Ricerca sviluppata in collaborazione con …..

Giuseppe Foffi

Piero Tartaglia

Emanuela Zaccarelli

Wolfgang Goetze, Mattias Sperl, Thomas Voigtmann

Schema del seminario

- Sfere dure, un modello per particelle colloidali
- Colloidi con corto range di interazione (SR)

  un nuovo asse nello spazio delle fasi e una nuova lunghezza di localizzazione
- Predizioni della teoria di accoppiamento tra I modi (MCT) per colloidi SR

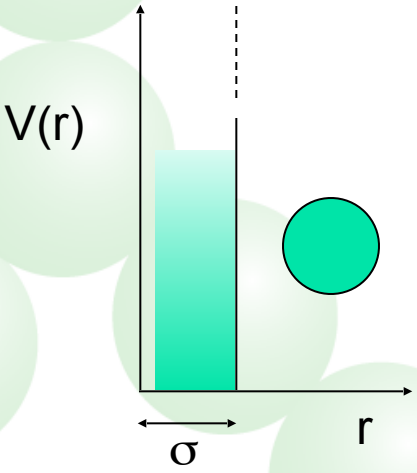
  Simulazioni

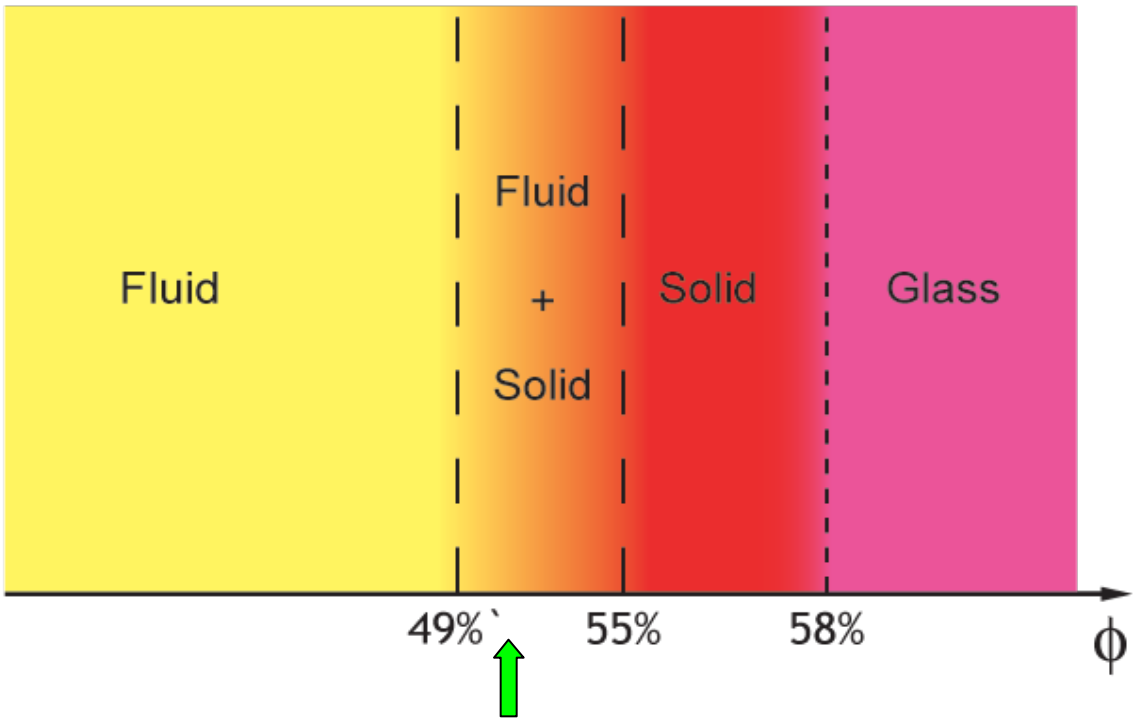
  Esperimenti
- La Dinamica vicino il punto A_4
- Domande Aperte:
- vetri e gels… due faccie della stessa fisica?

Sfere Dure

Potenziale

(No temperatura, solo densita')



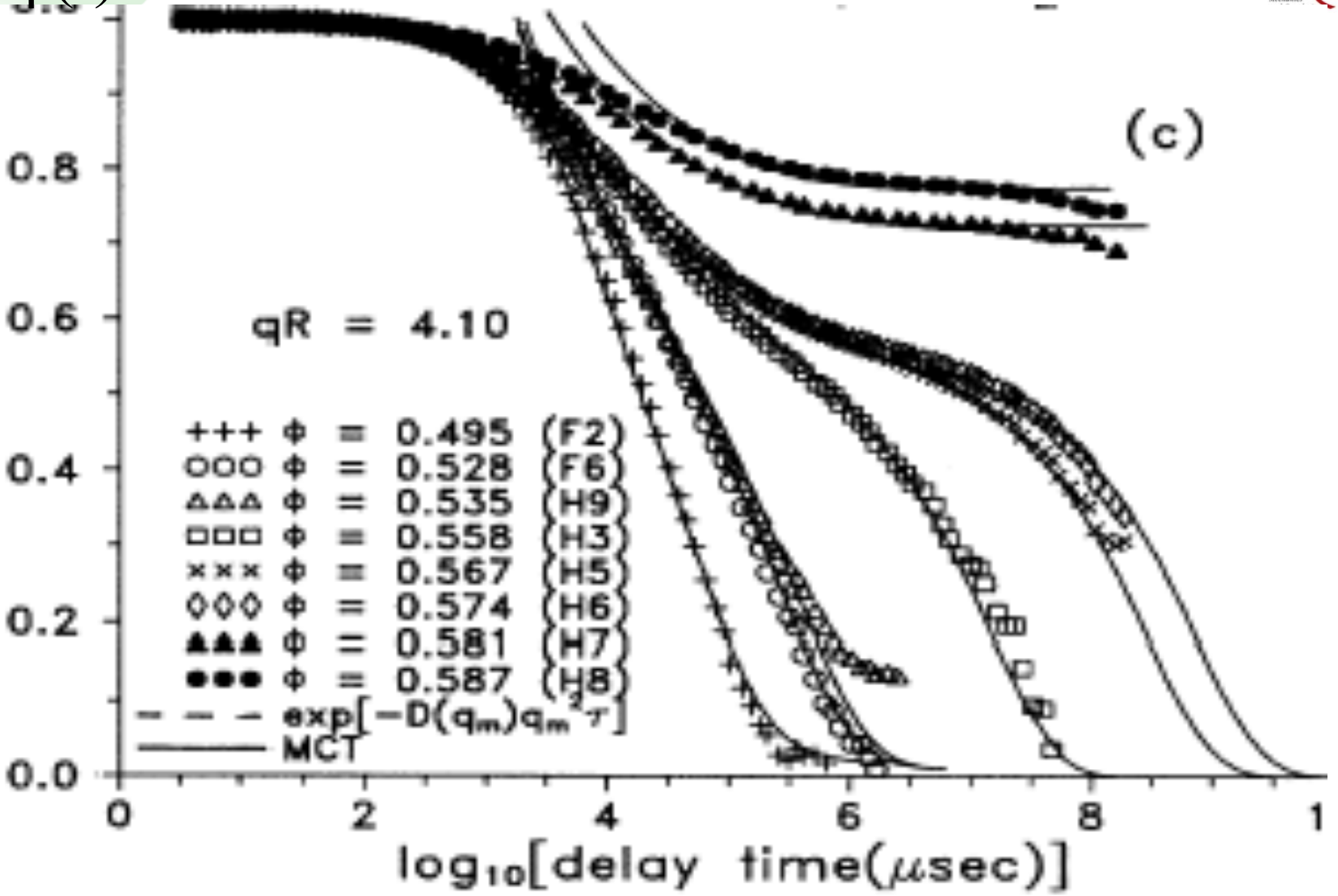


MCT transition
ϕ=51.6%

Sperimentalmente, a ϕ=0.58, la dinamica si arresta. La struttura del solido e' disordinata

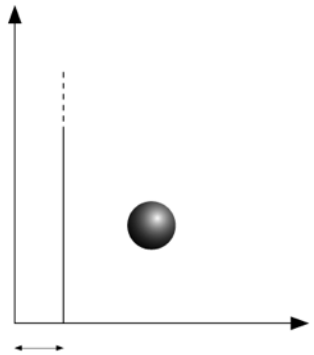
1. W. van Megen and P.N. Pusey *Phys. Rev.* A **43**, 5429 (1991)
2. U. Bengtzelius et al. *J. Phys.* C **17**, 5915 (1984)
3. W. van Megen and S.M. Underwood *Phys. Rev. Lett.* **70**, 2766 (1993)

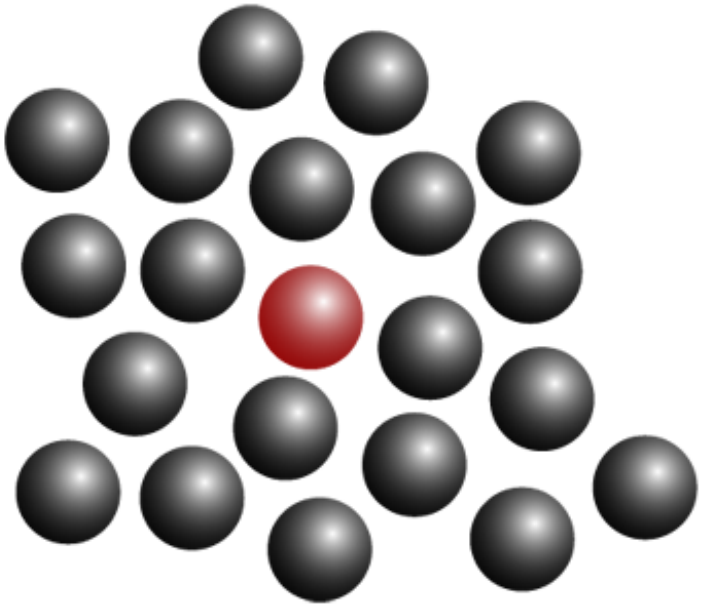
$\phi(t)$ HS (slow) dynamics

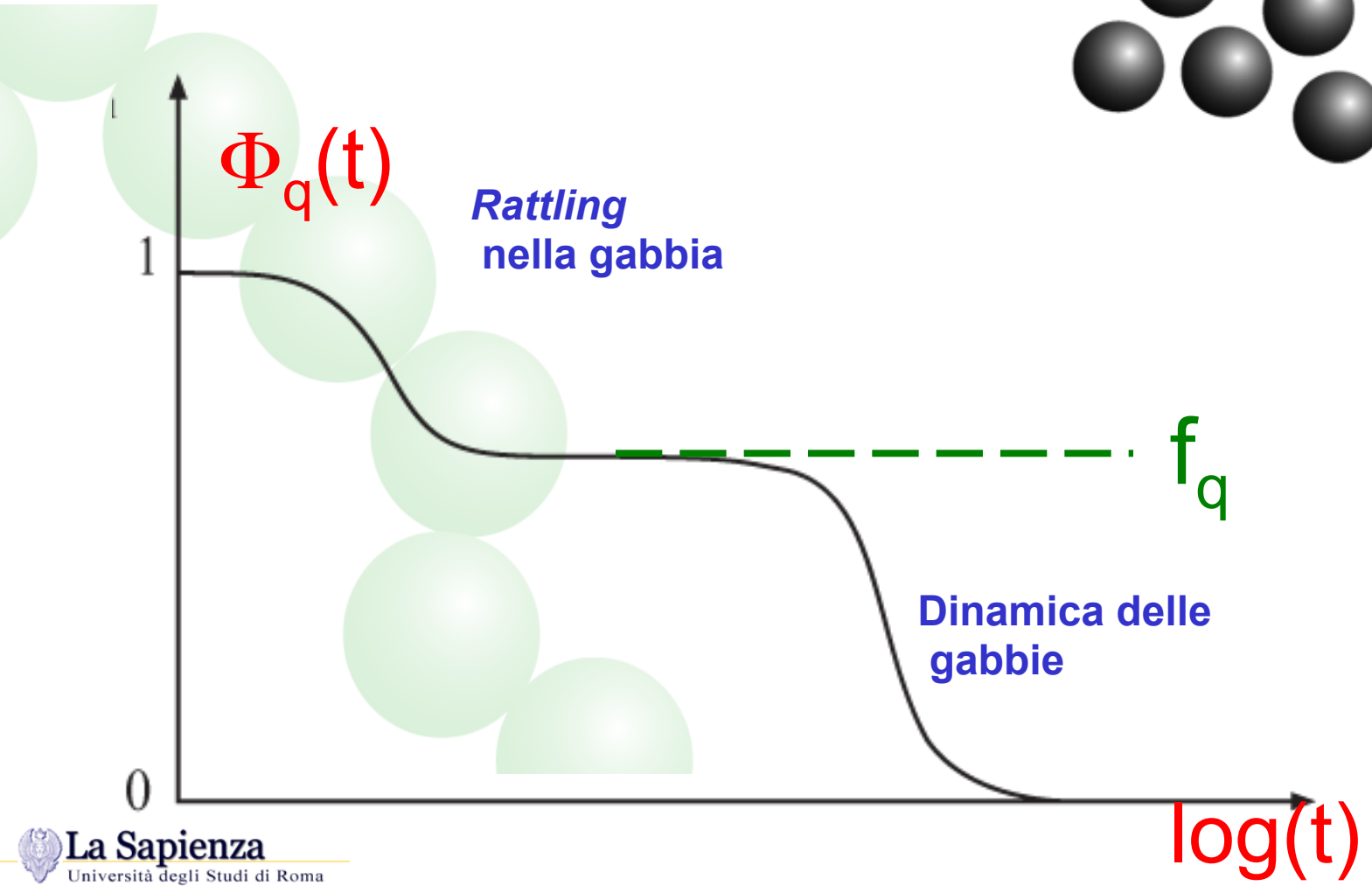


van Megen and S.M. Underwood *Phys. Rev. Lett.* **70**, 2766 (1993)

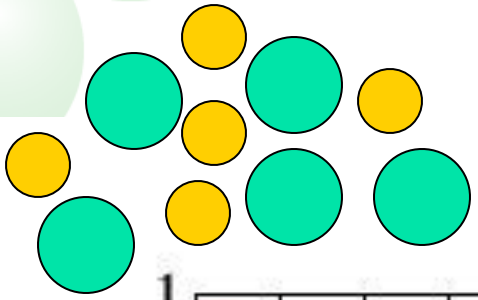
L'effetto gabbia (in Sfere Dure).







