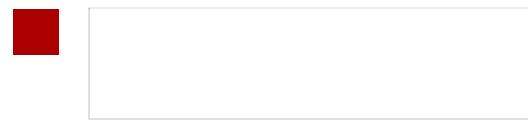
- ◆ Lattice-Gas

- ◆ OK up to heavy nuclei



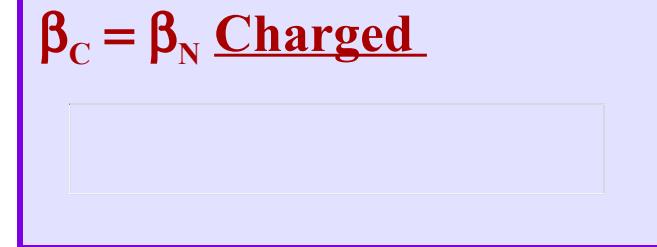
Gulminelli, PC, Comment to PRC66 (2002) 041601

# Statistical treatment of Non saturating forces interactions



- Effective charge  $q = 1$  charged system -
- Effective charge  $q = 0$  uncharged system -

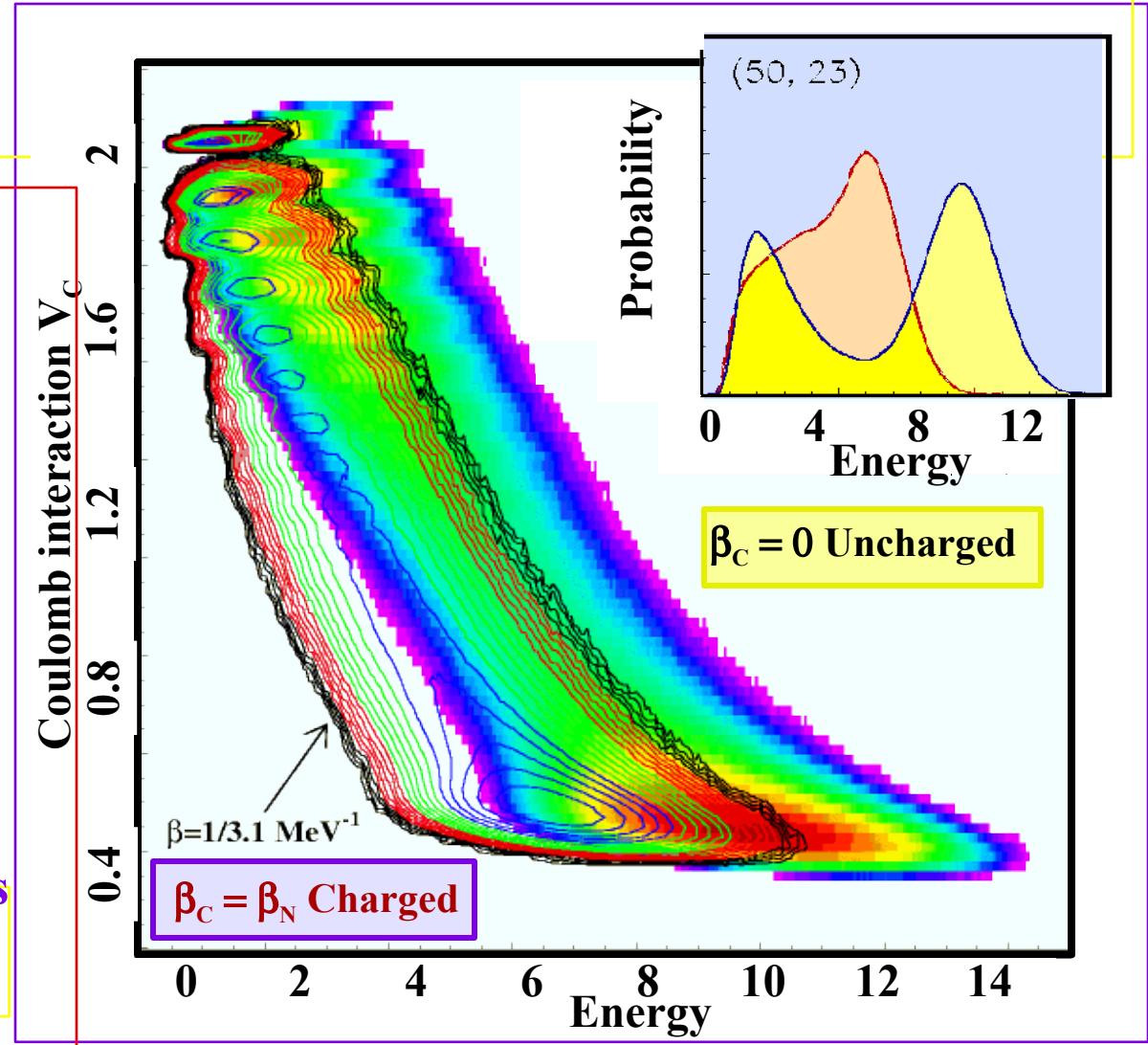
- A unique framework:  $e^{-\beta E} = e^{-\beta_N E_N} \cdot \beta_C V_C$ 
  - ◆ Introduce two temperatures  $\beta_N = \beta$  and  $\beta_C = q^2 \beta$
  - ◆ O two energies  $E_N$  and  $V_C$



# With and without Coulomb a unique

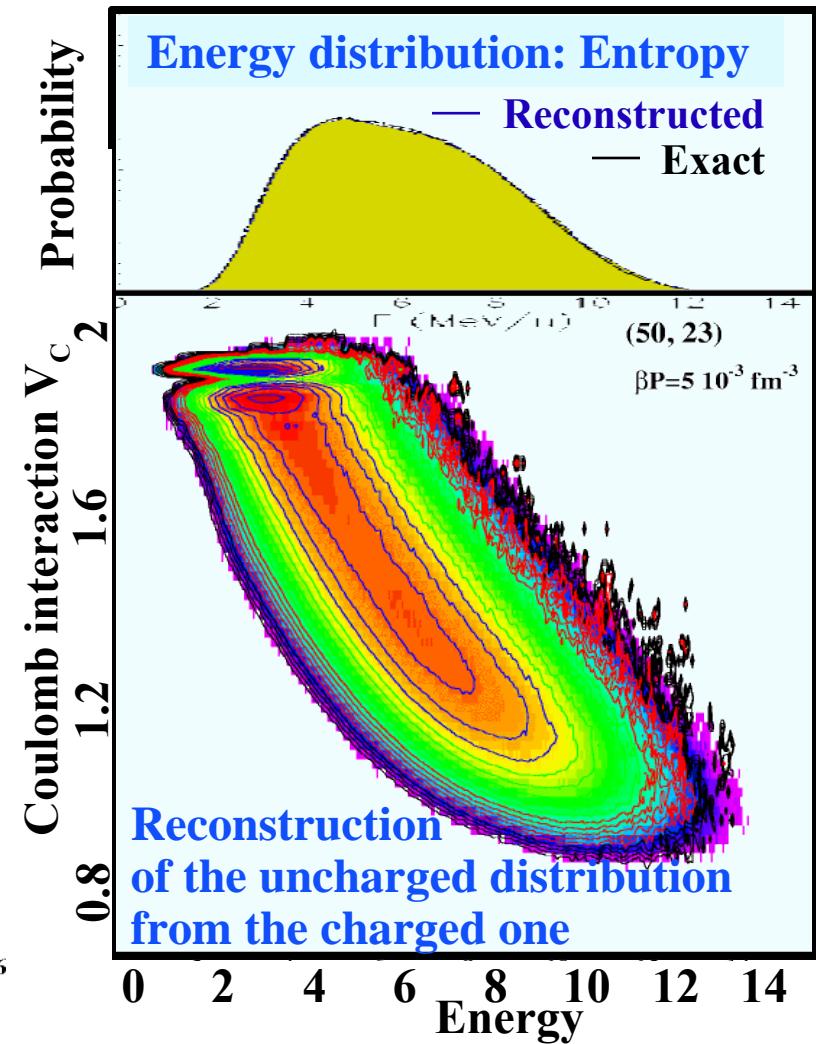
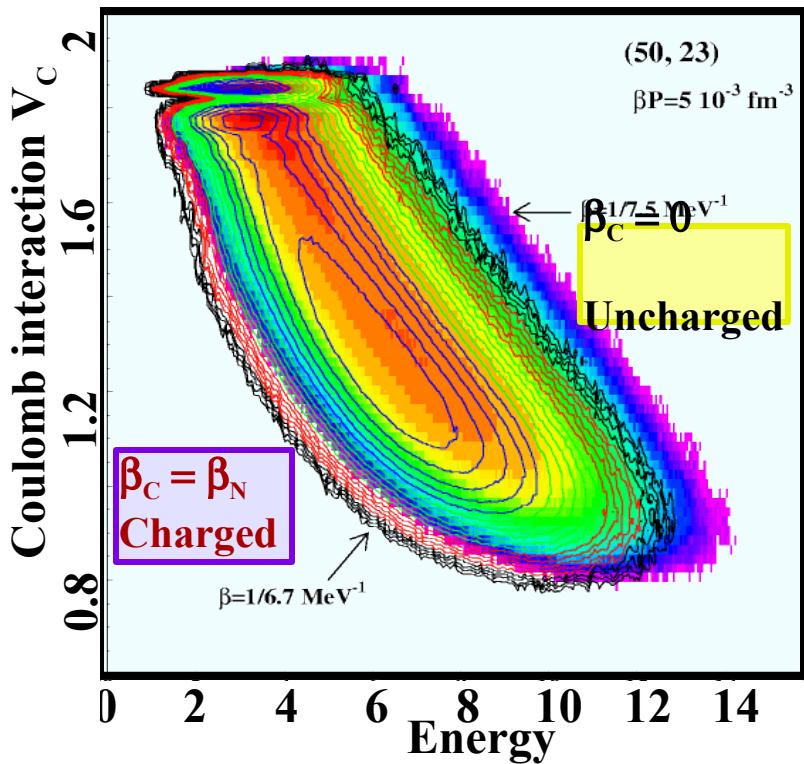
$$S(E_N, V_C)$$

- $(E_N, V_C)$  a unique phase diagram
  - Coulomb reduces E bimodality
    - ◆ different weight
    - ◆ rotation of E axis
- $E = E_N + V_C$ , charged  
 $E = E_N$ , uncharged



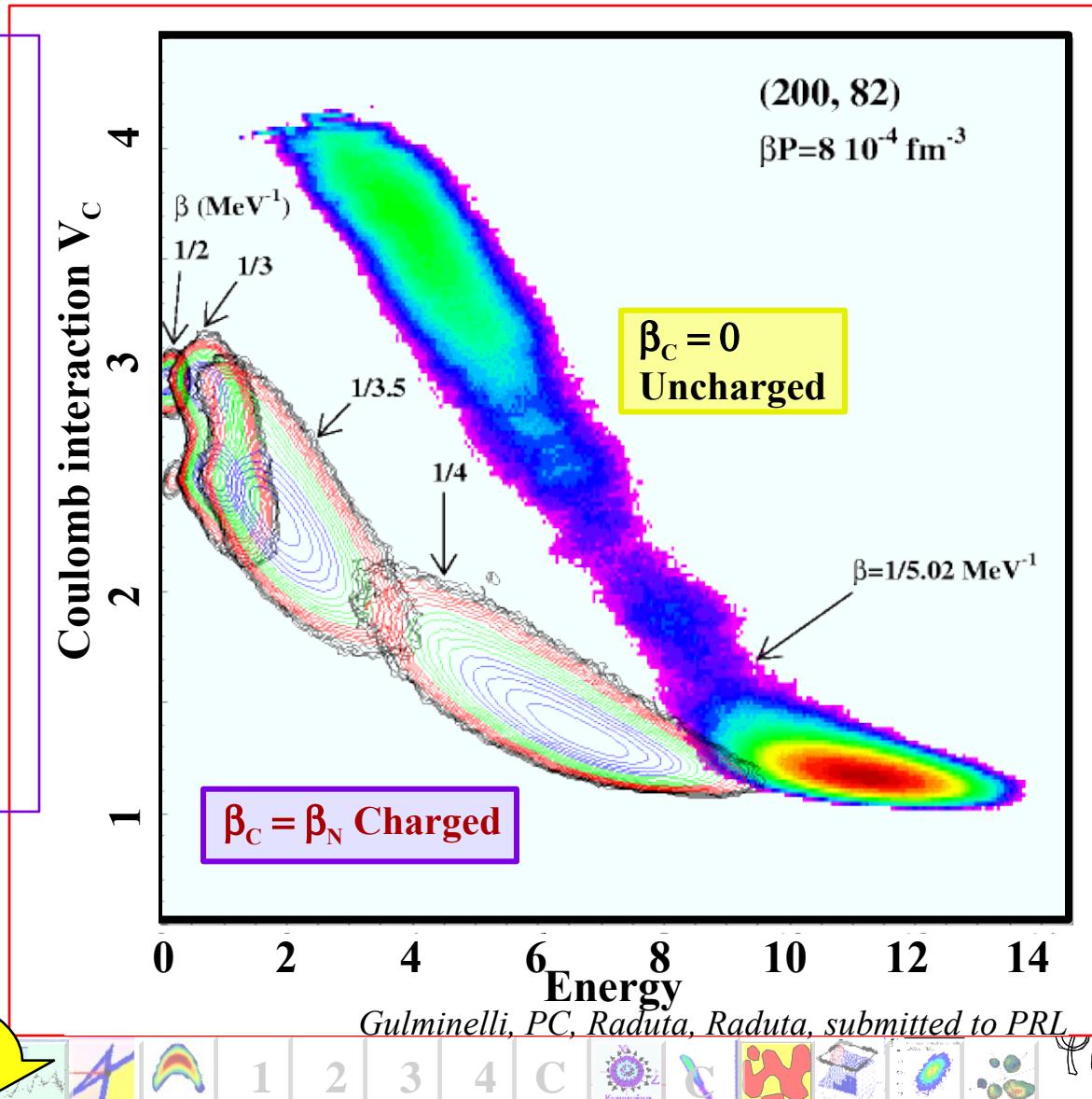
# Correction of Coulomb effects

- If events overlap



# Partitions may differ for heavy nuclei

- Channels are different  
(cf fission)
- Re-weighting impossible
- However, a unique phase diagram  
( $E_N$   $V_C$ )





# -Appendix - III -

## Equilibrium in finite systems

### ■ Macroscopic

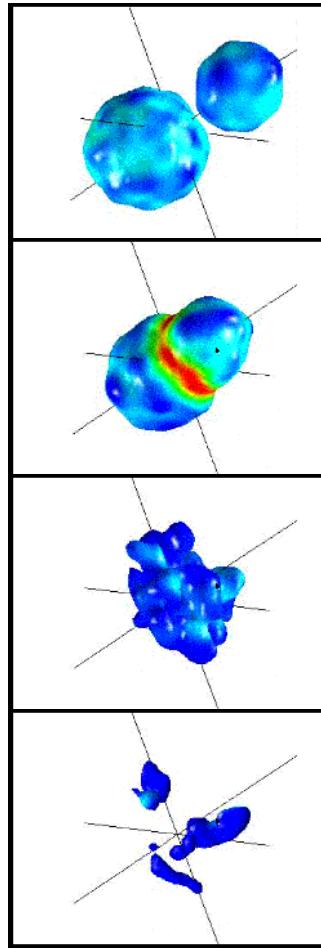
- ◆ One realization (event) at equilibrium

### ■ Microscopic

- ◆ Statistical ensemble and information
- ◆ Ergodicity versus mixing dynamics
- ◆ Multiplicity of equilibria
- ◆ What is temperature?



