Glassy Slowdown and Amorphous Order

Sho Yaida

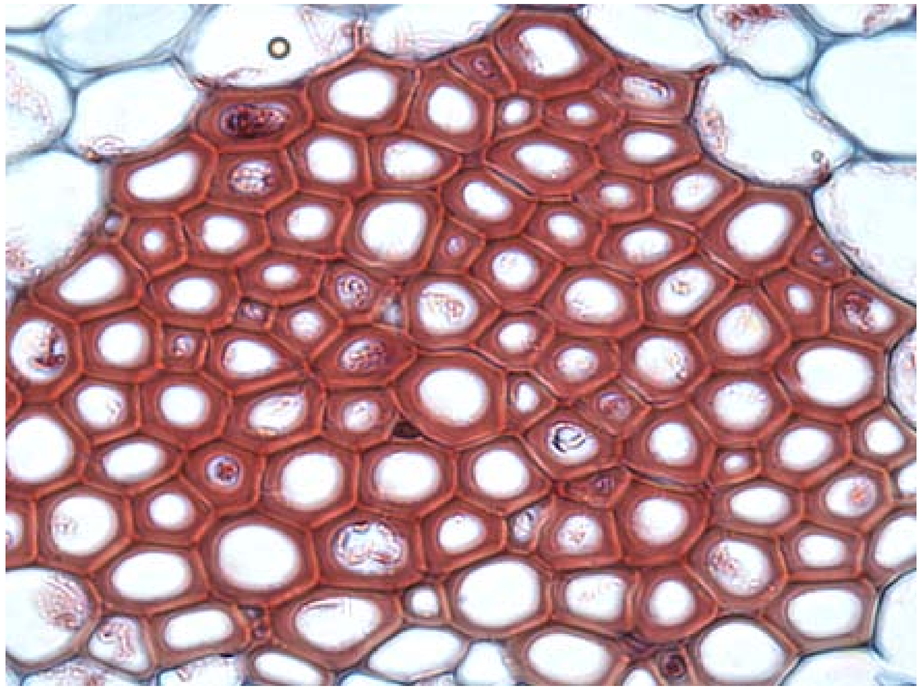
facebook
Artificial Intelligence Research

