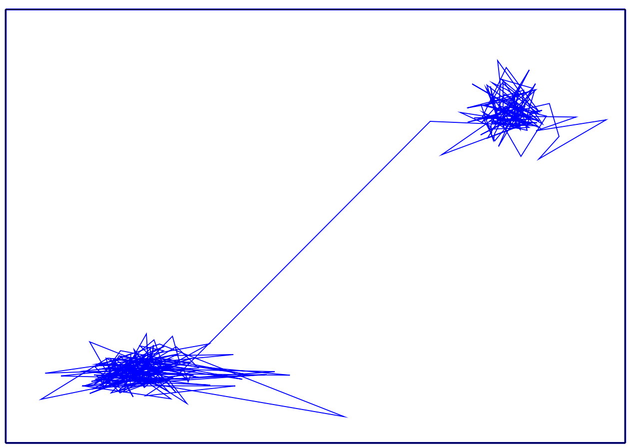
Single Particle Jumps in a Glass: Statistics and History Dependence

Katharina Vollmayr-Lee

Bucknell University, USA



thanks to:

A. Zippelius
K. Binder
J. Horbach
E. A. Baker

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Model

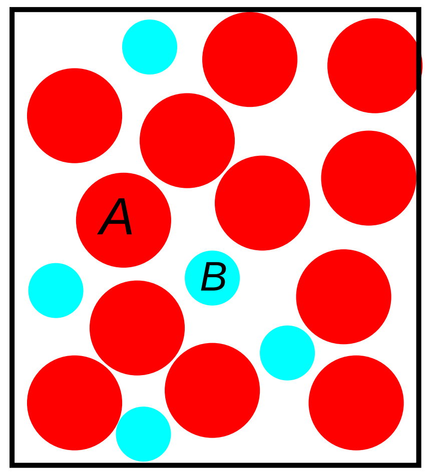
Binary Lennard-Jones System

$$V_{\alpha\beta}(r) = 4\,\epsilon_{\alpha\beta}\left(\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12} - \left(\frac{\sigma_{\alpha\beta}}{r}\right)^{6}\right)$$

$\sigma_{\mathrm{AA}} = 1.0 \quad \sigma_{\mathrm{AB}} = 0.8 \quad \sigma_{\mathrm{BB}} = 0.88$

$\epsilon_{\mathrm{AA}} = 1.0 \quad \epsilon_{\mathrm{AB}} = 1.5 \quad \epsilon_{\mathrm{BB}} = 0.5$

[W. Kob and H.C. Andersen, PRL 73, 1376 (1994)]



Simulations

Molecular Dynamics Simulations

(Velocity Verlet)

