FLUIDI METASTABILI E INSTABILI

P = cost
mono-componente

β

metastabile

α

binodale ←

spinodale ←

$\alpha = G$
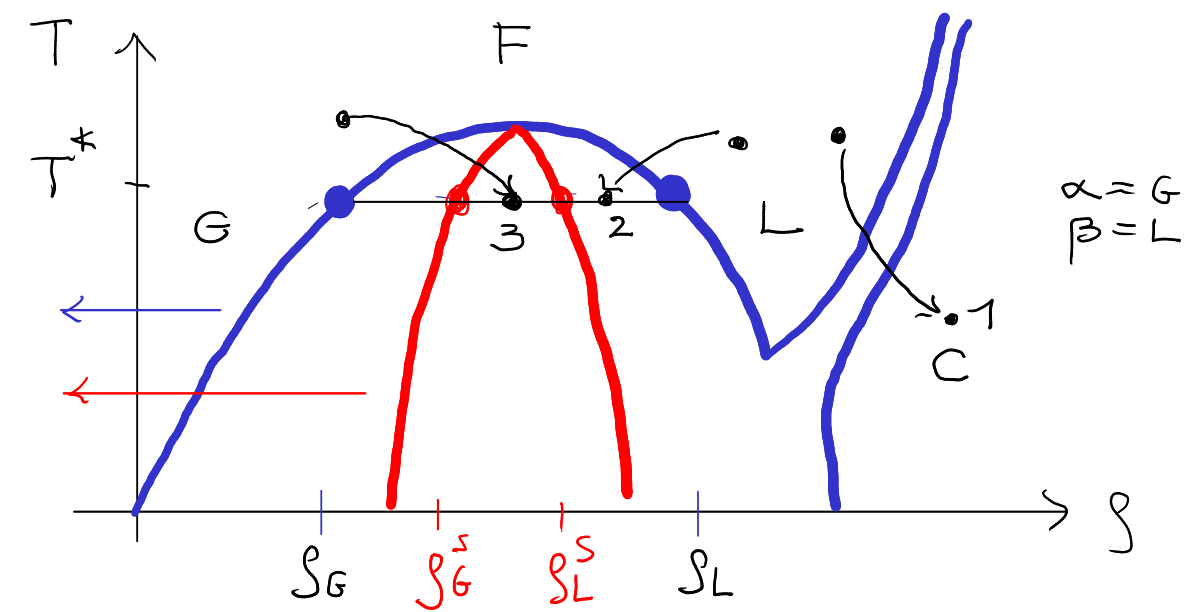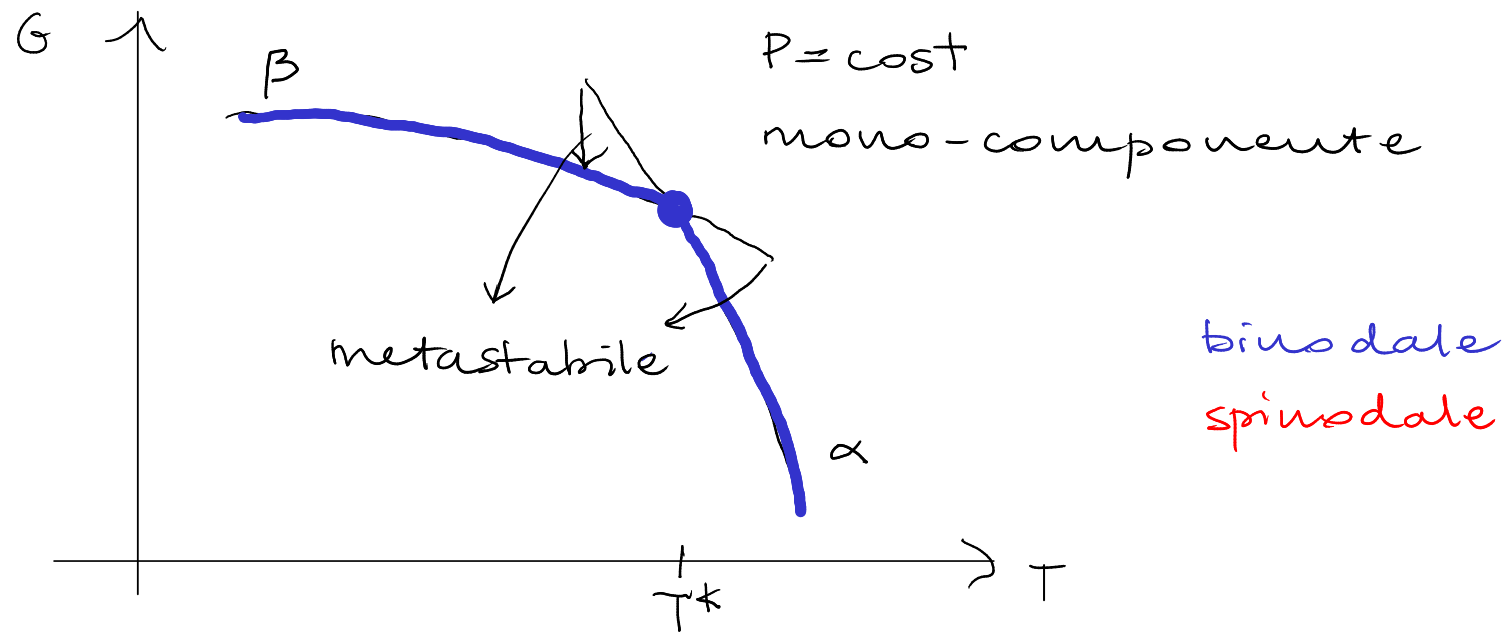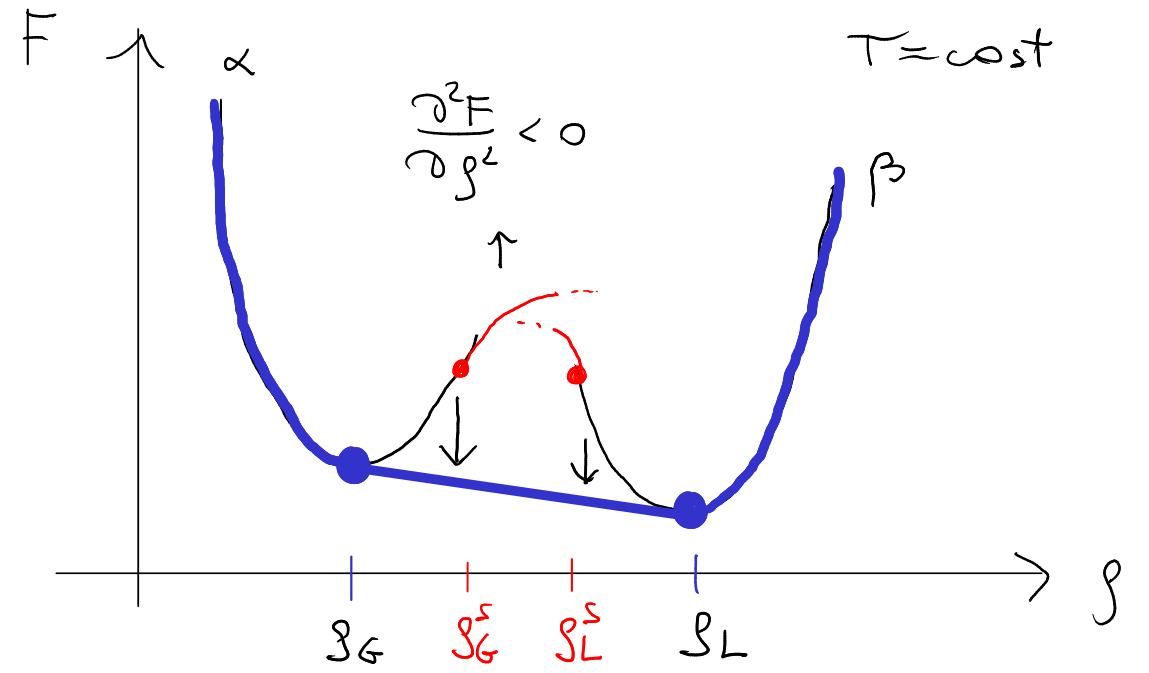$\beta = L$

1. metastabile rispetto a cristallo
2. metastabile rispetto a liquido + gas   } ①
3. instabile rispetto a liquido + gas   ②

① nucleazione + crescita

② decomposizione spinodale

T = cost

$\frac{\partial^2 F}{\partial \varrho^2} < 0$

1) Nucleazione

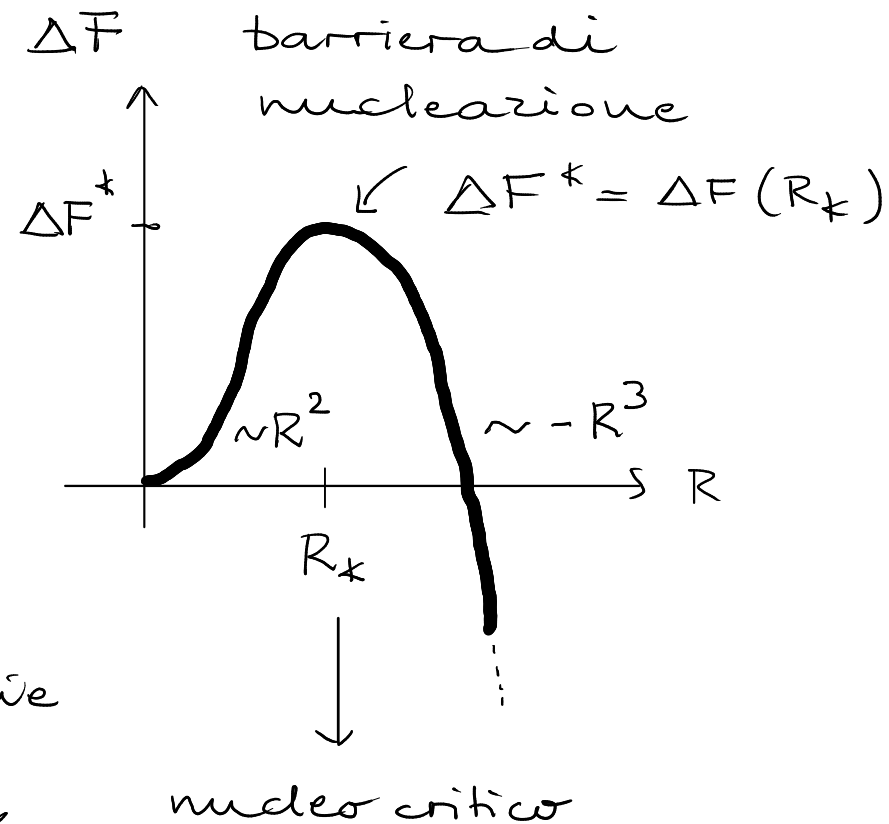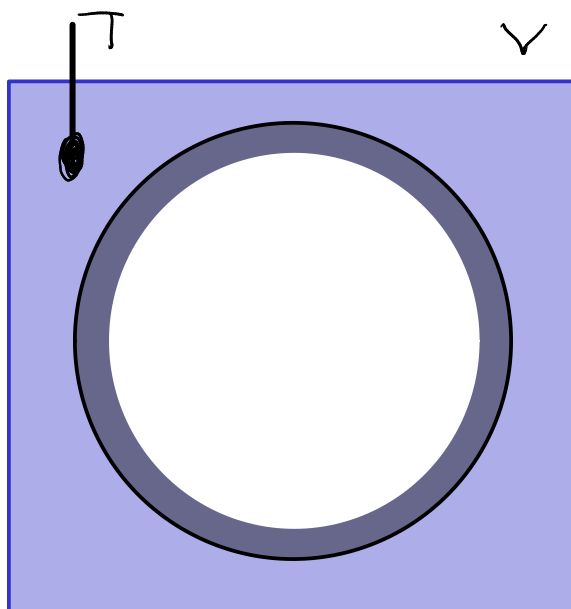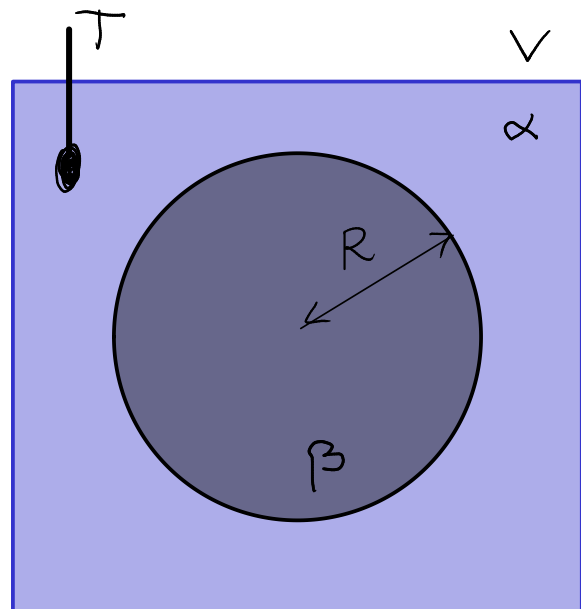CNT : fenomenologica α = metastabile β = stabile $f = \dfrac{F}{V}$ $f_\beta < f_\alpha$

$$\Delta f = f_\beta - f_\alpha$$

$$\Delta F = \frac{4}{3}\pi R^3 \Delta f + 4\pi R^2 \cdot \gamma \longrightarrow \text{tensione di superficie}$$