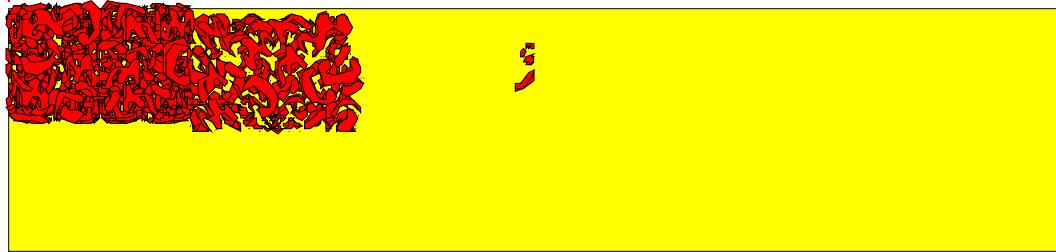
# Equilibrium : What Does It Mean?



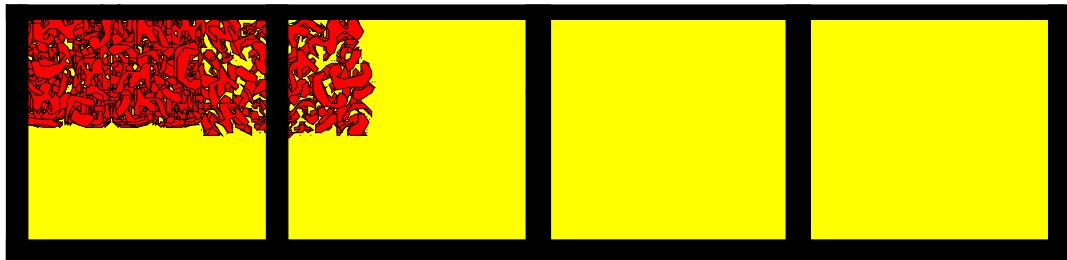
- Finite systems
  - ◆ In time
  - ◆ In space

- Isolated open systems
  - ◆ No reservoir or bath
  - ◆ No container

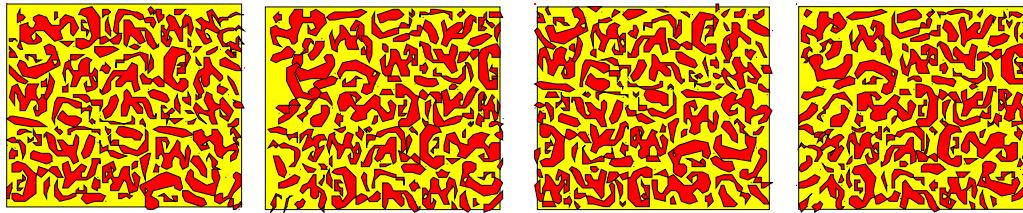
# Equilibrium : What Does It Mean?



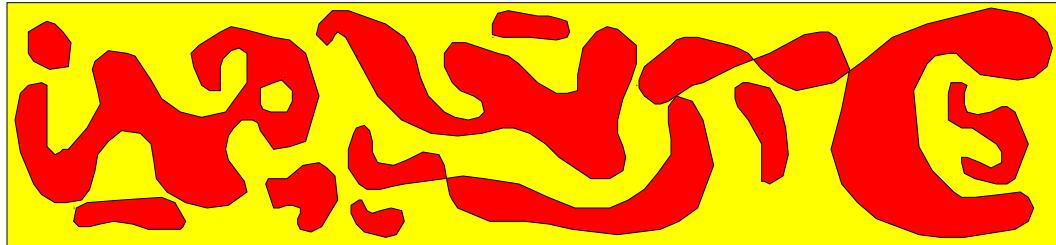
- Thermodynamics : infinite system



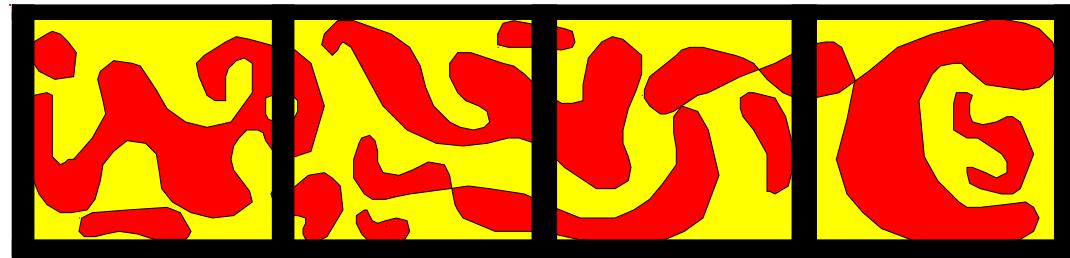
- One  $\infty$  system = ensemble of  $\infty$  sub-systems



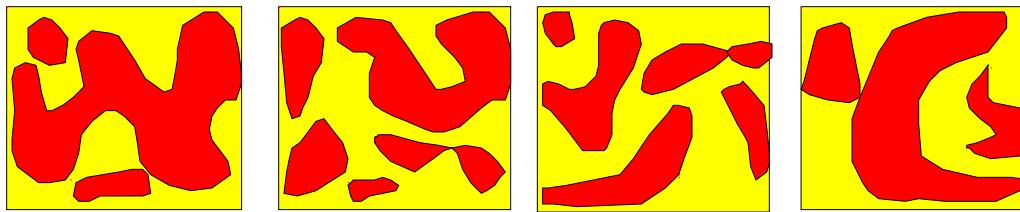
# Equilibrium : What Does It Mean?



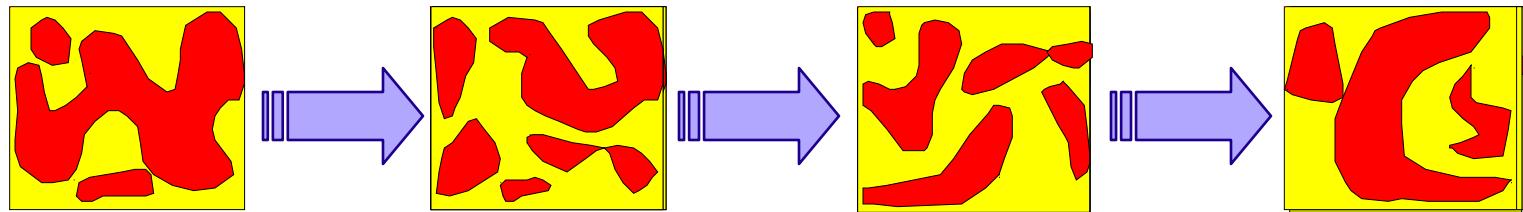
- Finite system



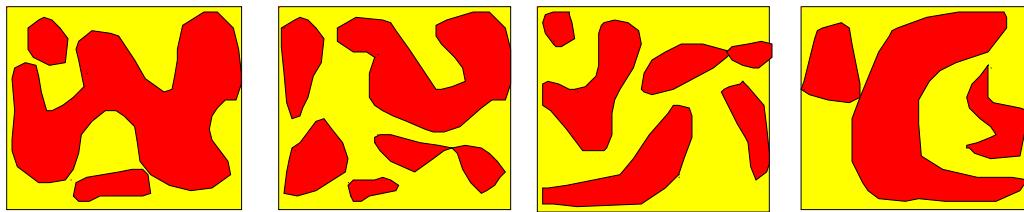
- Cannot be cut in sub-systems



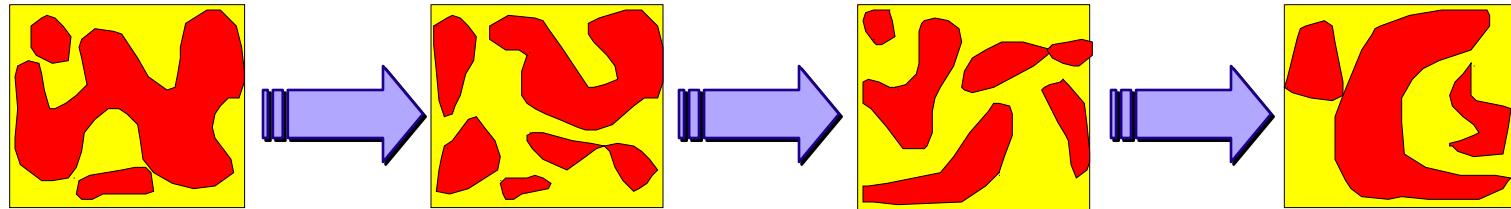
# Equilibrium : What Does It Mean?



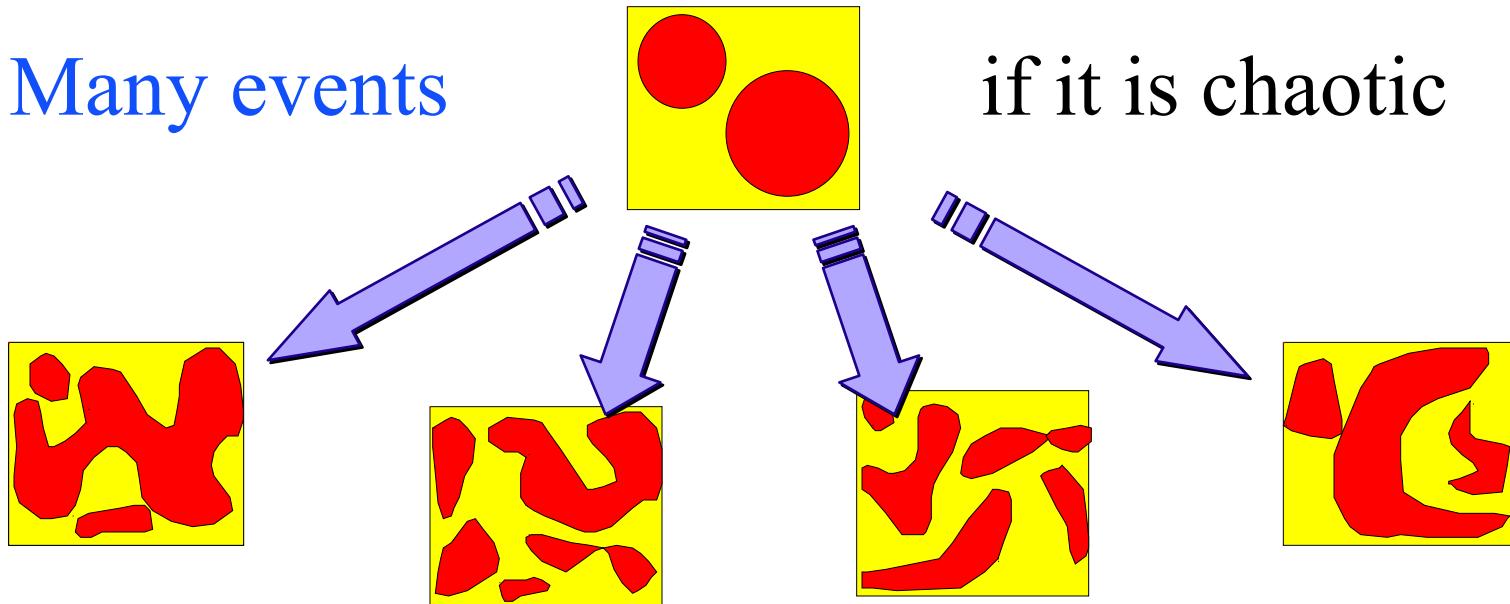
- One small system in time      if it is ergodic  
Is a statistical ensemble
- Cannot be cut in sub-systems



# Equilibrium : What Does It Mean?

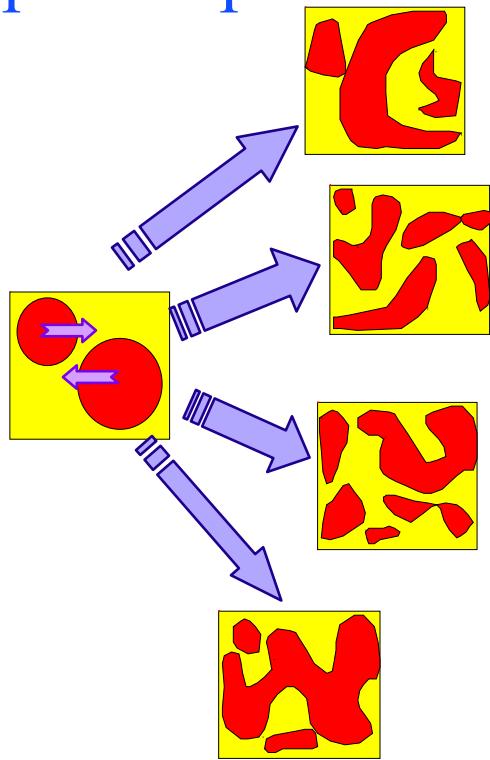


- One small system in time      if it is ergodic
- Many events                        if it is chaotic