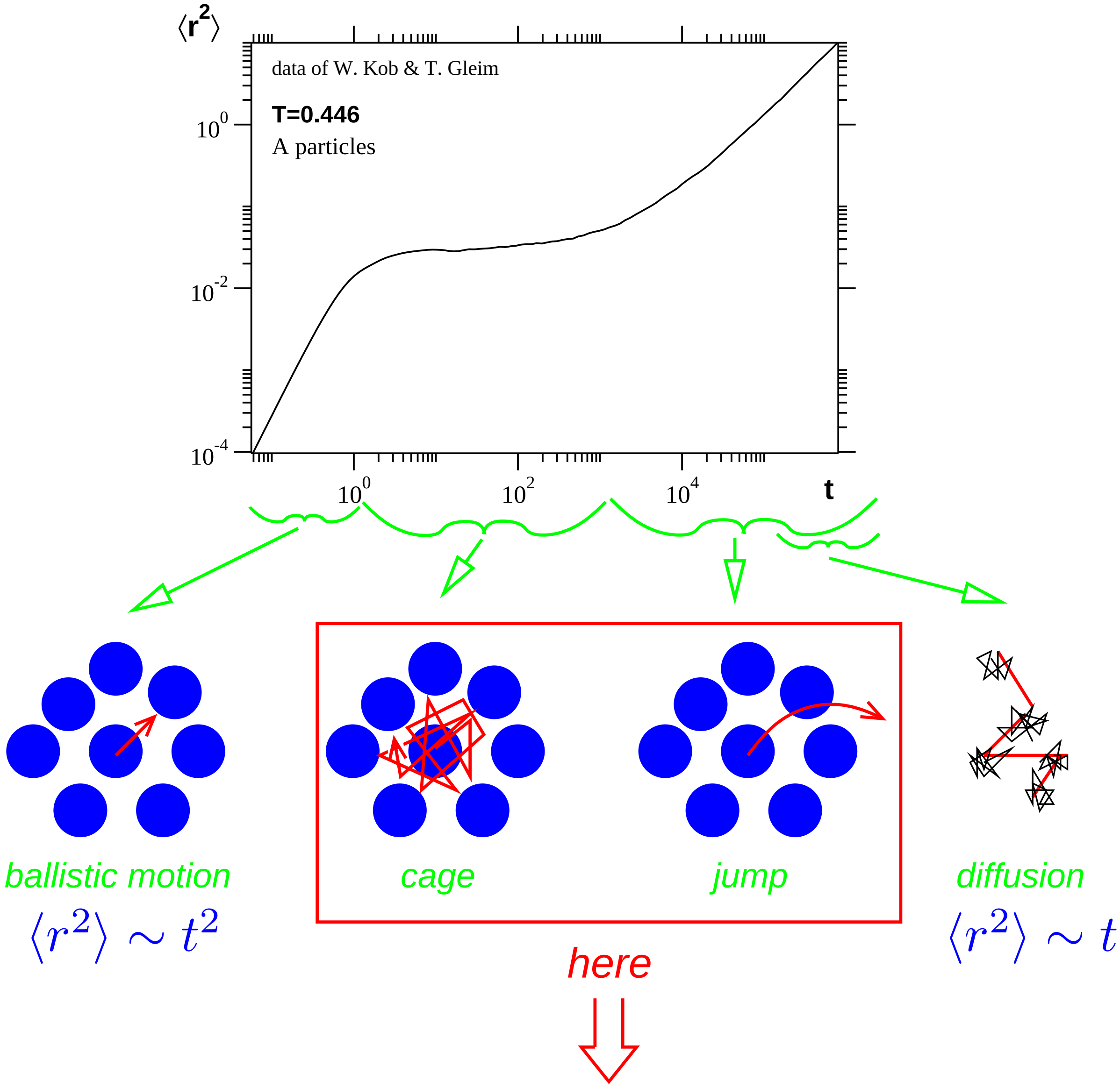
below glass transition:

$T = 0.15 - 0.43$ (MCT $T_{\mathrm{c}} = 0.435$)

Cage-Picture

Mean-Squared Displacement

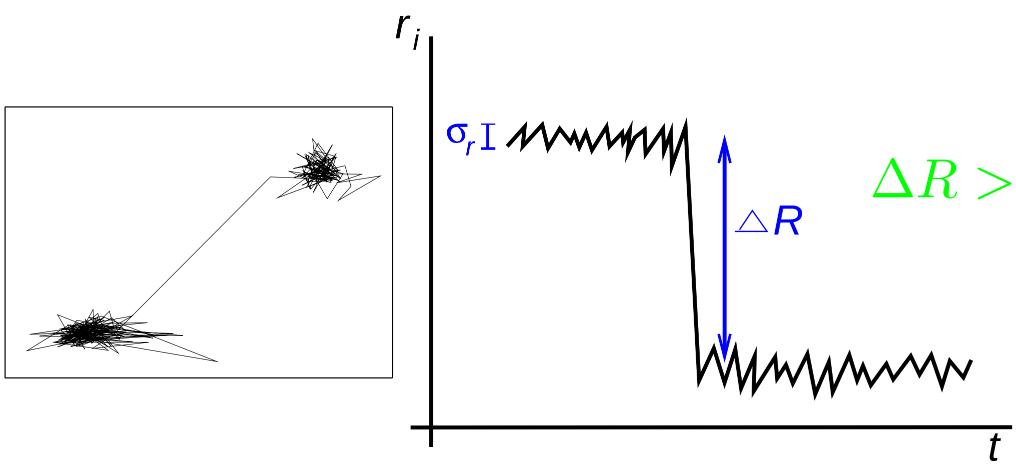
$$\langle r^2\rangle(t) = \left\langle \frac{1}{N}\sum_{i=1}^{N}\left(\underline{r}_i(t)-\underline{r}_i(0)\right)^2\right\rangle$$