ΔF barriera di nucleazione

$\Delta F^* \quad \swarrow \Delta F^* = \Delta F(R_*)$

$\sim R^2 \qquad \sim -R^3$

R_*

nucleo critico

$$\left.\frac{d\Delta F}{dR}\right|_{R^*} = 0 \; : \quad 4\pi R_*^2 \Delta f + 2 \cdot 4\pi R_* \gamma = 0 \;\Rightarrow\; R_* = -\frac{2\gamma}{\Delta f}$$

$$\Delta F^* = \frac{4}{3}\pi\left(-\frac{8\gamma^3}{\Delta f^3}\right)\Delta f + 4\pi \frac{4\gamma^2}{\Delta f^2}\gamma = \frac{4\pi}{3}\frac{12-8}{\Delta f^2}\gamma^3 = \frac{16\pi}{3}\frac{\gamma^3}{\Delta f^2} \sim \frac{1}{\Delta f^2}$$

Cinetica della nucleazione

- $\Delta F(R)$ paesaggio di energia
- 1 dof: R del nucleo
- particella browniana senza inerzia in campo esterno

Eq. Smoluchowski: $\Delta U \to \Delta F$, $x \to R$, $D = \dfrac{k_B T}{\xi} = D(R)$

BH 10.6 $\Rightarrow$ $p(R, t)$

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial R}\left[D(R) \frac{\partial p}{\partial R} + \frac{1}{\xi} \frac{d \Delta F}{dR} p \right] \qquad \Delta F^* \gg k_B T$$

Tempo di nucleazione τ_X (1 nucleo critico)

$=$ tempo di uscita

$$\tau_X = \frac{1}{D(R_*)} \cdot \frac{1}{\left(-\dfrac{1}{2\pi k_B T} \dfrac{d^2 \Delta F}{dR^2}\Big|_{R_*} \right)^{1/2}} \cdot \exp\left(\frac{\Delta F^*}{k_B T} \right) \quad \leftarrow \text{ fattore di Arrhenius}$$

$\uparrow$ fattore cinetico $\qquad \uparrow$ fattore termodinamico (Zeldovich)

ΔF

ΔF^*

R_*

R

problema di kramers

$\Delta U \gg k_B T$

Tasso di nucleazione :   nuclei / tempo / volume

$$I = \frac{N}{\tau_x} \cdot \frac{1}{V} = \frac{S}{\tau_x}$$

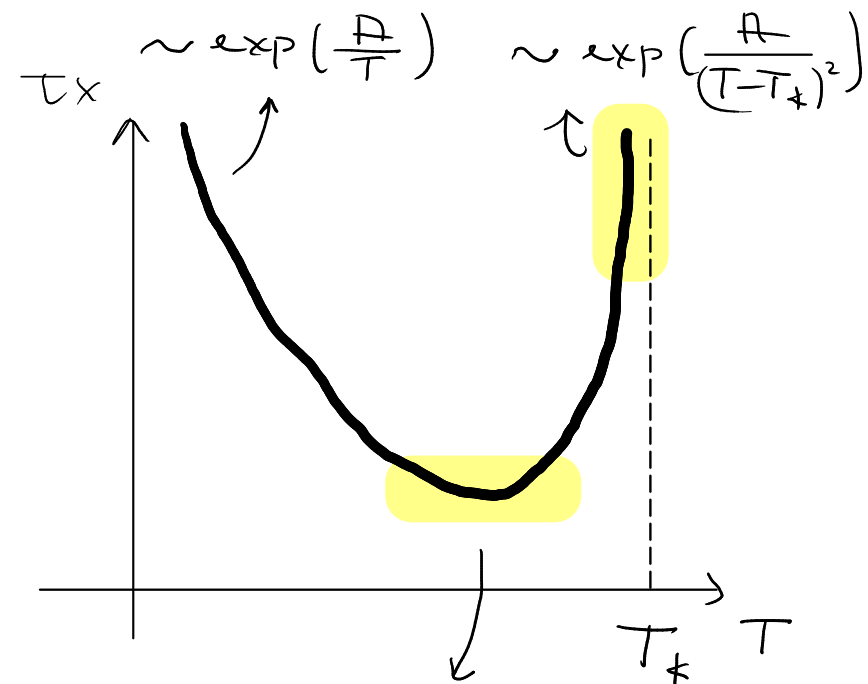Dipendenza di τ_x dalla temperatura

$T \ll T_k$: $D(R^k) \sim \exp\left(-\frac{\Delta E_d}{K_B T}\right)$

$$\tau_x \sim \exp\left(\frac{\Delta E_d}{K_B T}\right) \cdot \exp\left(\frac{\Delta F^k}{K_B T}\right)$$
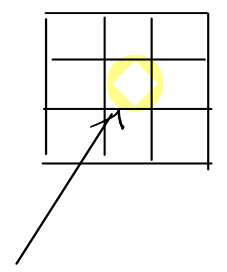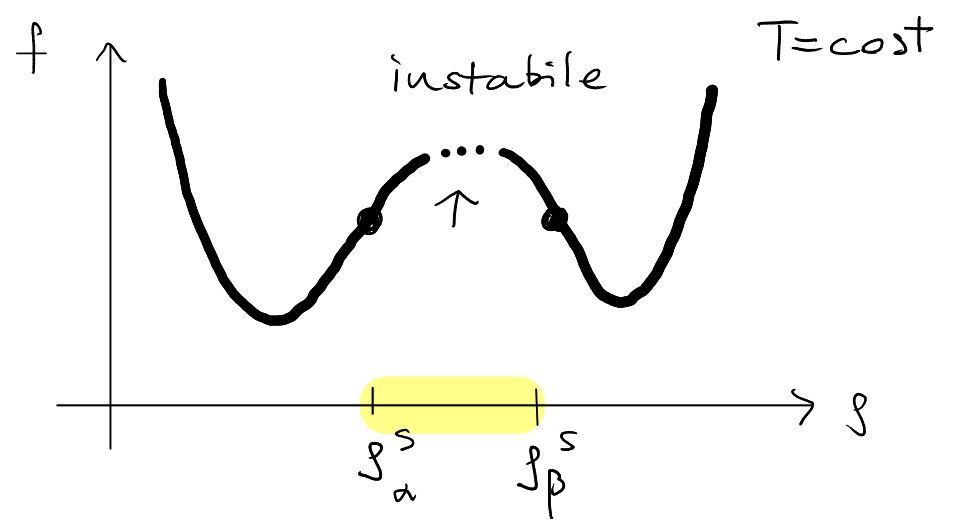
$T \approx T_k$: $\Delta f \sim (T - T_k)$

$$\Delta F^k \sim \frac{1}{\Delta f^2} \sim \frac{1}{(T-T_k)^2}$$
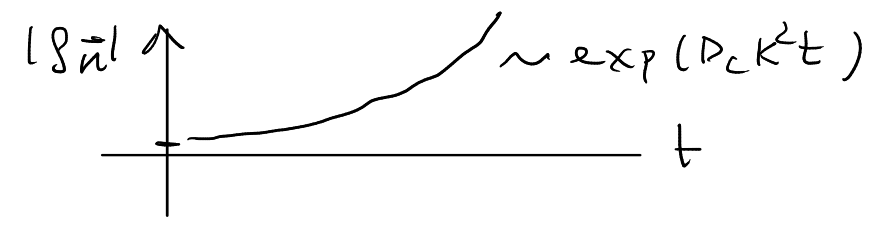
$$\tau_x \sim \exp\left(\frac{A}{T(T-T_k)^2}\right)$$

τ_x $\sim \exp\left(\frac{A}{T}\right)$ $\sim \exp\left(\frac{A}{(T-T_k)^2}\right)$

T_k T

nucleazione
+ rapida
omogenea

2) Decomposizione Spinodale

$$\frac{\partial F}{\partial N}\bigg|_T = \mu = \frac{\partial f}{\partial \rho}\bigg|_T$$

$$\frac{\partial^2 f}{\partial \rho^2}\bigg|_T = \frac{\partial \mu}{\partial \rho}\bigg|_T < 0 \quad \Rightarrow \quad D_C < 0 \;!!$$
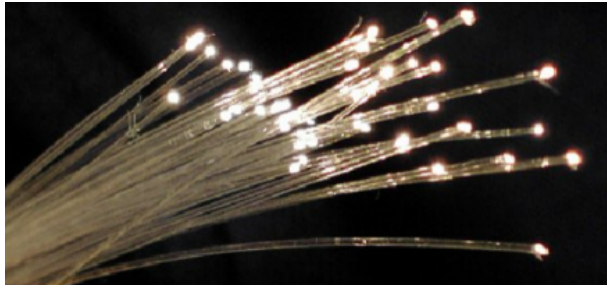
$$\frac{\partial \rho}{\partial t} = D_C \vec{\nabla} \rho \quad \Rightarrow \quad \rho_{\vec{k}}(t) = \rho_{\vec{k}}(0) \, \exp(- D_C k^2 t) = \rho_{\vec{k}}(0) \, \exp(+ |D_C| k^2 t)$$

$$\text{Cahn - Hilliard :} \quad \frac{\partial \rho}{\partial t} = \frac{L_{NN}}{T} \nabla^2 \left[\frac{\partial^2 f}{\partial \rho^2} \rho_N - \frac{k_B T \, \xi_0^2}{\rho} \nabla^2 \rho \right]$$

$$\rho_N(\vec{r}, t) = \rho(\tilde{r}, t)$$

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \left(L_{NN} \vec{\nabla}\left(-\frac{\mu}{T}\right) \right)$$

$$= \vec{\nabla} \cdot \left(\frac{L_{NN}}{T} \vec{\nabla} \mu \right)$$

$$\mu = \mu[\rho(\vec{r}, t)] \quad = \vec{\nabla} \cdot \left(\underbrace{\frac{L_{NN}}{T} \frac{\partial \mu}{\partial \rho}}_{D_C} \vec{\nabla} \rho \right)$$

Formatori di vetro

ossidi

Silicati : SiO_2 (silice)

B_2O_3

gorilla glass ©

vetro da finestre

SiO_2 : 70%
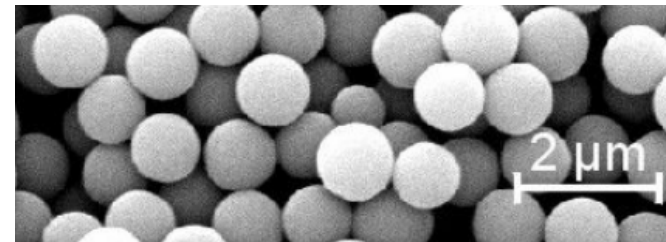NaO_2 : 20%
CaO : 10%

Polimeri
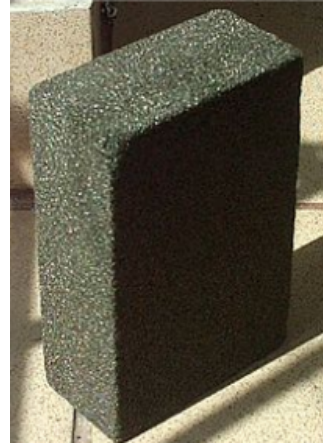
polistirene

PMMA

Metallici

Colloidi

2 µm

organici

Substance	T_g
SiO_2	1473[g]
B_2O_3	532[m]
nPOH	97[h]
PropGlyc	167[d]
3-MePent	77[f]
3-Br-P	108[a]
glycerol	190[d]
BMPC	243[h]
salol	220[a]
MTHF	91[a]
OTP	246[h]
PropCarb	158[i]
triPhenPhos	203[k]
CKN	333[g]

Richert & Angell JCP 1998
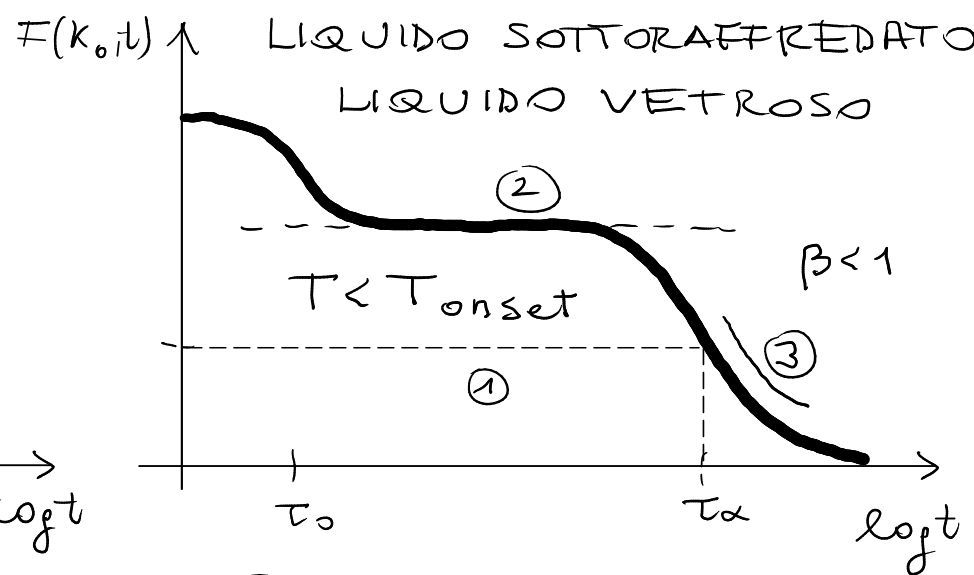
Liquido sottoraffreddato : $T < T_m$ Vetro : $T < T_g$

