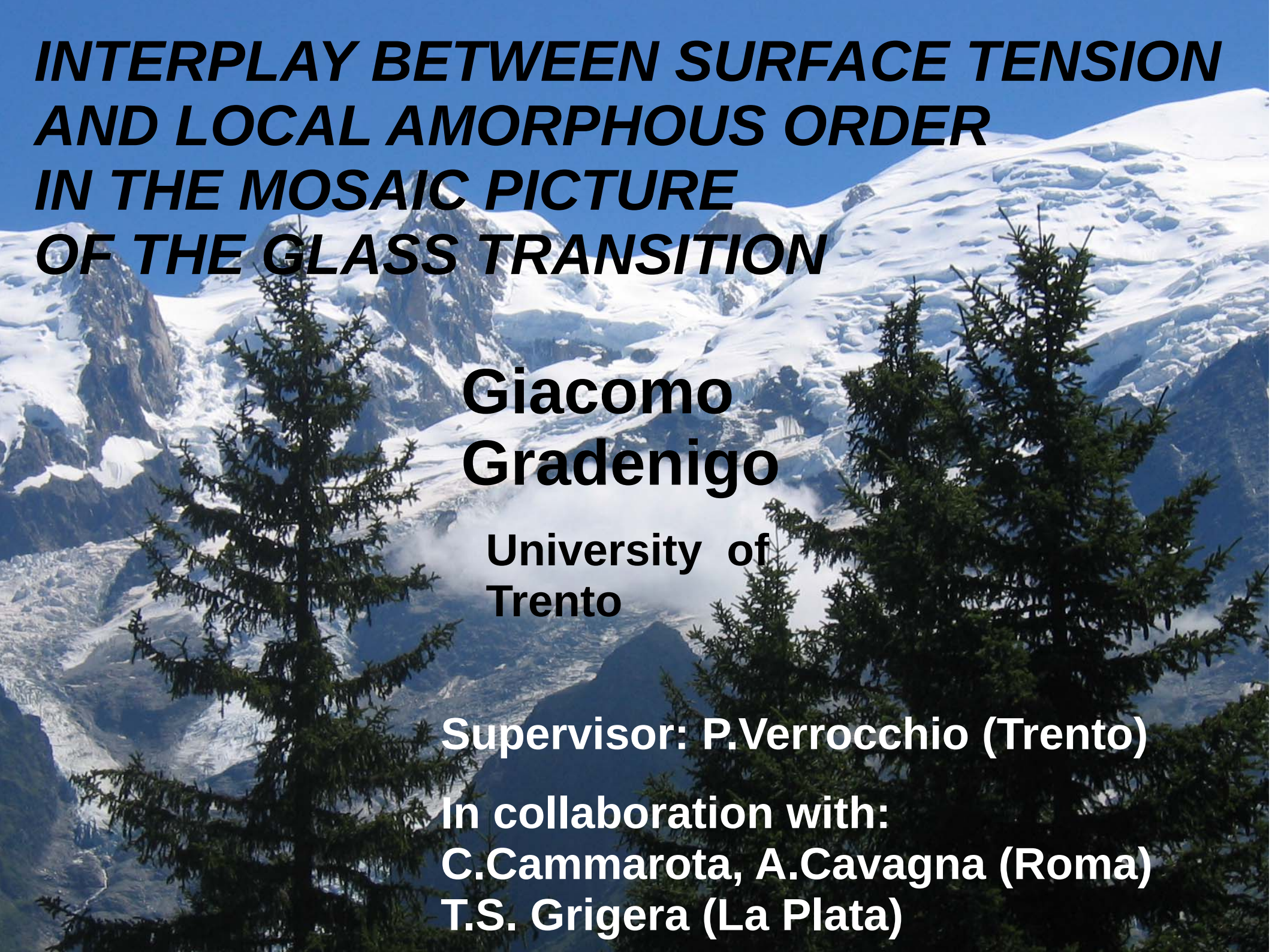

INTERPLAY BETWEEN SURFACE TENSION AND LOCAL AMORPHOUS ORDER IN THE MOSAIC PICTURE OF THE GLASS TRANSITION

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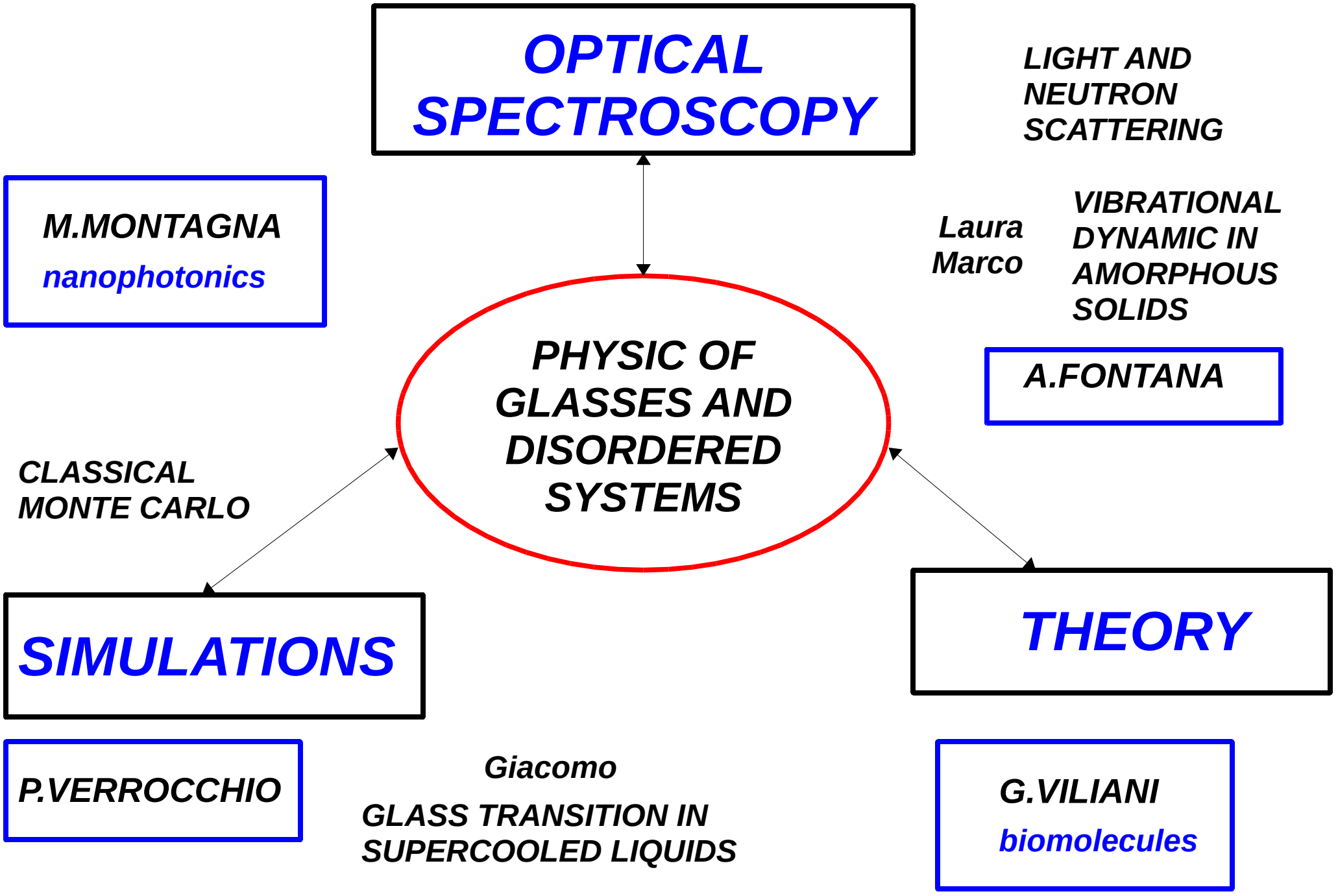
Supervisor: P.Verrocchio (Trento)