Definitions

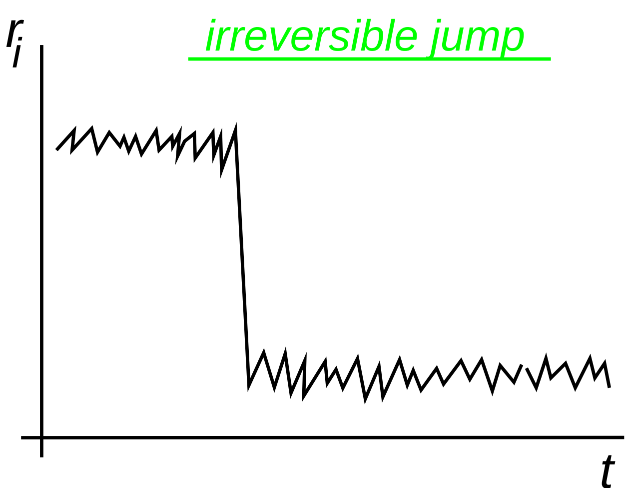
Jump-Occurrence

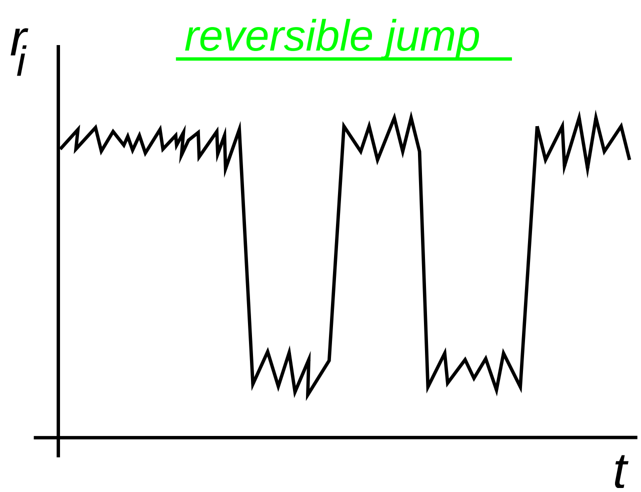
Single Particle Trajectories



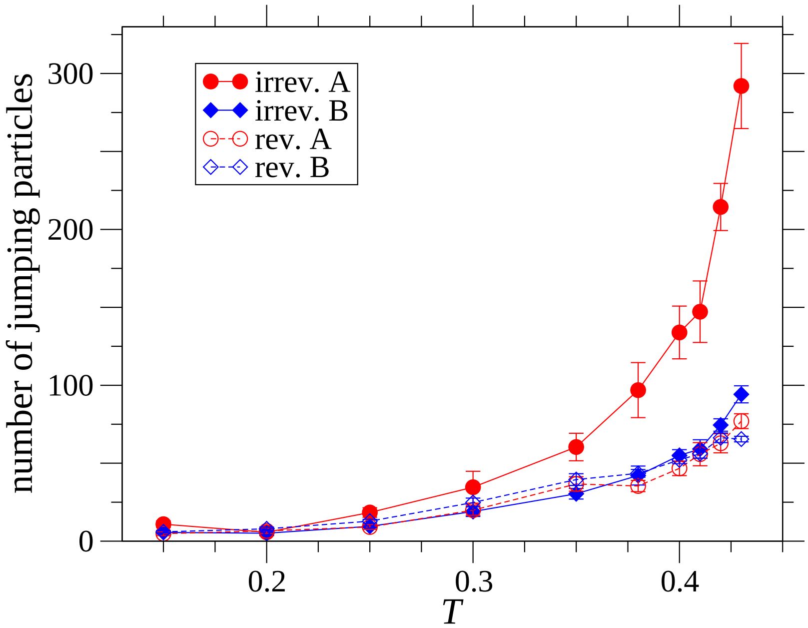
$$\Delta R > \sqrt{20}\,\sigma_r$$

Jump-Type



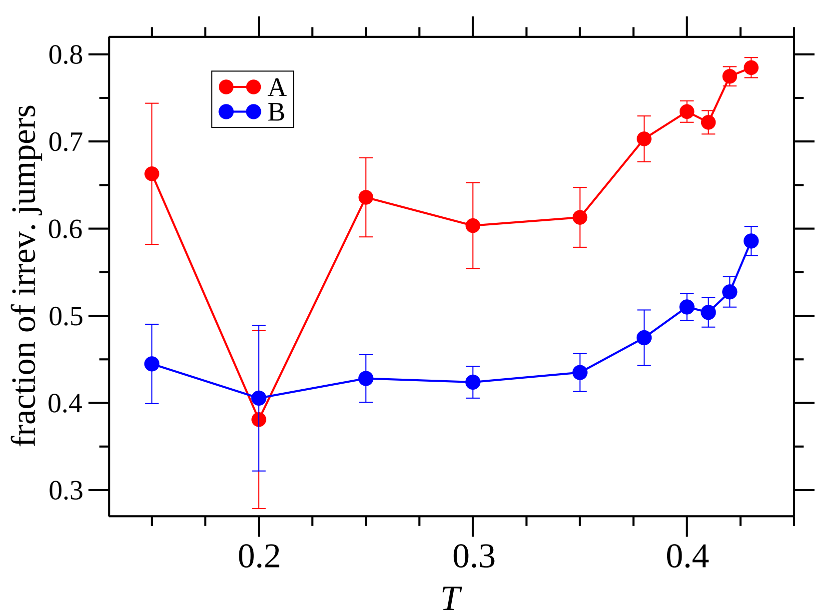


Number of Jumping Particles