1) Tempo di rilassamento strutturale

$$F(k,t) = \frac{\langle \hat{S}_{\vec{k}}(t)\, \hat{S}_{-\vec{k}}(0) \rangle}{\langle \hat{S}_{\vec{k}}(0)\, \hat{S}_{-\vec{k}}(0) \rangle}$$
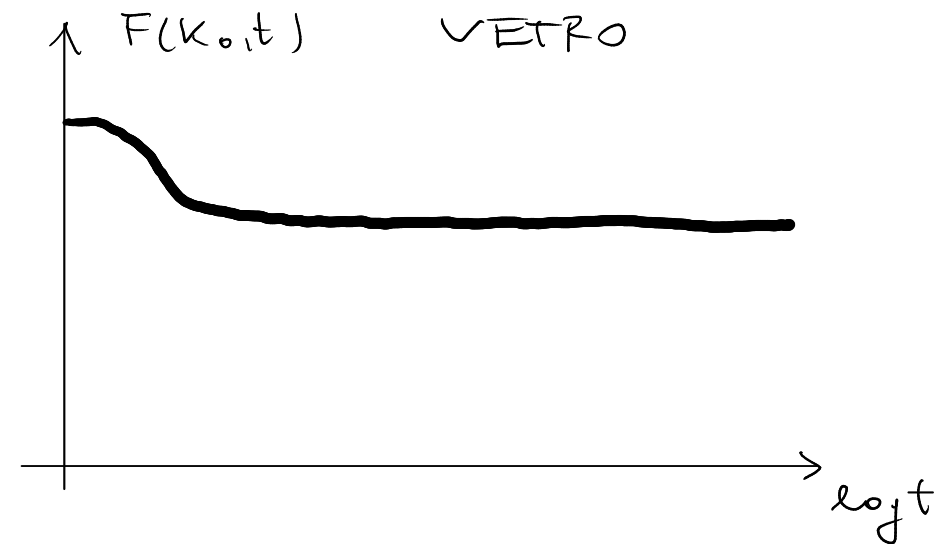
$$k_0 \approx \frac{2\pi}{z_0}$$

z_0

LIQUIDO NORMALE

$$F(k_0, \tau_\alpha) = \frac{1}{e}$$

LIQUIDO SOTTORAFFREDATO
LIQUIDO VETROSO

② $T < T_{onset}$ $\beta < 1$ ③

①

VETRO

τ_0 τ_α $\log t$

τ_0 τ_α $\log t$

$\log t$
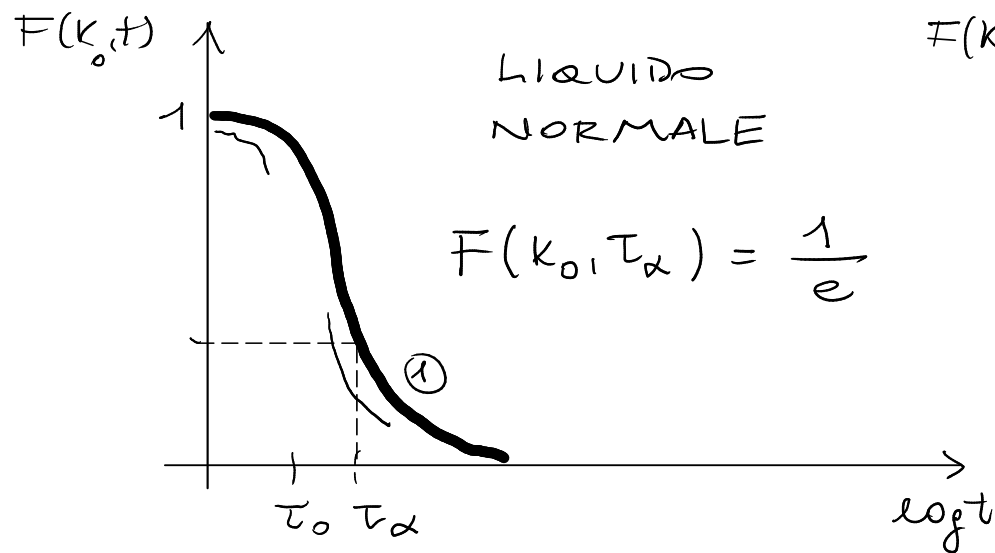
① $F(k_0, t) \sim \exp\left(-t/\tau_\alpha\right)$

① $\tau_\alpha \gg \tau_0$

② two-step

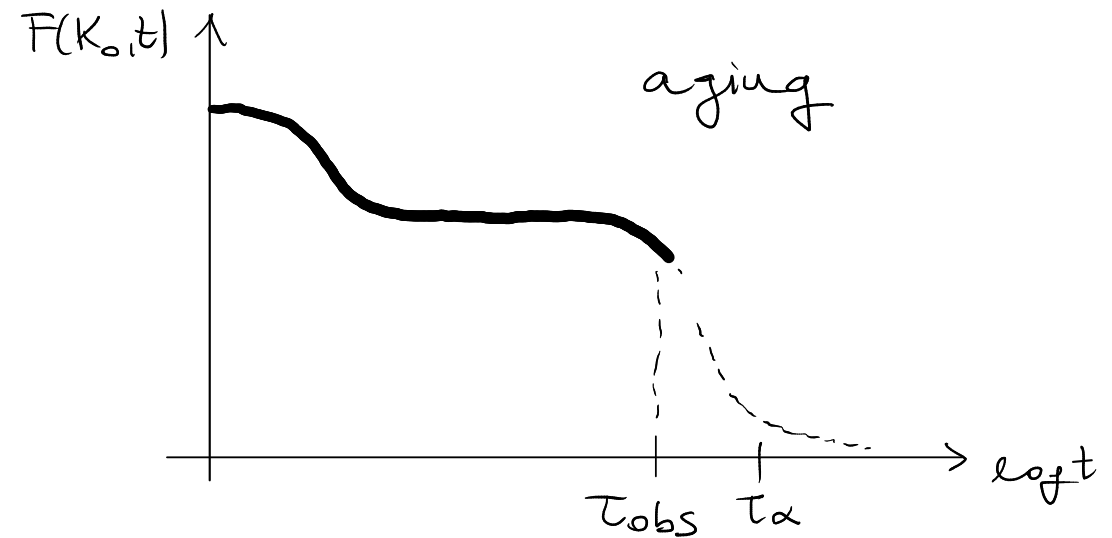③ $F(k_0, t) \sim \exp\left(-\left(t/\tau_\alpha\right)^\beta\right)$

Relazione Maxwell

$$\eta = G_0 \tau_\alpha$$

$1/T$

2) **Tempo di osservazione : τ_{obs}**

$F(K_0, t)$ ... τ_α ... τ_{obs} ... $\log t$

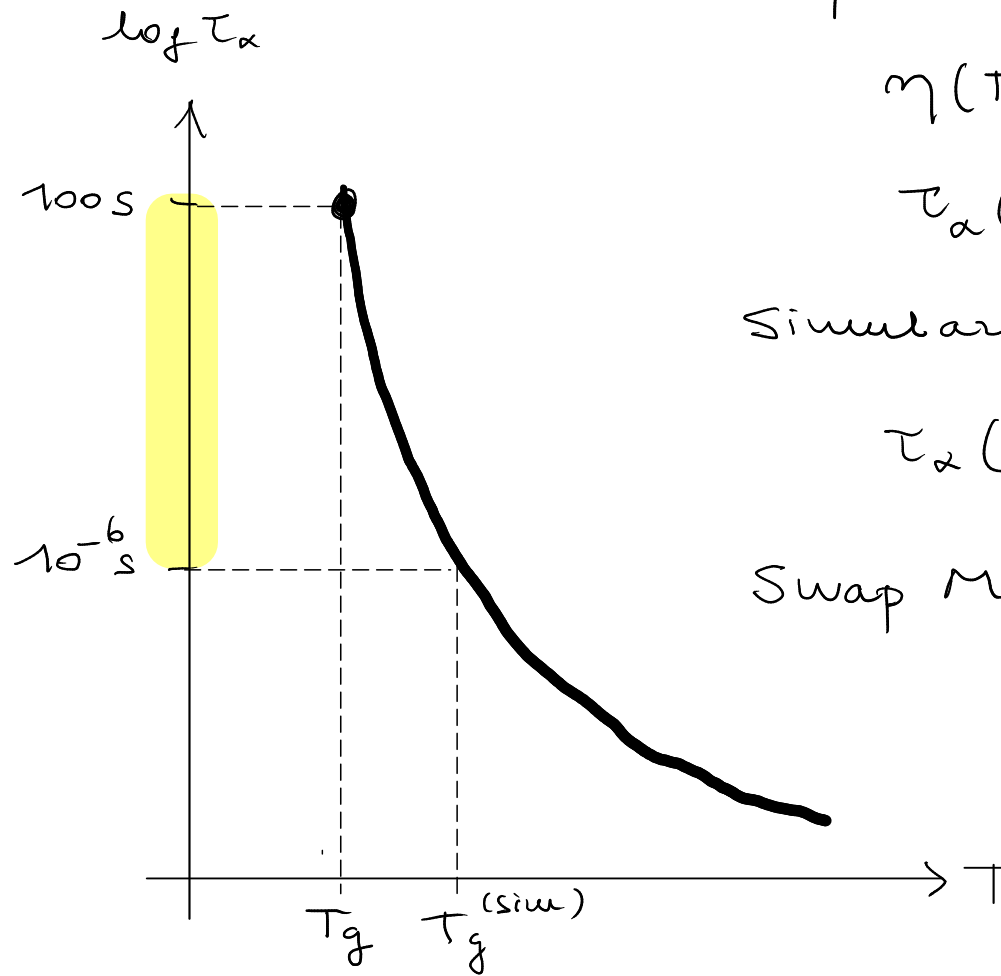$F(K_0, t)$ ... aging ... τ_{obs} τ_α ... $\log t$
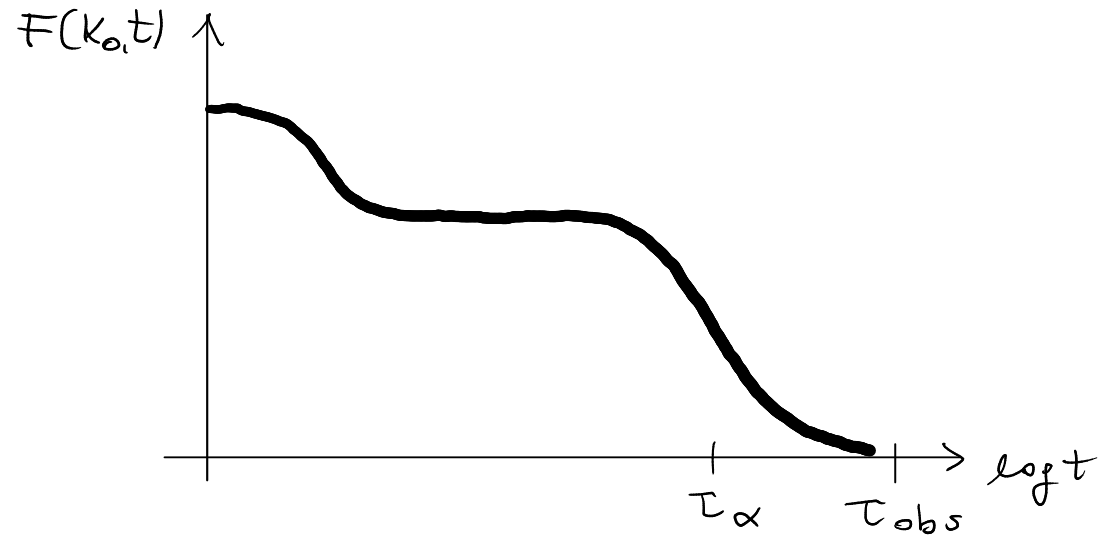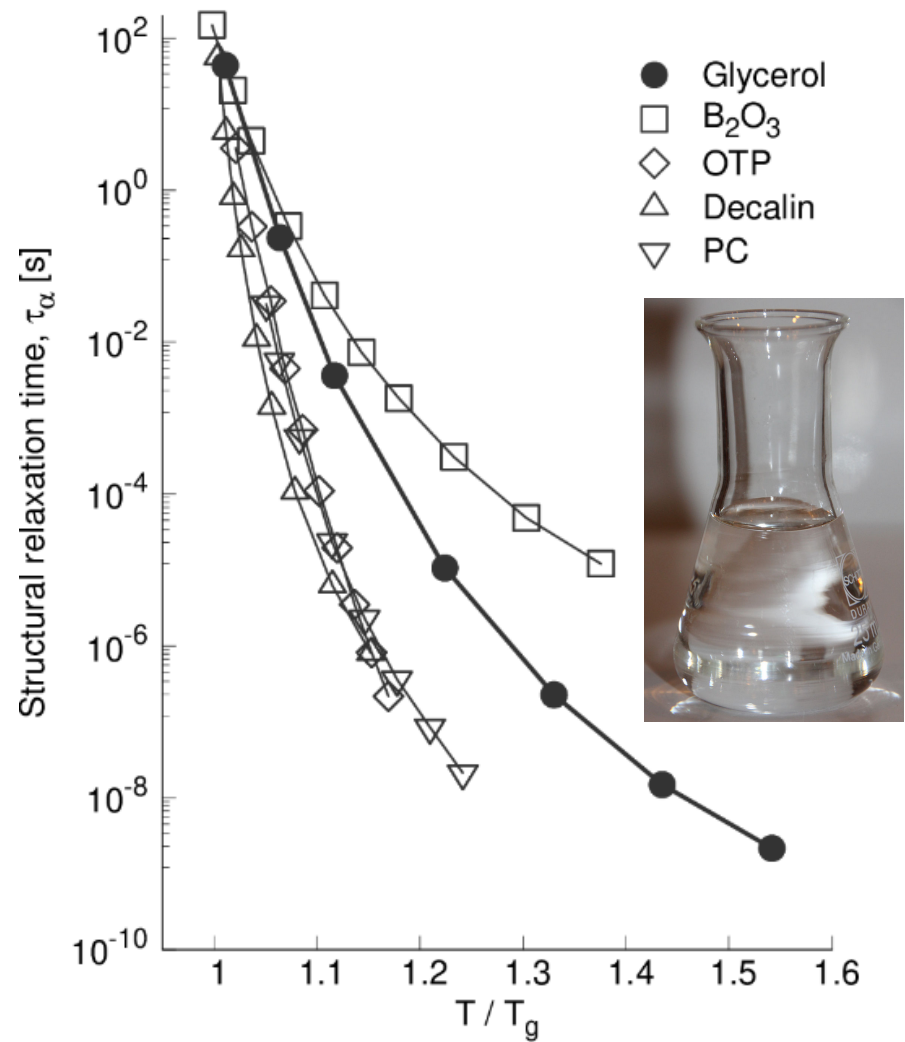
non-ergodico
fuori-equilibrio