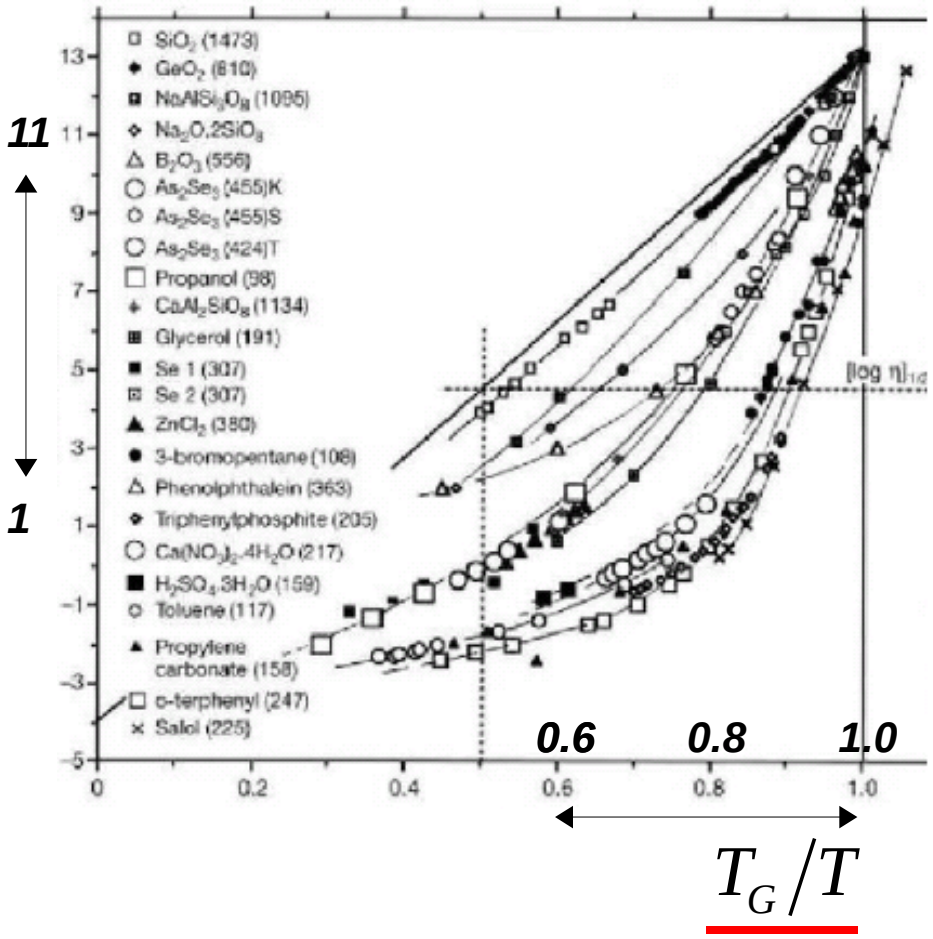
In collaboration with:
C.Cammarota, A.Cavagna (Roma)
T.S. Grigera (La Plata)


OPTICAL SPECTROSCOPY
LIGHT AND NEUTRON SCATTERING
M.MONTAGNA
nanophotonics
Laura Marco
VIBRATIONAL DYNAMIC IN AMORPHOUS SOLIDS
A.FONTANA
PHYSIC OF GLASSES AND DISORDERED SYSTEMS
CLASSICAL MONTE CARLO
SIMULATIONS
THEORY
P.VERROCCHIO
Giacomo
GLASS TRANSITION IN SUPERCOOLED LIQUIDS
G.VILIANI
biomolecules
SPING GLASS COMMUNITY (ROME, G.PARISI)

STRUCTURAL GLASSES

Physic ruled by classical thermodynamic

$$\log(\eta)$$



Strong glasses

$$\eta = \eta_0 \exp\left(\frac{A}{T}\right)$$

$$\tau = \tau_0 \exp\left(\frac{A}{T}\right)$$

Ahrrenius

Fragile glasses

$$\eta = \eta_0 \exp\left(\frac{A}{T - T_0}\right)$$

$$\tau = \tau_0 \exp\left(\frac{A}{T - T_0}\right)$$

Volger-Fulchner

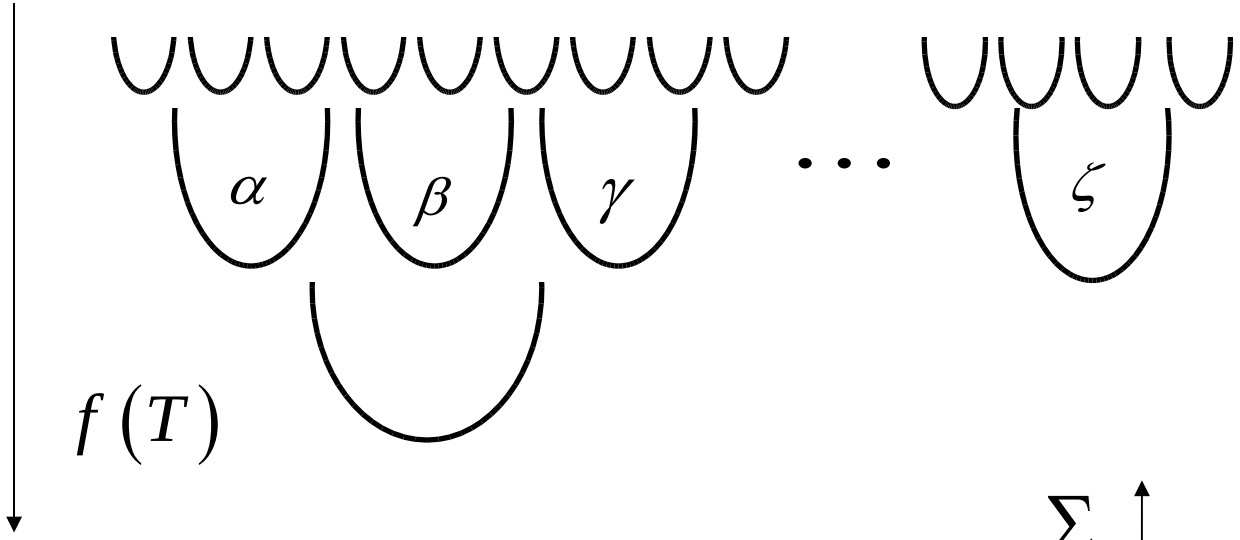
Diverging timescales

? Thermodynamic transition ?