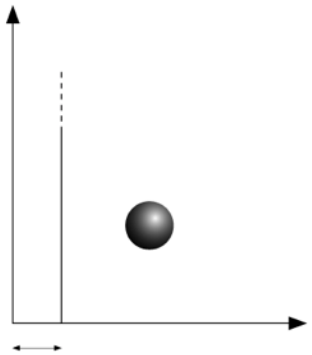
MCT --- confronto simulazioni/teoria per miscela binaria HS



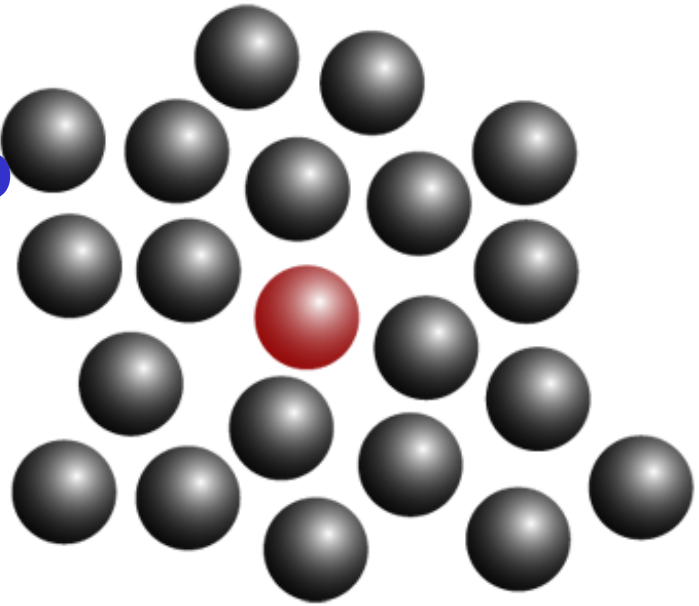
σ_A=1

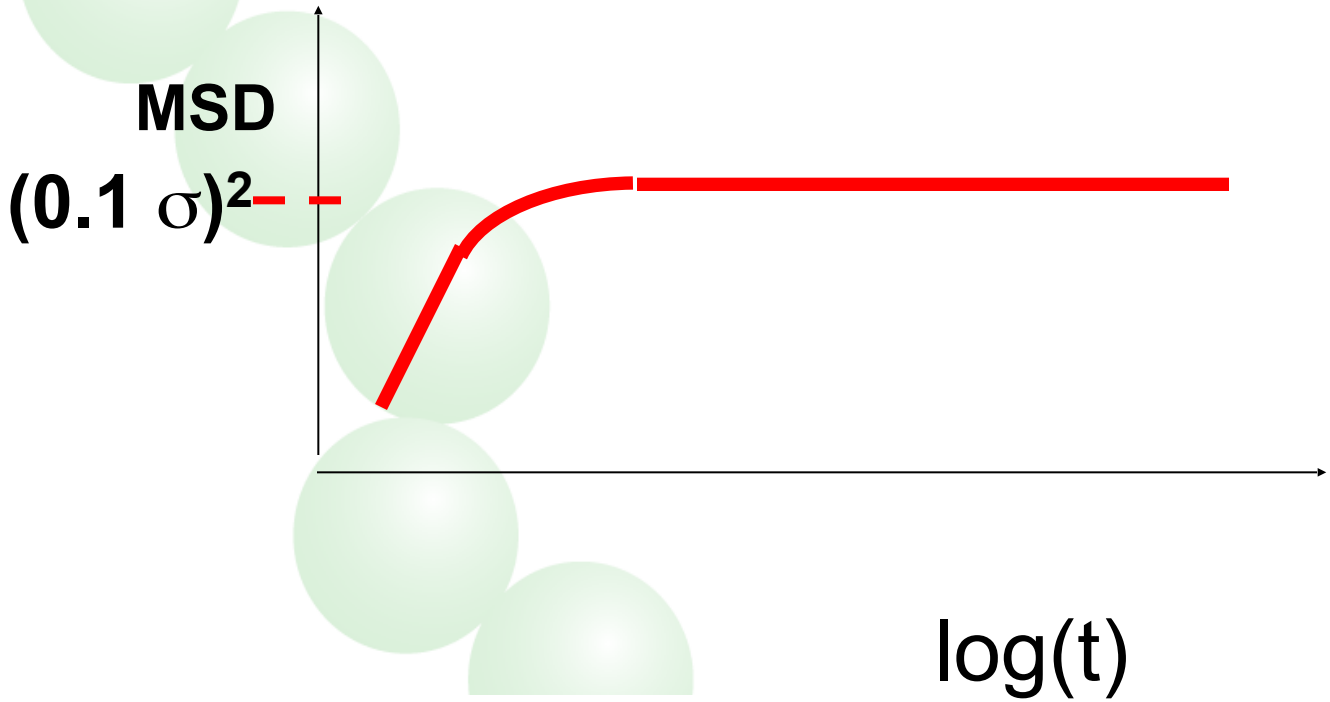
σ_B=0.6

Foffi et al Prl 2003



Lo spostamento quadratico medio (nel vetro)



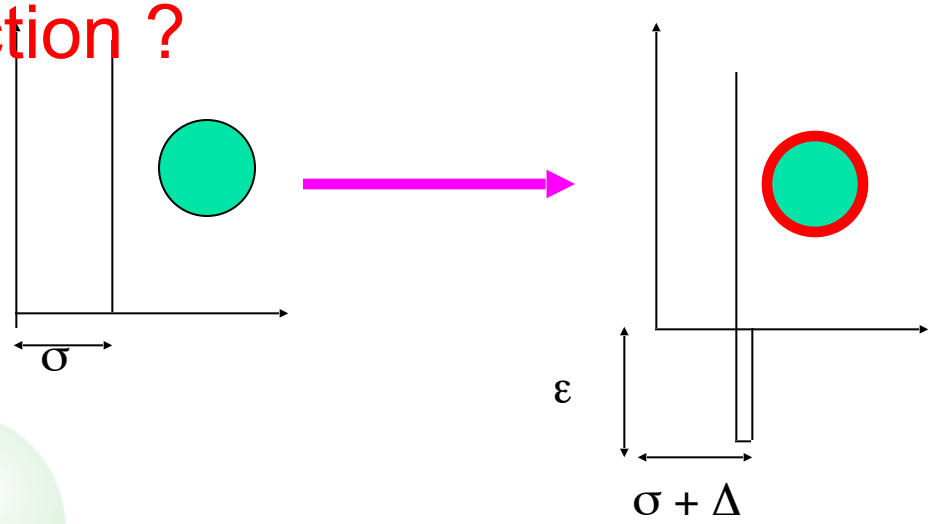


log(t)

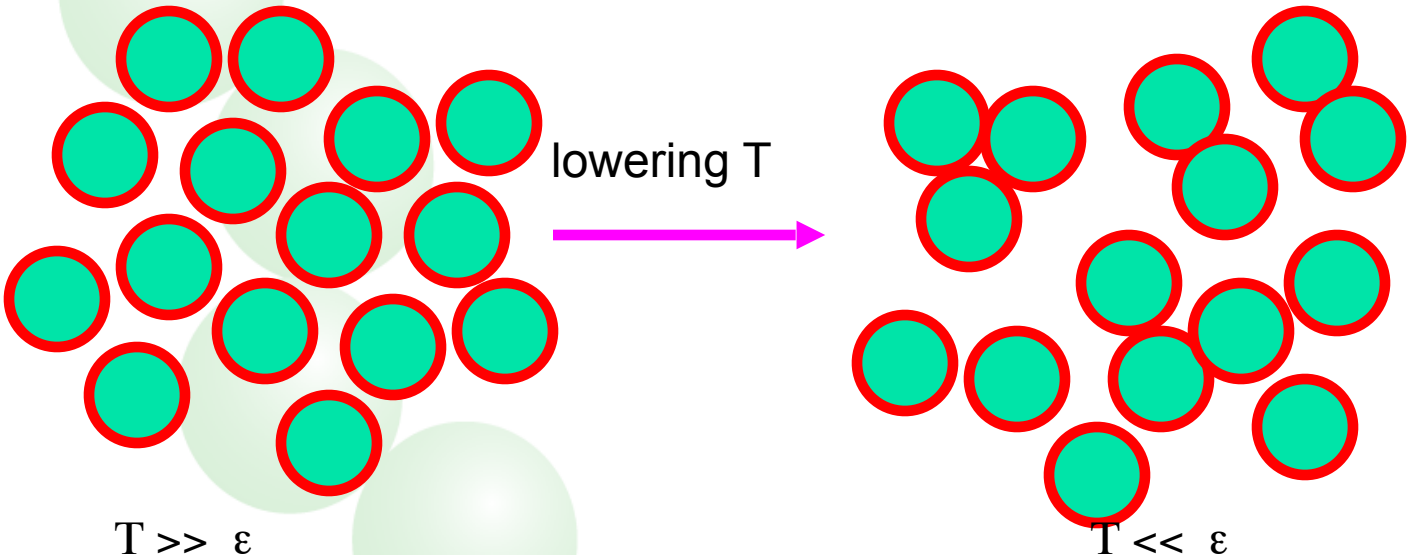
Can the localization length be controlled in a different way ?

What if we add a short-range attraction ?

Hard Spheres Potential

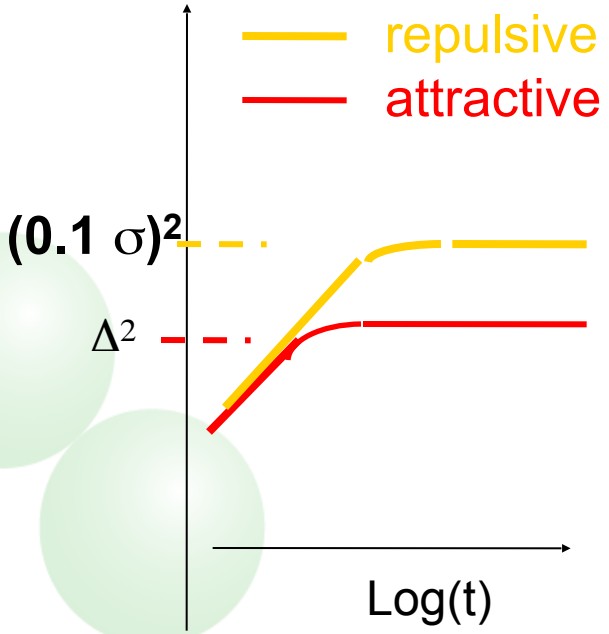


Square-Well short range attractive Potential



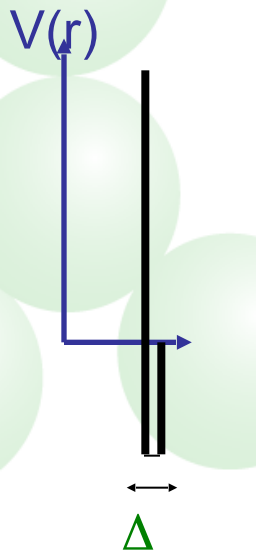
A model with two different localization length