Def. di equilibrio di Feynman : " when all the fast things have happened
and all the slow ones not "

Det. operativa della transizione vetrosa :

$$\tau_\alpha (T_g) = \tau_{obs} \qquad \tau_\alpha = \tau_\alpha (T)$$

Right panel (hand-drawn plot):

$\log \tau_\alpha$

$100\,s$ · · · · · ●

$10^{-6}\,s$ · · · · ·

T_g $T_g^{(sim)}$ → T

Right column (handwritten notes):

Esperimenti :

$$\eta(T_g) = 10^{12}\ Pa\cdot s$$

$$\tau_\alpha(T_g) \approx 10^2\ s$$

Simulazioni :

$$\tau_\alpha\left(T_g^{(sim)}\right) \approx 10^{-6}\ s$$

Swap MC PRX 2017

Bottom row (handwritten):

$$timestep = \frac{\tau_o}{100}$$

$$\tau_o \sim 10^{-12}\ s$$

$$10^{-6}\ \frac{s}{step\cdot part}$$

$$N = 10^3$$

$$t_1 = 10^{-3}\,s$$

$$\frac{t_1^{reale}}{timestep} \approx 10^{-3} \times 10^{14}$$

$$= 10^9$$

3) <mark>Tempo di cristallizzazione</mark> : τ_x

$$\tau_x \sim \frac{1}{D(R_k)} \exp\left(\frac{\Delta F^*}{K_B T}\right)$$

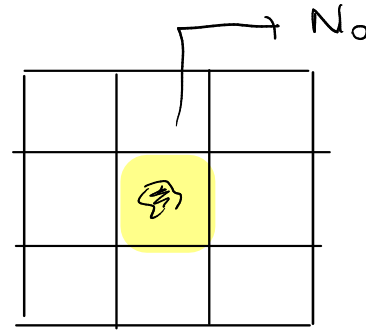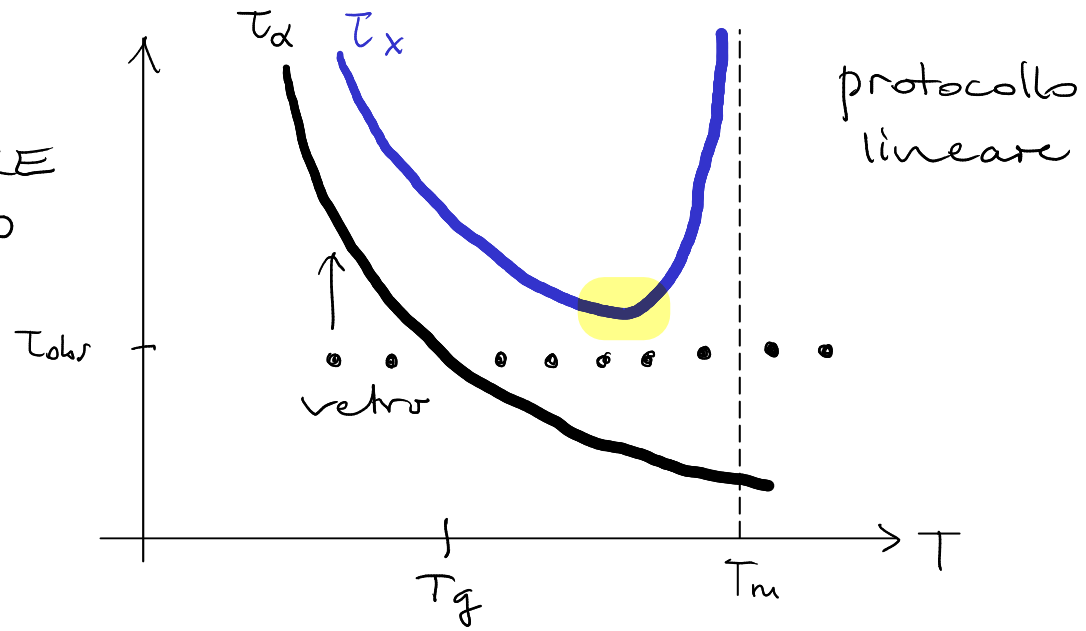$$\tau_{x,N} \sim \frac{1}{N}$$

$$\exists\, N_0 : \tau_{x,N_0} = \tau_x$$

Diagramma tempo – temperatura – trasformazione (TTT)

① rilassare defs lenti ($\hat{S}_{\overline{n}_0}$) ② evitare cristallo
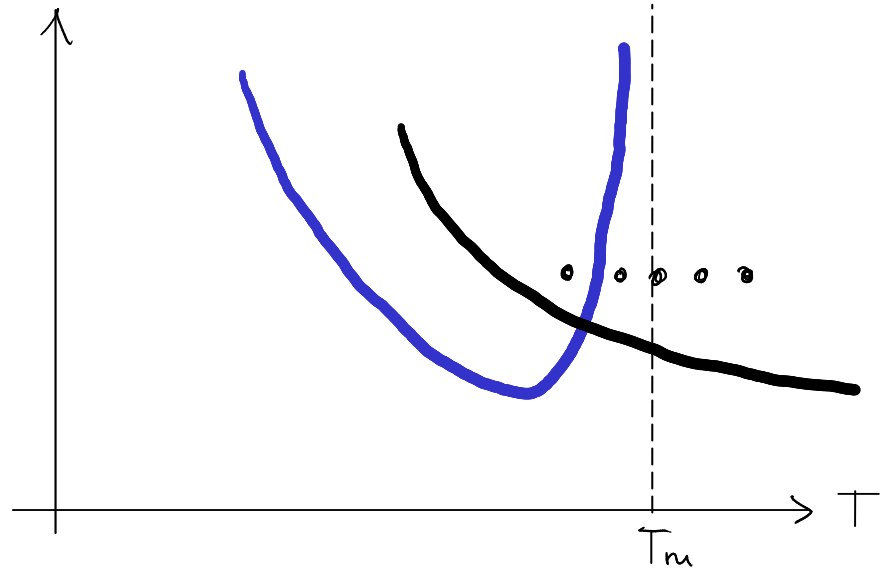
$\tau_\alpha < \tau_{obs} < \tau_x$