⟹ both A & B particles jump

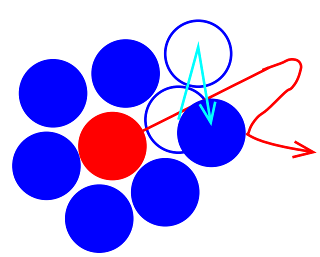
⟹ irrev. & reversible jumps at all temperatures T



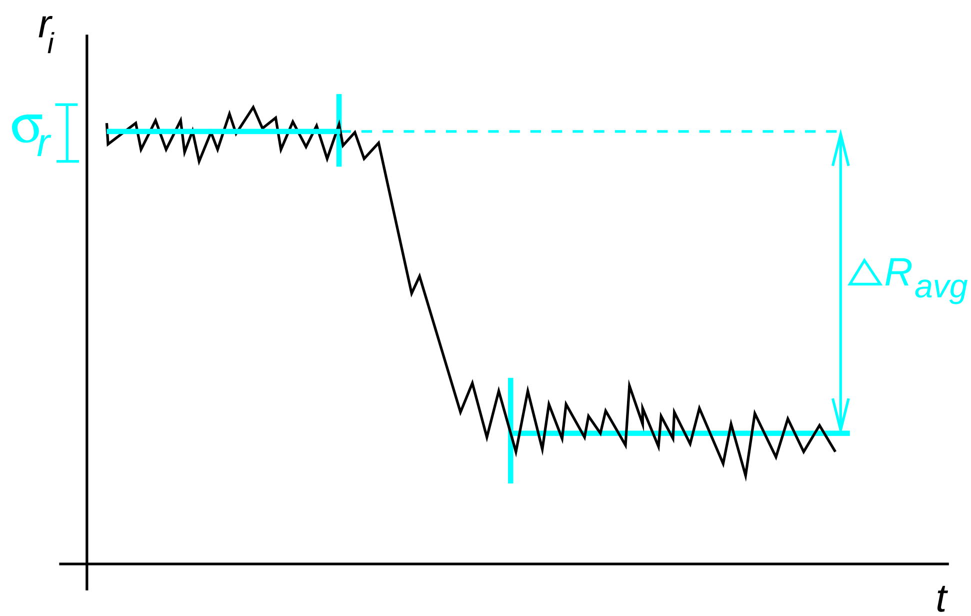
⟹ fraction of irrev. jumpers increases with increasing T

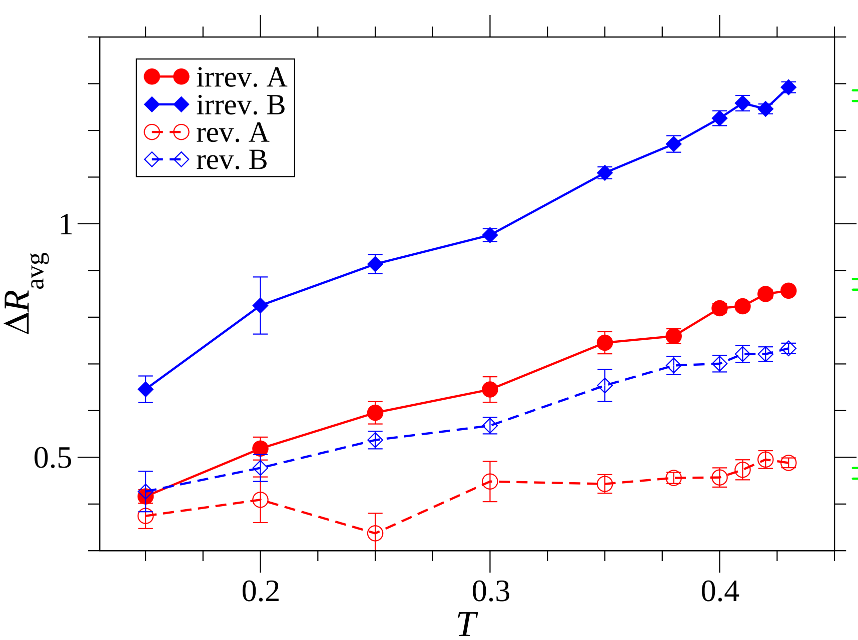
interpretation:

door closing



Jump Size



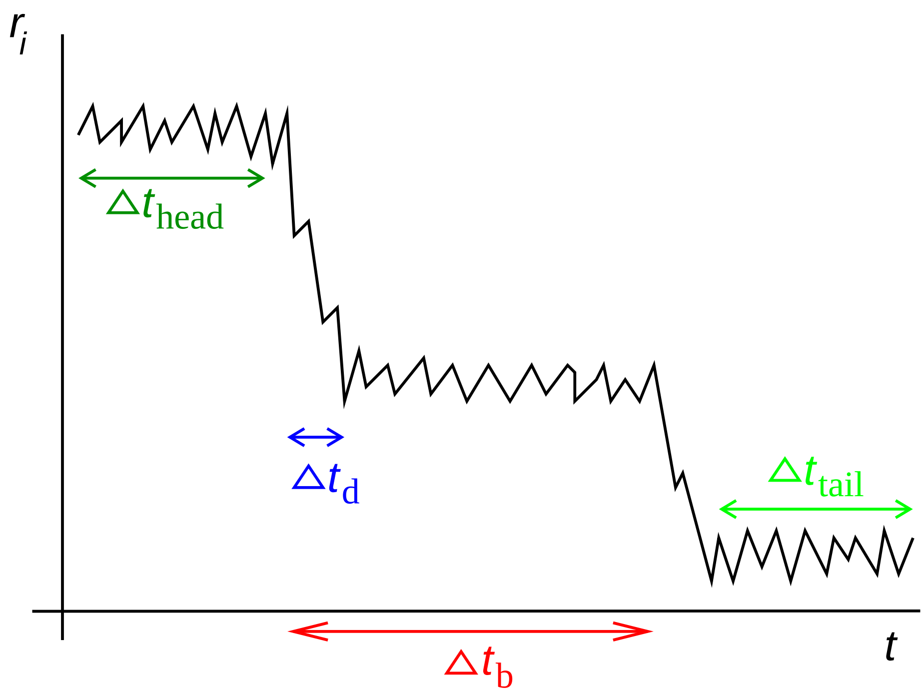


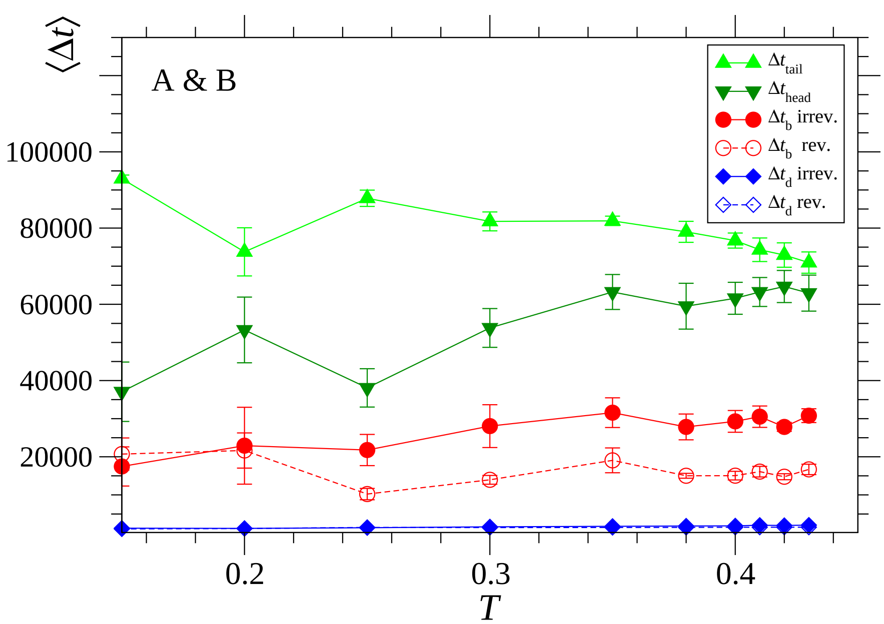
⟹ increasing with incr. T

⟹ (smaller) B-part. jump farther

⟹ irrever. jumps farther

Time Scale