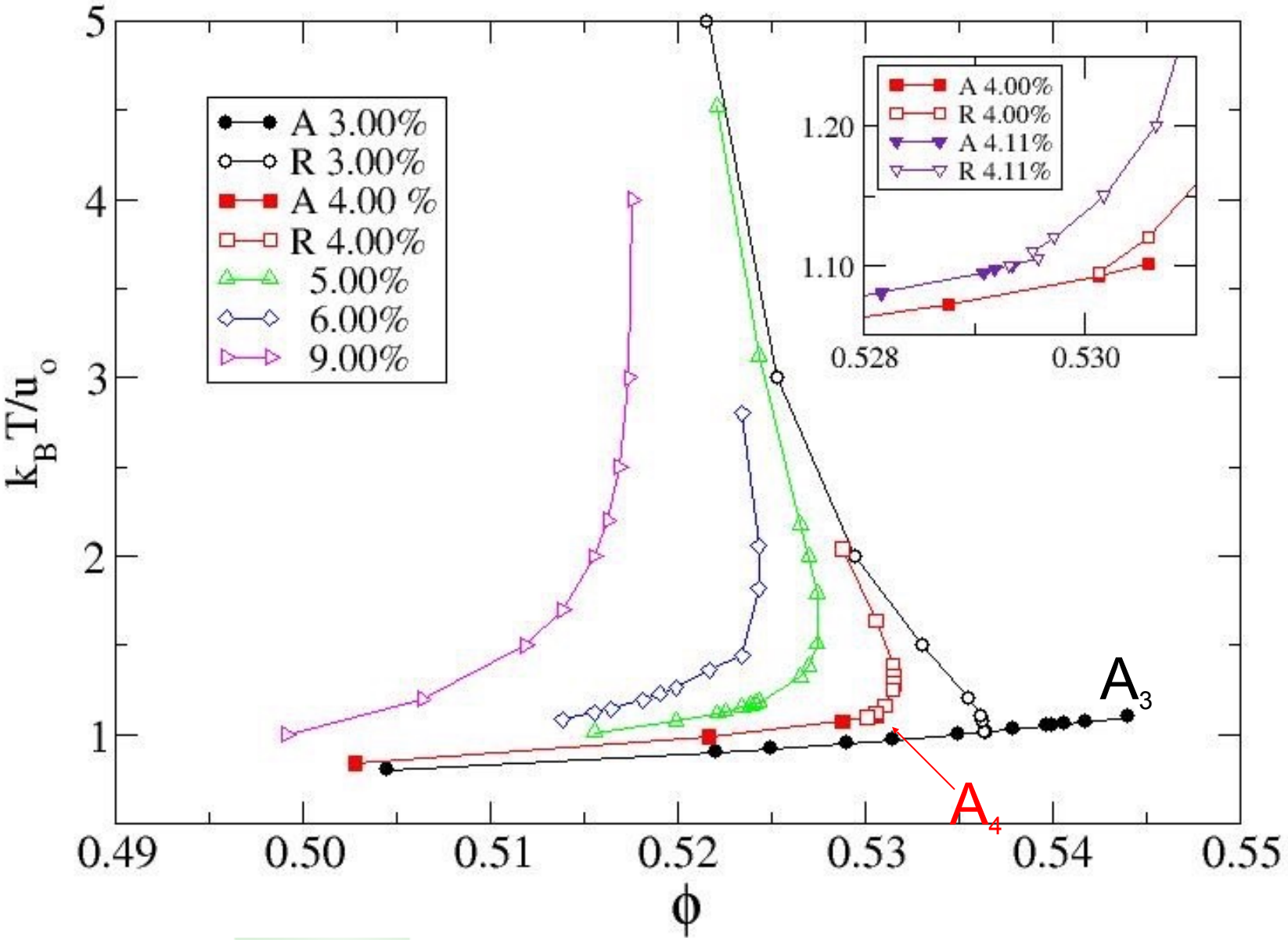
Mean squared displacement



How does the system change from one (glass) to the other ?

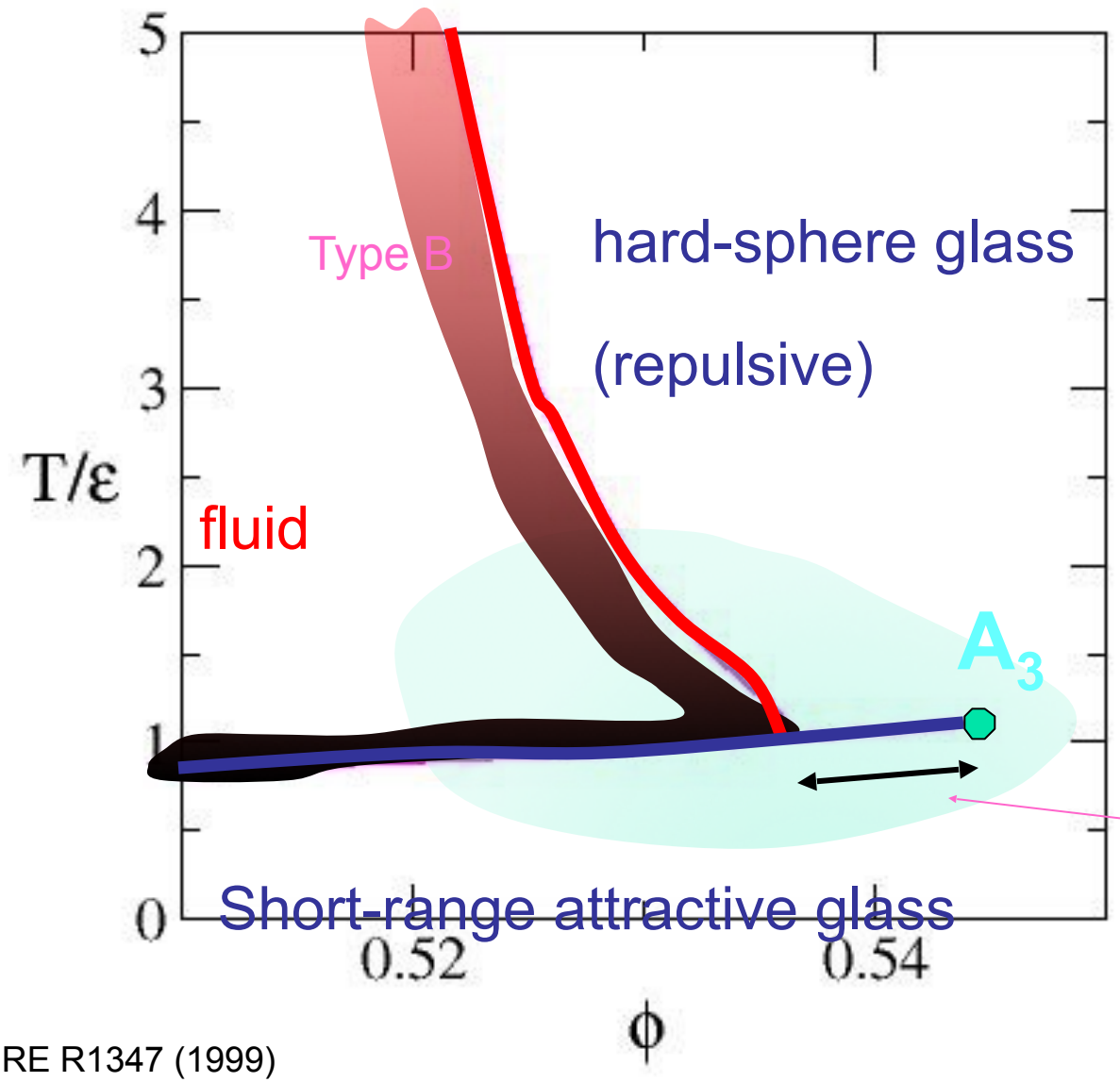
MCT IDEAL GLASS LINES (PY) - SQUARE WELL MODEL - CHANGING Δ

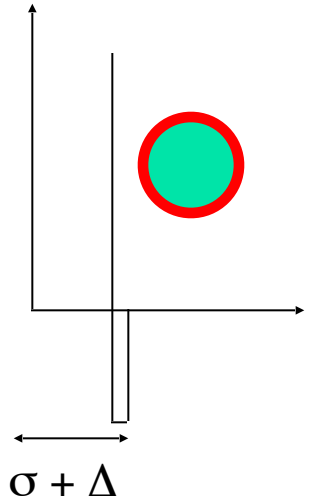




PRE-63-011401-2001

MCT predictions for short range attractive square-well





Controlled by Δ/σ

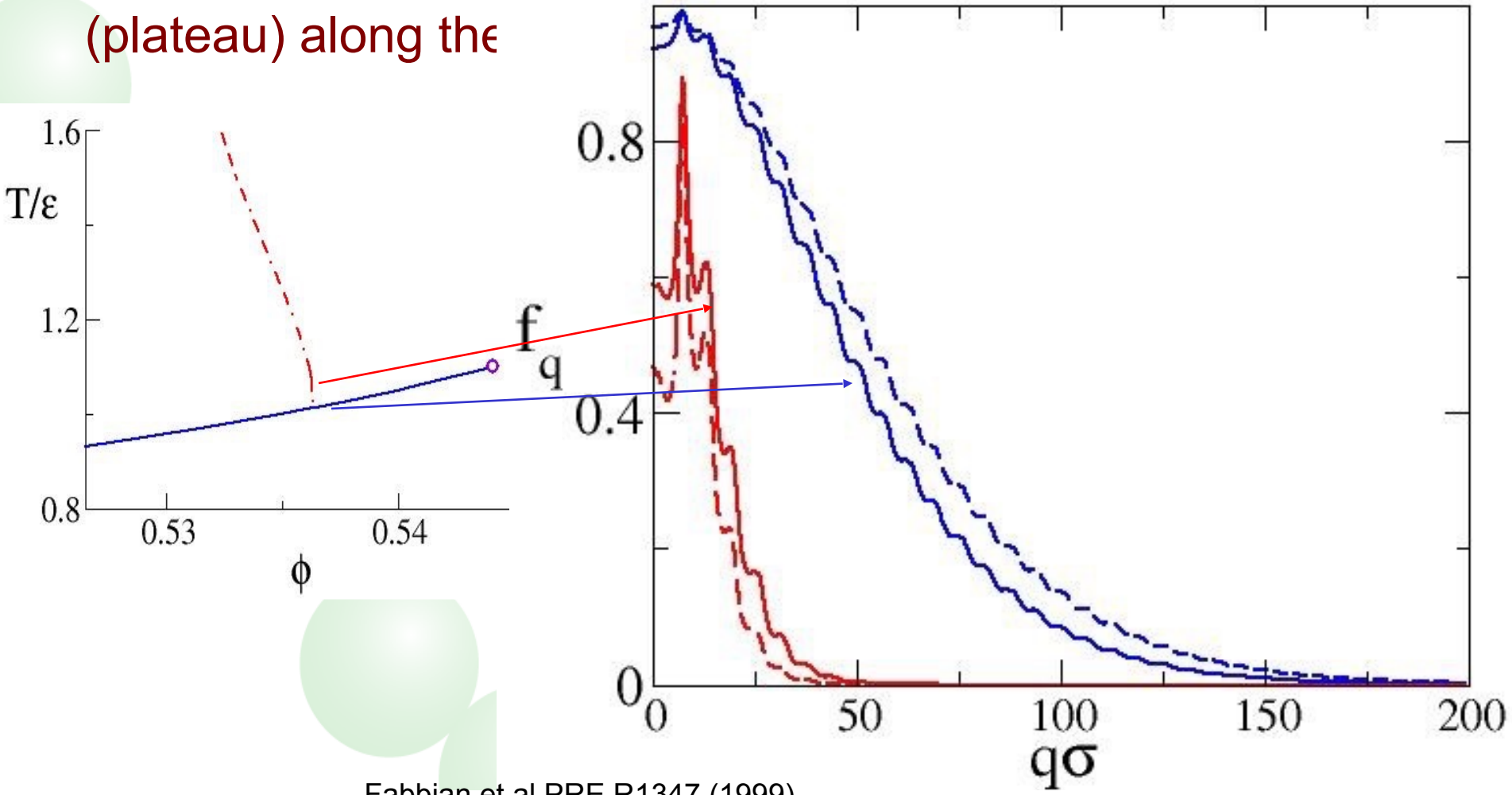
Fabbian et al PRE R1347 (1999)
Bergenholtz and Fuchs, PRE 59 5708 (1999)

Fluid-Glass on cooling and heating !!