BUON FORMATORE DI VETRO

τ_α τ_x

protocollo lineare

τ_{obs}

vetro

T_g T_m T

protocollo non-lineare

$\tau_{obs} \sim \tau_\alpha$

T_g T_m T

CATTIVO FORMATORE DI VETRO

T_m T

H_2O Patm

160 K – 230 K

NO MAN'S LAND T_m T

$$\log \langle |\Delta \vec{r}|^2 \rangle$$

$$\delta^2 = \langle |\Delta \vec{r}(t_o)|^2 \rangle$$

$$\delta^2 \leftrightarrow T \quad \underline{es.}$$

$\sim t$

δ^2

$\sim t^2$

t_o

$\log t$

cage effect

$\delta \sim 0.2 \, \xi_o$

ξ_o

$$F_s(K,t)$$

$\log t$
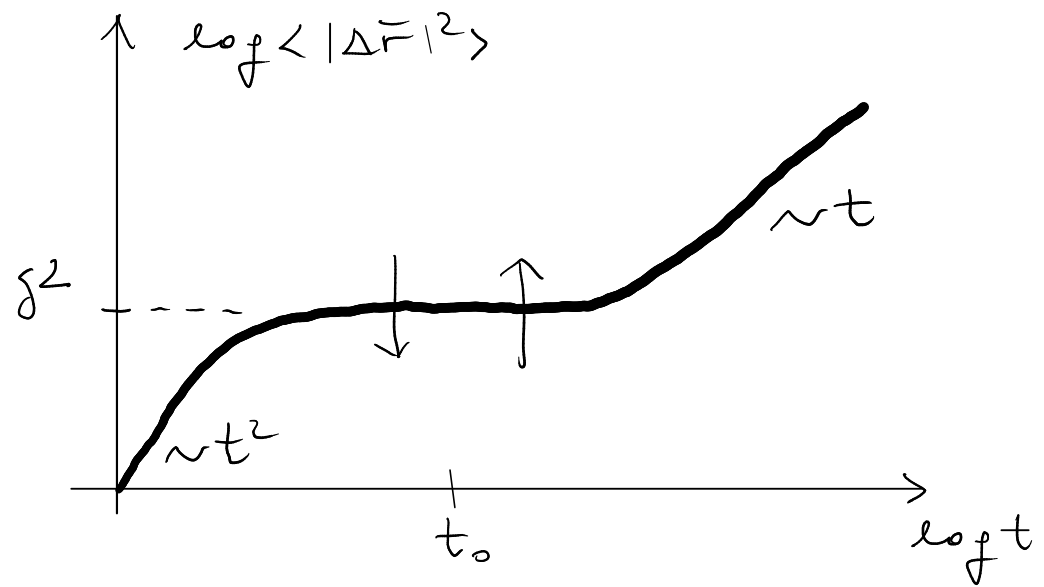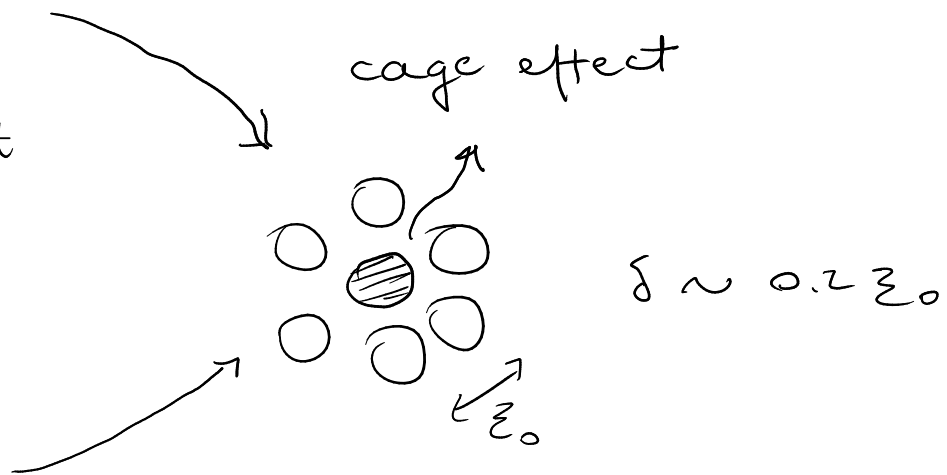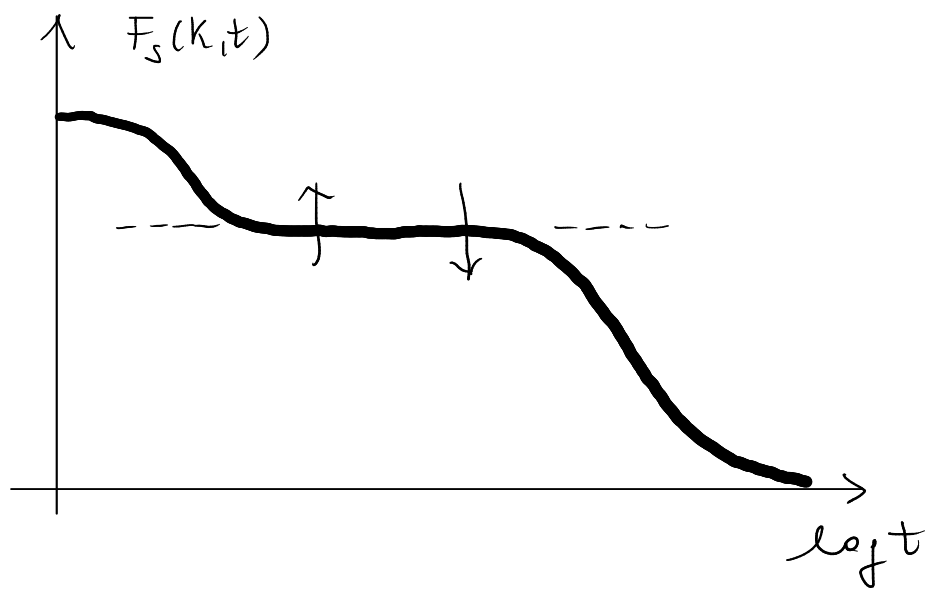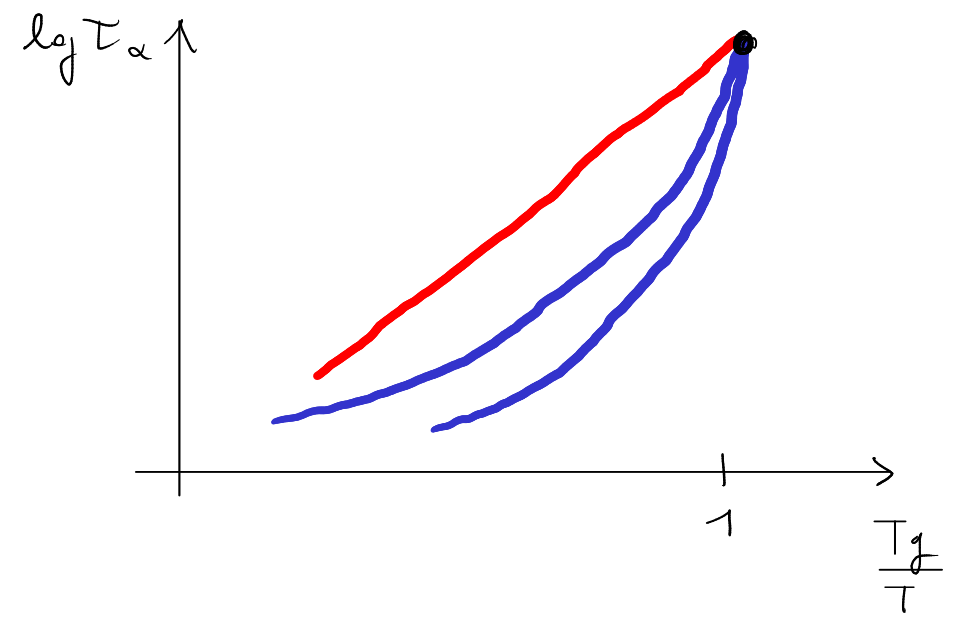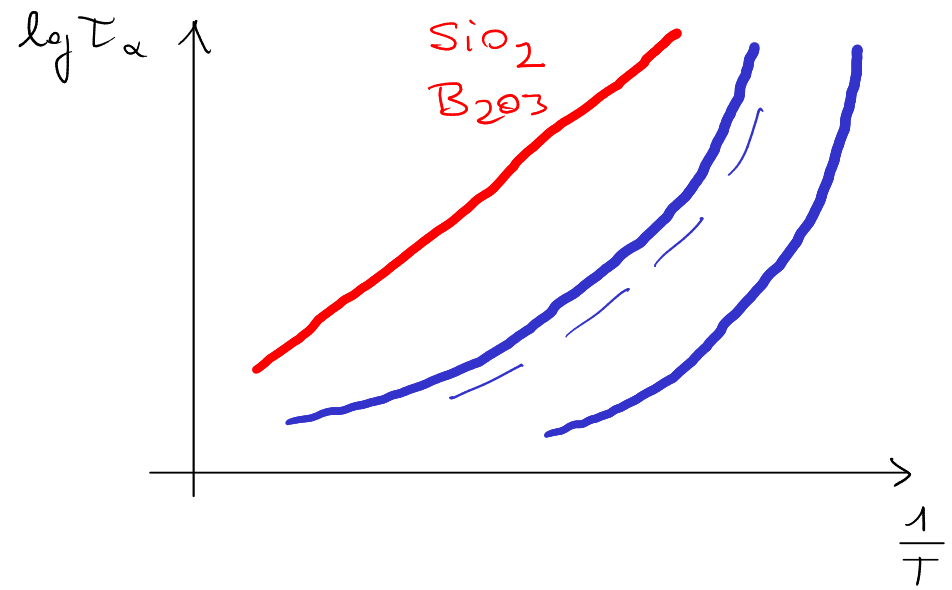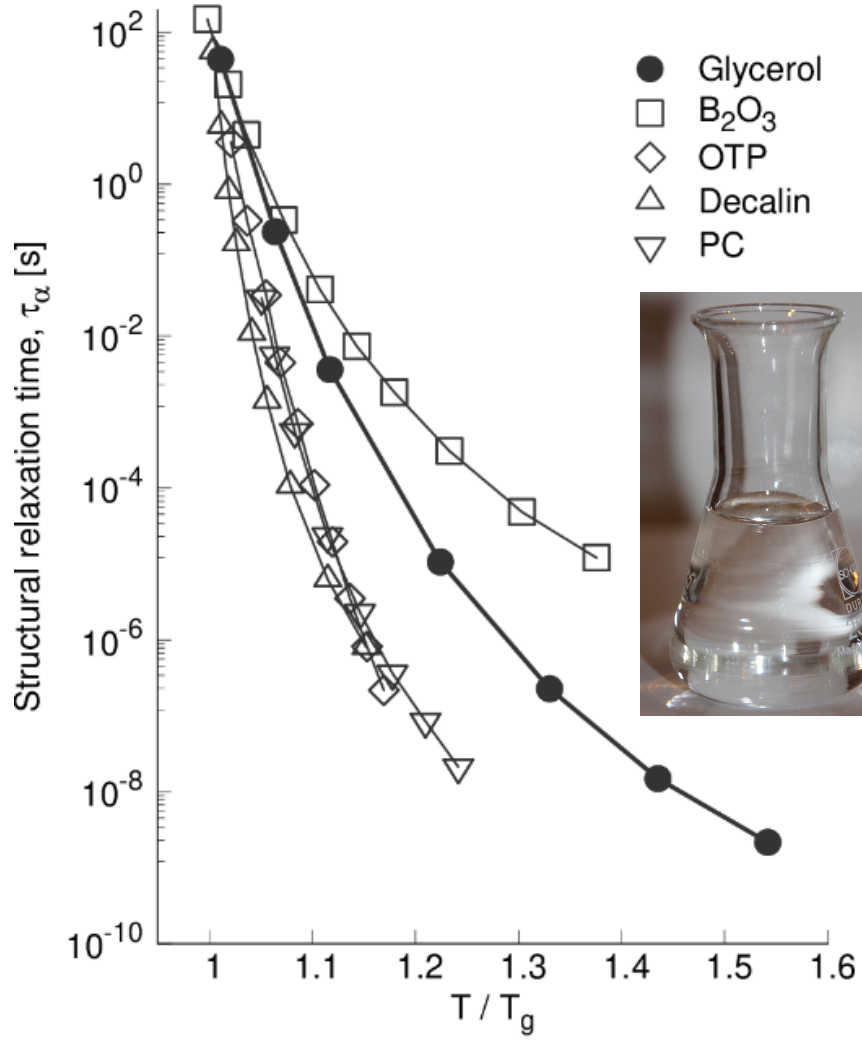
Arrhenius

$$\tau_\alpha \sim \exp\left(\frac{\Delta E}{k_B T}\right)$$

STRONG

Super-Arrhenius

$$\tau_\alpha \sim \exp\left(\frac{\Delta E(T)}{k_B T}\right)$$

$\Delta E \uparrow \quad T \searrow$
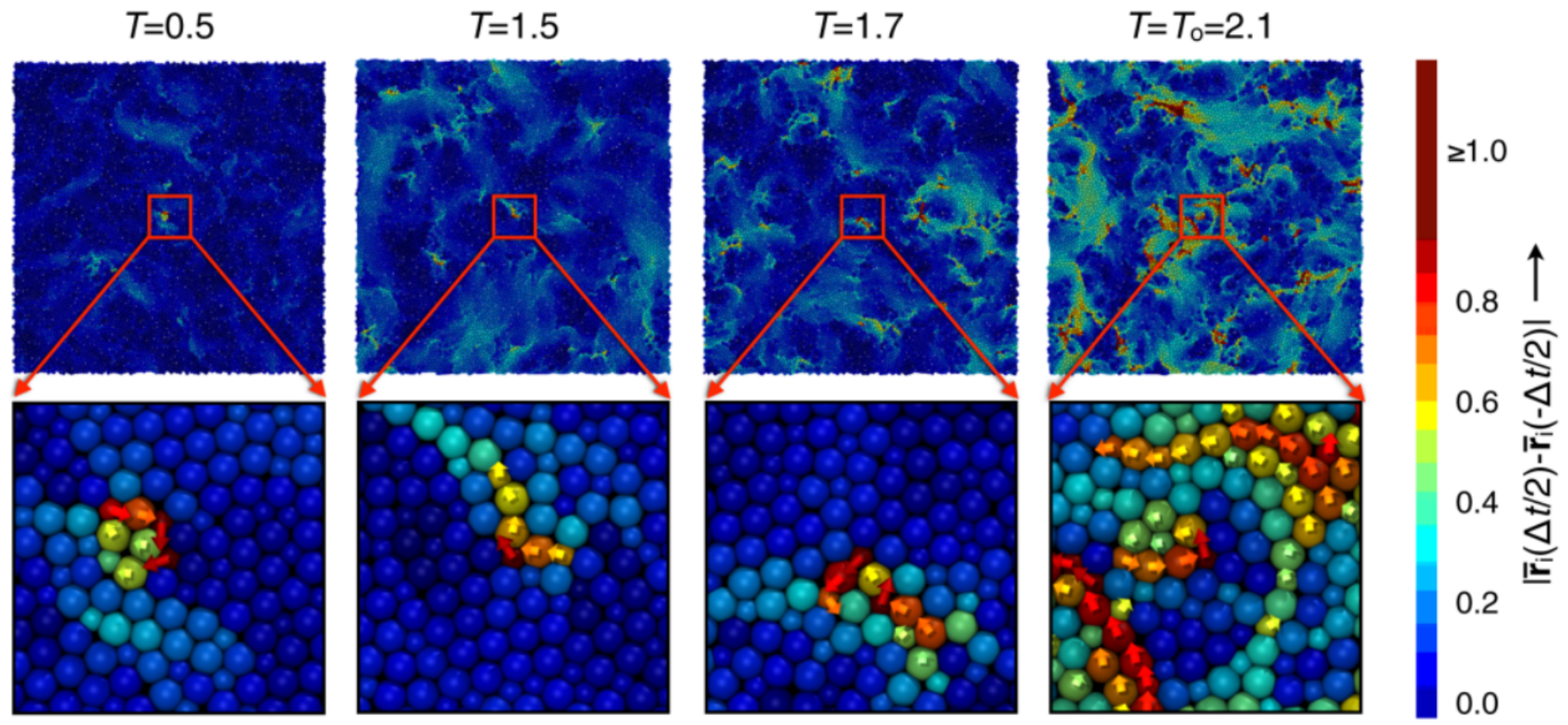
FRAGILE