? Diverging lenghtscale ?

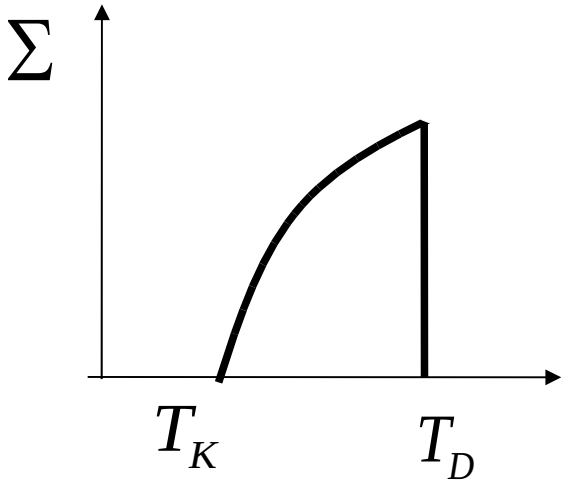
MOSAIC

EXPONENTIAL NUMBER OF VALLEYS: COMPLEXITY



Multistate scenario : many amorphous phases

$$\mathcal{N}(f) = e^{N\Sigma(f)}$$



$f - T\Sigma(f)$

Entropic contribution to free energy

$T \le T_K$

Glass

$T_K < T \le T_D$

Supercooled liquid

$T > T_D$

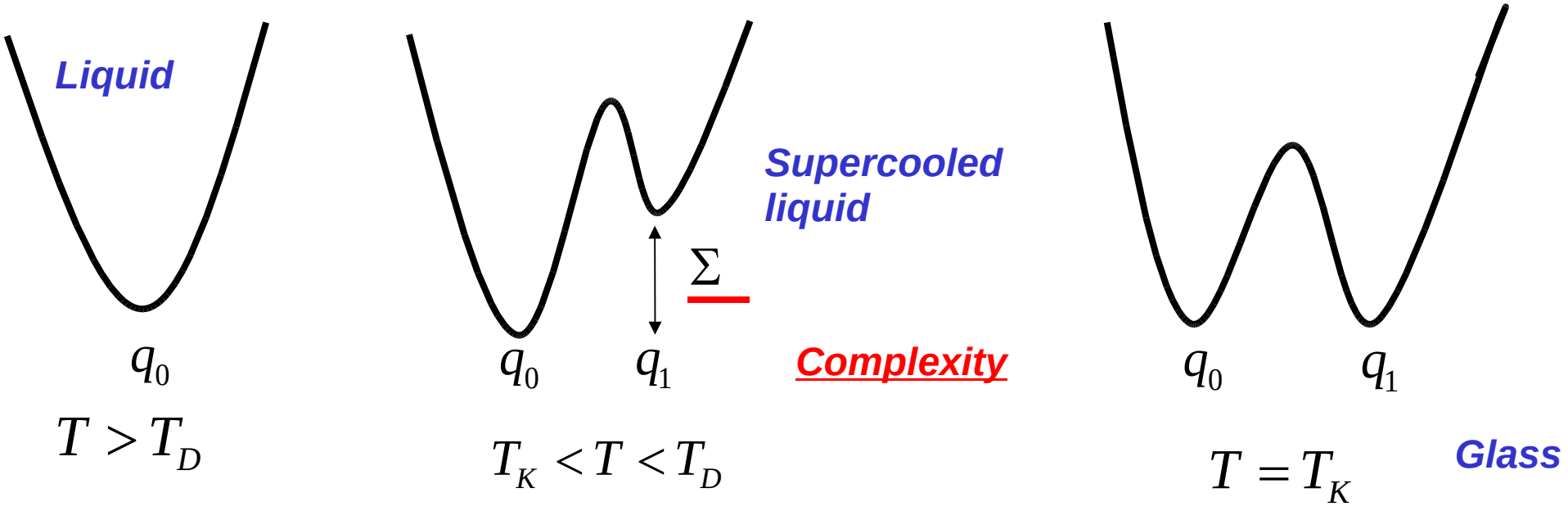
Liquid

OVERLAP AS ORDER PARAMETER

$q(C_1, C_2)$ **Overlap function = measure of similarity**

$V(q)$

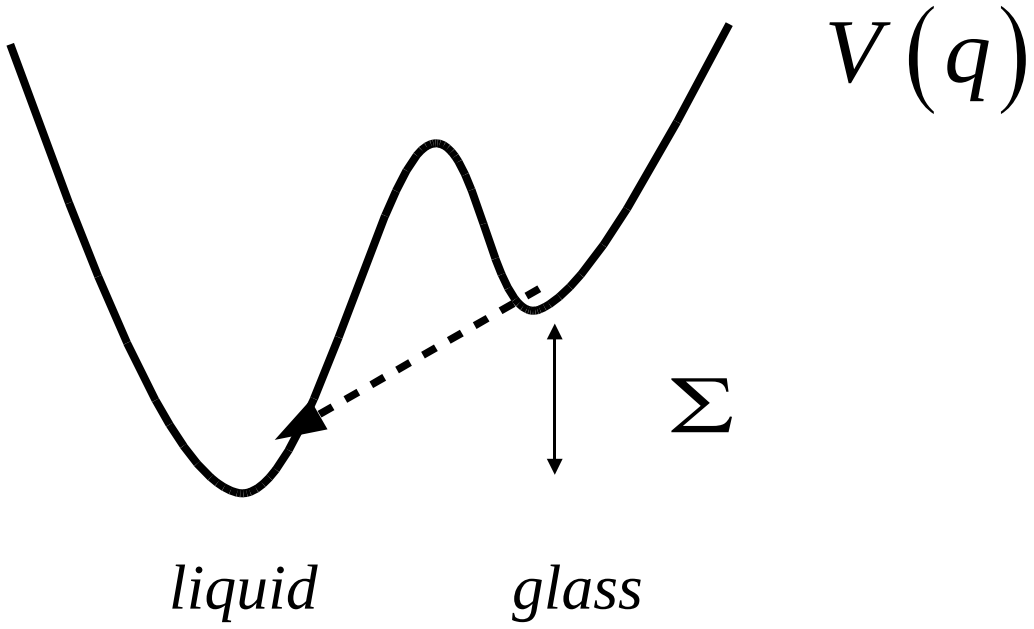
Minima are phases relevant for thermodynamic