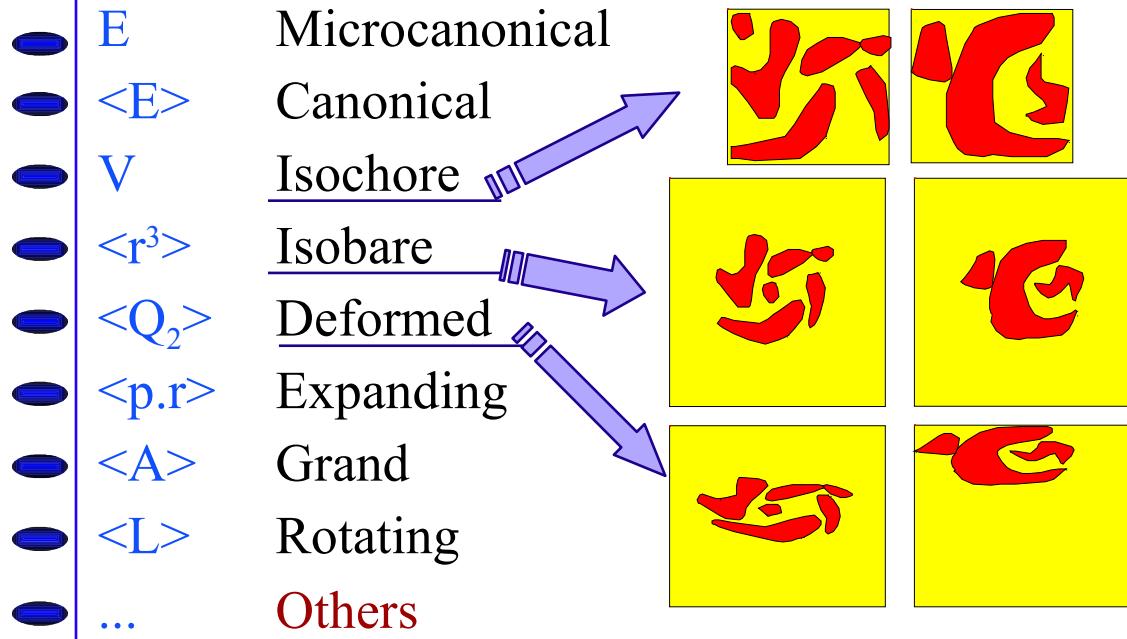
# Statistics from minimum information

- “Chaos” populates phase space

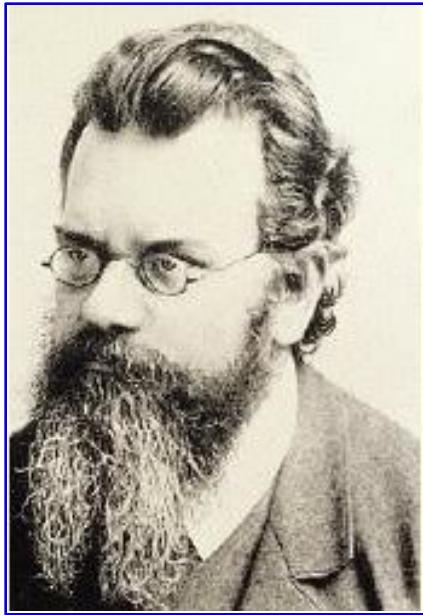


- Dynamics: global variables
- Statistics: population

◆ Many different ensembles



# What is temperature ?



L. Boltzmann

■  $W$  equiprobable microstates



Entropy = disorder (-information)

■  $T$  is the entropy increase



R. Clausius

# What is temperature ?

## ■ The microcanonical temperature

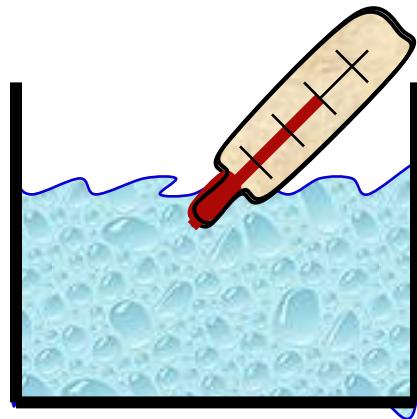
$$S = k \log W$$

$$\delta S = T^{-1} \delta E$$



# What is temperature ?

- It is what thermometers measure.



$$E = E_{\text{thermometer}} + E_{\text{system}}$$

- The microcanonical temperature

$$S = k \log W$$

$$\delta S = T^{-1} \delta E$$

# What is temperature ?

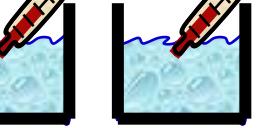
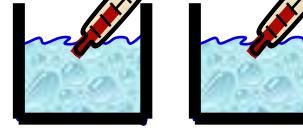
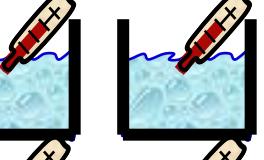
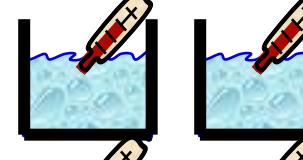
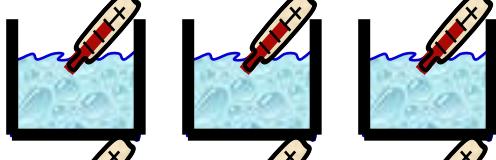
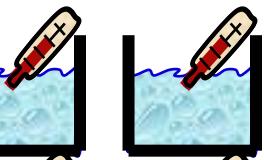
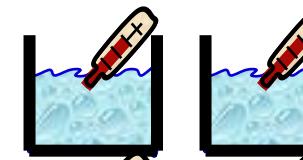
- It is what thermometers measure.



$$E = E_{\text{thermometer}} + E_{\text{system}}$$



Distribution of microstates



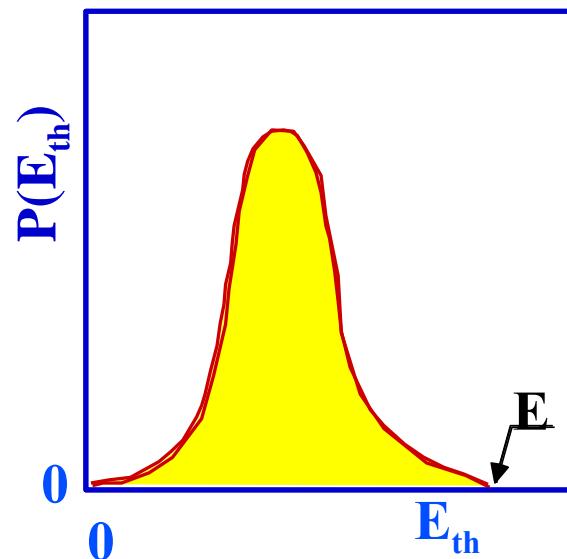
- The microcanonical temperature

$$S = k \log W$$

$$\delta S = T^{-1} \delta E$$

# What is temperature ?

- It is what thermometers measure.



$$E = E_{\text{th}} + E_{\text{sys}}$$

Distribution of microstates

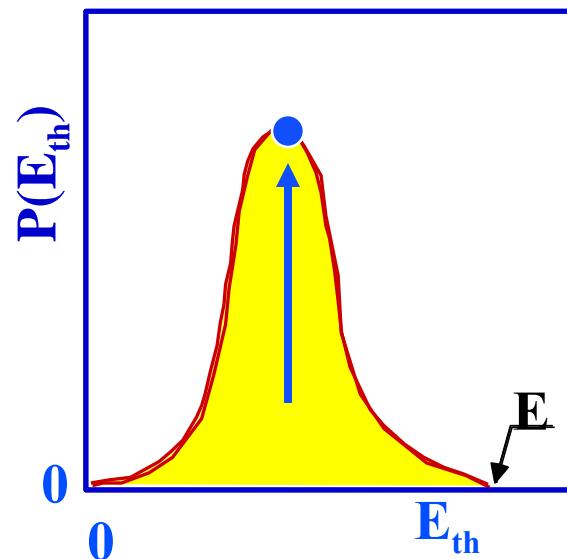
- The microcanonical temperature

$$S = k \log W$$

$$\delta S = T^{-1} \delta E$$

# What is temperature ?

- It is what thermometers measure.



$$E = E_{\text{th}} + E_{\text{sys}}$$

Equiprobable microstates

$$P(E_{\text{th}}) \propto W_{\text{th}}(E_{\text{th}})^* W_{\text{sys}}(E-E_{\text{th}})$$
$$\max P \Rightarrow \delta \log W_{\text{th}} - \delta \log W_{\text{sys}} = 0$$

$$\max P \Rightarrow \delta S_{\text{th}} - \delta S_{\text{sys}} = 0$$

**Most probable partition:  $T_{\text{th}} = T_{\text{sys}}$**

- The microcanonical temperature

$$S = k \log W$$

$$\delta S = T^{-1} \delta E$$



# -Appendix -IV-

## C<0 in Liquid gas transition

- Negative heat capacity in fluctuating volume ensemble
  - ◆ Difference between  $C_p$  and  $C_v$
- Difference between C and E(T)
  - ◆ Role of the thermo transformation
- Negative heat capacity in statistical models and Channel opening



- a -

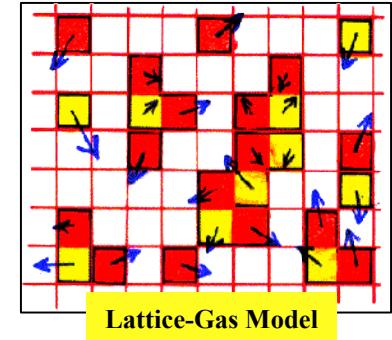
# Role of volume fluctuations

Fixed volume  $C_v > 0$  but  $K < 0$

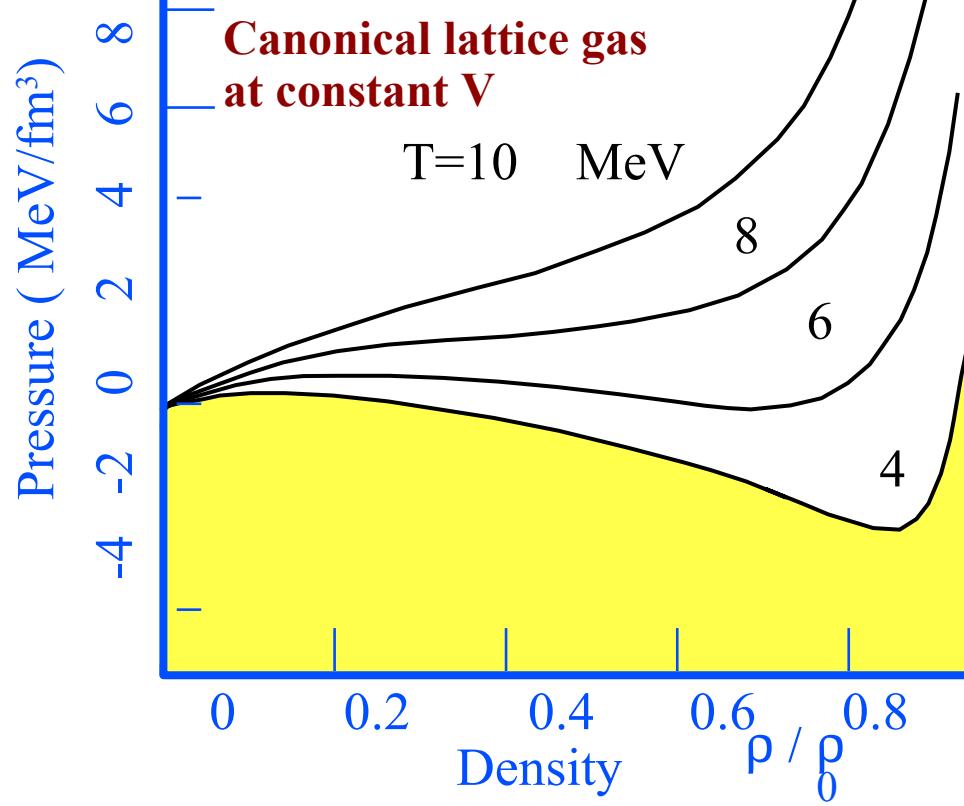
Open systems  $C_p < 0$

# Volume: order parameter

## L-G in a box: $V=\text{cst}$



Lattice-Gas Model

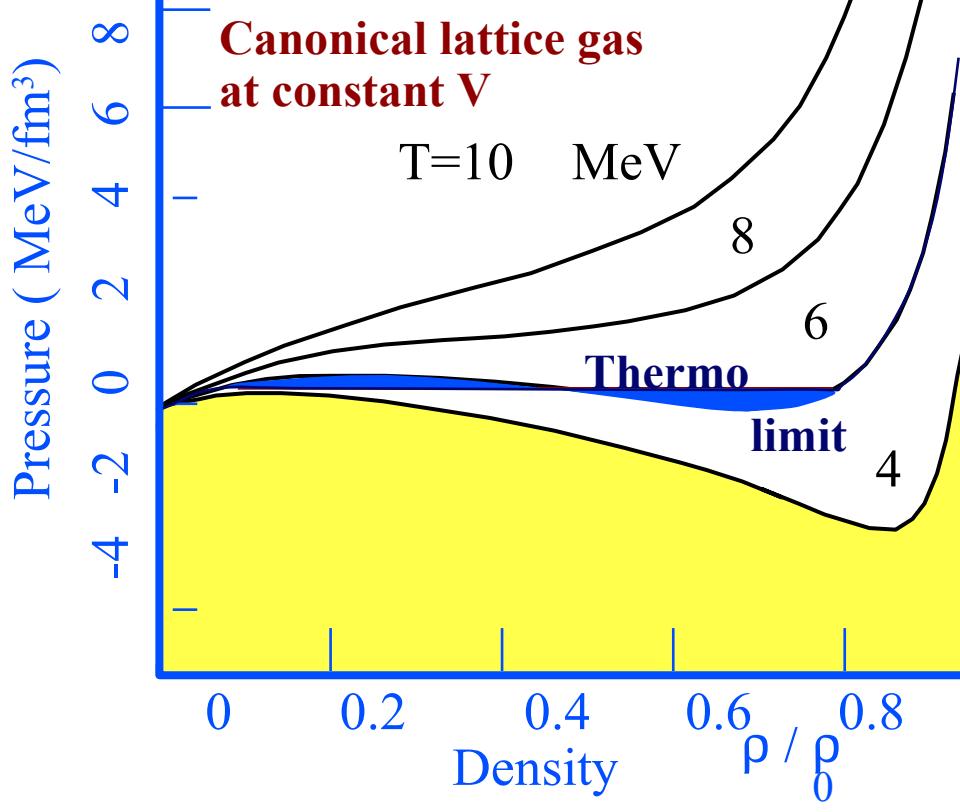
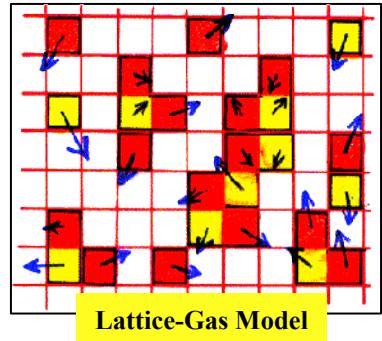