MCT Predictions:

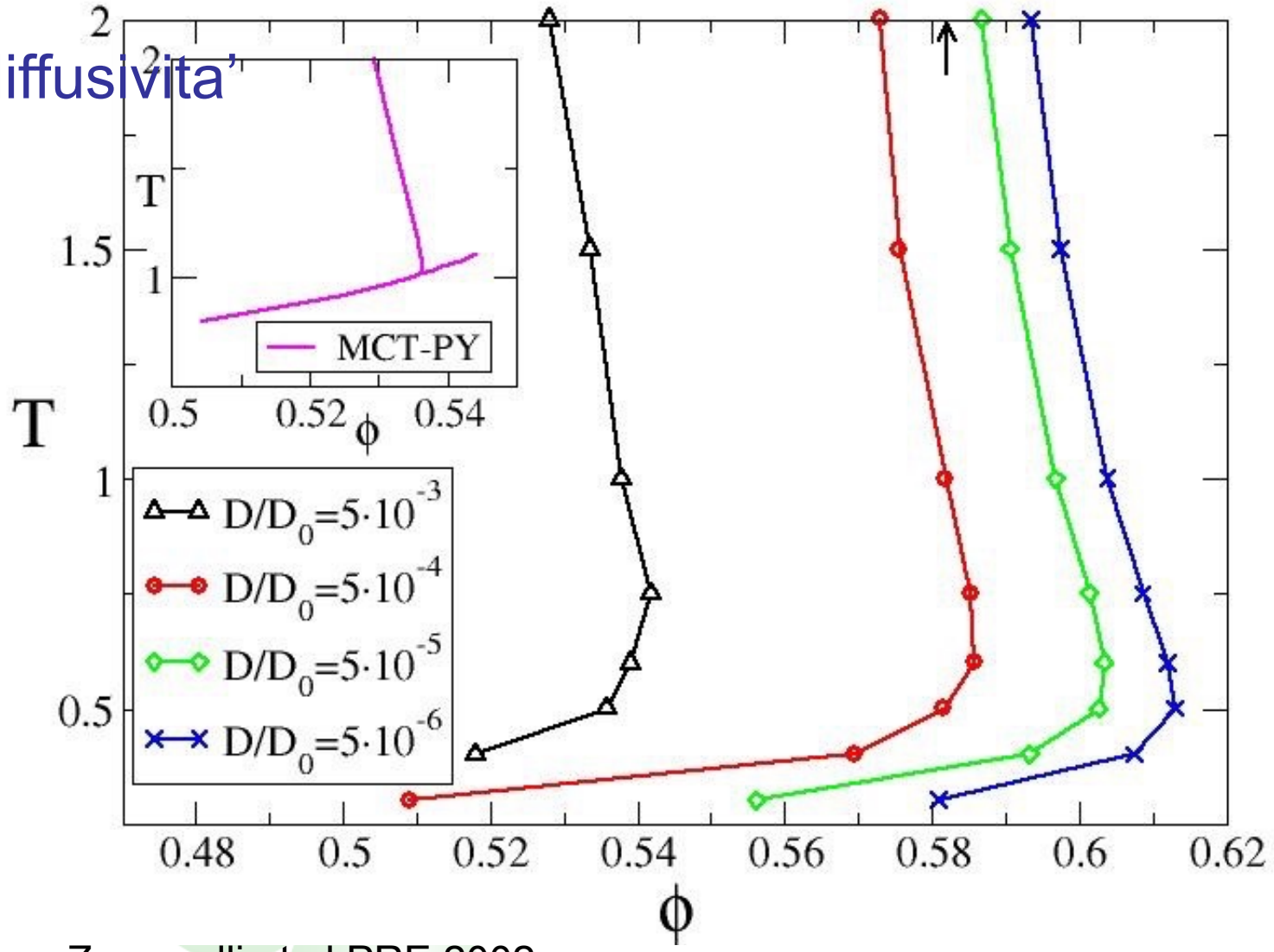
Wavevector dependence of the non ergodicity parameter

(plateau) along the



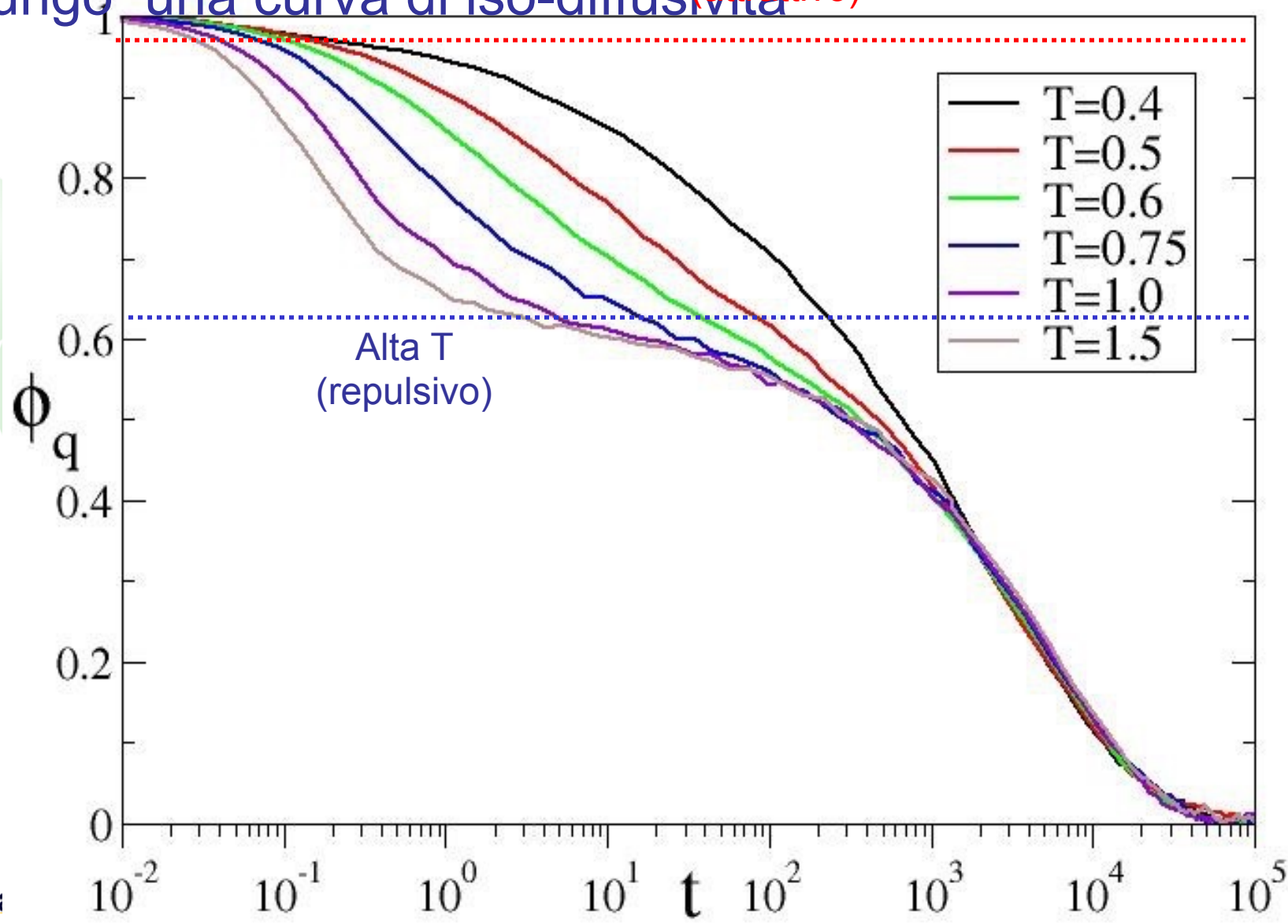
Fabbian et al PRE R1347 (1999)
Bergenholtz and Fuchs, PRE 59 5708 (1999)

Confronto con le simulazioni…. Curve iso-diffusivita’

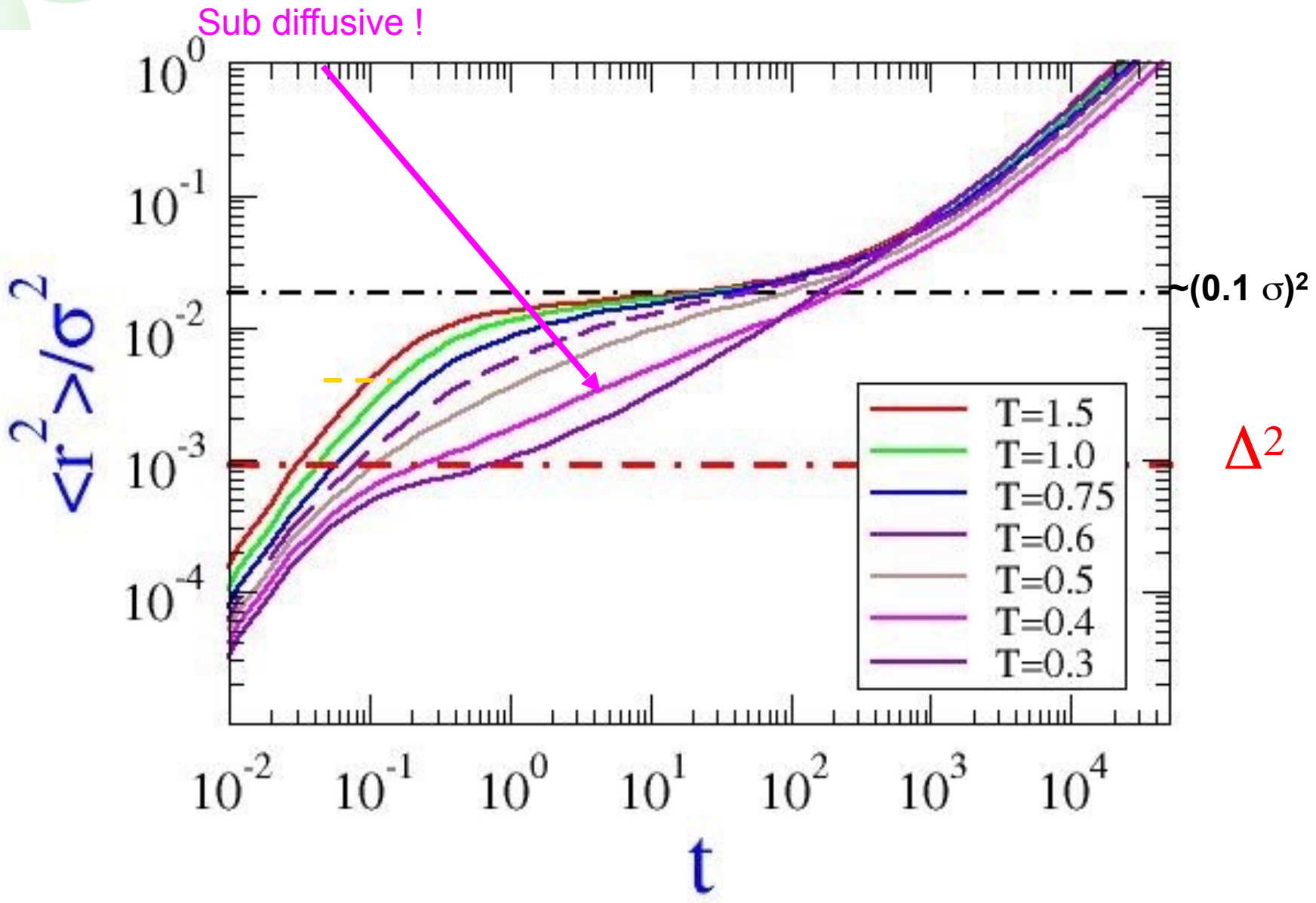


Zaccarelli et al PRE 2002

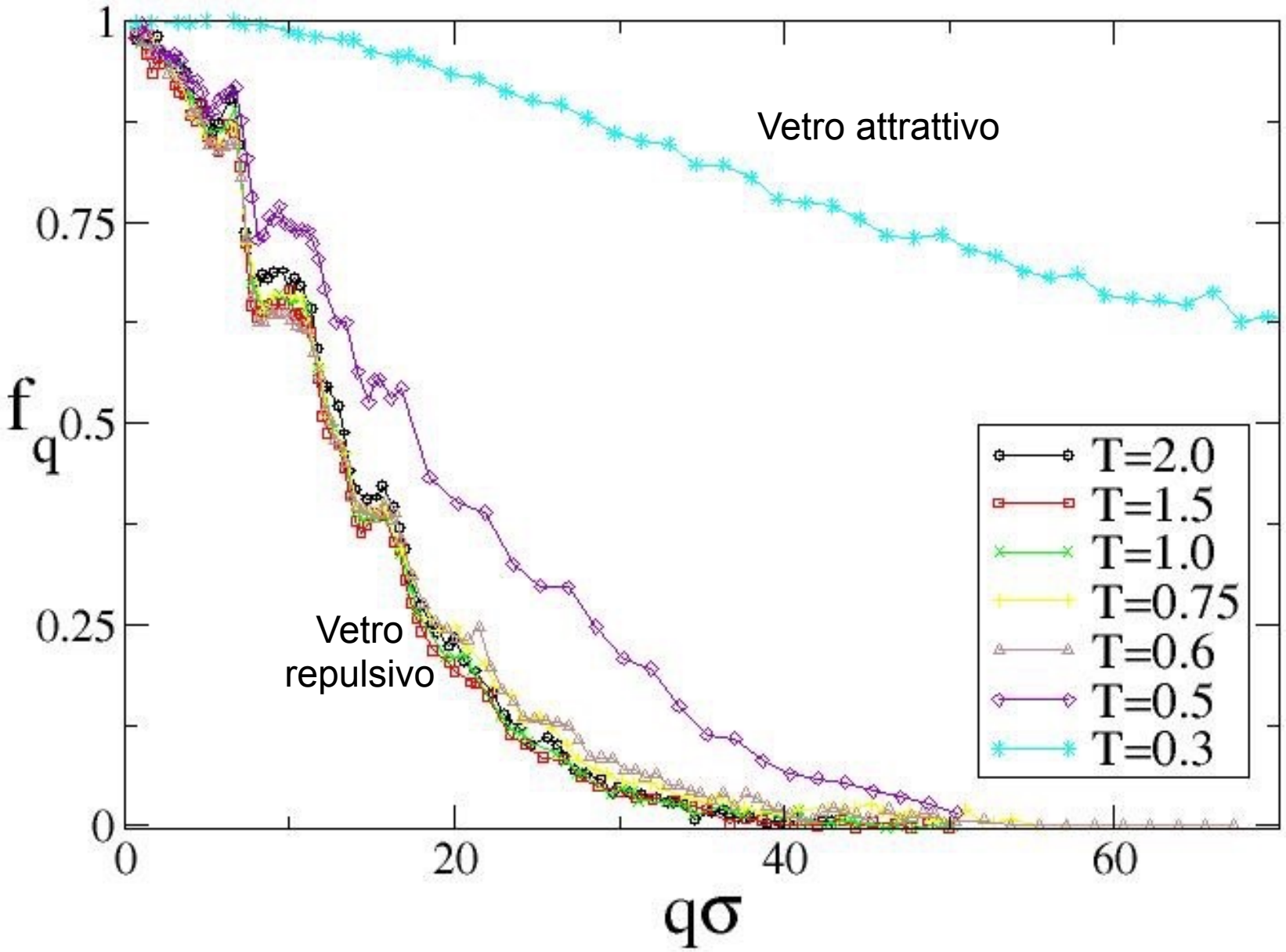
Simulazioni: Funzioni di correlazione della densita'lungo una curva di iso-diffusività