Classificazione di Angell : fragilità

$$m = \frac{d \log \tau_\alpha}{d(T/T_g)}\bigg|_{T=T_g}$$

Eterogeneità dinamiche

T=0.5   T=1.5   T=1.7   T=T_0=2.1

≥ 1.0

0.8

0.6

$|\bar{r}_i(\Delta t/2) - \bar{r}_i(-\Delta t/2)| \longrightarrow$

0.4

0.2

0.0

keys et al. PRX 2011

Termodinamica

Energia interna: E

Capacità termica: $C_V = \left.\dfrac{\partial E}{\partial T}\right|_V$
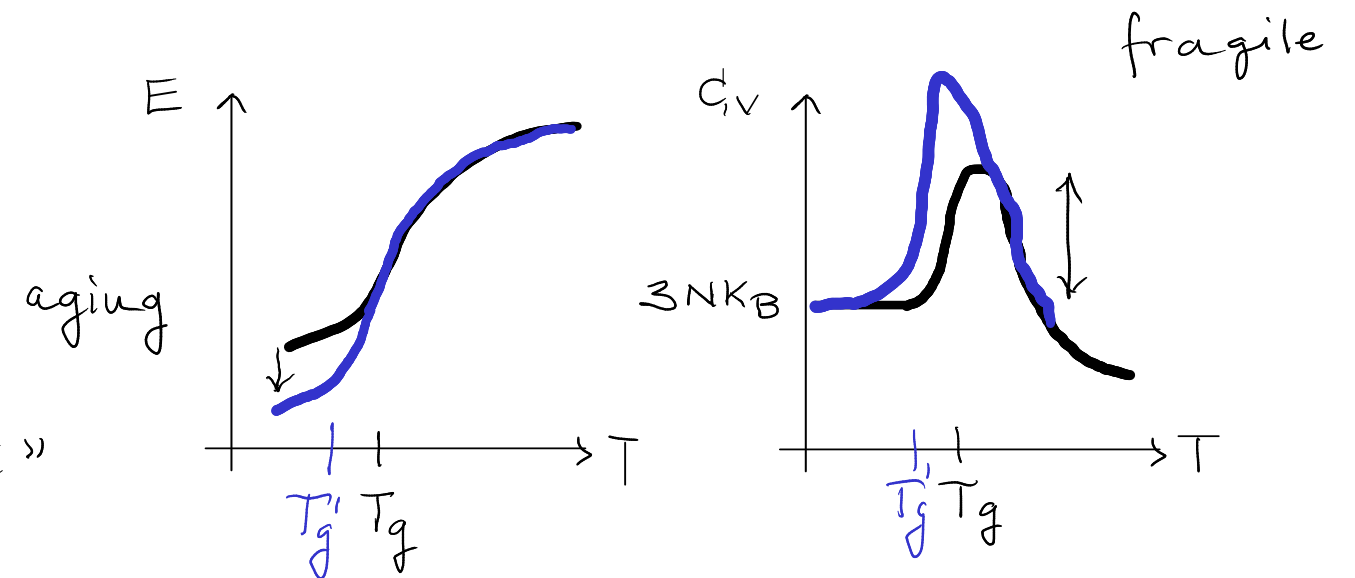
Approx armonica: $E \approx 3NK_BT$

Congelamento di defs "configurazionali"

aging

T_g' T_g

C_V

fragile

$3NK_B$

T_g' T_g

$N = \text{cost}$ $V = \text{cost}$

Entropia: $dS = \dfrac{1}{T} dE - \underset{\approx 0}{\dfrac{P}{T} dV} + \underset{\approx 0}{\dfrac{\mu}{T} dN}$

$$S(T) = S(T_0) + \int_{T_0}^{T} \frac{1}{T} dE = S(T_0) + \int_{T_0}^{T} \frac{C_V}{T} dT$$

$\Big\langle$ gas perfetto   integrazione
  solido armonico   termodinamica

▢ cristallo perfetto : $S = S_{vib}$

▢ cristallo + difetti : $S = S_{vib} + S_c$

▢ liquido : S

▢ liquido sotto raffredato : $S \approx S_{vib} + S_c$

$$\Delta S = S_{liq} - S_{crist} \approx (S_{vib} + S_c) - (S_{vib}) \approx S_c$$
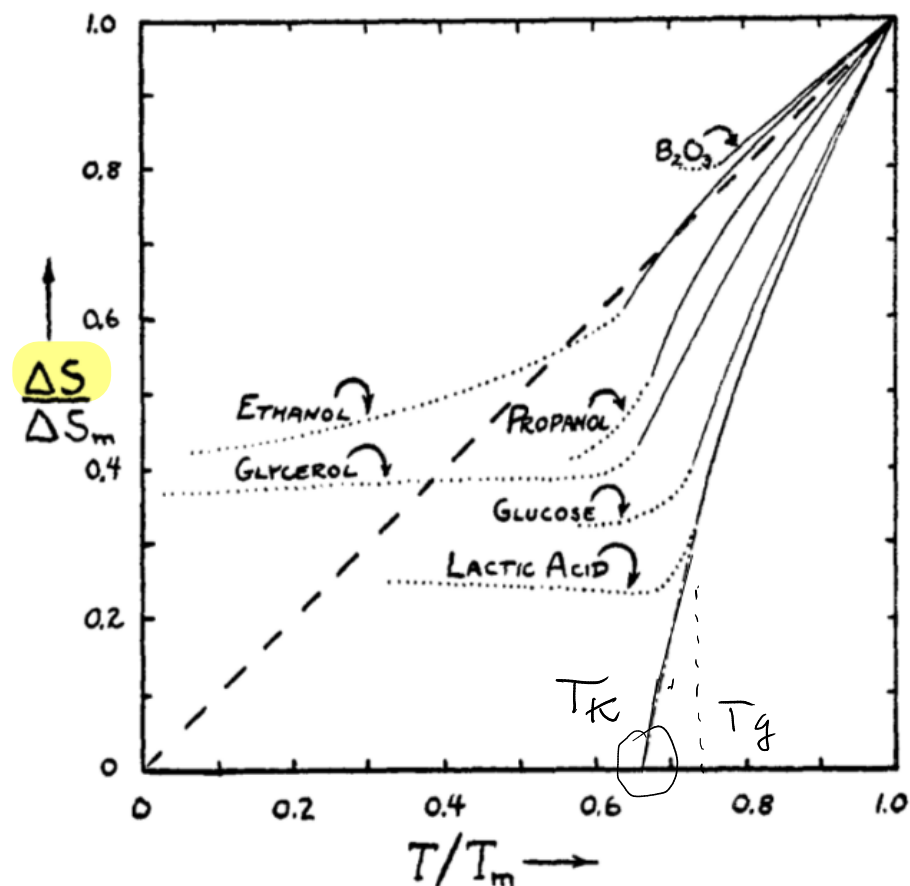
4. Differences in entropy between the supercooled liquid and crystalline ph

Kauzmann Chemical Reviews 1948

Paradosso di Kauzmann

"Entropy crisis"

Then how are these curves to be extrapolated below T_0? Certainly it is unthinkable that the entropy of the liquid can ever be very much less than that of the solid.[7] It therefore seems obvious that the "true" or "non-vitreous" curves

[7] It could conceivably become slightly less at finite temperatures because of a "tighter" binding of the molecule in the highly strained liquid structure, with consequent higher frequencies of vibration and a lower density of vibrational levels.
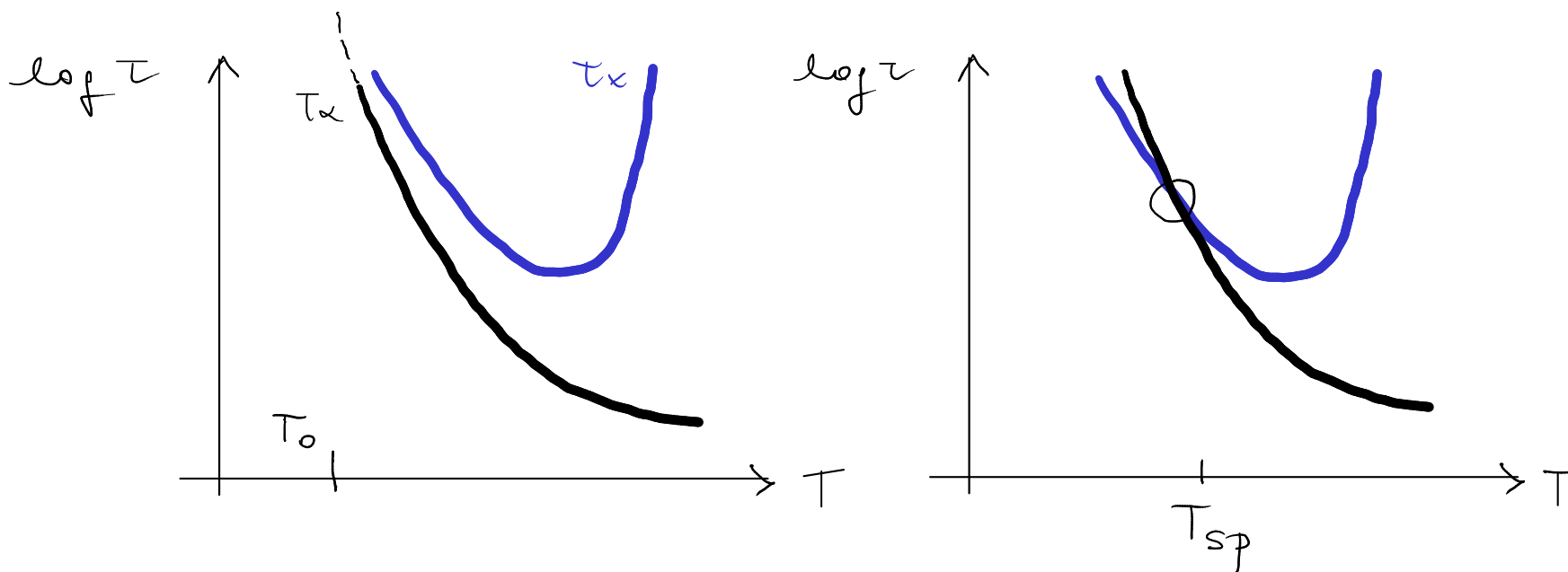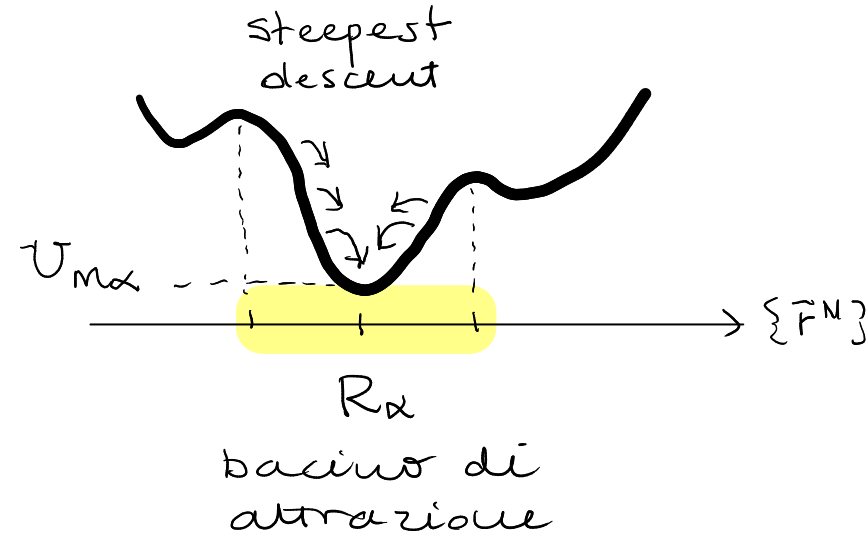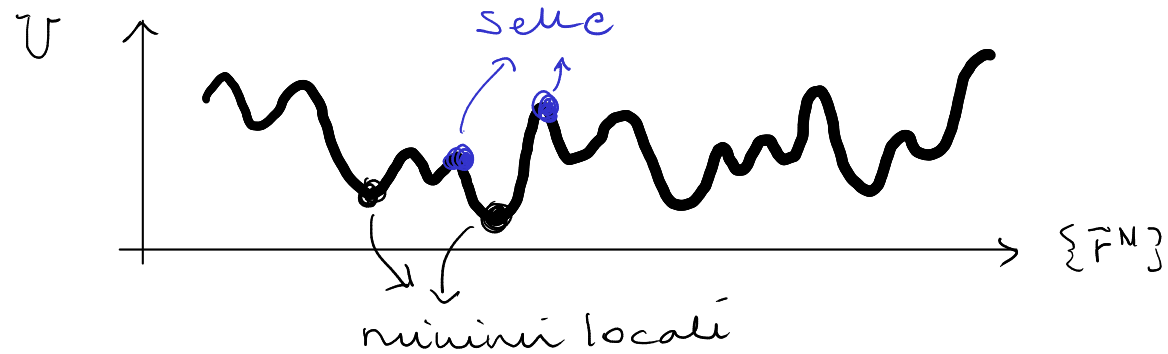

$$\tau_\alpha \sim \exp\left(\frac{A}{T-T_0}\right)$$

Vogel-Fulcher

① vetro ideale

① cristalizzazione

TEORIE E MODELLI DELLA TRANSIZIONE VETROSA

Energy landscape (PEL)

$$\tilde{U} = U(\{\vec{r}^N\})$$

Stillinger Weber '80

"struttura inerente"

punti stazionari : $\vec{\nabla} U = \vec{0}$

Hessiana : $\mathcal{H} = \left(\dfrac{\partial^2 U}{\partial r_{i\alpha} \partial r_{j\beta}} \right)$ $\quad i,j = 1,\dots,N$ $\quad \alpha,\beta = x,y,z$

$N = \text{cost}$ $\quad V = \text{cost}$ $\quad \Lambda = \dfrac{h}{\sqrt{2\pi m k_B T}}$

$$Z(T) = \text{Tr}\left[\exp\left(-\beta H(\{\vec{r}^N, \vec{p}^N\}) \right) \right] = \sum_\alpha \dfrac{1}{\Lambda^{3N}} e^{-\beta U_{m\alpha}} \int_{R_\alpha} d\vec{r}^N \, e^{-\beta\left[U(\{\vec{r}^N\}) - U_{m\alpha} \right]}$$

$$u_{m\alpha} = \dfrac{U_{m\alpha}}{N} \qquad U(\{\vec{r}^N\}) = \left(U(\{\vec{r}^N\}) - U_{m\alpha} \right) + U_{m\alpha}$$

$$Z(T) = \sum_\alpha e^{-\beta U_{m\alpha}} \dfrac{1}{\Lambda^{3N}} \int_{R_\alpha} d\vec{r}^N \, e^{-\beta\left[U(\{\vec{r}^N\}) - U_{m\alpha} \right]}$$