■ Negative compressibility

Gulminelli & PC PRL 82(1999)1402

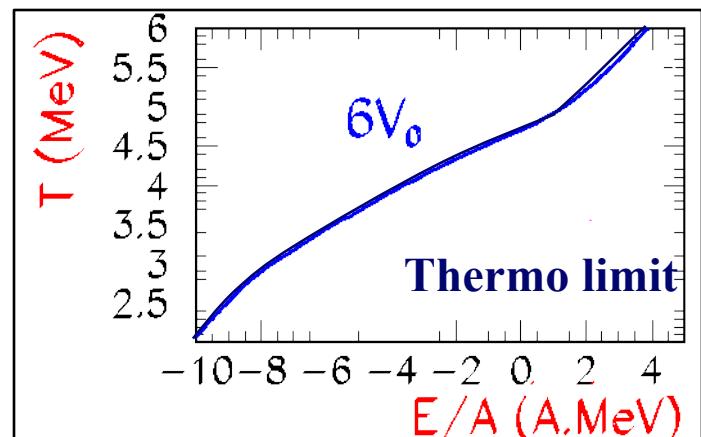
# Volume: order parameter

## L-G in a box: $V=\text{cst}$



■ Negative compressibility  
*Gulminelli & PC PRL 82(1999)1402*

■  $C_V > 0$



See specific discussion for large systems

Pleimling and Hueller, *J.Stat.Phys.* 104 (2001) 971

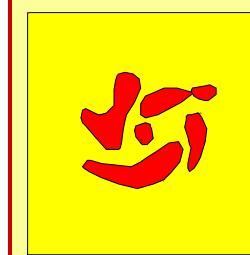
Binder, *Physica A* 319 (2002) 99.

Gulminelli et al., *cond-mat/0302177*, *Phys. Rev. E*.

# Open systems (no box)

## Fluctuating volume

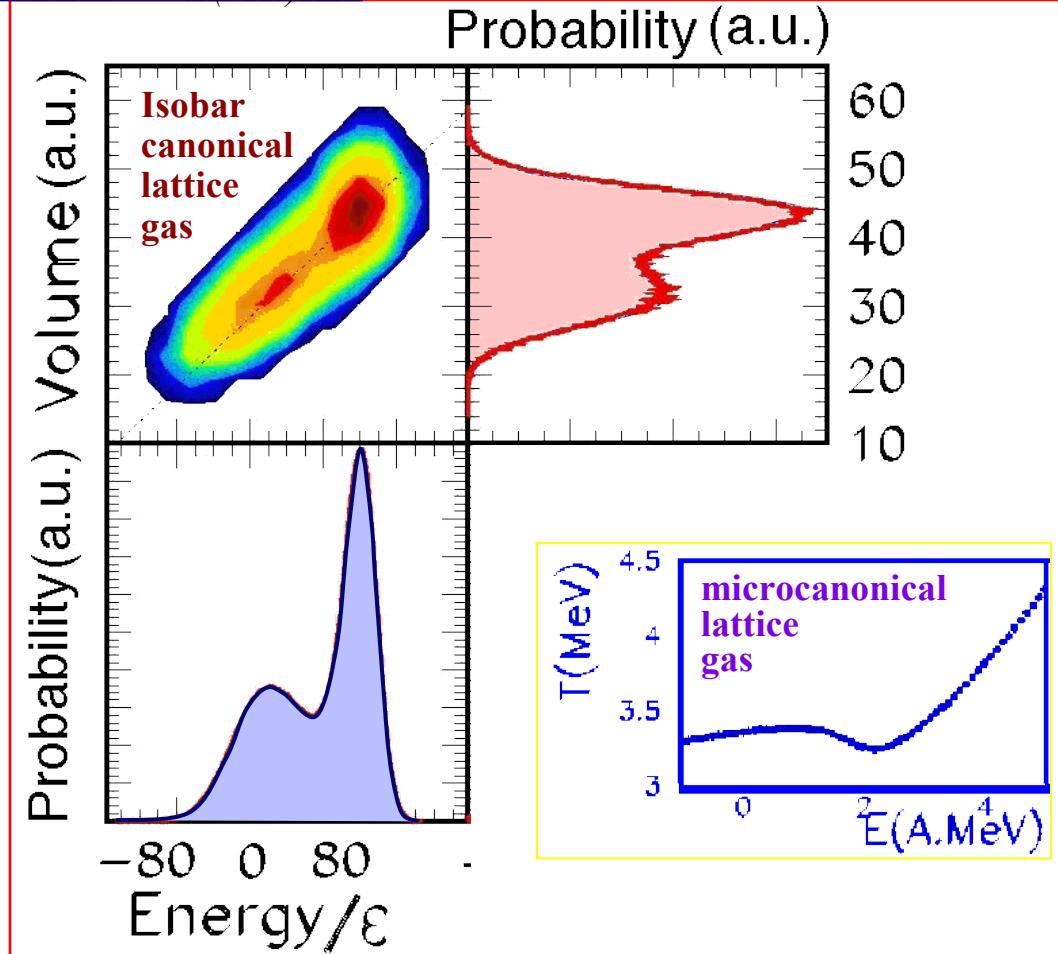
PC, Duflot & Gulminelli PRL 85(2000)3587



Isobar  
ensemble

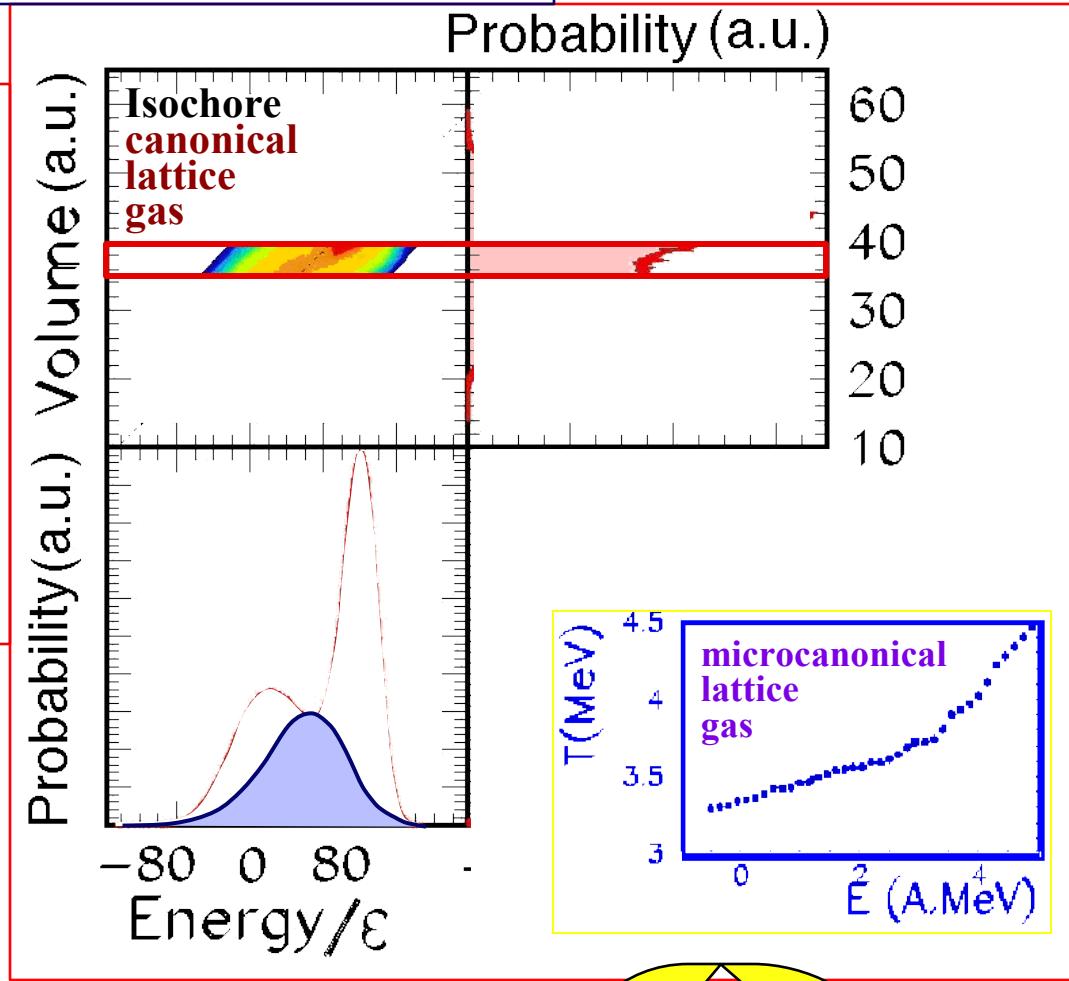
$$P^{(i)} \propto \exp -\lambda V^{(i)}$$

- Bimodal  $P(V)$ 
  - ◆ Negative compressibility
  
- Bimodal  $P(E)$ 
  - ◆ Negative heat capacity  $C_p < 0$



# Constrain on V i.e. on order parameter

- Suppresses bimodal  $P(E)$ 
  - ◆ No negative heat capacity  $C_V > 0$



See specific discussion for large systems

Pleimling and Hueller, J.Stat.Phys.104 (2001) 971

Binder, Physica A 319 (2002) 99.

Gulminelli et al., cond-mat/0302177, Phys. Rev. E.