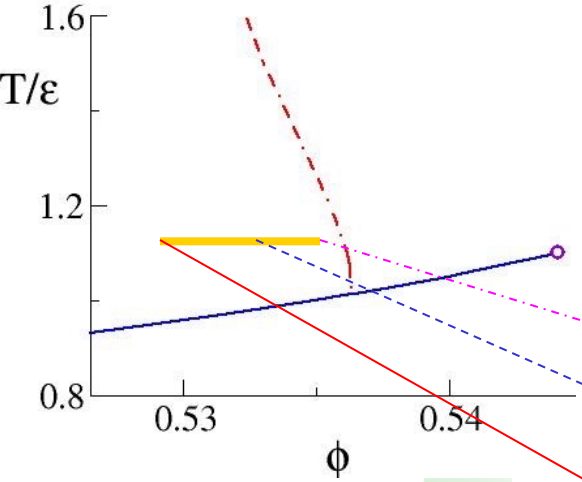


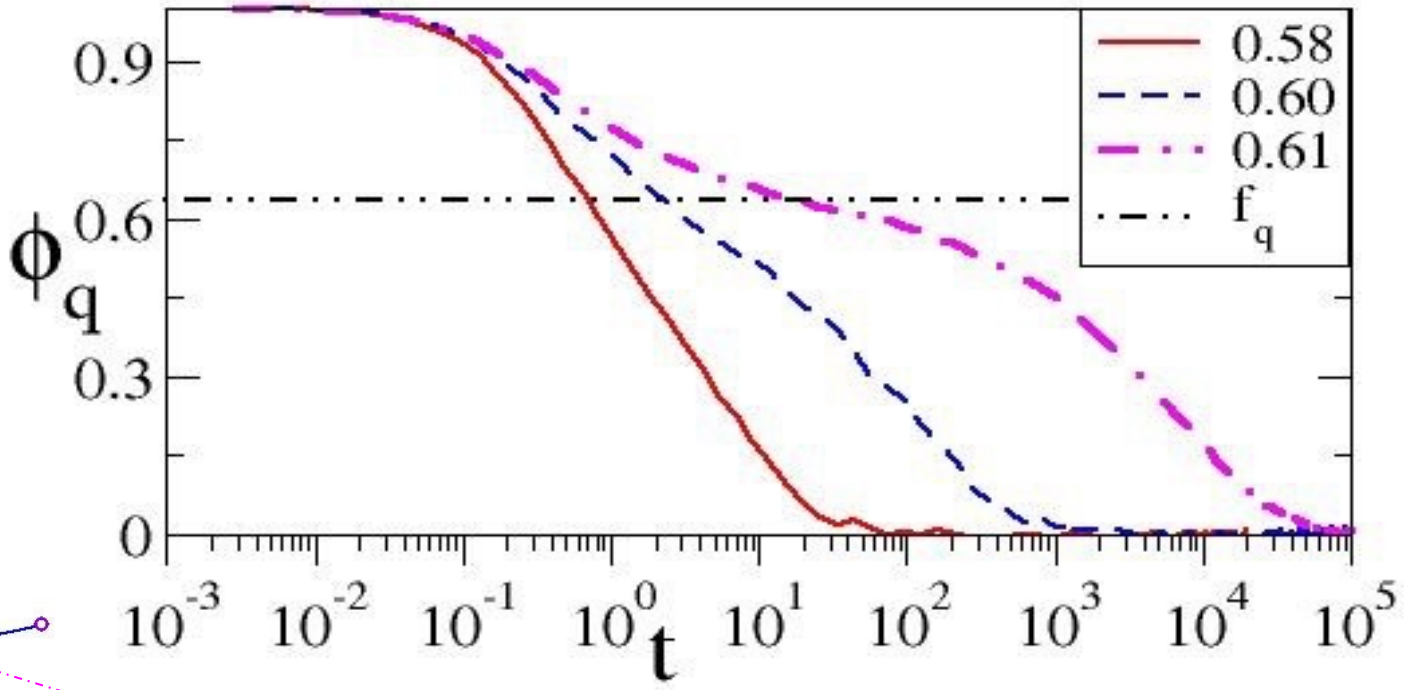
Simulazioni: Spostamento quadratico medio lungo curva isocrona

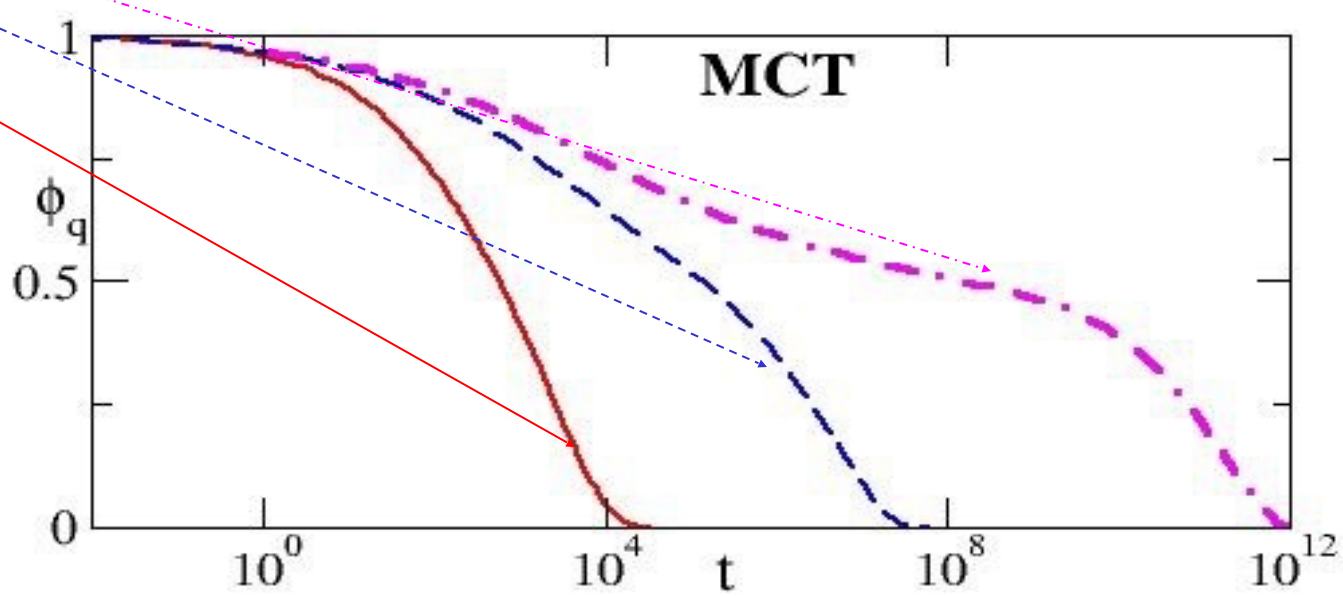


Simulazioni: Parametro di non ergodicita' lungo curva isocrona

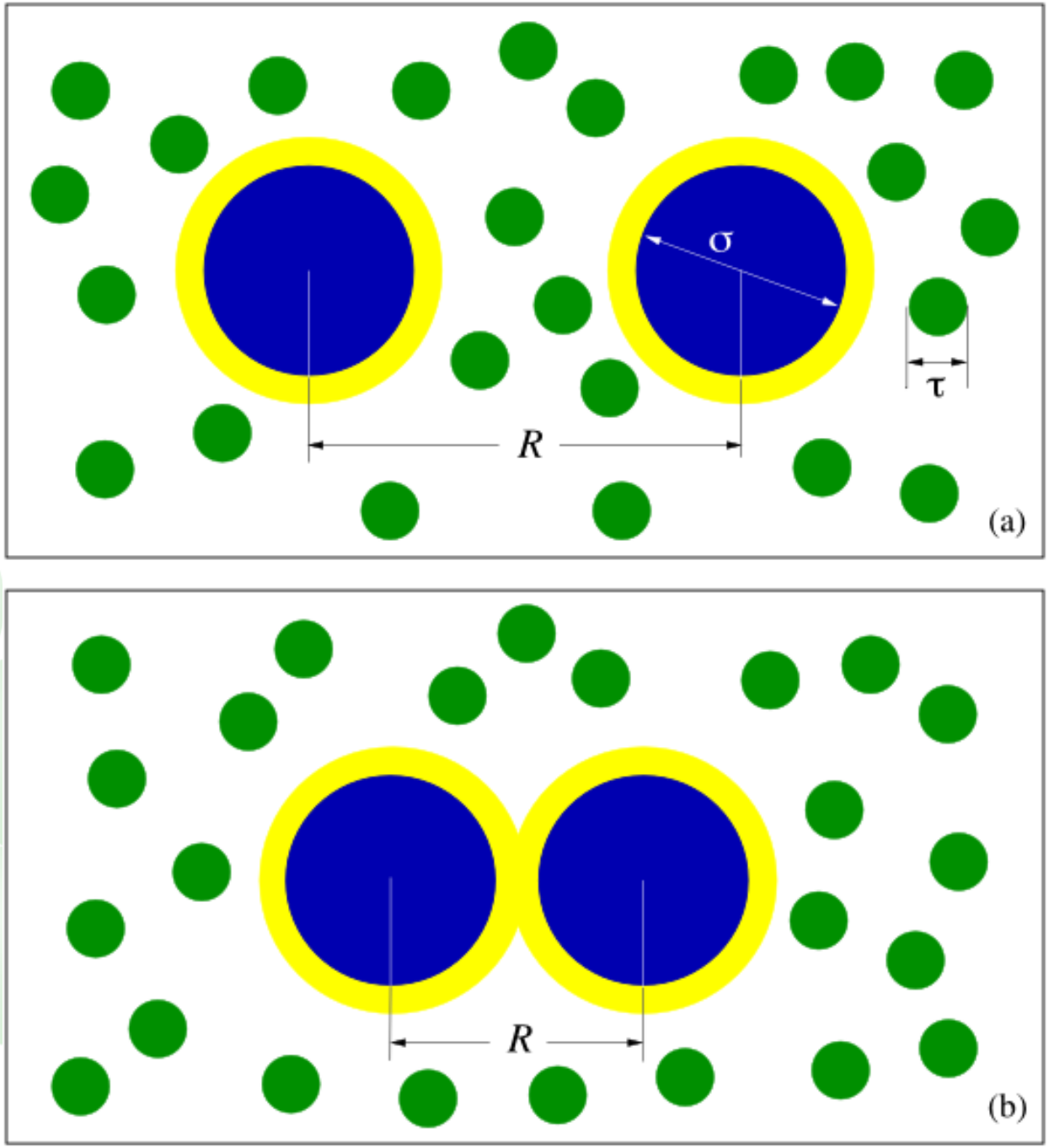



1.6
T/ε
1.2
0.8
0.53
0.54
ϕ


0.9
0.6
0.3
0
ϕ_q
10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{1} 10^{2} 10^{3} 10^{4} 10^{5}
t
0.58
0.60
0.61
f_q