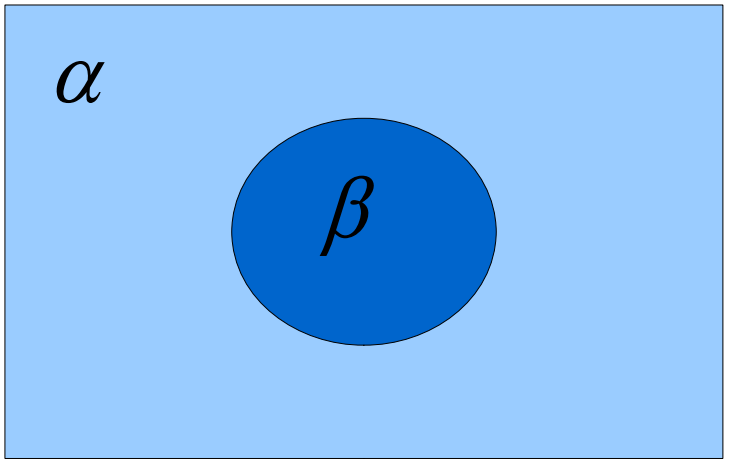
$q_1 \approx 1$ **System in glassy state**

$q_0 \approx 0$ **System in liquid state**

RELAXATION FROM METASTABILITY
RANDOM FIRST ORDER



α **Amorphous state**



β **New amorphous state**

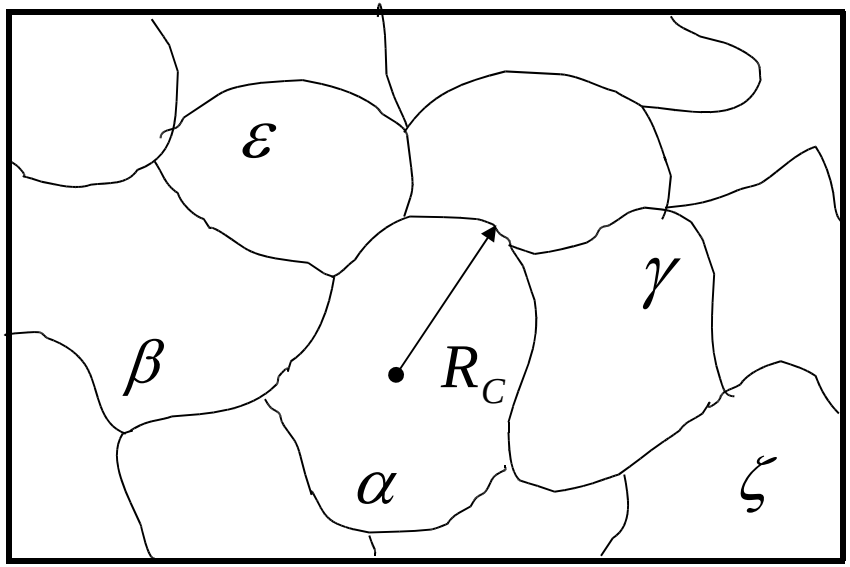
Random First Order

$$\Delta f = \Upsilon R^{\theta} - T\Sigma R^{3}$$

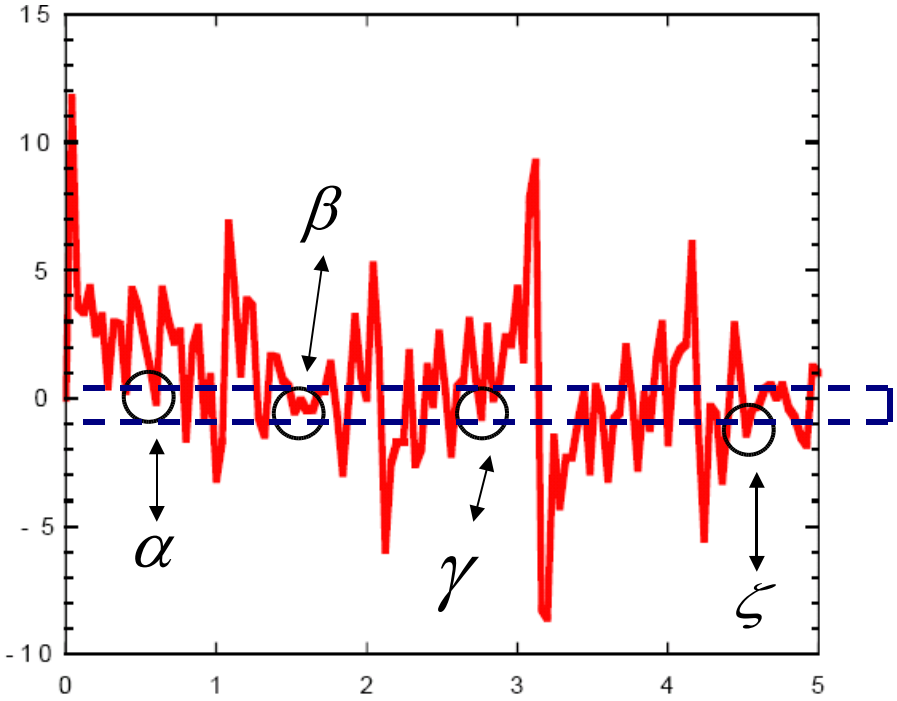
Standard First Order

$$\Delta f = \Upsilon \beta R^{2} - \delta f R^{3}$$

MOSAIC OF STATES



Free Energy Landscape



$\Sigma \neq 0$

DIVERGING CORRELATION LENGHT

$$\Delta f = \Upsilon R^{\theta} - T\Sigma R^{3} = 0 \qquad \Upsilon R^{\theta} = T\Sigma R^{3}$$

$$R_C = \left(\frac{\Upsilon}{T\Sigma} \right)^{\frac{1}{3-\theta}}$$

Approaching glass transition

$\Sigma \downarrow \Rightarrow R_C \uparrow$

G.Biroli, J.-P. Bouchaud, J.Chem.Phys, 121, 7347, (2004)

G.Biroli,J-P Bouchaud, A. Cavagna, T.S. Grigera and P.Verrocchio, Nature Phys. (2008)