- b -

Pressure dependent EOS  
Caloric Curves not EOS  
Fluctuations measure EOS

# Volume dependent T(E)

■ 2-D EOS

$$\begin{array}{c} E \longrightarrow T \\ V \longrightarrow P \end{array}$$

Temperature

Energy

Pressure



# Volume dependent T(E)

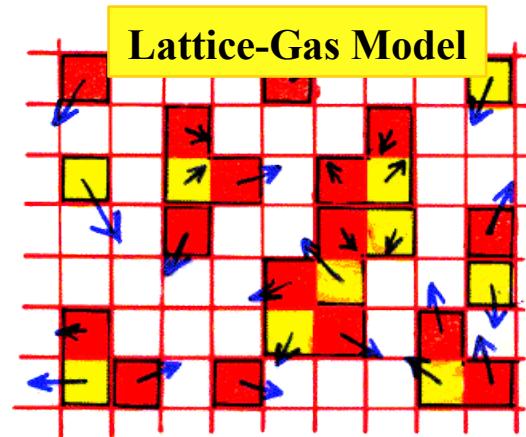
■ 2-D EOS

$$\begin{array}{c} E \longrightarrow T \\ V \longrightarrow P \end{array}$$

Temperature

Energy

Pressure



# Volume dependence of T<sub>CF</sub>

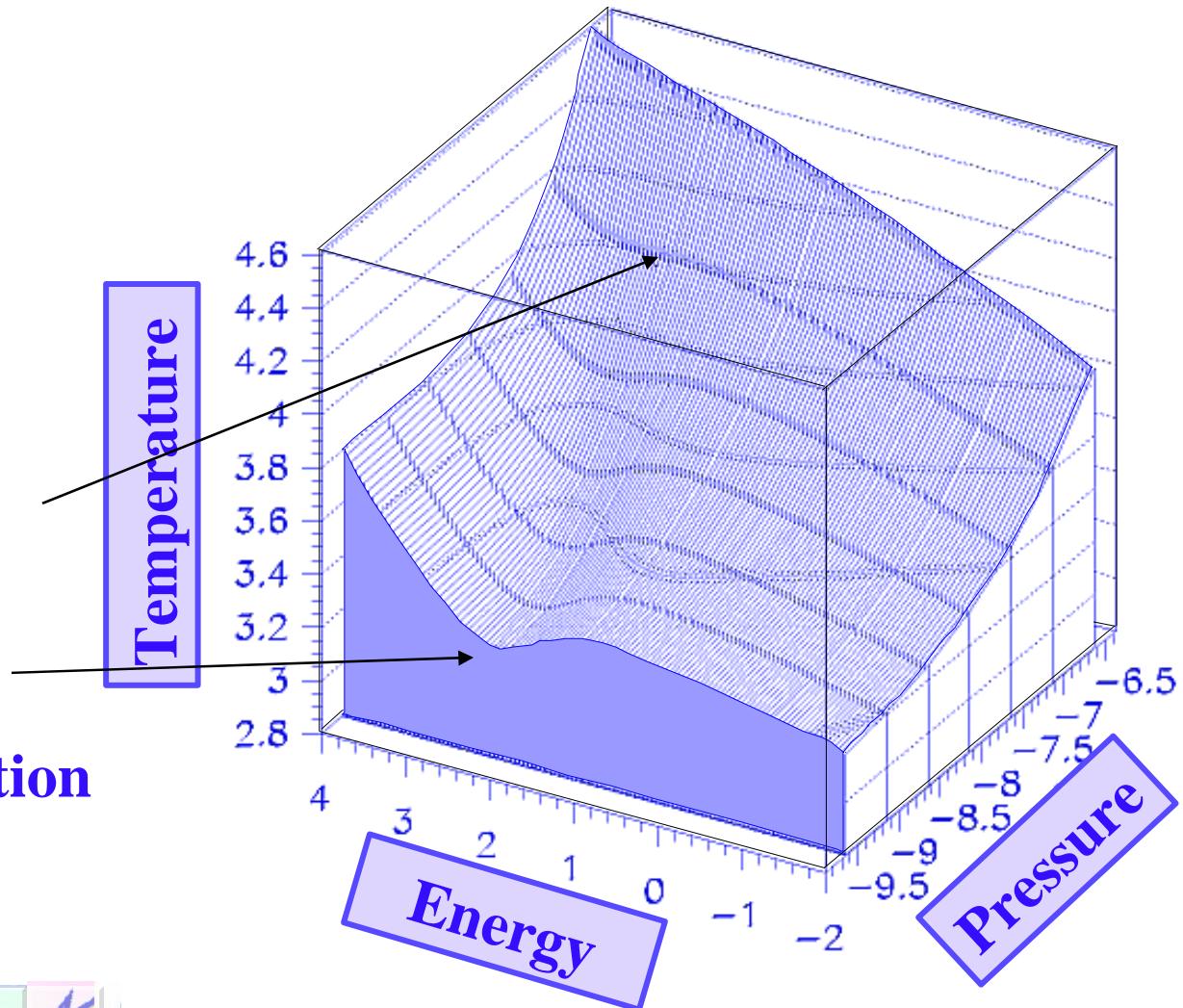
## ■ 2-D EOS

$$E \longrightarrow T$$

$$V \longrightarrow P$$

■ Critical point

■ First order  
Liquid gas  
Phase Transition

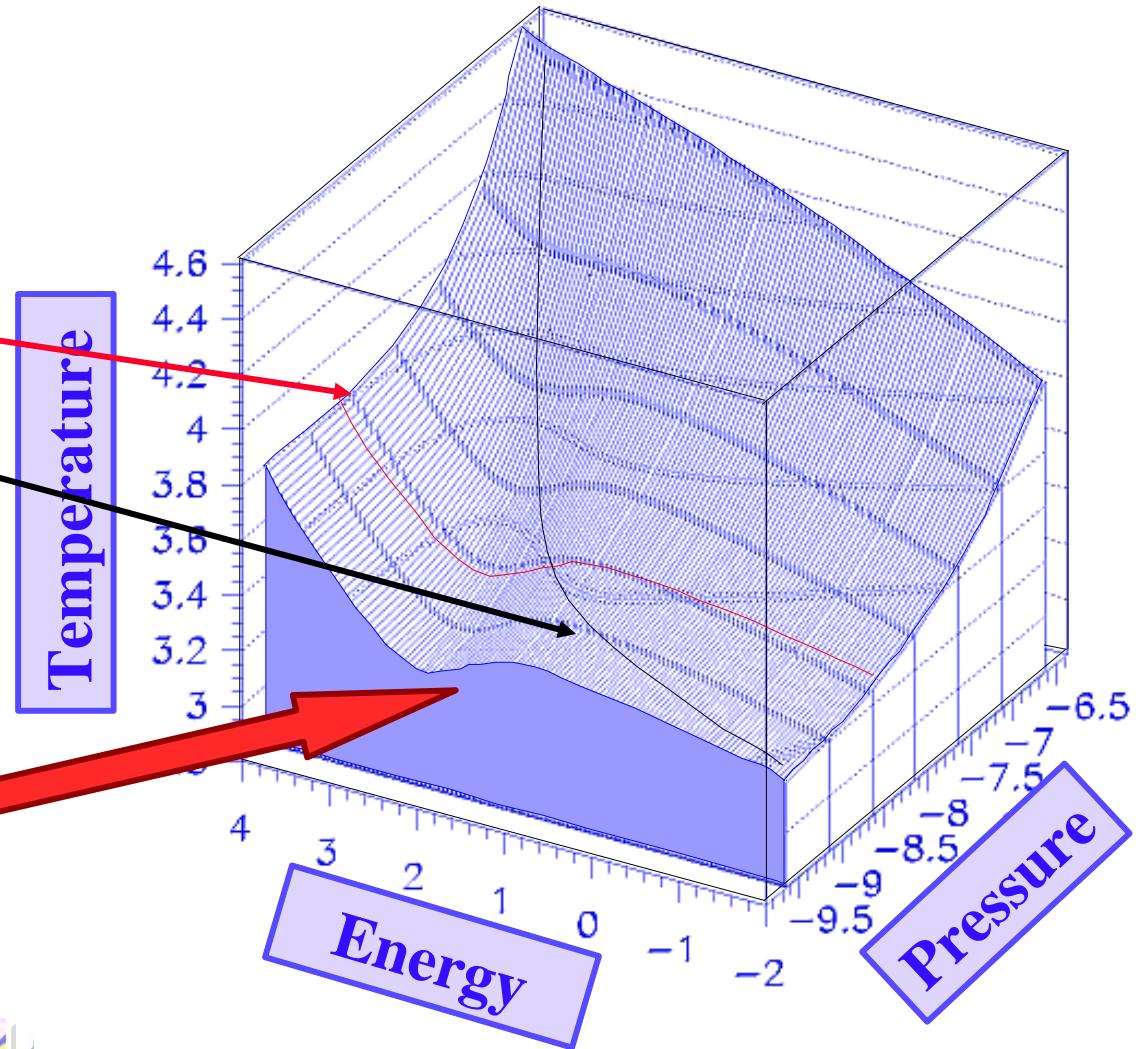


# Volume dependent TCFs

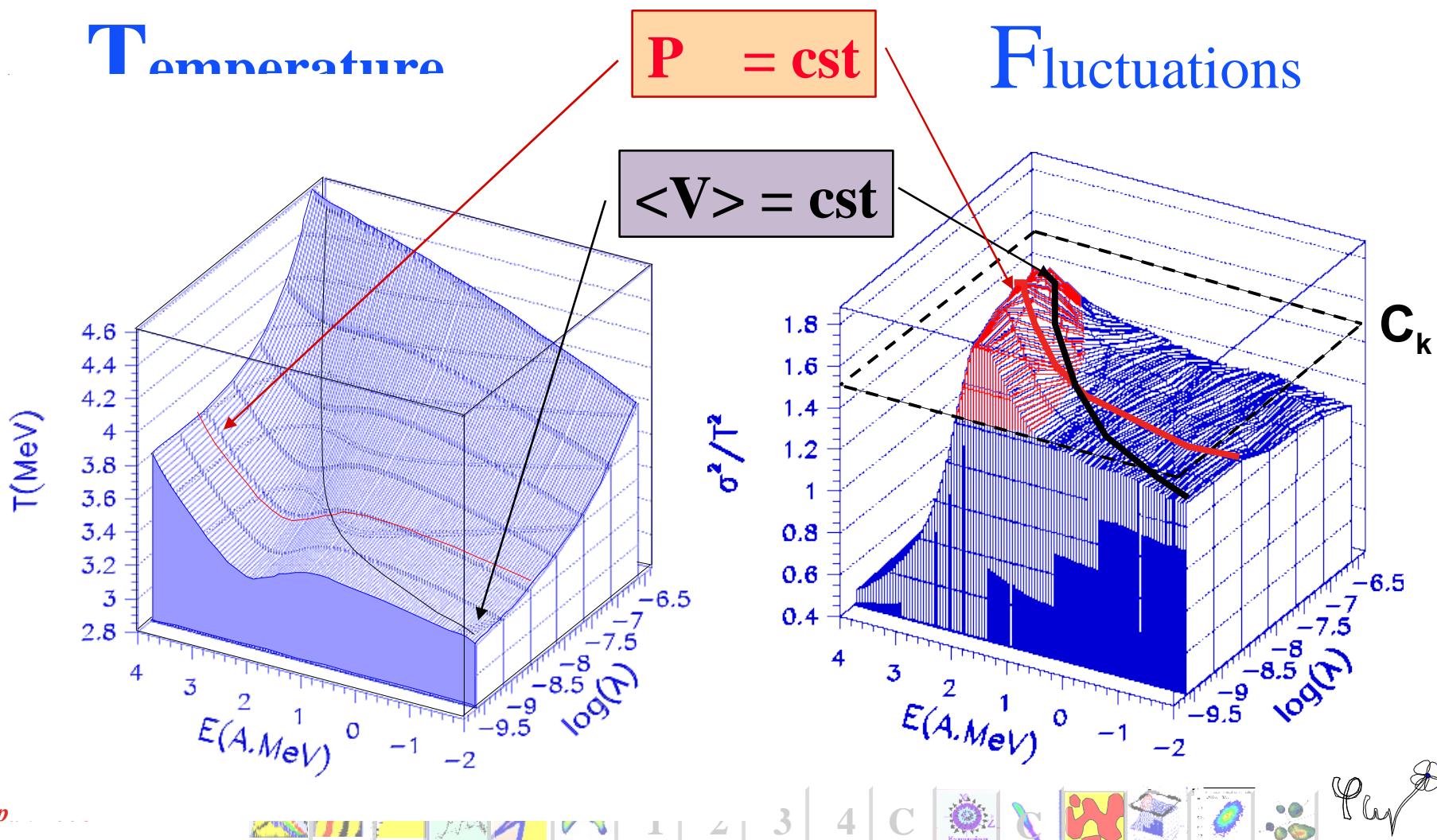
## ■ Transformation dependent Caloric Curve