Densità di stati : $\Omega(u_m)$ $\qquad$ $\Omega(u_m) \, du_m$: n. minimi con energia tra

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ u_m e $u_m + du_m$

$$Z(T) = \int du_m \, \Omega(u_m) \, e^{-\beta N u_m} \, Z(u_m, T)$$

$\qquad\qquad\qquad\qquad\qquad\qquad$ $\hookrightarrow$ funzione di partizione vincolata

$$F_{basin}(u_m, T) = -K_B T \ln[Z(u_m, T)] \qquad f_{basin} = \frac{F_{basin}}{N}$$

$$= \int du_m \, \Omega(u_m) \, e^{-\beta N (u_m + f_{basin})}$$

Entropia configurazionale :

$$S_c = K_B \ln \Omega(u_m) \qquad\qquad s_c = \frac{S_c}{N} \qquad \triangle$$

$$Z(T) = \int du_m \, e^{-\beta N (u_m + f_{basin} - T s_c)}$$

1) Approx armonica:

$$f_{basin} \approx f_{vib} \qquad \frac{\partial f_{vib}}{\partial u_m} \approx 0$$

2) $N \to \infty$ Approx di punto sella (metodo di Laplace)

$$\int_a^b e^{Nf(x)} dx \qquad f \text{ ha un massimo in } x_o \qquad \text{per } N \to \infty$$

$$\approx \int_a^b e^{N\left[f(x_o) - \frac{1}{2}|f''(x_o)|(x-x_o)^2 \right]} dx = e^{Nf(x_o)} \int_{-\infty}^{\infty} e^{-\frac{1}{2}N|f''(x_o)|(x-x_o)^2} dx$$

$$\approx \sqrt{\frac{2\pi}{N|f''(x_o)|}} \ e^{Nf(x_o)}$$

$$\nwarrow \text{①}$$

$$Z(T) \approx \int du_m \ e^{-\beta N (u_m + f_{vib} - T s_c)} \qquad N \to \infty$$

$$\begin{cases} Z(T) \approx A(N)\, e^{-\beta N(u_m + f_{vib} - Ts_c)} & \swarrow \textcircled{2} \\[4mm] 1 + \dfrac{\partial f_{vib}}{\partial u_m} - T\dfrac{\partial s_c}{\partial u_m} = 0 \end{cases}$$

$$\underset{\textcircled{1} \approx 0}{\uparrow}$$

$$\begin{cases} Z(T) \approx e^{-\beta N(u_m + f_{vib} - Ts_c)} \qquad \Rightarrow \quad \text{termodinamica} \\[4mm] \dfrac{\partial s_c}{\partial u_m} = \dfrac{1}{T} \end{cases}$$

$$s_c = s_c(u_m)$$

1) $\quad S_c = 0 \qquad u_m \lesssim u_K$

2) $\quad \dfrac{\partial S_c}{\partial u_m}\Big|_{u_K} = \dfrac{1}{T_K}$

Supercooled liquids, glass transitions, and the Kauzmann paradox

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Many liquids have heat capacities that substantially exceed those of the corresponding crystal, and this discrepancy magnifies in the supercooled regime. Thus, liquid entropy declines more rapidly with temperature than does crystal entropy, and the former paradoxically seems to fall below the latter for temperatures below the Kauzmann point T_K. Although laboratory glass transitions inevitably intervene to prevent observation of this entropy crossing, it has often been argued that a second-order "ideal glass transition" in principle should occur at T_K. The inherent structure theory of condensed phases has been modified to describe supercooled liquids, and has been applied to this Kauzmann paradox. The conclusion is that an ideal glass transition of the type normally associated with the Kauzmann phenomenon cannot occur for substances of limited molecular weight and with conventional intermolecular interactions. This result also subverts theoretical expressions for shear viscosity (such as the Tamman–Vogel–Fulcher and the mode-coupling formulas) that diverge to infinity at an ideal glass transition temperature.
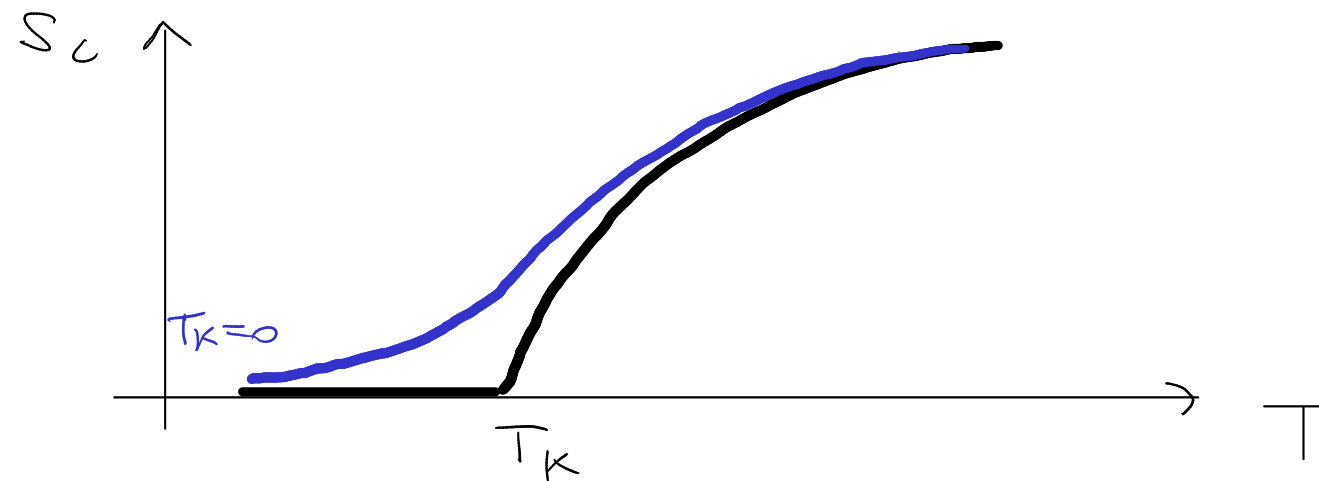
Modello di Adam e Gibbs (1965)

CRR = regioni che rilassano in modo cooperativo
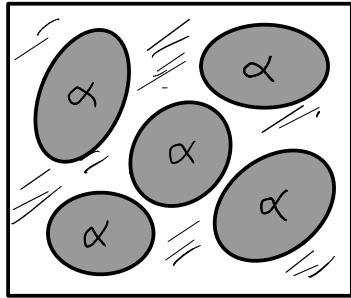
N particelle

n particelle / CRR

α n. stati / CRR

N. stati accessibili

$$\Omega = \alpha^{N/n}$$

Entropia configurazionale per particella

$$S_c = \frac{1}{N} k_B \ln \Omega = \frac{k_B}{n} \ln \alpha \sim \frac{1}{n} \qquad n \sim \frac{1}{S_c}$$

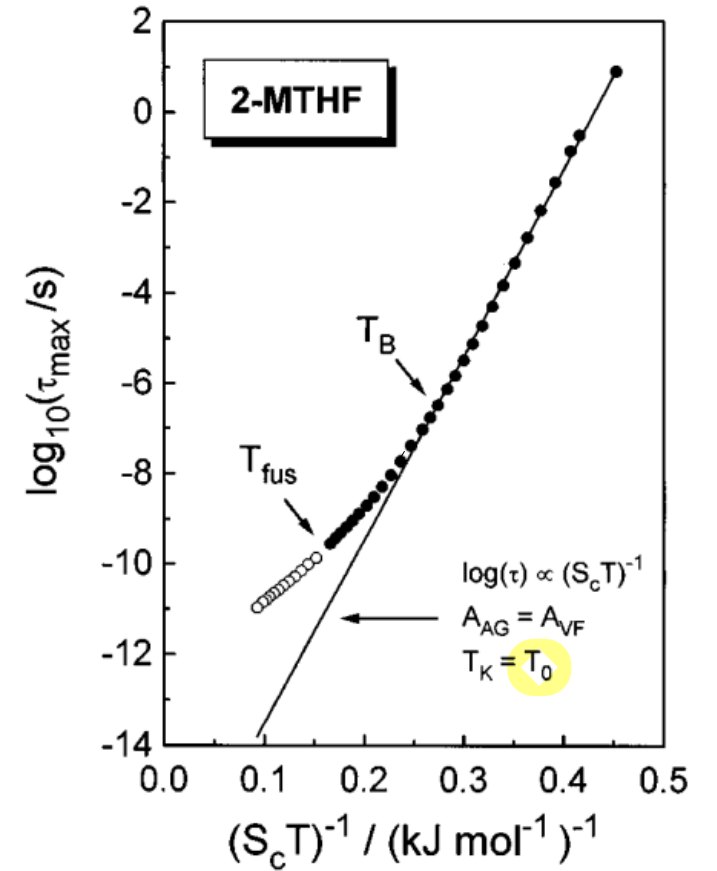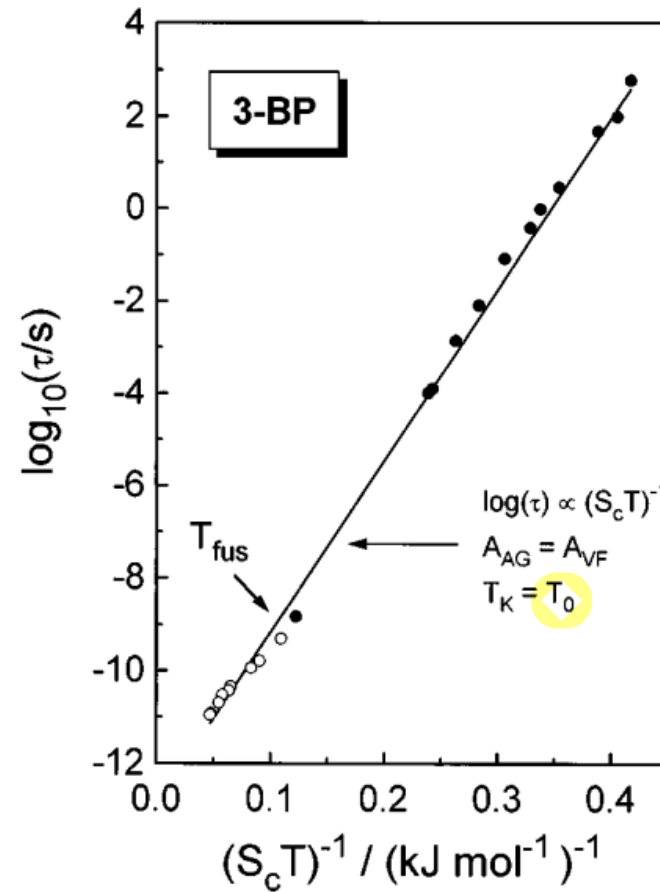Rilassamento termicamente attivato $\Delta E \sim n \sim \frac{1}{S_c}$

$$\tau_\alpha = \tau_0 \exp\left(\frac{\Delta E}{k_B T}\right) = \tau_0 \exp\left(\frac{A}{T S_c}\right) \qquad \text{relazione di Adam \& Gibbs}$$

Transizione ideale T_K : $T \simeq T_K \gg 0$

$$S_c \sim \frac{1}{T_K} (T - T_K)$$

$$\tau_\alpha \approx \tau_0 \exp \left(\frac{T_K B}{T(T - T_K)} \right)$$

$$\begin{cases} \tau_\alpha \approx \tau_0 \exp \left(\frac{C}{T - T_K} \right) \\ \text{Vogel - Fulcher} \qquad \nwarrow T_0 \end{cases}$$

$$\log(\tau) \propto (S_c T)^{-1}$$
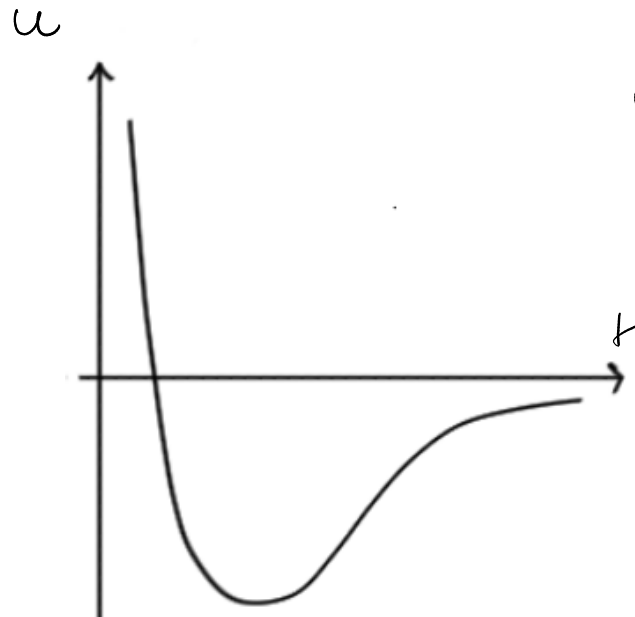$$A_{AG} = A_{VF}$$
$$T_K = T_0$$