Υ ***Really exhist ??***

Σ ***Analitically computed in mean field models***

Computed numerically for short range interactions

INHERENT STRUCTURES APPROXIMATION

FREE ENERGY MINIMA → ***POTENTIAL ENERGY MINIMA*** **Inherent Structures**

Fragile Liquid Former ***Soft spheres*** $1/r^{12}$

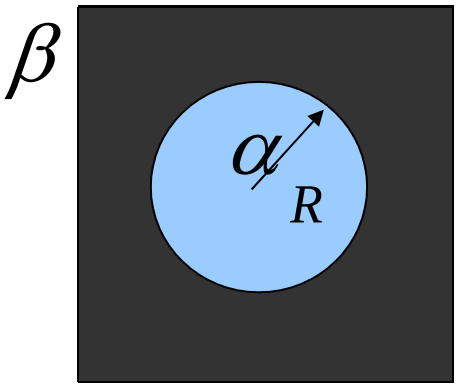
For a given T

Quench from equilibrium

$$E_\alpha \approx E_\beta$$

$$q\left(C_\alpha, C_\beta\right) \approx 0$$

β α

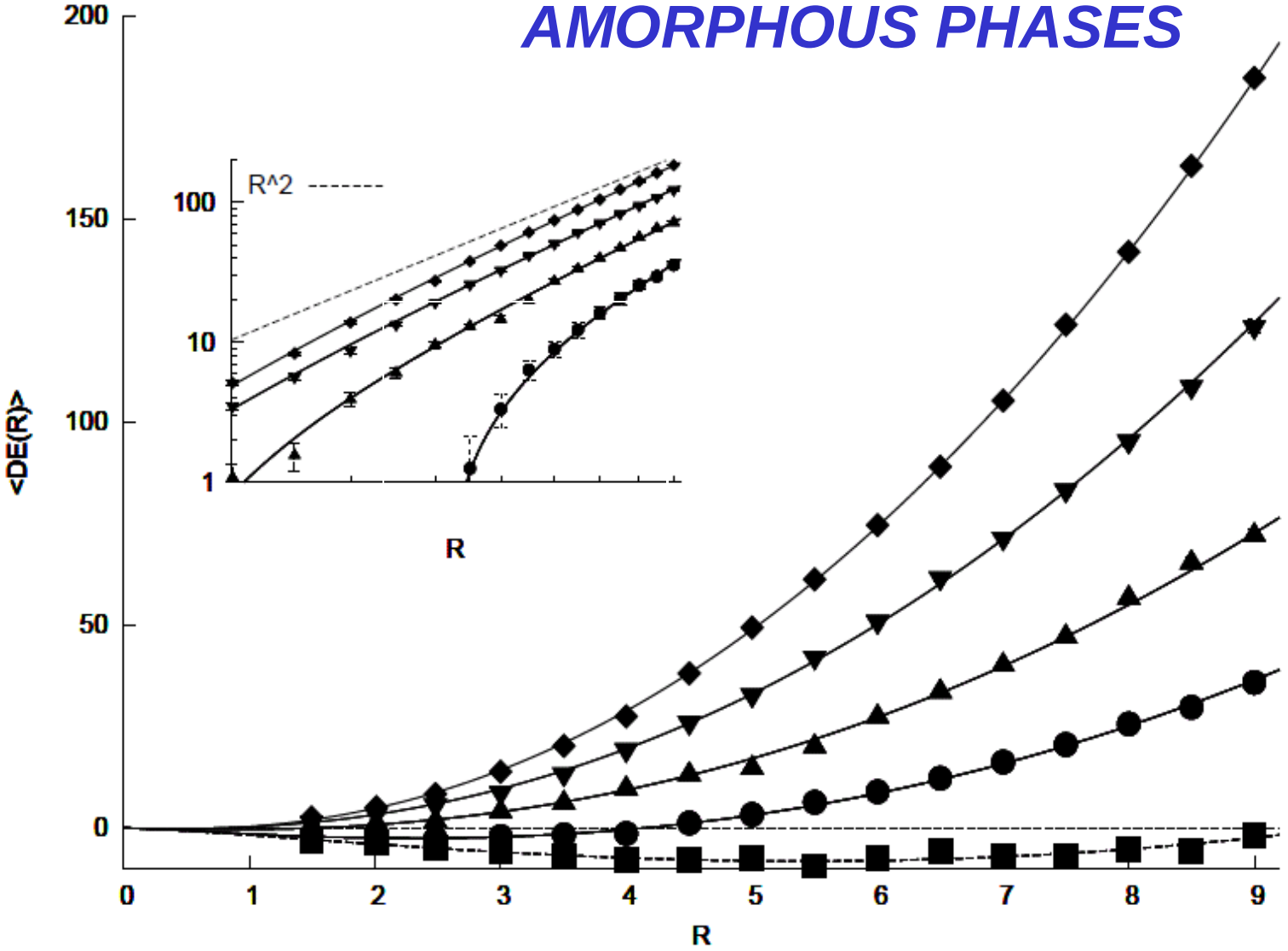


Quench

$\alpha\beta$

$$DE\left(R\right) = E_{\alpha\beta} - \frac{E_\alpha + E_\beta}{2}$$

EXHISTENCE OF SURFACE TENSION BETWEEN AMORPHOUS PHASES



$T = 0.9\,T_D$

$T = 1.3\,T_D$

$$DE = \Upsilon R^2 - \delta R^{\omega}$$

Standard surface cost

Small size correction

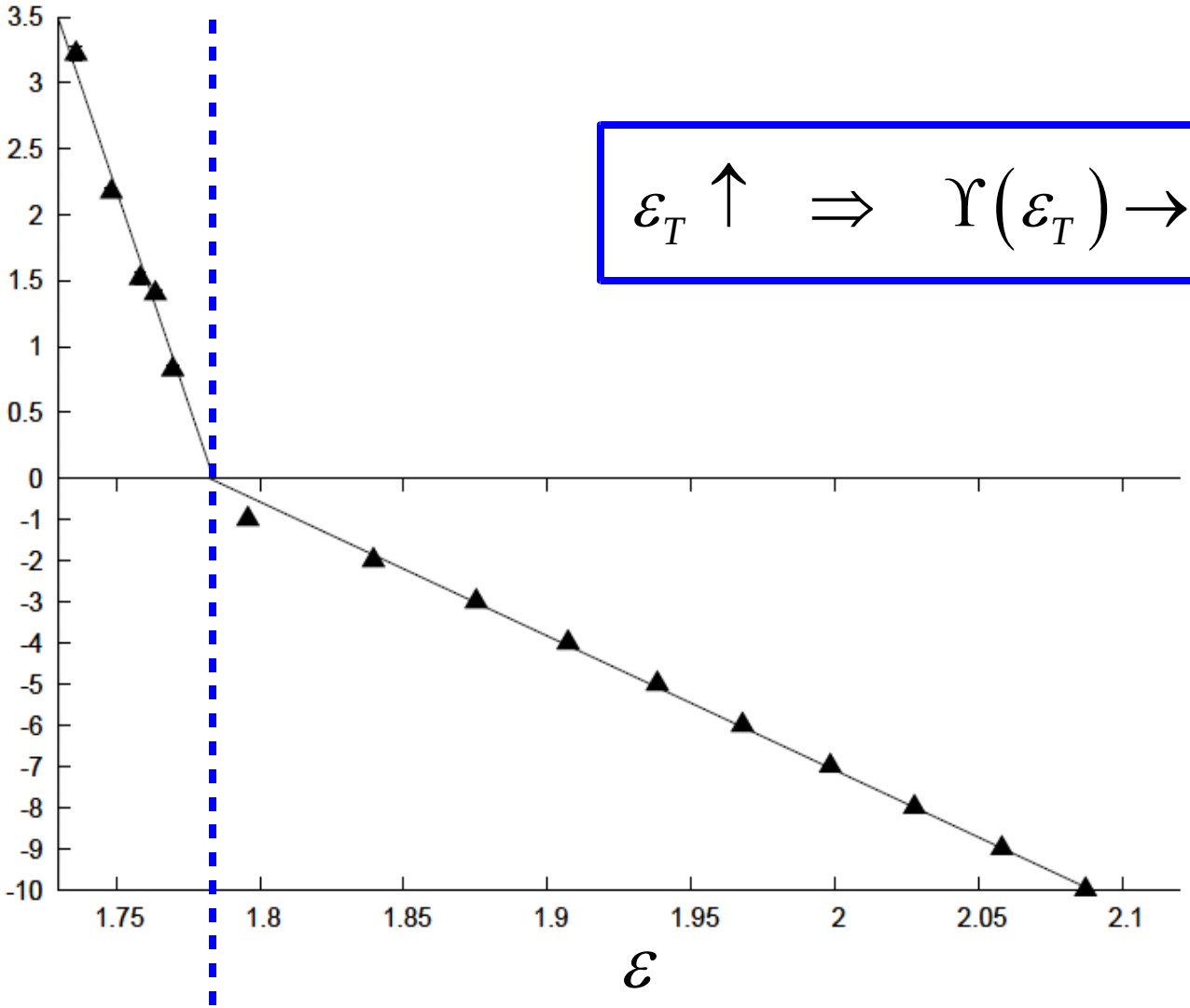
$\omega < 2$

Roughening of surface between amorphous phases