MCT
1
0.5
0
ϕ_q
10^{0} 10^{4} 10^{8} 10^{12}
t

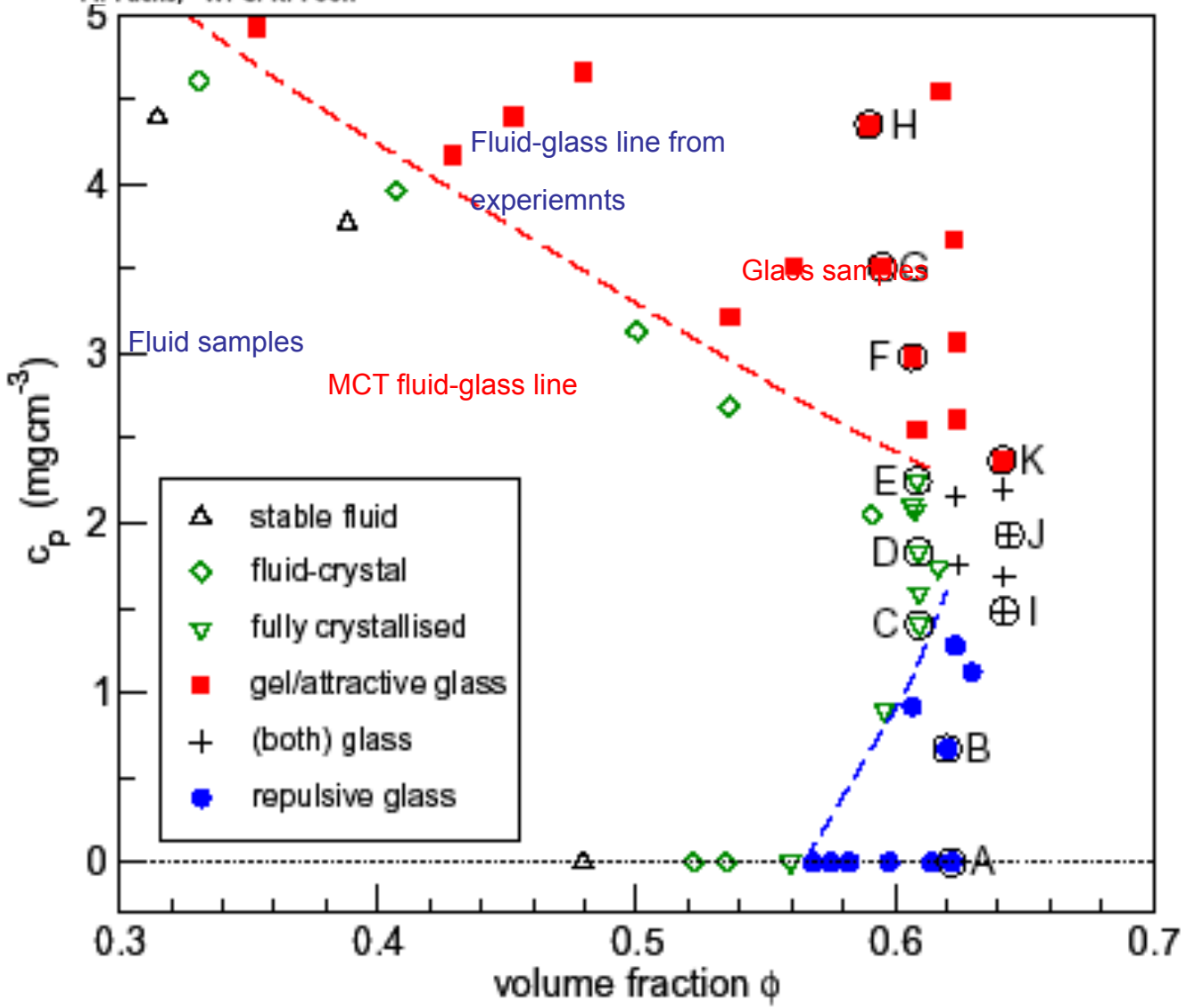
Depletion Interaction: A Cartoon



Multiple Glassy States in a Simple Model System

N. Pham,[1] A. M. Puertas,[1,2] J. Bergenholtz,[3] S. U. Egelhaaf,[1]
A. Moussaïd,[1] P. N. Pusey,[1] A. B. Schofield,[1] M. E. Cates,[1]
M. Fuchs,[1] W. C. K. Poon[1*]

Temperature



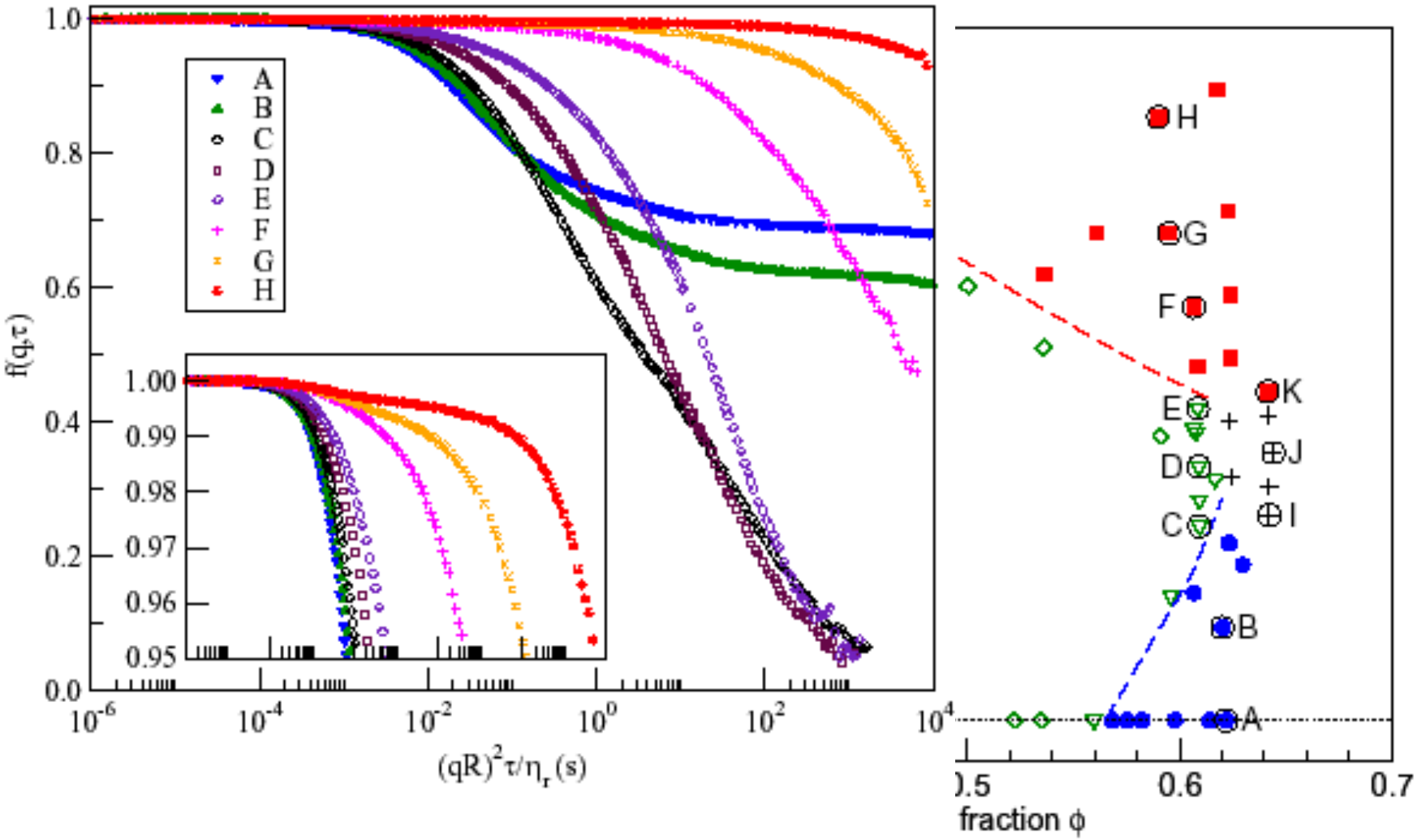


FIG. 6: Collective dynamic structure factors at $qR = 1.50$ from samples A–H spanning the re-entrant region. The time axis is scaled to dimensionless length scale $(qR)^2$ and relative polymer solution viscosity η_r. The inset shows the same plots on an expanded vertical axis.

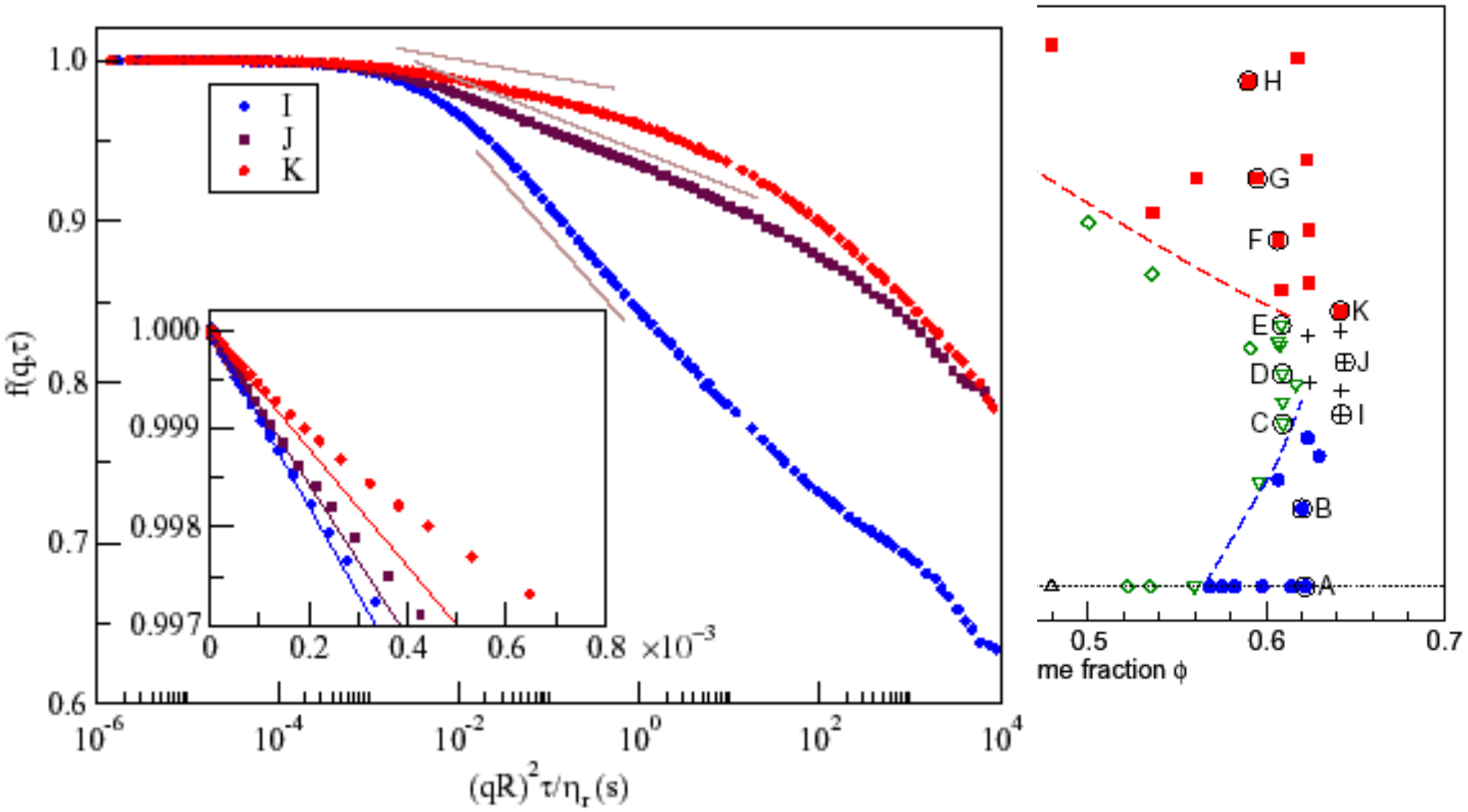
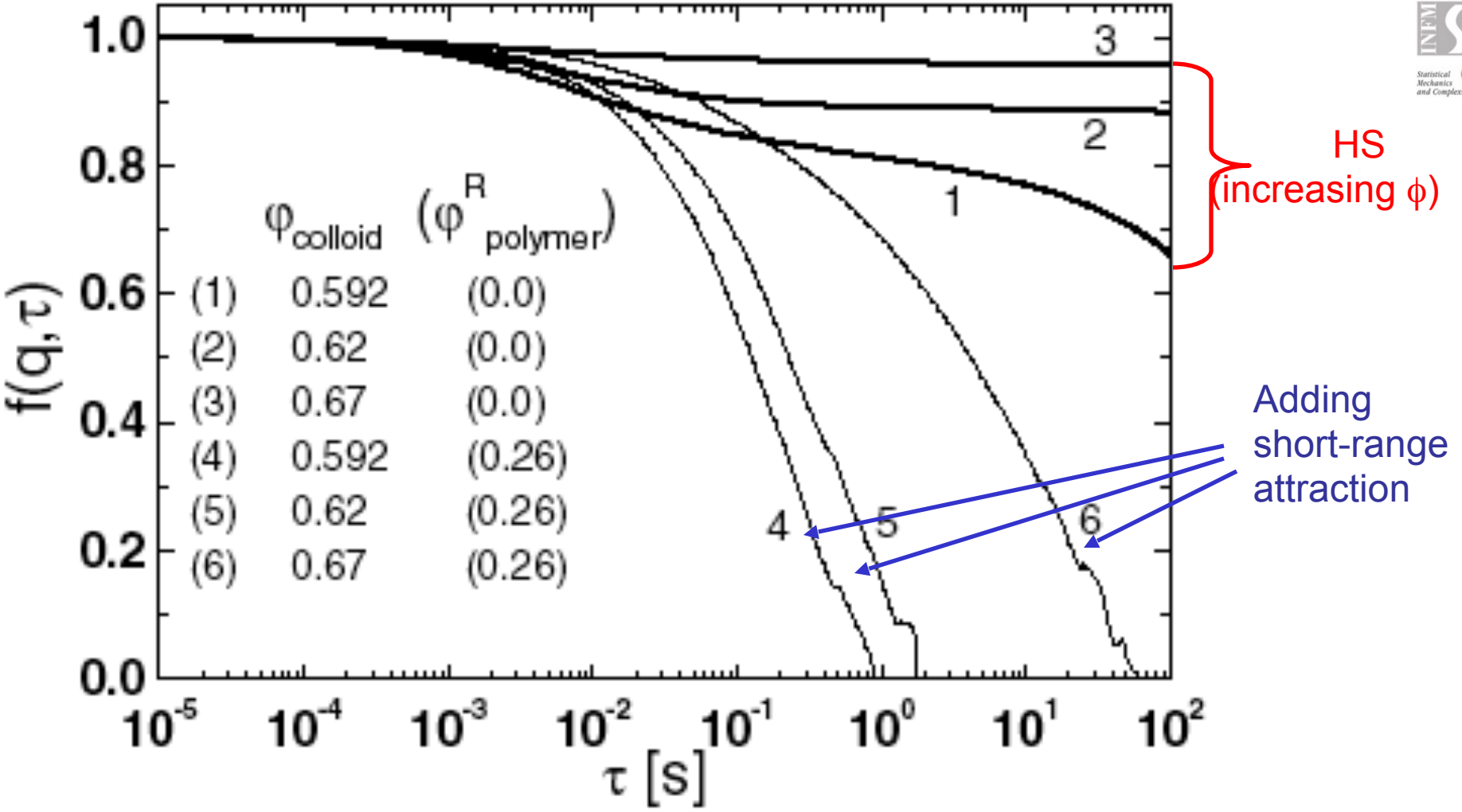