- $P = \text{cst}$
- $\langle V \rangle = \text{cst}$

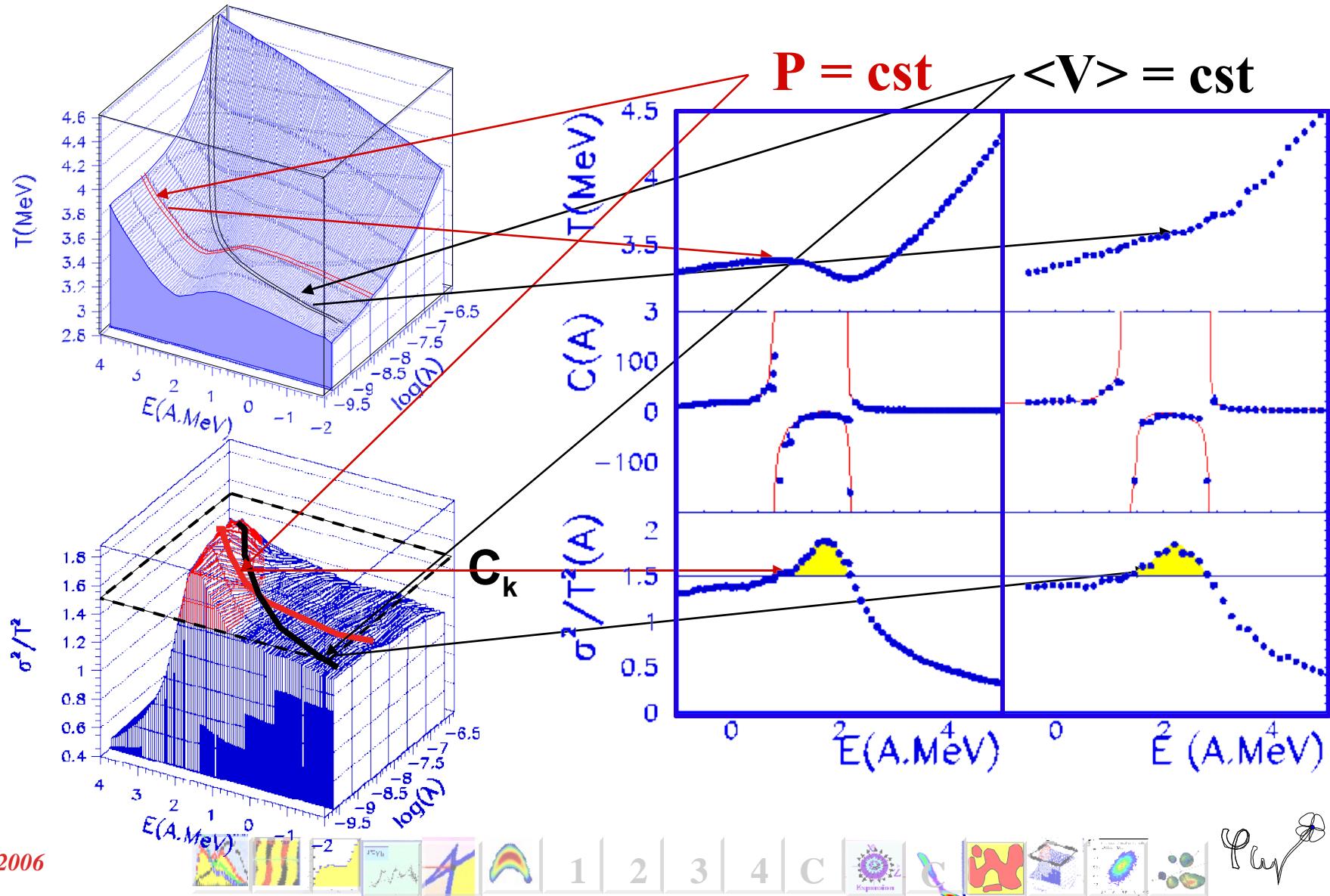
## ■ Negative Heat Capacity



# Volume dependent EOS

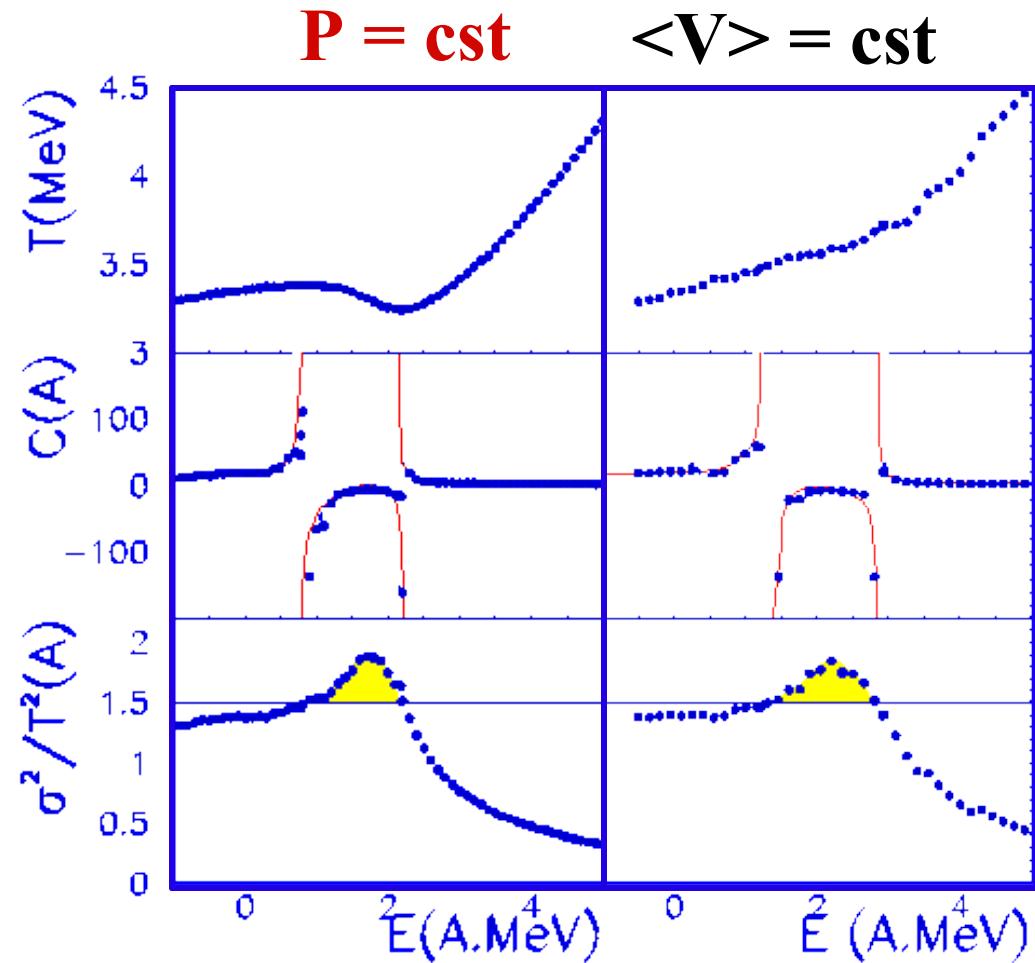


# Volume dependent EOS



# Volume dependent EOS

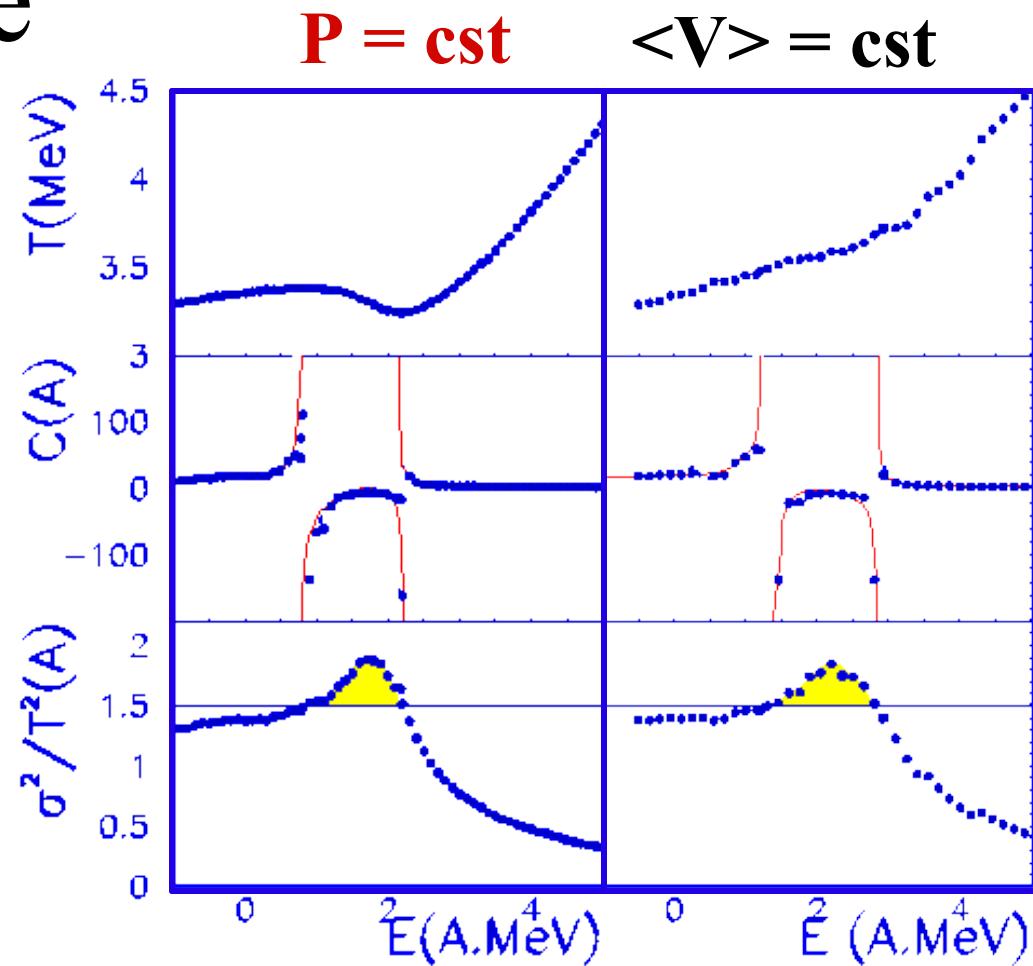
- The Caloric curve depends on the transformation
- $C$  is not  $dT/dE$
- $\sigma^2$  measures EOS Abnormal in Liquid-Gas



# Caloric curve are not EOS

## Fluctuations are

- The Caloric curve depends on the transformation
- $C$  is not  $dT/dE$
- $\sigma^2$  measures EOS
- $\sigma^2$  abnormal in Liquid-Gas



- C -

# Negative curvatures

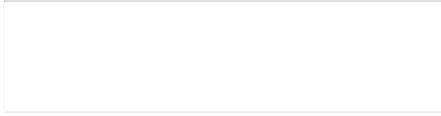
## Channel opening

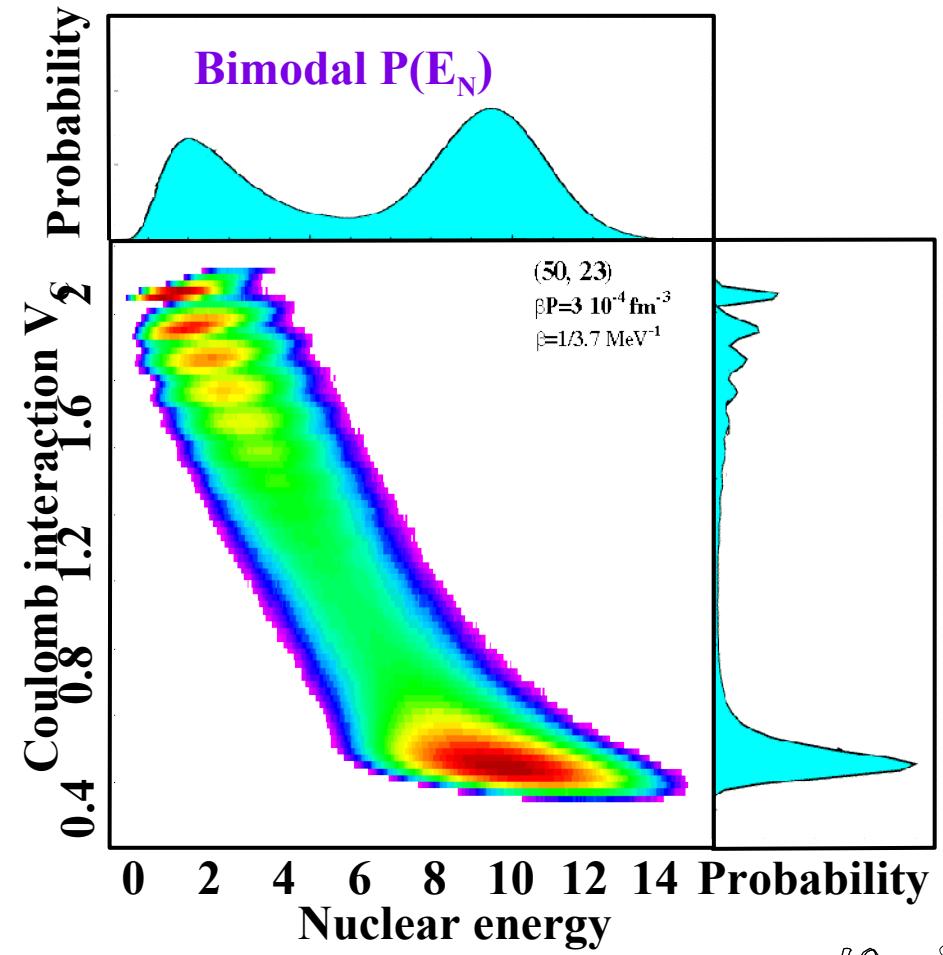
### Ex: Statistical models



# C<0 in statistical models

## Liquid-gas and channel opening

- 
- ◆  $q = 0 \Rightarrow$   
no-Coulomb
- Many channel opening
- One Liquid-Gas transition ( $V_c$  related to  $V$ )





# -Appendix -V-

## How to progress

- Correcting errors in  $\sigma$  reconstruction
  - ◆ Iterative procedure
- C from other observables
  - ◆ Using correlated observables



# Correction of experimental errors

## ■ Heat capacity from fluctuations



## ■ $\sigma_{\text{can}}$ can be “filtered”

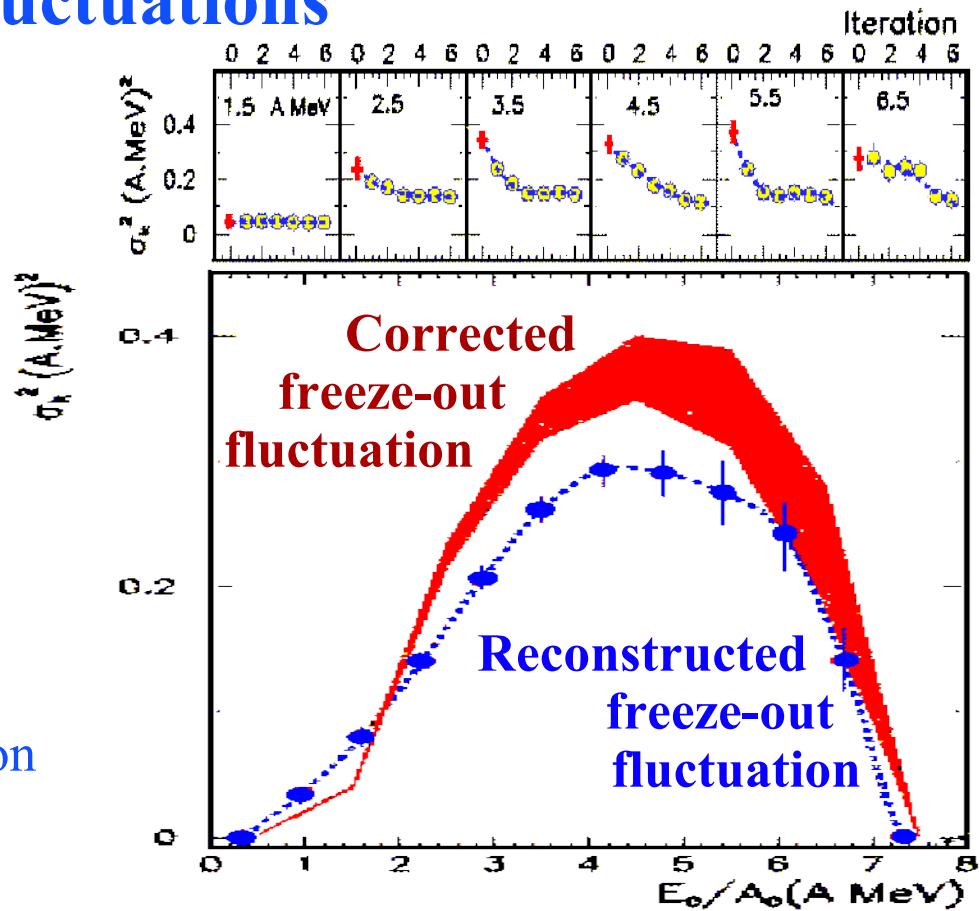
- ◆ (apparatus and procedure)

# Correction of experimental errors

## ■ Heat capacity from fluctuations



- $\sigma_{\text{can}}$  can be “filtered”
  - ◆ (apparatus and procedure)
- $\sigma_k$  can be corrected
  - ◆ Iterate the procedure
    - ◆ Freeze-out reconstruction
    - ◆ Decay toward detector