VANISHING SURFACE TENSION: FROM MINIMA TO SADDLES

$\Upsilon(\varepsilon)$

$-k(\varepsilon)$



$$\varepsilon_T \uparrow \quad \Rightarrow \quad \Upsilon(\varepsilon_T) \to 0$$

Saddles instability index

T.S.Grigera, J.Chem.Phys. 124, (2006)

Supercooled liquid | ***Liquid***

Minima | ***Saddles***

Activated dynamic | ***Non activated dynamic***

CONCLUSIONS

***Exhistence of surface tension** among “states” in supercooled liquids.*

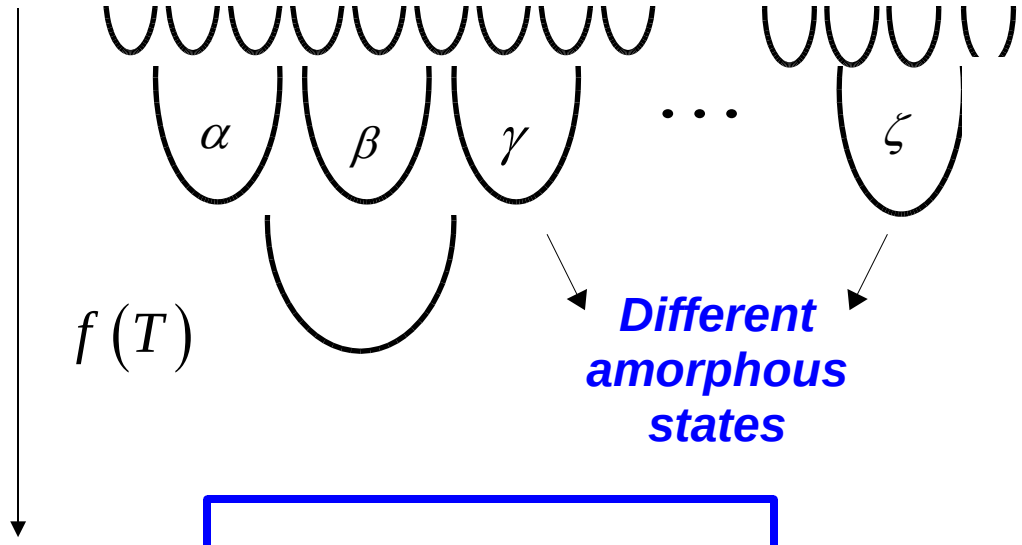
Our result are consistent with a crossover from activated (supercooled liquid) to non activated (liquid) relaxational dynamic.

PLANS

Study of thermodynamic stability of interfaces in supercooled liquids using constrained MonteCarlo simulations.

Calculation of the surface tension term from the partition function of a liquid using a replica formulation of the problem.