FIG. 12: The DSFs at $qR = 1.50$ for samples I–K with $\phi \sim 0.64$. Extremely stretched relaxation is found in all three samples with logarithmic decay over long ranges of τ (straight lines). The inset shows the short-time dynamics, which deviate from the diffusive regime from very early times.

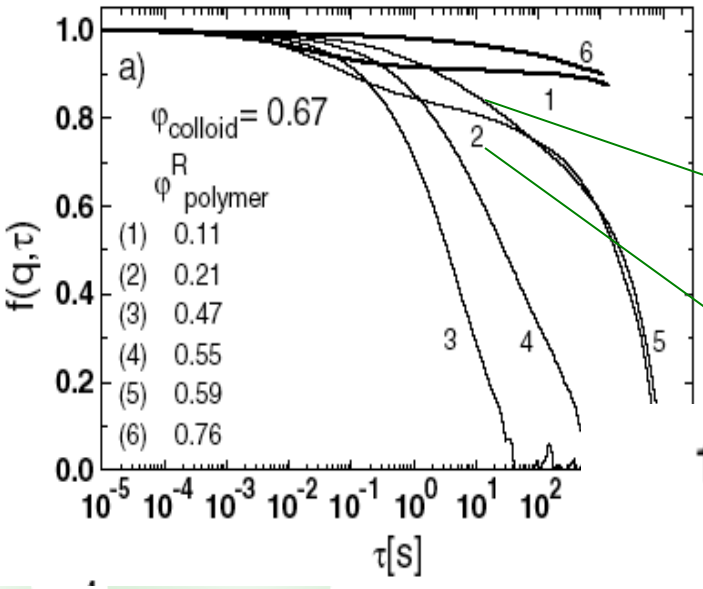


T. Eckert and E. Bartsch

Colloidal-Polymer Mixture with Re-entrant Glass Transition in a Depletion Interactions

Phys.Rev. Lett. 89 125701 (2002)

FIG. 1. Comparison of the density autocorrelation functions $f(q, \tau)$ of a hard sphere colloidal suspension (see text) before (thick solid lines) and after (thin solid lines) the addition of linear polymer chains (size ratio $\delta = R_{g,\text{polymer}}/\langle R_{\text{colloid}}\rangle = 0.054$). The colloid volume fractions of each set of $f(q, \tau)$ increase from left to right as indicated in the figure. The dynamics is probed at a scattering vector corresponding to the peak maximum of $S(q)$ of the pure colloid suspension at its glass-transition volume fraction $\varphi_g \approx 0.595$ [22].



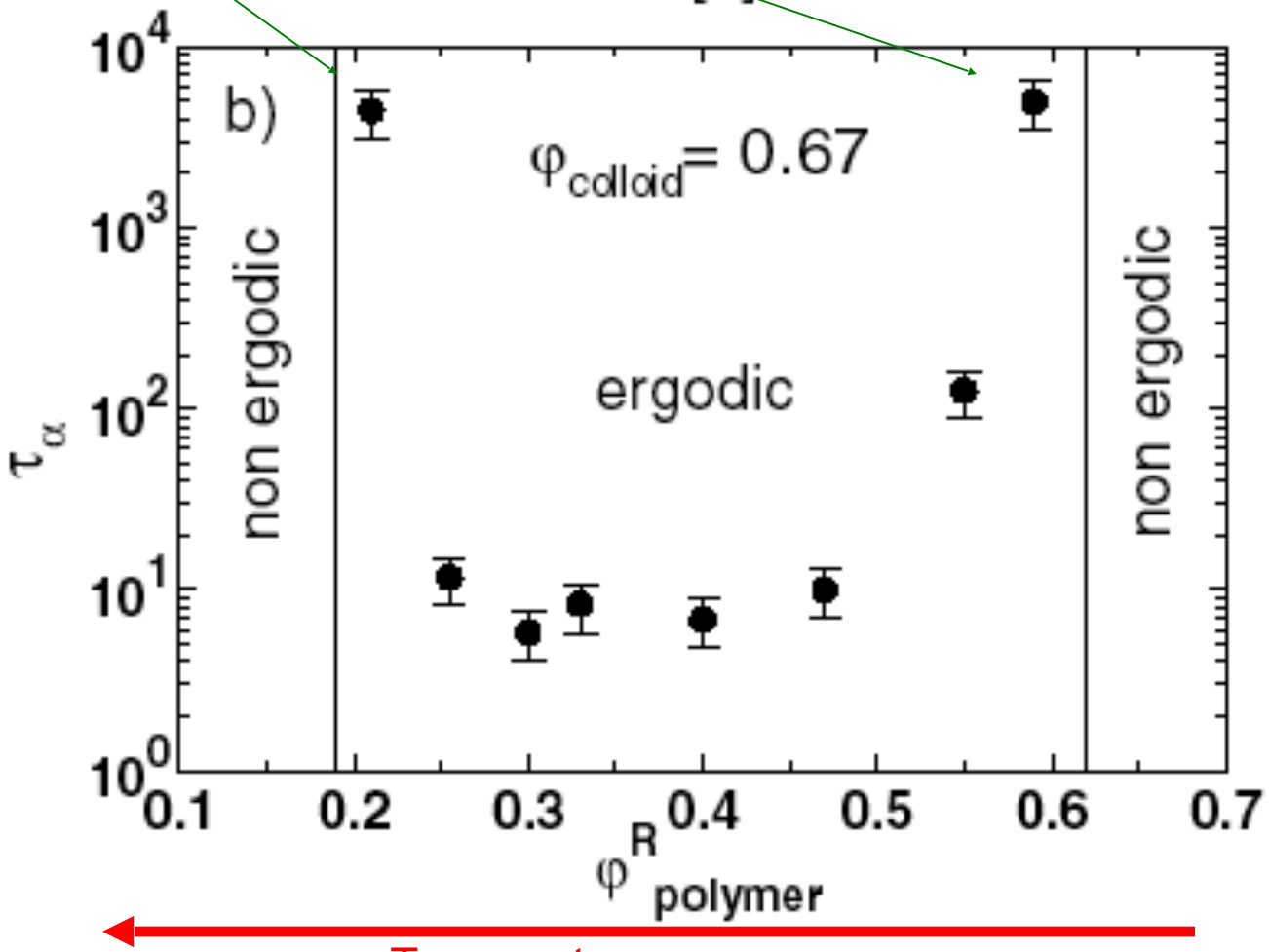
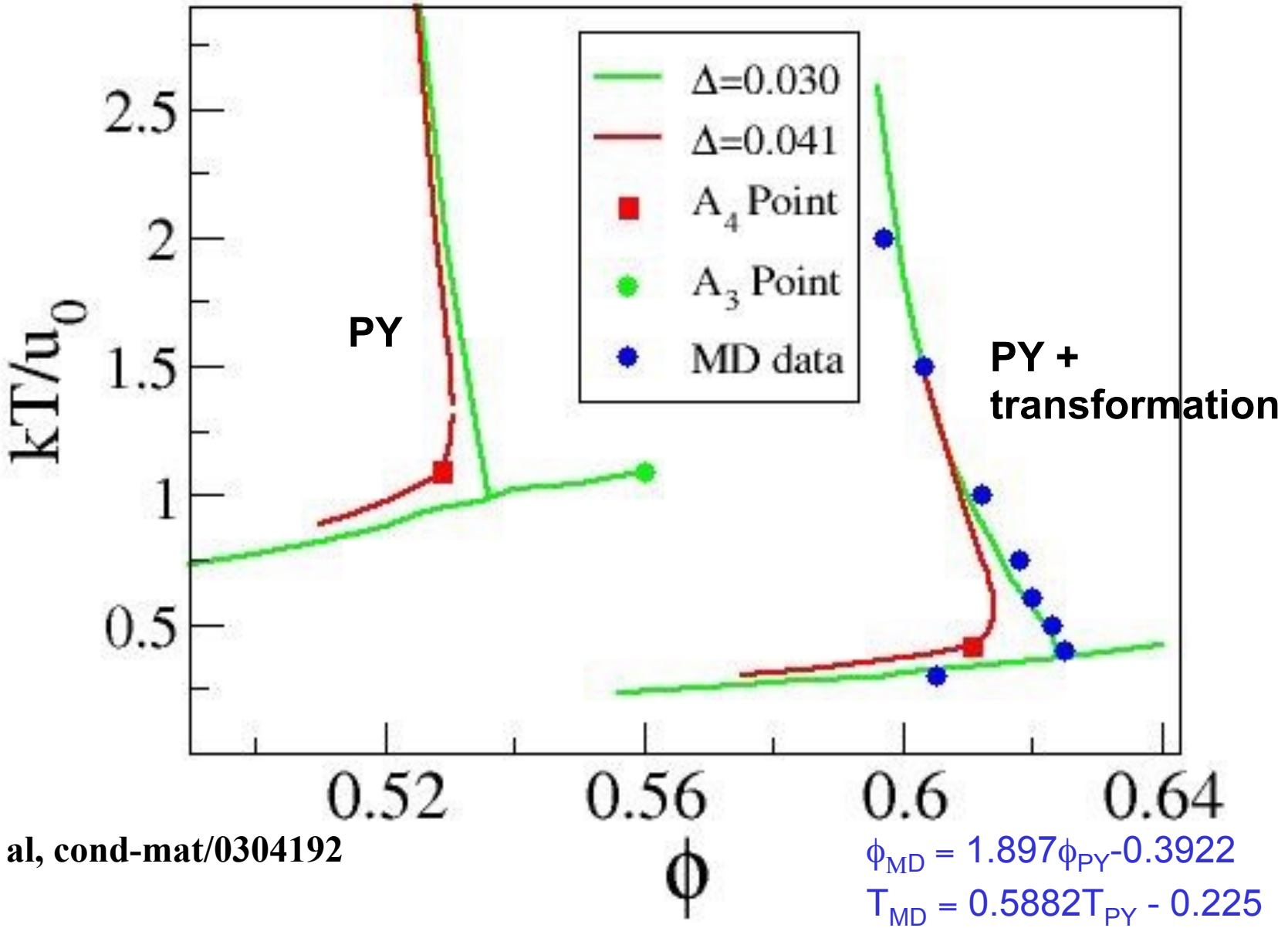


FIG. 3. Effect of increasing the free polymer volume $\varphi^R_{polymer}$ on the dynamics of a colloid suspension in state close to random close packing ($\varphi_{colloid} = 0.67$) in the phenomenon of re-entrant melting. (a) Density au lation functions $f(q, \tau)$ (probed at the same scattering v in Fig. 1). The polymer reservoir volume fractions indicated by the numbers at the curves. The thi lines correspond to nonergodic (glassy) sample (b) Structural relaxation times τ_α versus polymer r volume fraction $\varphi^R_{polymer}$. The vertical lines schematic dicate the transition lines to the respective nonergodic