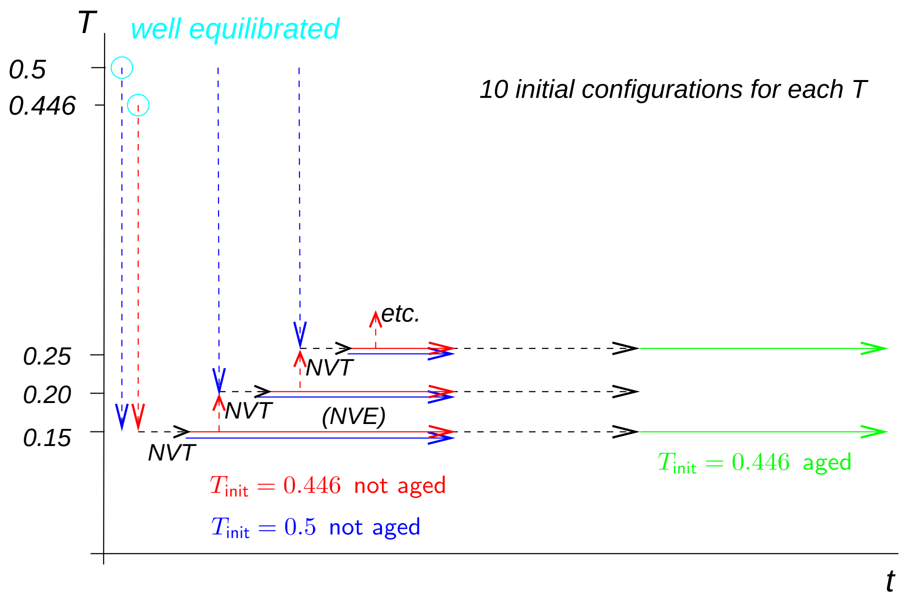
$\Longrightarrow$ $\Delta t_{\text{b}} \gg \Delta t_{\text{d}}$

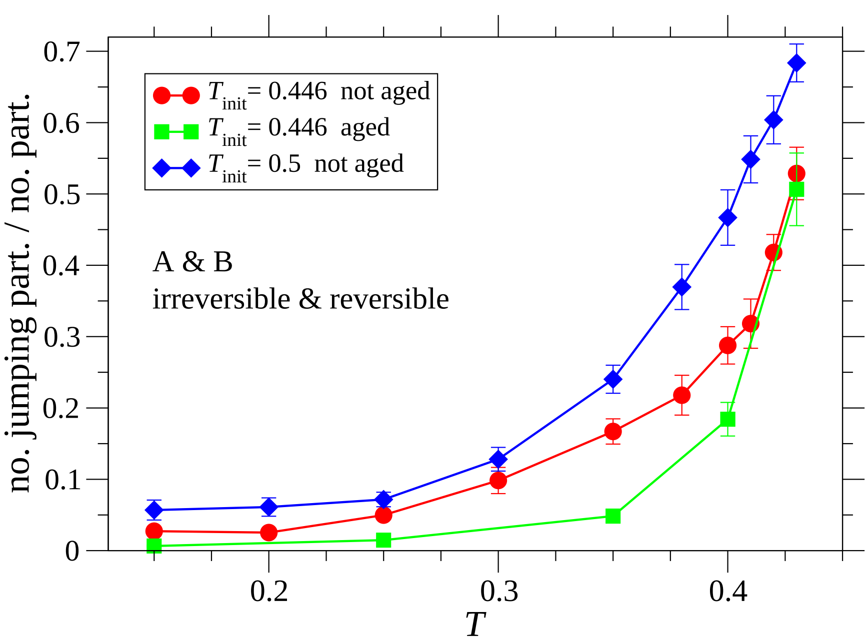
$\Longrightarrow$ Δt_{b} indep. of temperature at increasing T relaxation not via higher frequency