CONFIGURATIONAL ENTROPY : MULTISTATE SCENARIO



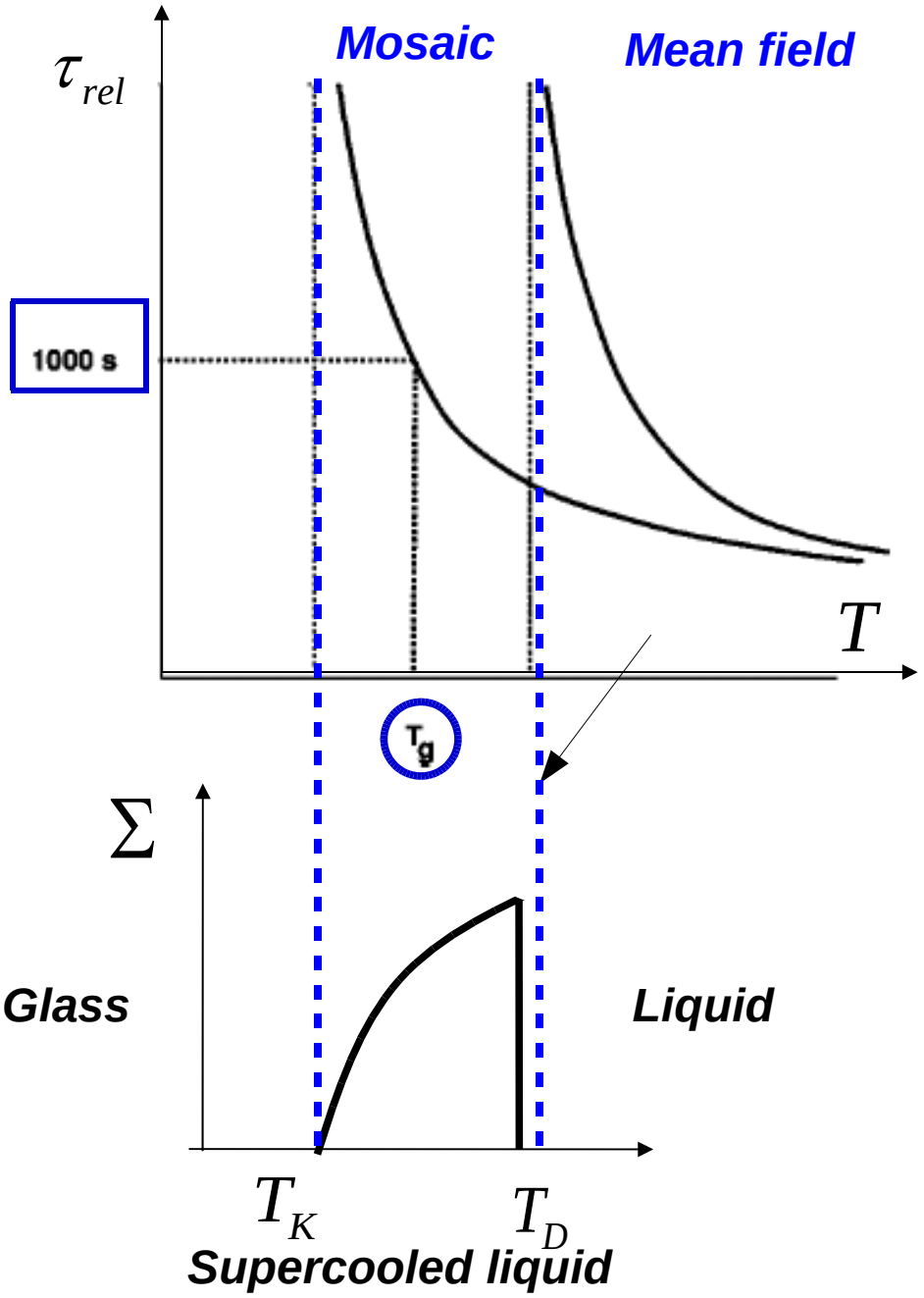
$$\mathcal{N}(f) = e^{N\Sigma(f)}$$

$$f - T\Sigma(f)$$

$T > T_D$ **Liquid**

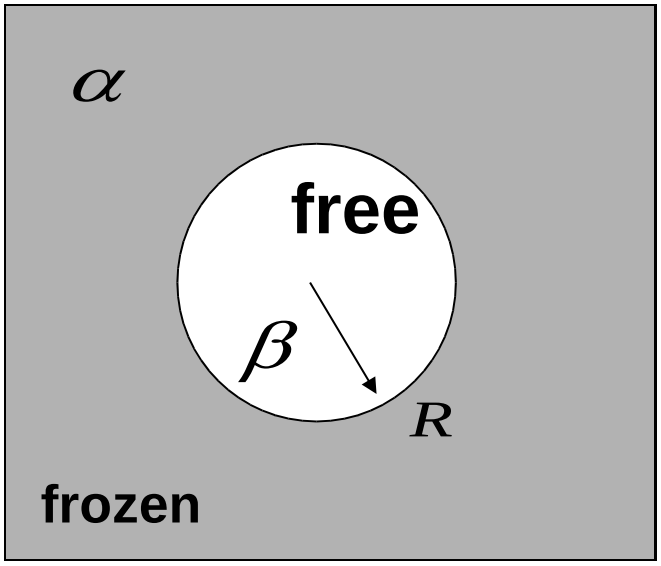
$T_K < T \leq T_D$ **Supercooled liquid**

$T \leq T_K$ **Glass**



CRITICAL SIZE OF DOMAINS

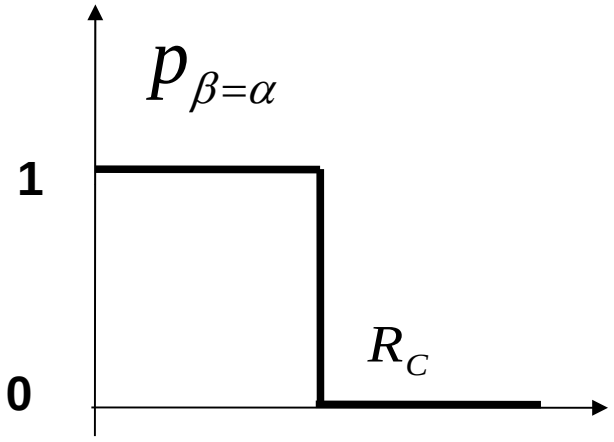
G.Biroli,J-P Bochaud,
J.Chem.Phys, 121, 7347, (2004)



$$\beta(t=0)=\alpha \qquad \beta(t=\infty)=?$$

$$Z_S = e^{-\beta f R^3} + e^{R^3\Sigma(f)-\beta f R^3-\beta\Upsilon R^\theta}$$

$$Z_S = Z_{\beta=\alpha} + Z_{\beta\neq\alpha}$$



$$p_{\beta=\alpha} = \frac{Z_{\beta=\alpha}}{Z_S} = \frac{1}{e^{-\beta(\Upsilon R^\theta - T\Sigma R^3)}+1}$$

$$p_{\beta\neq\alpha} = 1 - p_{\beta=\alpha}$$

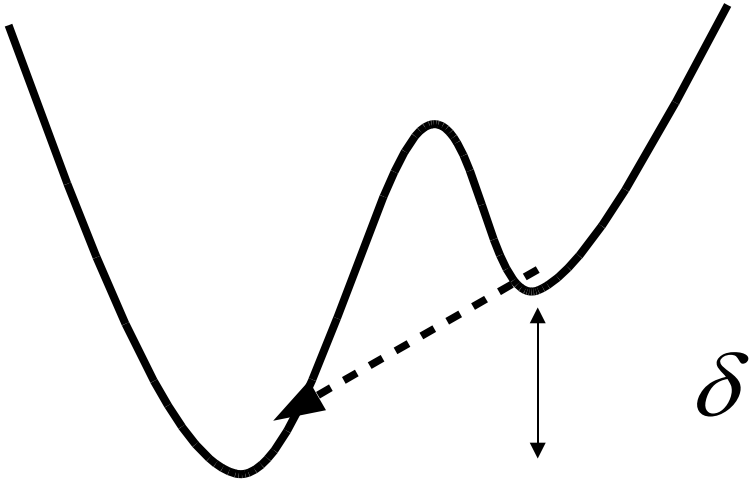
Free energy cost to nucleate a new phase

$$R_C = \left(\frac{\beta\Upsilon}{\Sigma}\right)^{\frac{1}{3-\theta}} \qquad \theta \leq 2$$