Tracing the A_4 point: Theory and Simulation



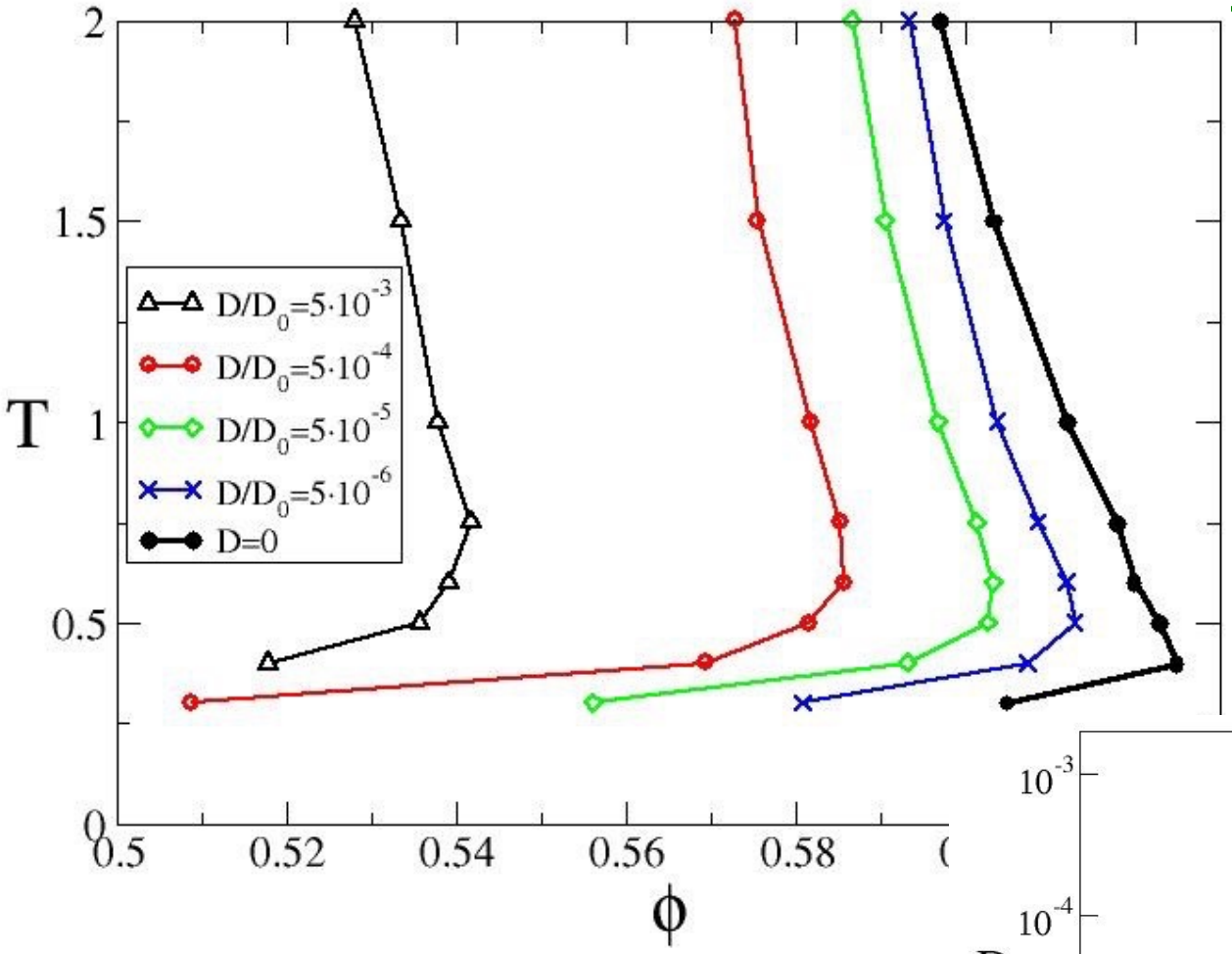
FS et al, cond-mat/0304192

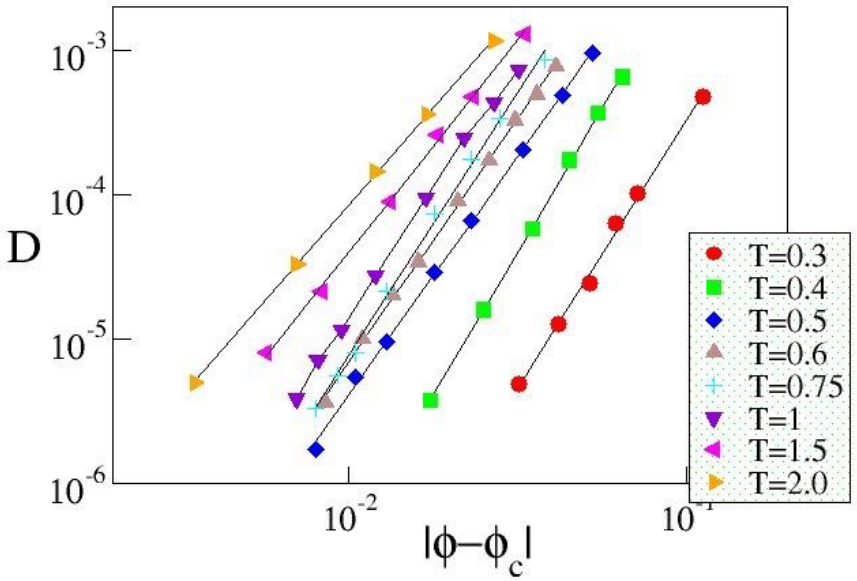
$\phi_{MD} = 1.897\phi_{PY} - 0.3922$

$T_{MD} = 0.5882T_{PY} - 0.225$

PY-MCT overestimates ideal attractive glass T by a factor of 2

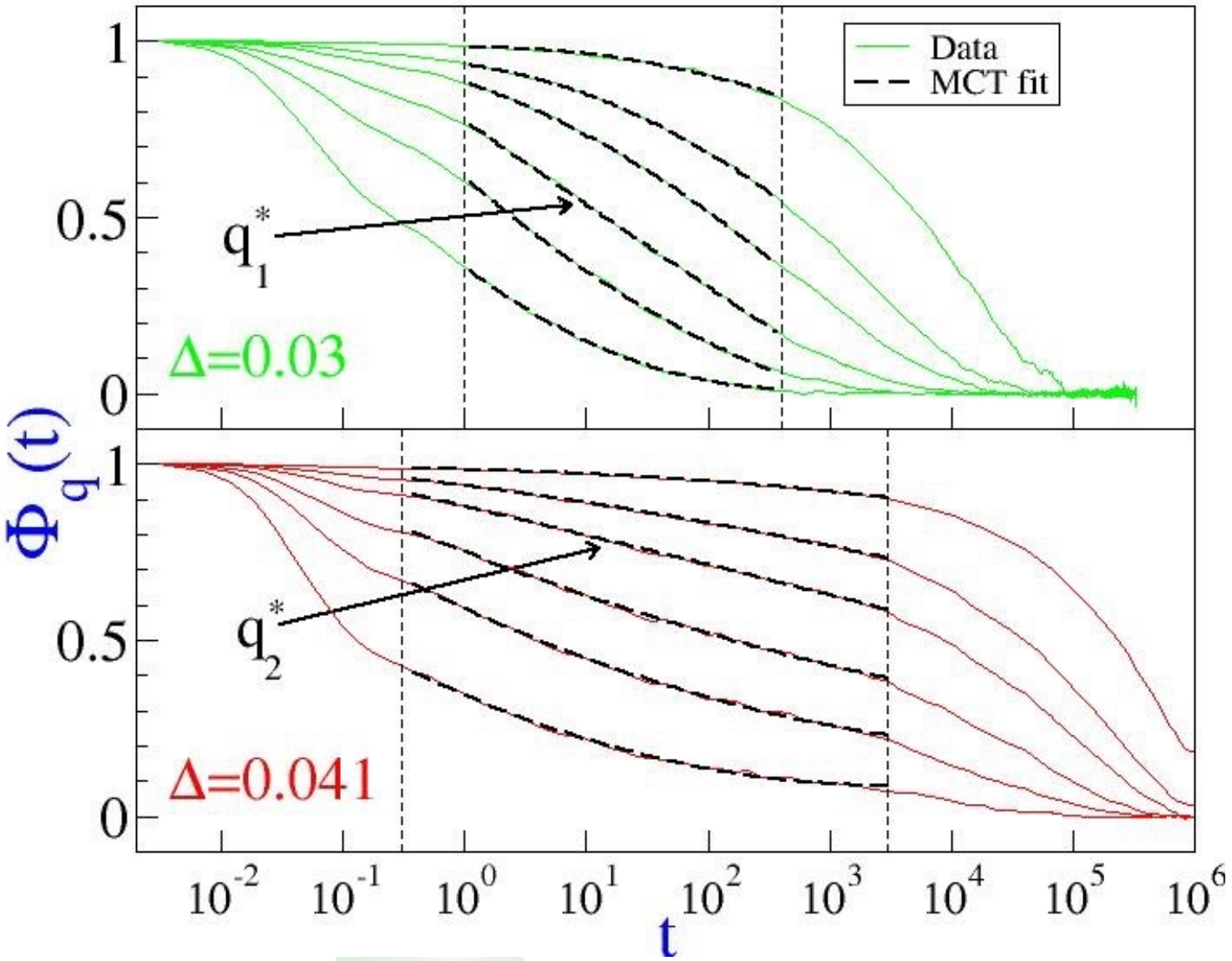
Isodiffusivity curves (MD Binary Hard Spheres)





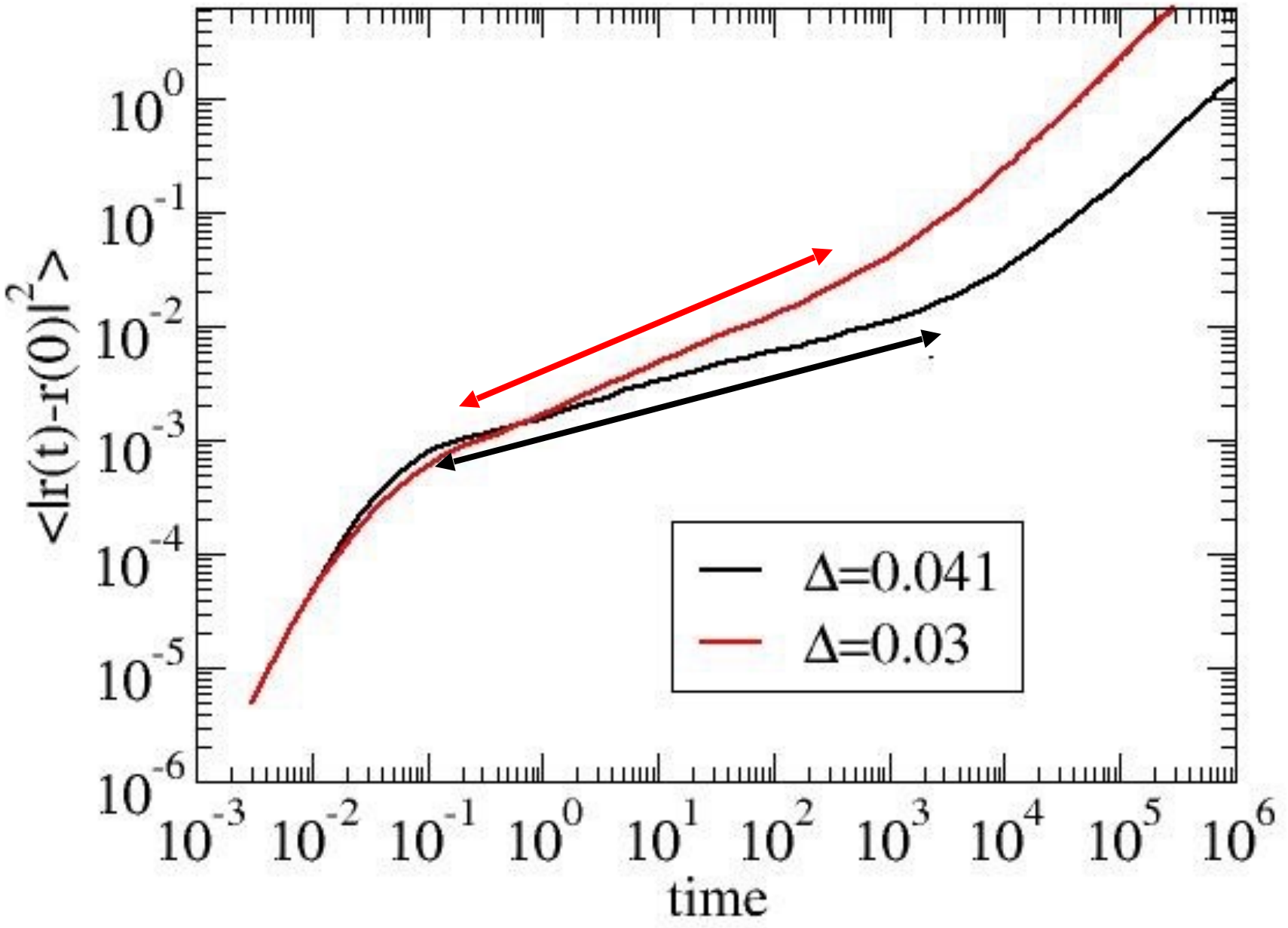
Zaccarelli et al PRE **66**, 041402 (2002).

Same T and ϕ, different Δ



$$\Phi_q(t)=f_q-h_q\,[B^{(1)}\ln(t/\tau) + B^{(2)}_q \ln^2(t/\tau)].$$

5 decadi di genuino comportamento sub-diffusivo !



Un Riassunto (ed i problemi aperti) !