# Heat capacity from any fluctuation

## ■ From kinetic energy



# Heat capacity from any fluctuation

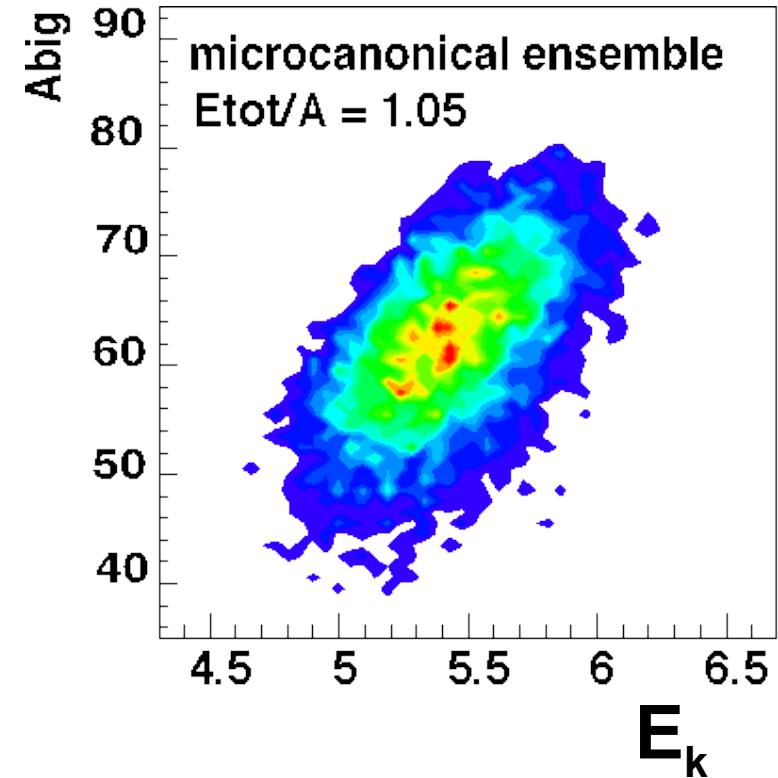
## ■ From kinetic energy



## ■ From any correlated observable (Ex. $A_{\text{big}}$ )

- ◆ 
$$\frac{X_k}{X} = 1 - \frac{\sigma_A^2}{\sigma_{A0}^2} \frac{1}{\rho^2}$$

- ◆  $\rho = \sigma_{kA} / \sigma_k \sigma_A$  correlation



- ◆  $\sigma_{A0}$  “canonical” fluctuations



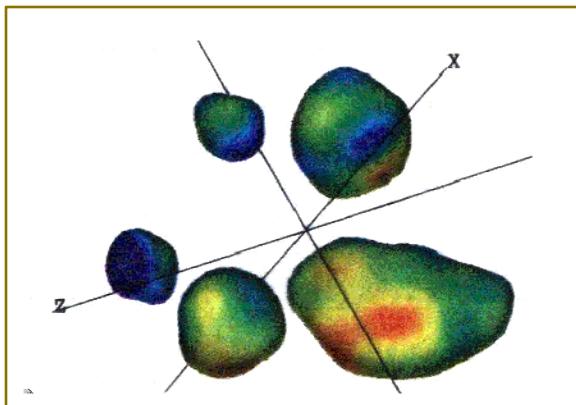
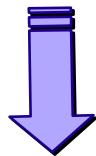
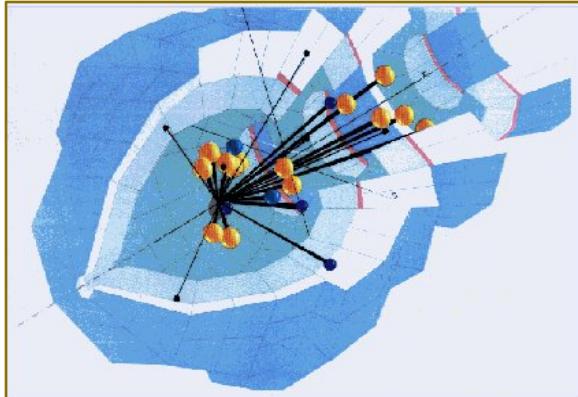
# -Appendix -VI-

## Test of freeze-out reconstruction

- Volume
  - ◆ Coulomb boost
- Temperature
  - ◆ Isotope ratios
  - ◆ Particle-fragment correlations
- Alternative extraction



# Multifragmentation experiment



**S**ort events in energy  
(Calorimetry)

**R**econstruct a freeze-out  
partition

**1-** Primary fragments:  $m_i$

**2-** Freeze-out volume:  $E_{coul}$

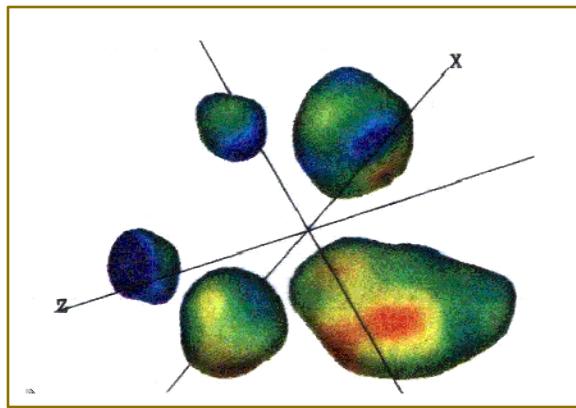
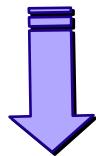
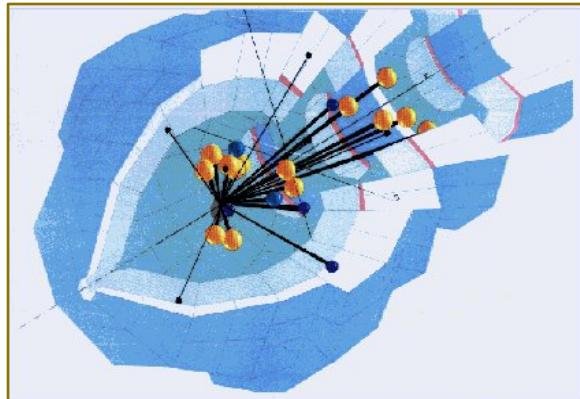
$$\bullet E_2 = \sum_i m_i + E_{coul}$$

$$\bullet E_1 = E^* - E_2 \Rightarrow \langle E_1 \rangle, \sigma_1$$

**3-** Kinetic EOS:  $T, C_1$

$$\bullet \langle E_1 \rangle = \langle \sum_i a_i \rangle T^2 + 3/2 \langle M-1 \rangle T$$

# Multifragmentation experiment



Sort events in energy  
(Calorimetry)

Reconstruct a freeze-out  
partition

1- Primary fragments:  $m_i$

2- Freeze-out volume:  $E_{coul}$

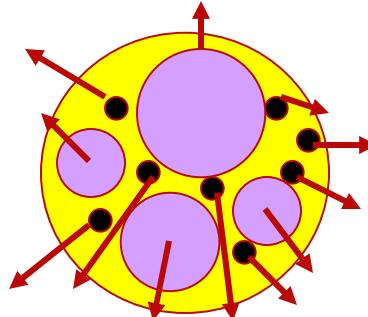
$$\bullet E_2 = \sum_i m_i + E_{coul}$$

$$\bullet E_1 = E^* - E_2 \Rightarrow \langle E_1 \rangle, \sigma_1$$

3- Kinetic EOS:  $T, C_1$

$$\bullet \langle E_1 \rangle = \langle \sum_i a_i \rangle T^2 + \frac{3}{2} \langle M-1 \rangle T E^*$$

# Volume

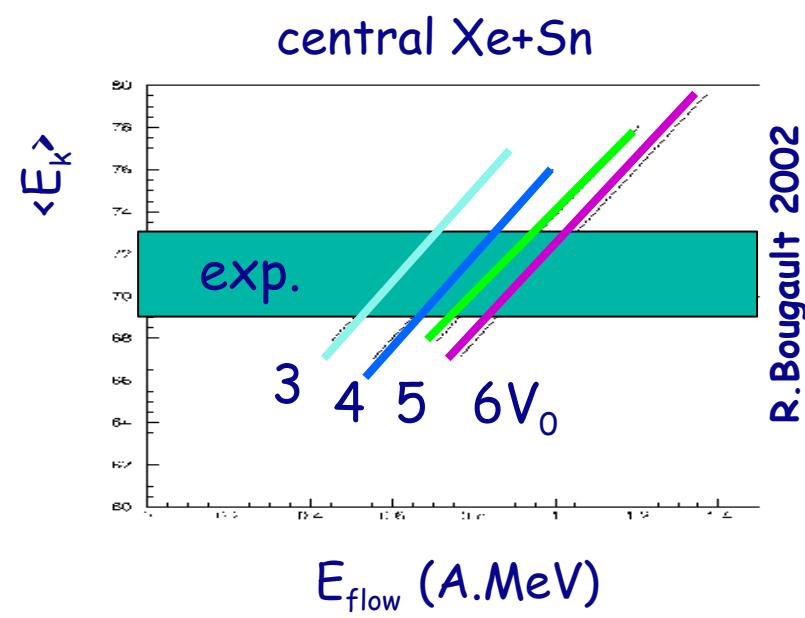
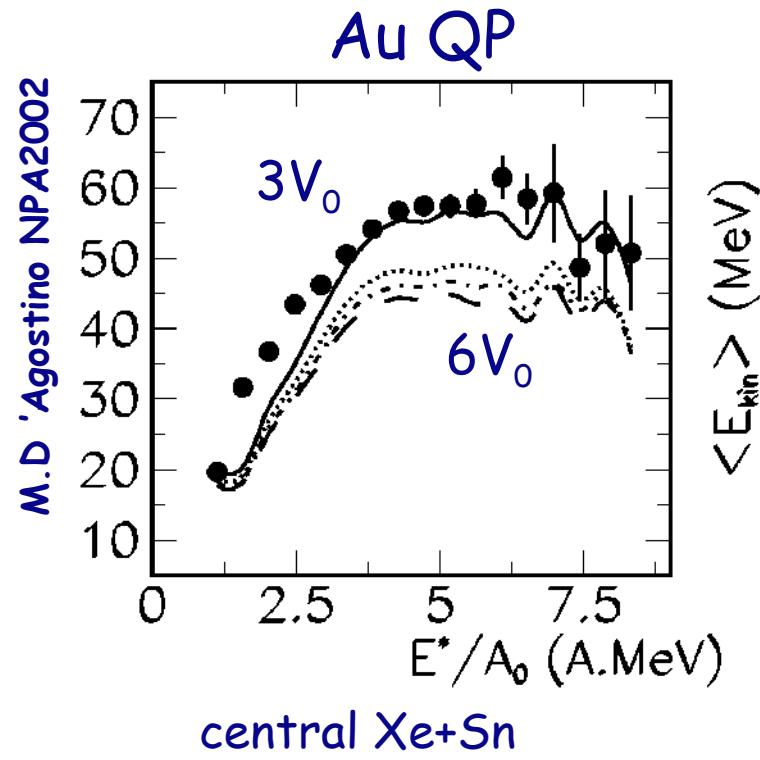
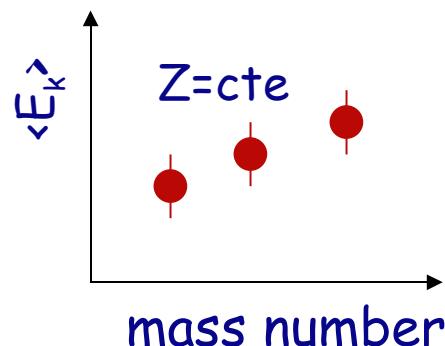


## From Coulomb boost

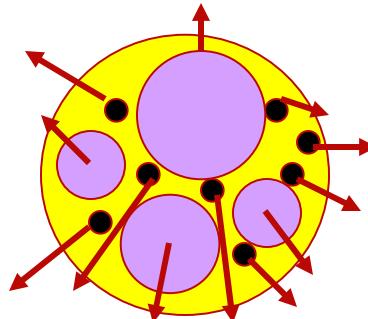
- ◆ C Weakly sensitive to V

## Ambiguity with expansion

- ◆ Need isotopic resolution
- ◆ Tiny influence on C



# Volume

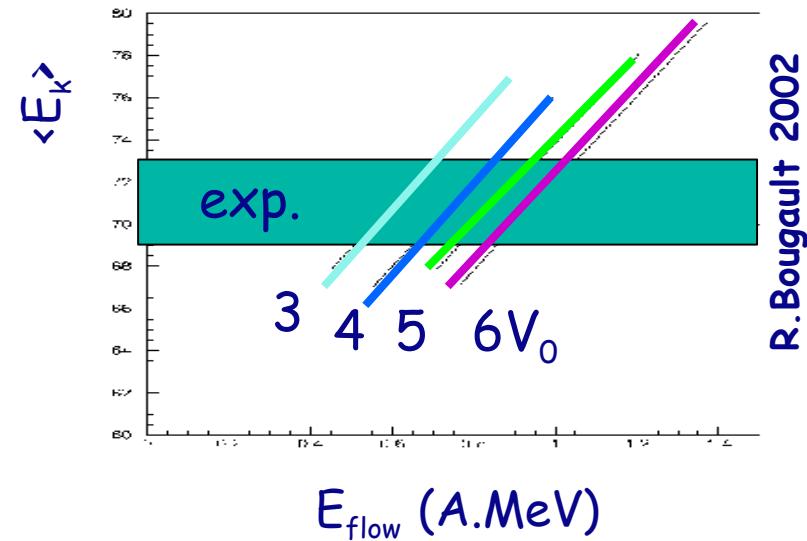
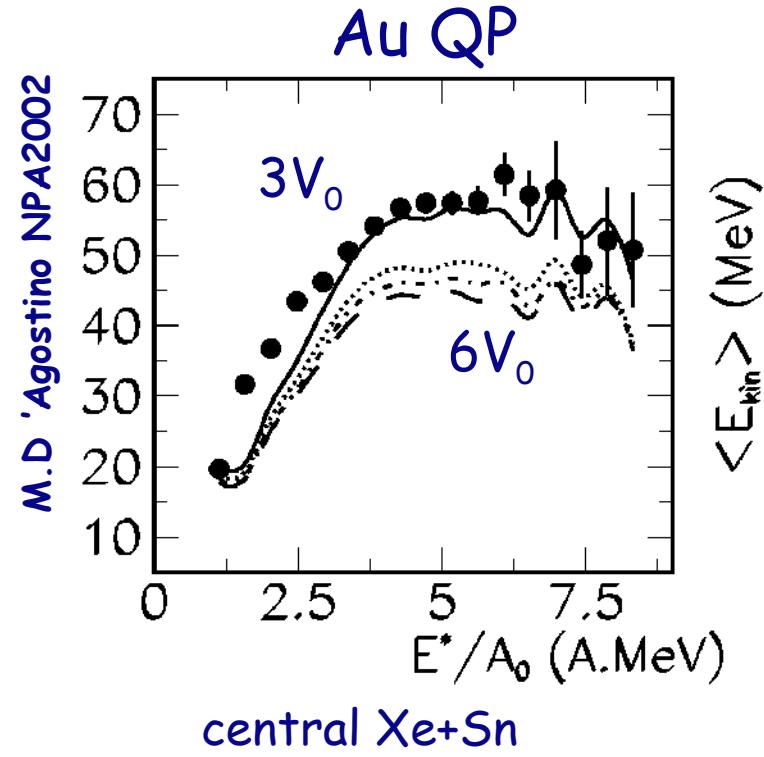
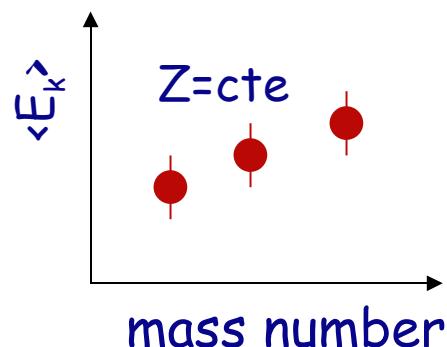