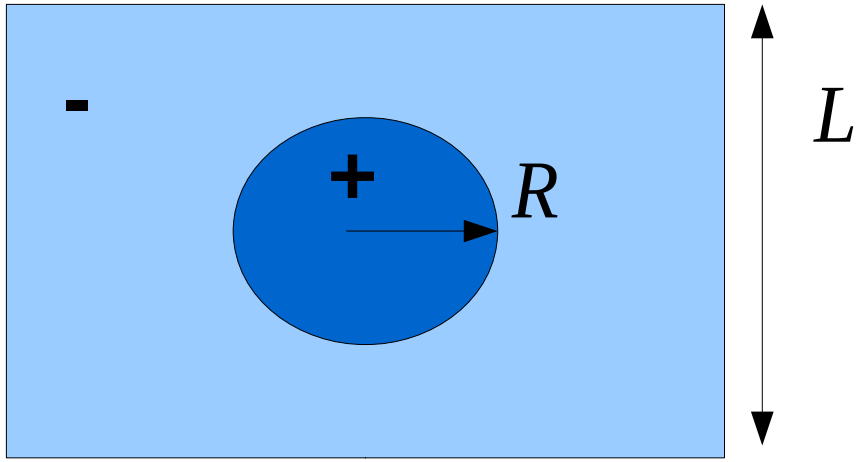
$$\Sigma \downarrow \Rightarrow R_C \uparrow$$

Growing correlation length benchmark of glass transition

FIRST ORDER PHASE TRANSITIONS



$m = +1 \quad m = -1$



Up magnetic field

Ising Model

$$-\sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

Nearest neighboors

$$\Delta f = \Upsilon R^2 - T \delta f \, R^3$$

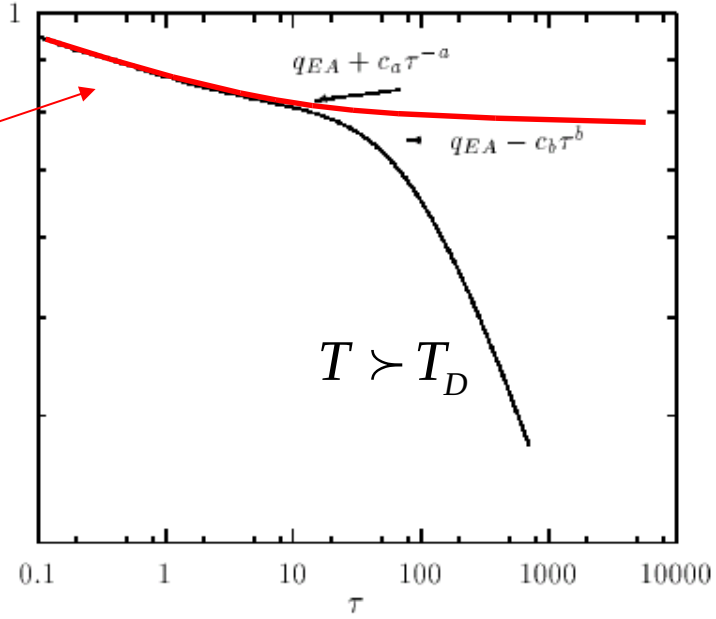
$$\Delta f = 0 \Longrightarrow R_C = \left(\frac{\beta \Upsilon}{\delta f} \right)$$

$$-\sum_{i,j} S_i S_j - h \sum_i S_i$$

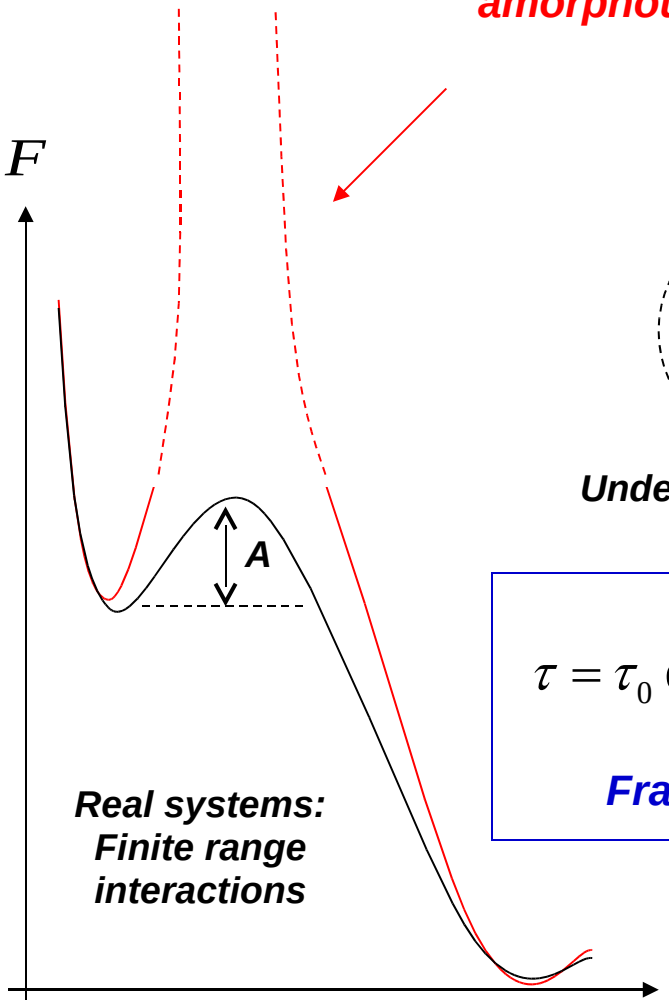
All to all

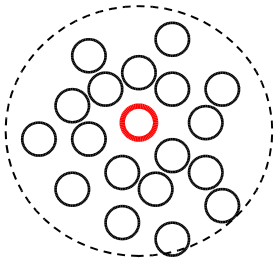
$$\Delta f = \alpha L^{\theta} - T \delta f \, R^3$$

Mean Field Predictions

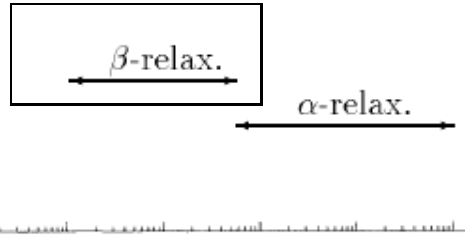


Mean field approximation: infinite energy barriers between different amorphous states





Undercooled Liquids



$$\tau = \tau_0 \exp\left\{\frac{A}{T - T_K}\right\}$$

Fragile systems