Complex landscapes in everyday life

Glass

Plastic

Sand



Tissue

Ecosystem

Learning

Outline

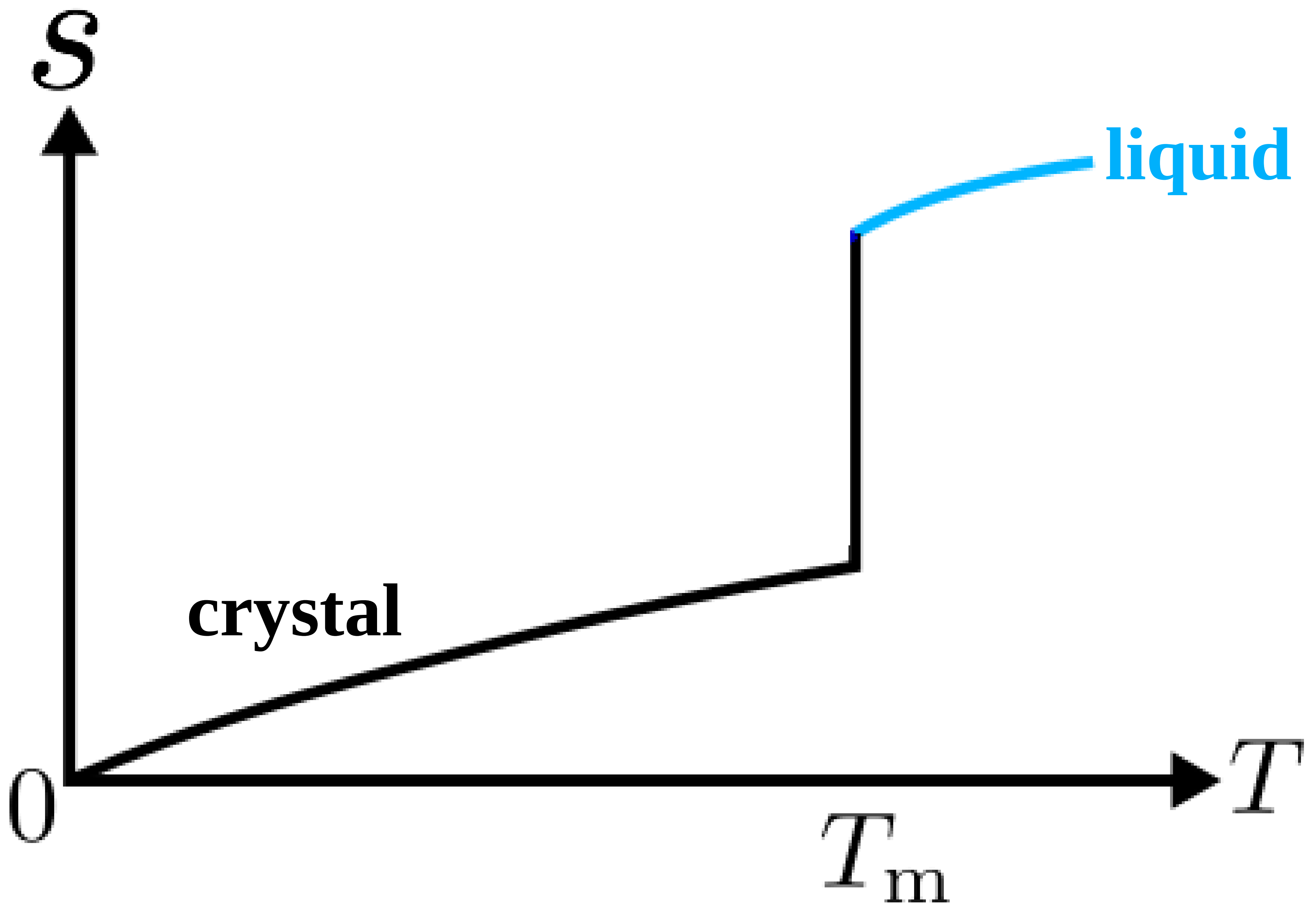
1 **Review of glass phenomenology**

2 **Amorphous order**

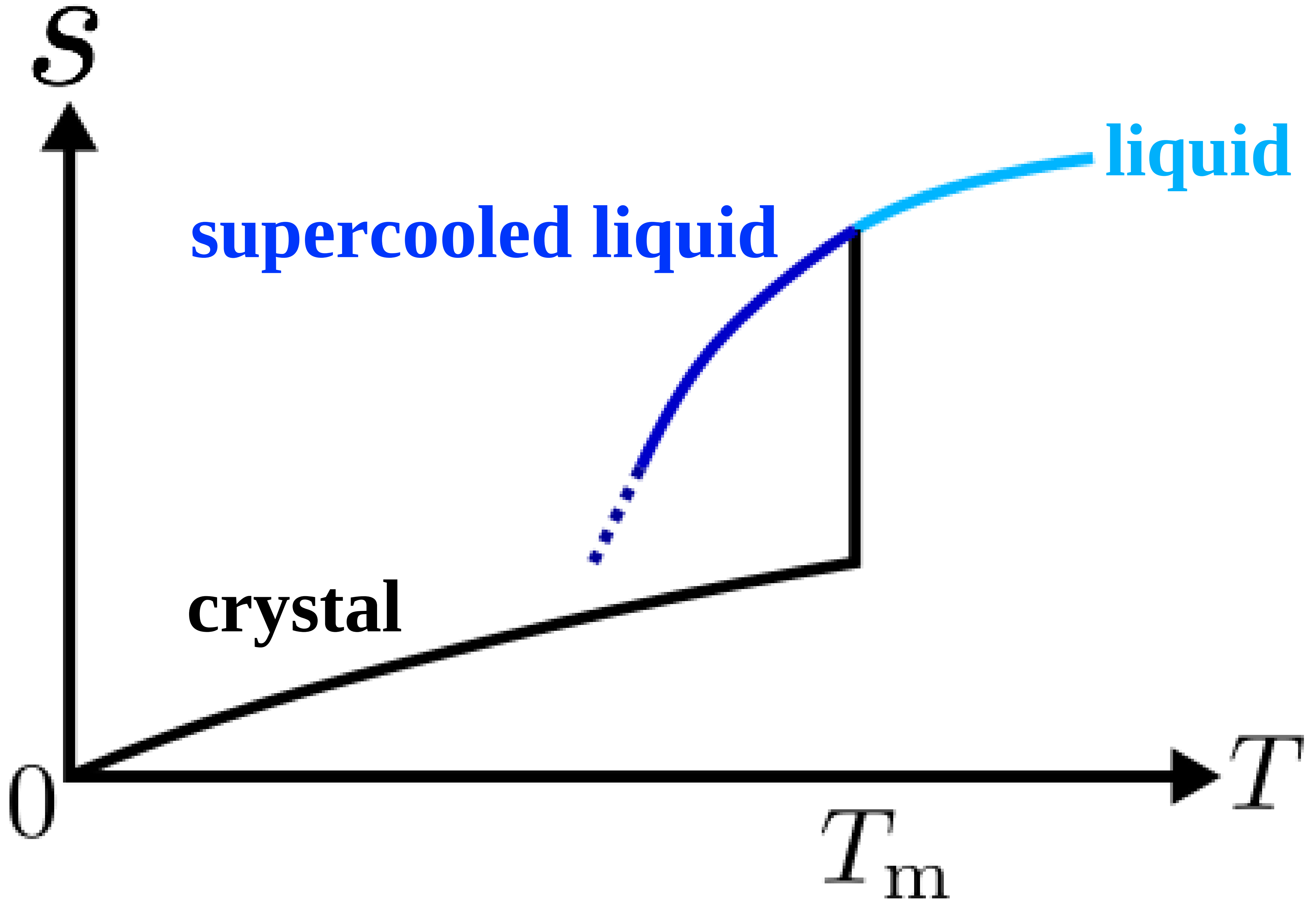
3 **Beyond the glass ceiling**