$\Longrightarrow$ $\Delta t_{\text{tail}} > \Delta t_{\text{head}}$ aging

History Dependence

History of Production Runs

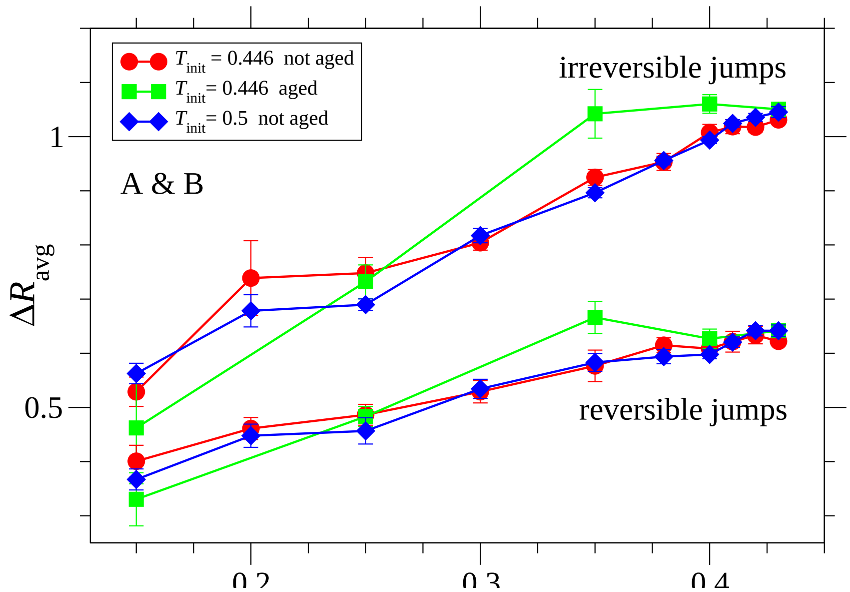




Number of Jumping Particles:

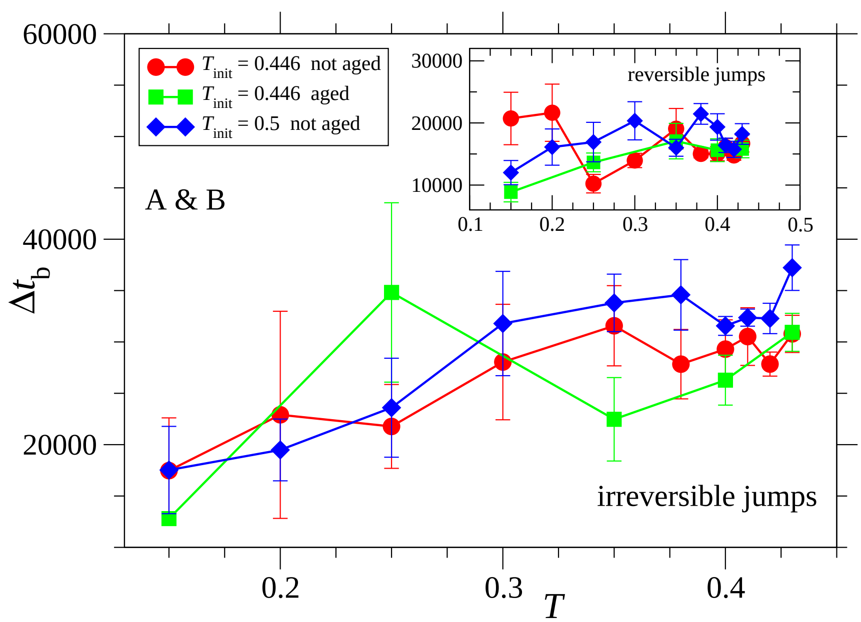
$\Longrightarrow$ qualitatively history independent

$\Longrightarrow$ quantitatively history dependent



Jump Size:

$\Longrightarrow$ history independent



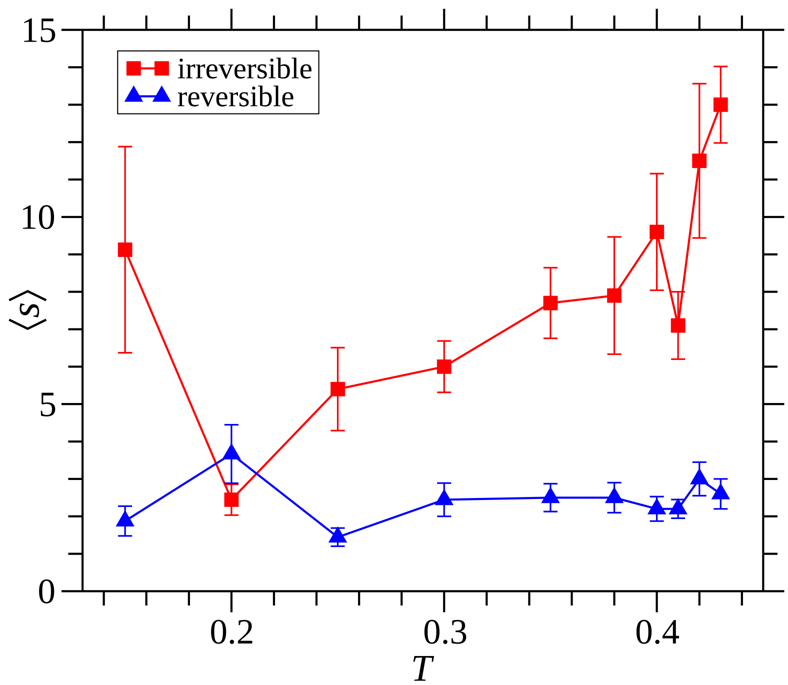
Time Between Jumps:

$\Longrightarrow$ history independent

Spatial Correlations

Definition:

Largest cluster of simultaneously jumping particles.



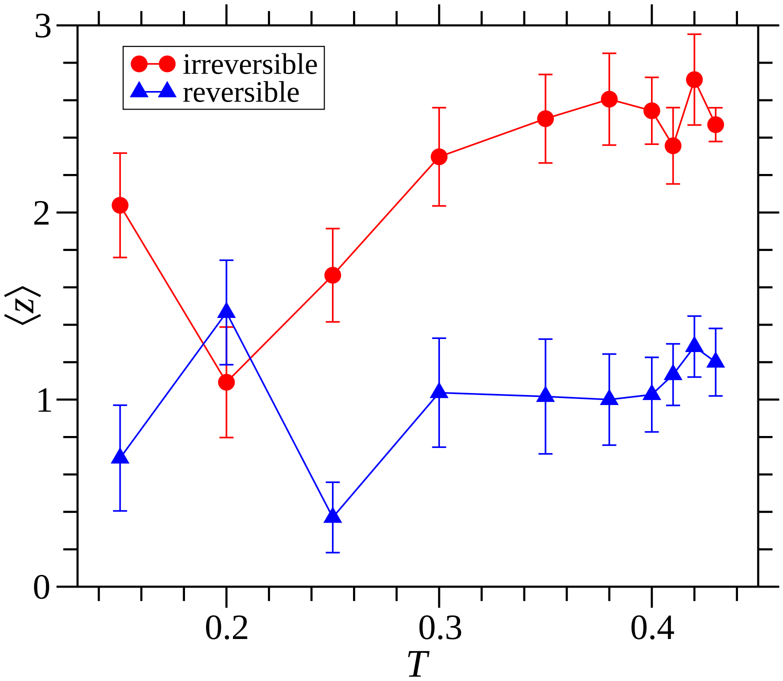
Number of Part. In a Cluster s:

$\Longrightarrow$ irreversible: $\langle s \rangle = 2 - 13$

incr. with incr. T

$\Longrightarrow$ reversible: $\langle s \rangle = 2 - 3$

independent of T



Coordination Number z:

$\Longrightarrow$ irreversible: $\langle z \rangle = 2 - 3$
even at largest T
$\Longrightarrow$ string-like

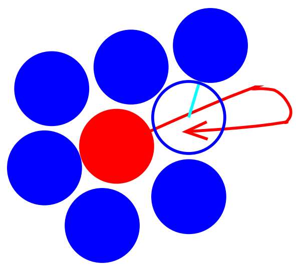
$\Longrightarrow$ reversible: $\langle z \rangle \approx 1$
independent of T

[E. A. Baker, KVL, K1.00081]

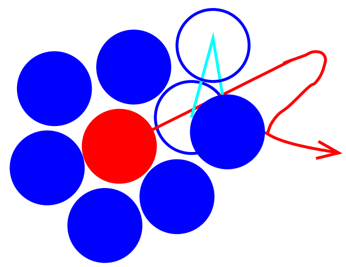
Summary

(Picture of Jump)

1. reversible & irreversible jumps



reversible jump



irreversible jump

2. irreversible jumps become more likely at larger T

3. At larger temperature relaxation:
   - not via Δt_{b} (indep. of T) (history independent)
   - via larger jumpsizes (history independent)
   - via more jumping particles (history dependent)
   - irreversible jumpers form string-like clusters

Acknowledgments:

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