## From Coulomb boost

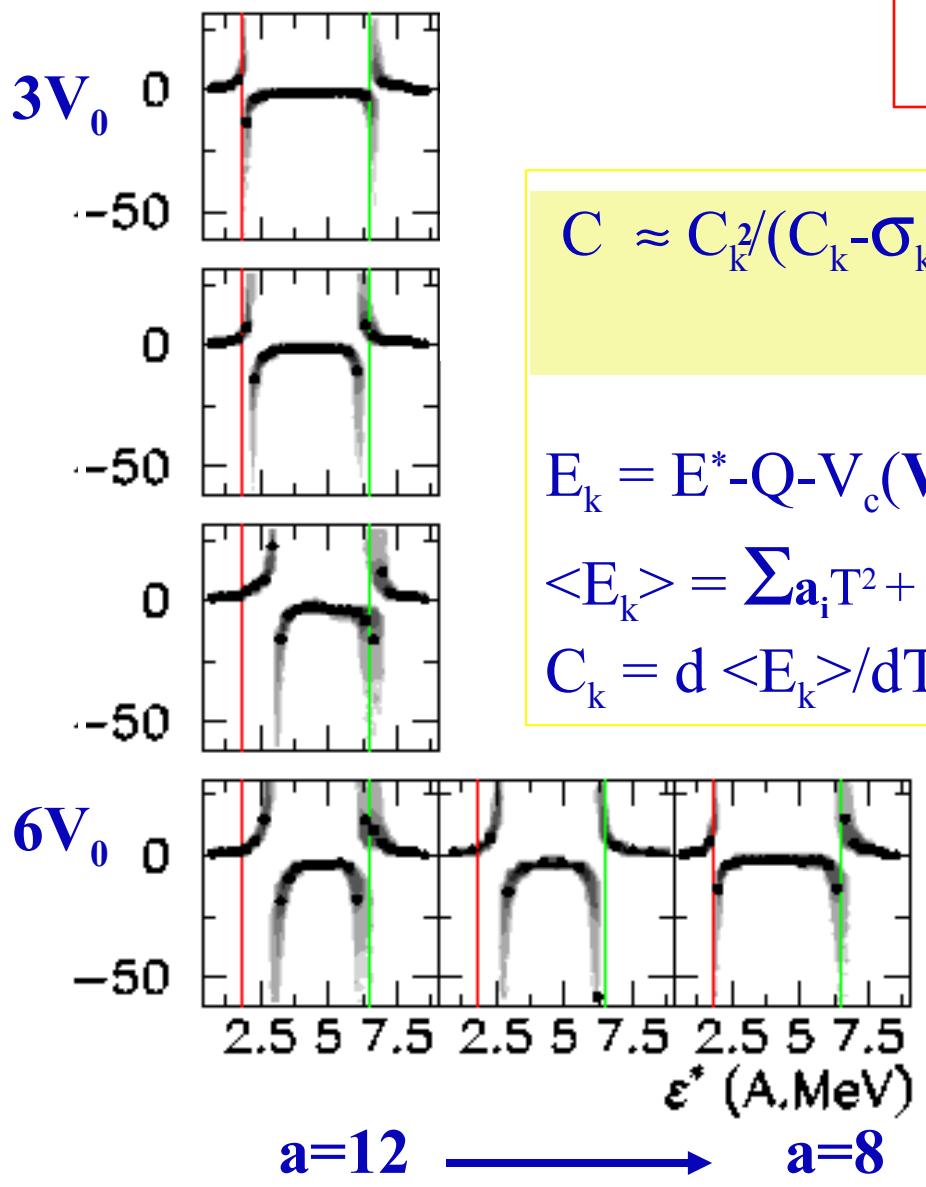
- ◆ C Weakly sensitive to V

## Ambiguity with expansion

- ◆ Need isotopic resolution
- ◆ Tiny influence on C



# Influence on C



$$C \approx C_k^2 / (C_k - \sigma_k^2 / T^2)$$

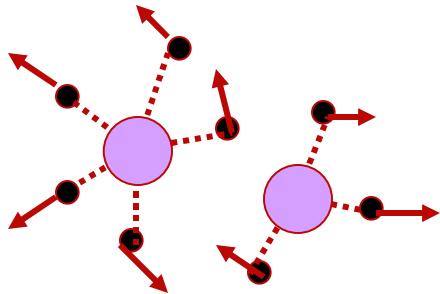
$$E_k = E^* - Q - V_c(V)$$

$$\langle E_k \rangle = \sum a_i T^2 + 3/2(\langle m \rangle - 1)T$$

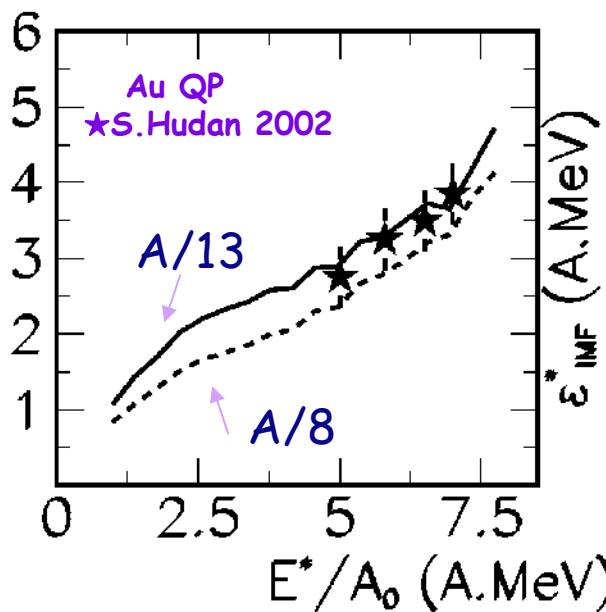
$$C_k = d \langle E_k \rangle / dT \quad C_k < 1.5 A_{\text{tot}}$$

Au+Au 35 A.MeV  
MULTICS data

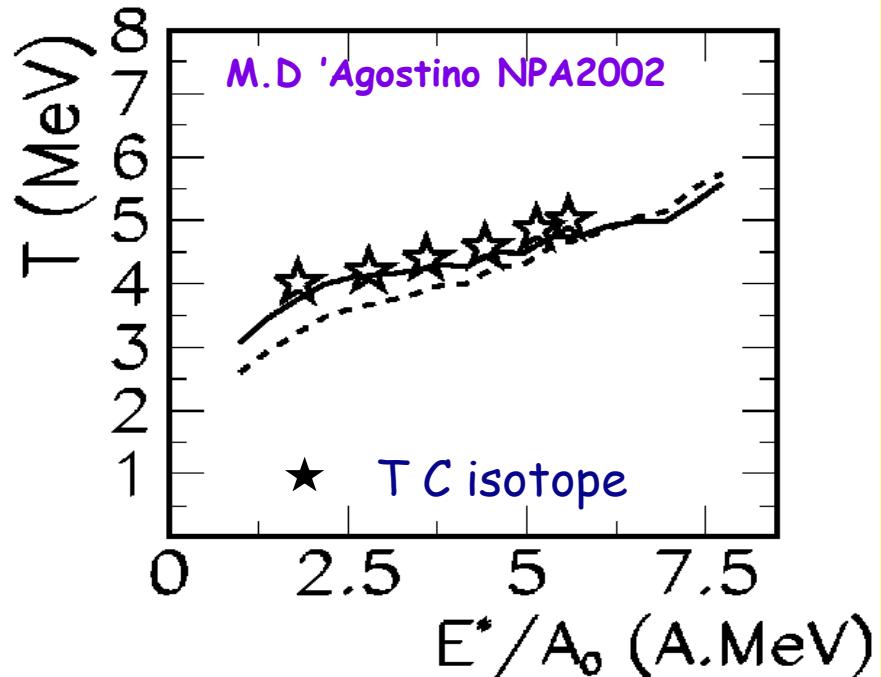
# Evaporation and temperature



## ■ Correlation



$$\langle E_k \rangle = \sum a_i(T) T^2 + 3/2(\langle m \rangle - 1)T$$



## ■ Consistency of T

# Heat capacity from the translational energy

$$T = \left\langle \frac{E_{tr}}{(3/2)m - 1} \right\rangle$$

$$\frac{1}{C} = 1 - T^2 \left\langle \frac{((3/2)m - 1)((3/2)m - 2)}{E_{tr}^2} \right\rangle$$

E.M.Pearson 1985, A.Raduta 2002

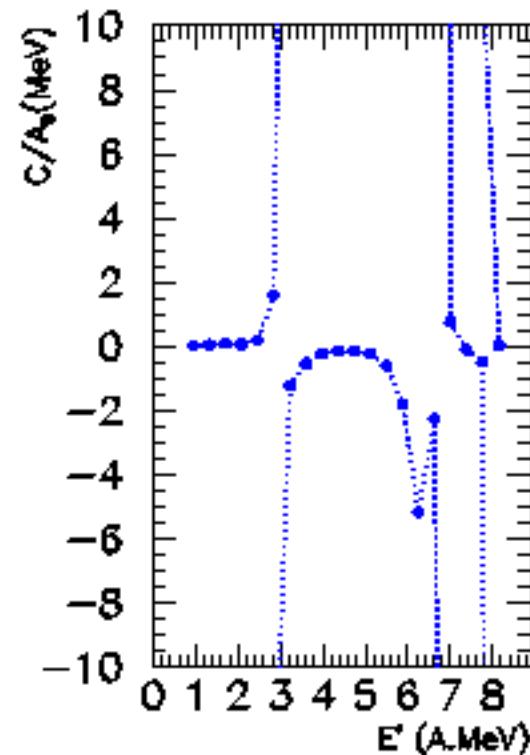
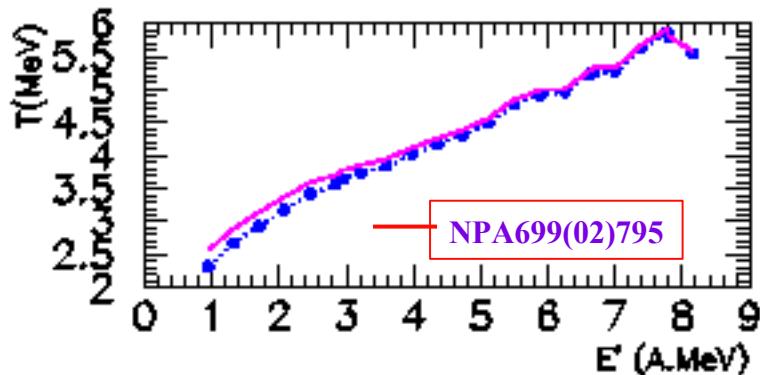
Coulomb trajectories

calorimetry

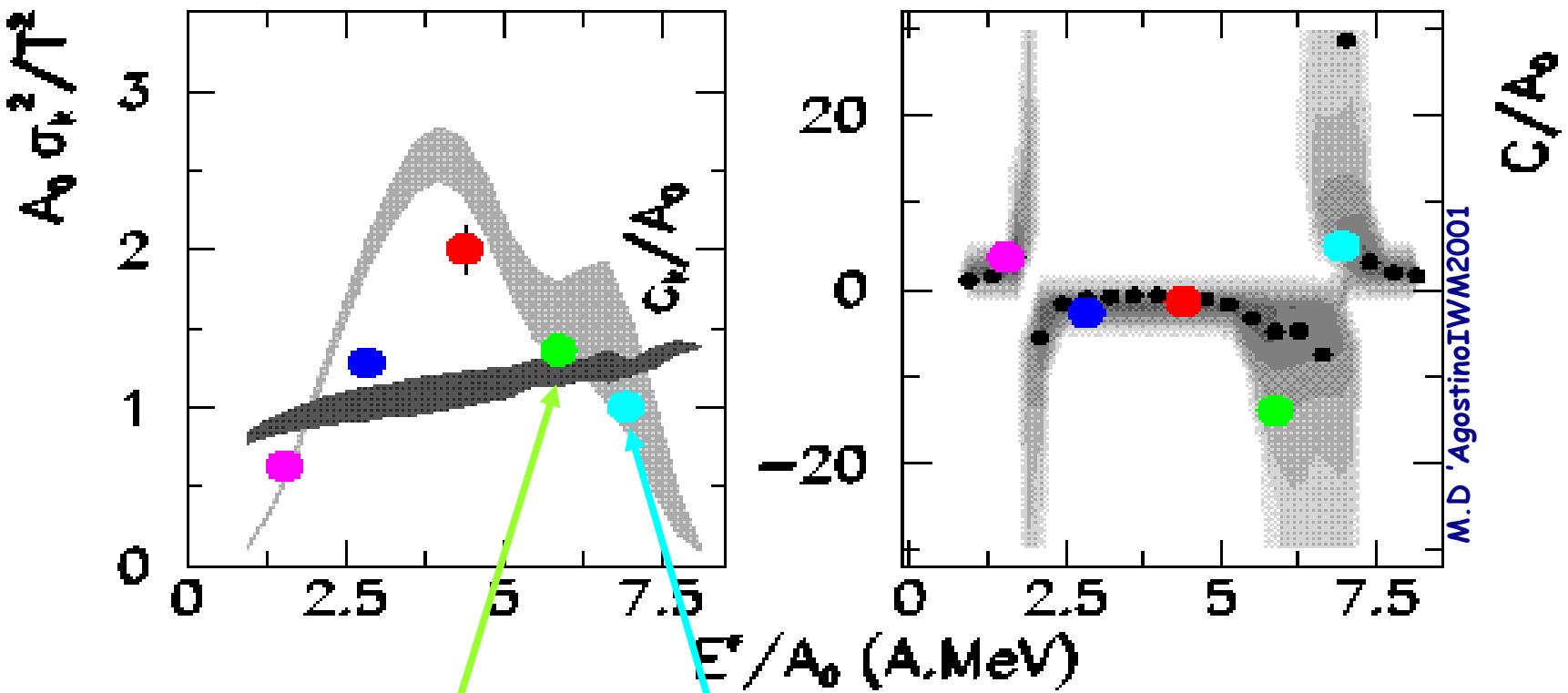
LCP-IMF correlations

Multics

Au+Au 35A.MeV



# Comparison central/peripheral



Au+Au 35  $E_F=1$

Au+Au 35  $E_F=0$

Up to  $\approx 35 A \cdot \text{MeV}$  the flow ambiguity  
is a small effect