Richert & Angell JCP 1998

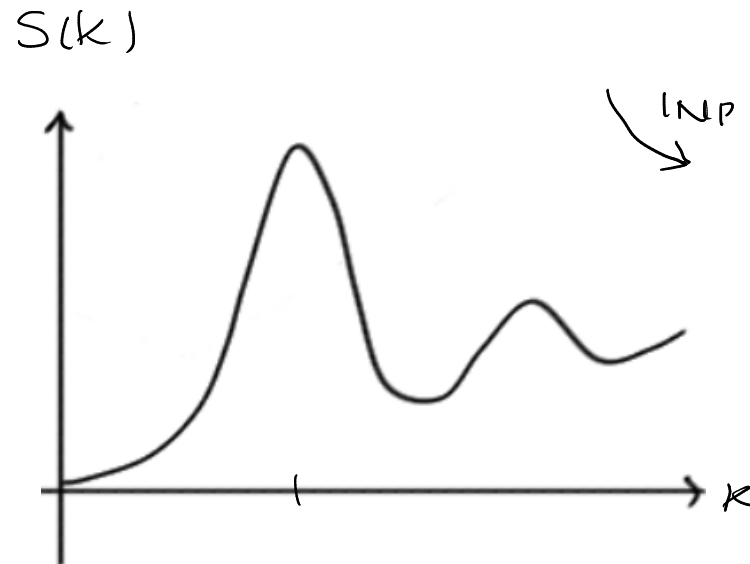Operatore di proiezione → Mori e Zwanzig ''1960

1984 Götze → transizione vetrosa

① 2-step relaxation + stretched exponential

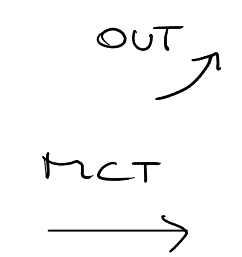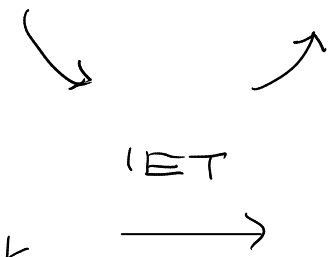② $\tau_\alpha (T)$ → vetro ideale

INTERAZIONI   STRUTTURA   DINAMICA

u $S(k)$ $F(k,t)$

IET   INP   OUT
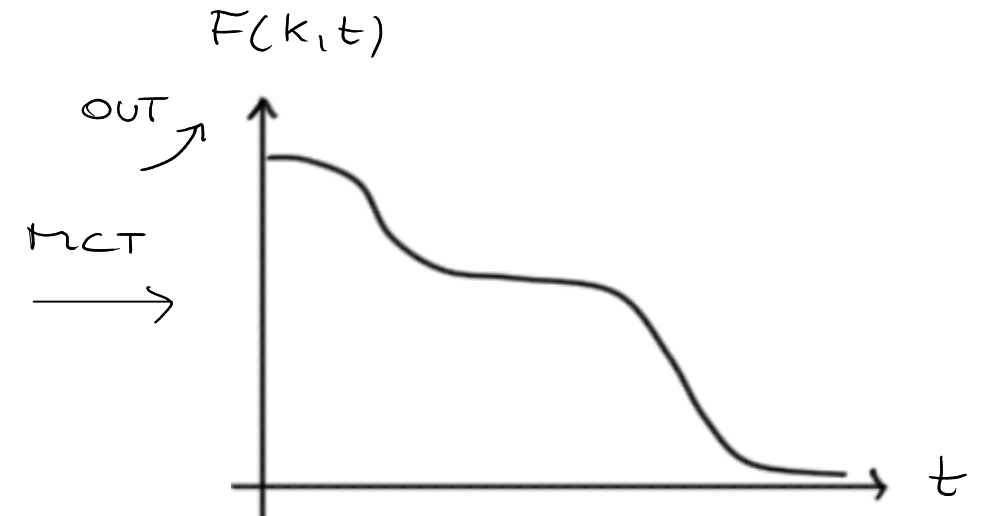   MCT

Variabile rilevante $A(t)$ $\{ A_1, \ldots, A_M \}$

$\quad$ lente $\hat{S}_{\vec{k}}(t)$, $\hat{\vec{J}}_{\vec{k}}(t)$ $\hat{\vec{J}}(\vec{r}, t) = \sum\limits_{i=1}^{N} \vec{v}_i \, \delta(\vec{r} - \vec{r}_i(t))$

$\quad$ resto

Prodotto Scalare

$\quad (B | A) \quad = \quad < A \, B^* > \qquad\qquad (\, < \delta A \, \delta B^* > \,)$

Eq. moto per A formalmente esatta : eq. Langevin generalizzata

$$\frac{dA}{dt} = i\,\Omega\,A(t) - \int_0^t ds \; M(t-s) \; A(s) \; ds + \Theta(t) \quad \leftarrow \text{forza stocastica}$$

$\qquad\qquad\qquad \uparrow \qquad\qquad\qquad\qquad \uparrow \qquad\qquad\qquad\qquad\qquad\qquad \downarrow$

$\qquad\qquad$ matrice delle $\qquad$ funzione di $\quad \sim \dfrac{(\Theta \,|\, \Theta(t))}{(A | A)} \qquad < \Theta(t)\, A^{\pm} > = 0$

$\qquad\qquad$ frequenze $\qquad\qquad$ memoria $\qquad\qquad\qquad\qquad\qquad\qquad (A | \Theta(t)) = 0$

$\qquad\qquad \sim \dfrac{(A | \mathring{A})}{(A | A)}$

Funzione di correlazione : $C(t) = \dfrac{< A(t) \, A^*(0) >}{< A(0) \, A^*(0) >}$

$$\frac{dc}{dt} = i\Omega c(t) - \int_0^t ds \, M(t-s) \, c(s) \, ds \qquad\qquad c(0) \to c(t)$$

Approssimazione mode-coupling : $\quad M \sim \hat{S}_{\bar{k}_1}(t) \, \hat{S}_{\bar{k}_2}(t) \quad \Rightarrow \quad F(k,t)$

$$\begin{cases} \dfrac{d^2 F}{dt^2} + \dfrac{k_B T \, k^2}{m \, S(k)} F(k,t) + \displaystyle\int_0^t ds \, M(k, t-s) \dfrac{dF}{ds}(k,s) = 0 \\[3em] M(k,t) = \dfrac{\rho \, k_B T}{16 \, \pi^3 \, m} \displaystyle\int d\bar{k}' \, |V_{\bar{k}, \bar{k}-\bar{k}'}|^2 \, F(k,t) \, F(|\bar{k}-\bar{k}'|, t) \end{cases}$$

$$\uparrow$$

vertici $\to S(k)$

Modello schematico : $\quad S(k) = \delta(k - k_0) \qquad \phi(t) = F(k_0, t)$

① $\quad \dfrac{d^2\phi}{dt^2} + \Omega^2 \phi + \lambda \displaystyle\int_0^t ds \, \phi^2(t-s) \dfrac{d\phi}{ds} = 0 \qquad \to$ memoria

② $\quad \dfrac{d^2\phi}{dt^2} + \Omega^2 \phi + \lambda \dfrac{d\phi}{dt} = 0 \qquad\qquad$ oscillatore armonico smorzato

②

ϕ

Sovrasmorzato

$\tau \sim x$

λ

t

Sottosmorzato

①

ϕ

$f = \phi(\infty)$

λ

t

$x < x_c : \quad f \simeq 0$
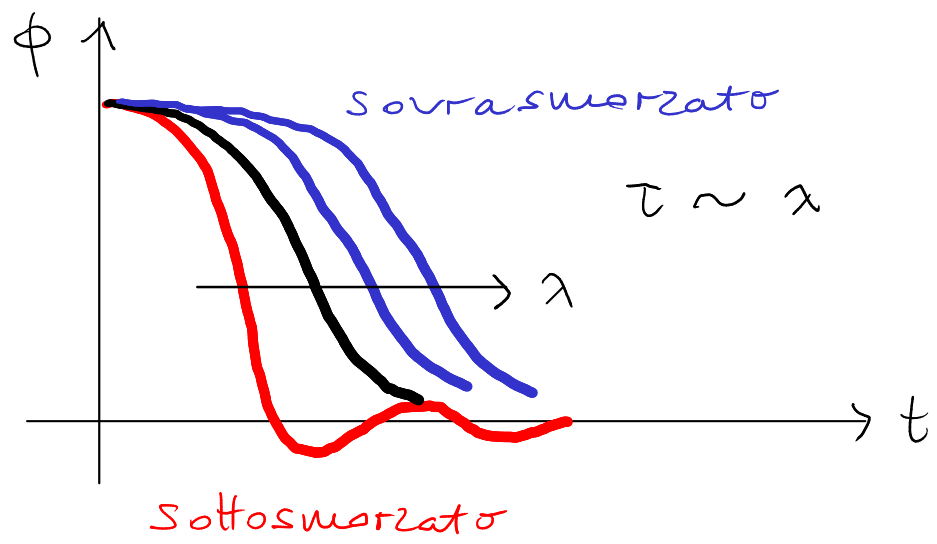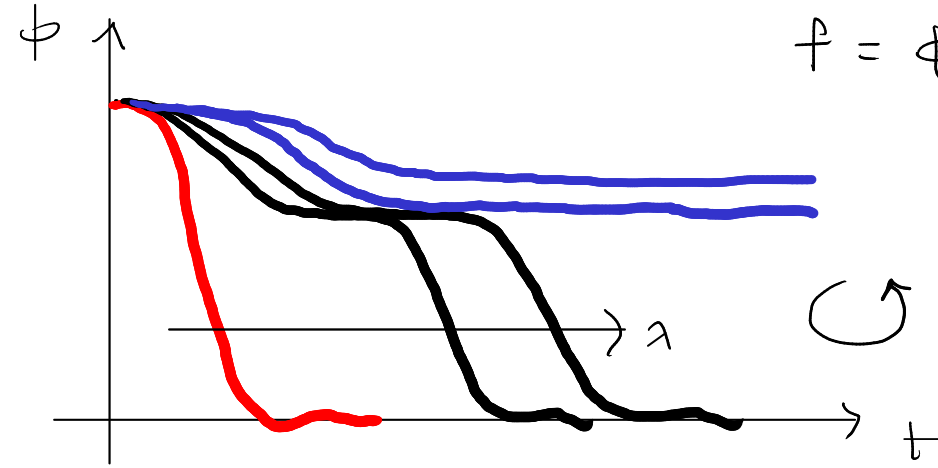
$x \geqslant x_c : \quad f > 0$

==Predizioni generali della MCT==

principi primi : $S(k) \rightarrow F(k,t)$ $\rightarrow$ numeriche

sviluppi asintotici in prossimità di T_c $\rightarrow$ analitiche

1] ==Two step relaxation== + ==stretched==

- β relaxation

$$F(k,t) \approx f(k) + |T - T_c| \, h(k) \, g_\pm \left(t/\tau_\beta \right)$$

$$g_+ = \left(t/\tau_\beta \right)^{-a} \qquad g_- \sim \left(t/\tau_\beta \right)^{b}$$

- α relaxation

$$F(k,t) \approx \exp\left(-\left(t/\tau_\alpha \right)^\beta \right) \qquad \beta \sim 0.6 - 0.7$$

2] ==$\tau_\alpha(t)$==

$$\tau_\alpha \sim \frac{1}{|T - T_c|^\gamma} \qquad \gamma \sim 2 \qquad a, b, \gamma$$

3] ==η, D, ---.==
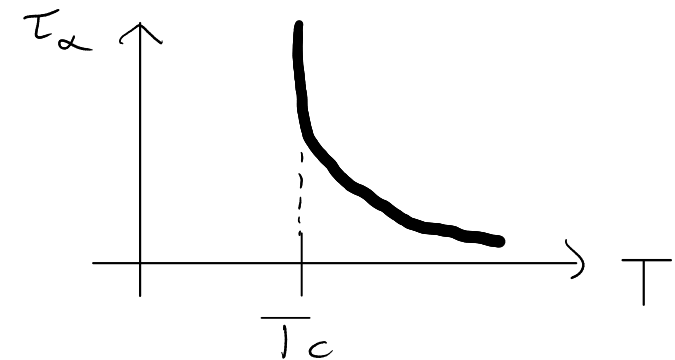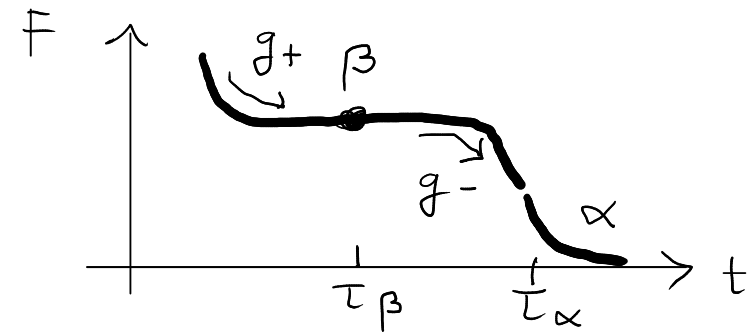
1) Principi primi : $S(k) \rightarrow F(k,t)$

2) Fit

miscela binaria
Kob - Andersen

$T_{onset} \sim 0.9 - 1.0$

$T_c^{(pp)} = \boxed{0.92}$

$T_c^{(fit)} = 0.435$

$T_g^{(sim)} = 0.4$