1 Review of glass phenomenology

Glass phenomenology

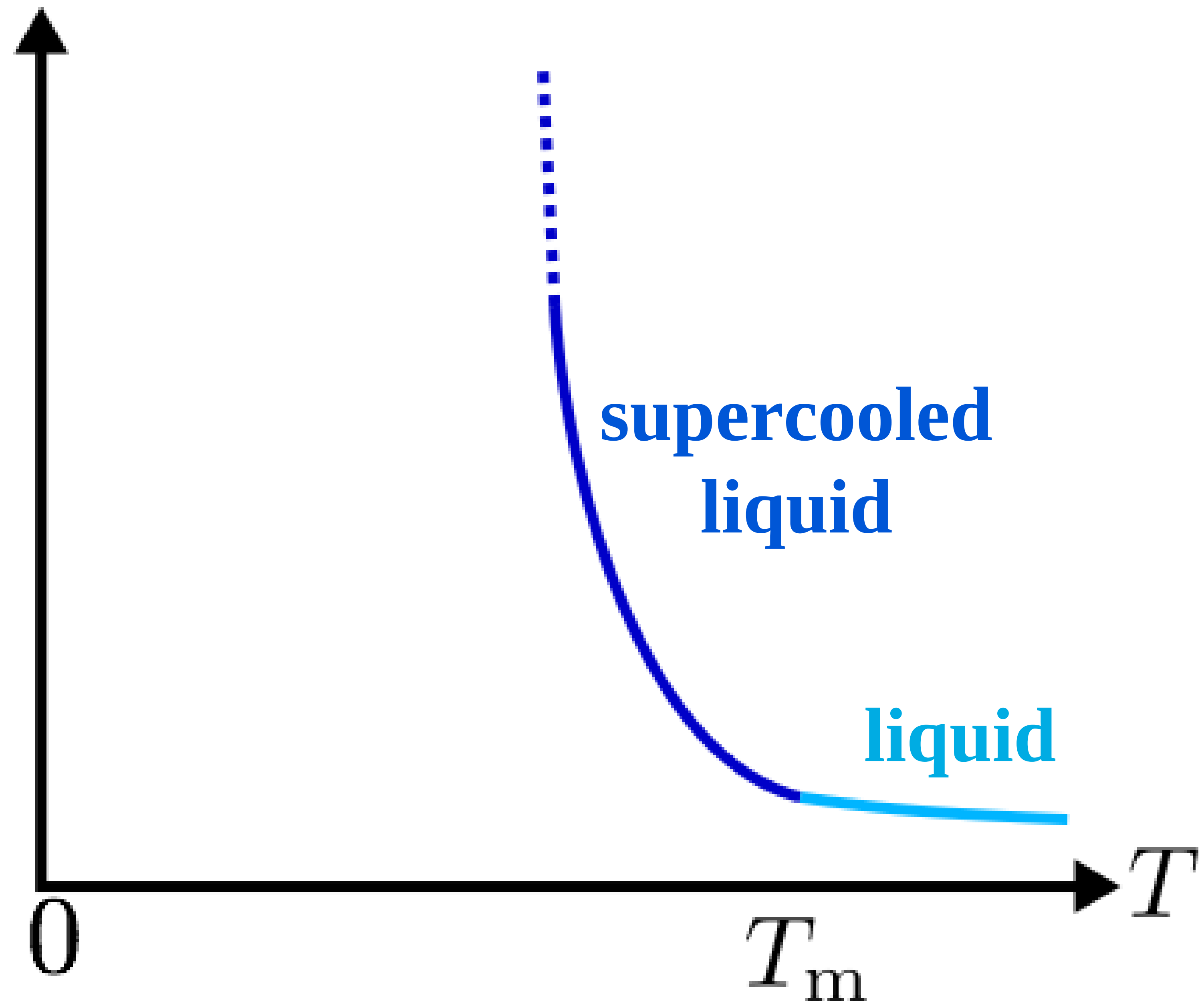


Glass phenomenology



Glass phenomenology

shear viscosity $\eta \sim t_{\mathrm{equilibration}}$



Glass phenomenology

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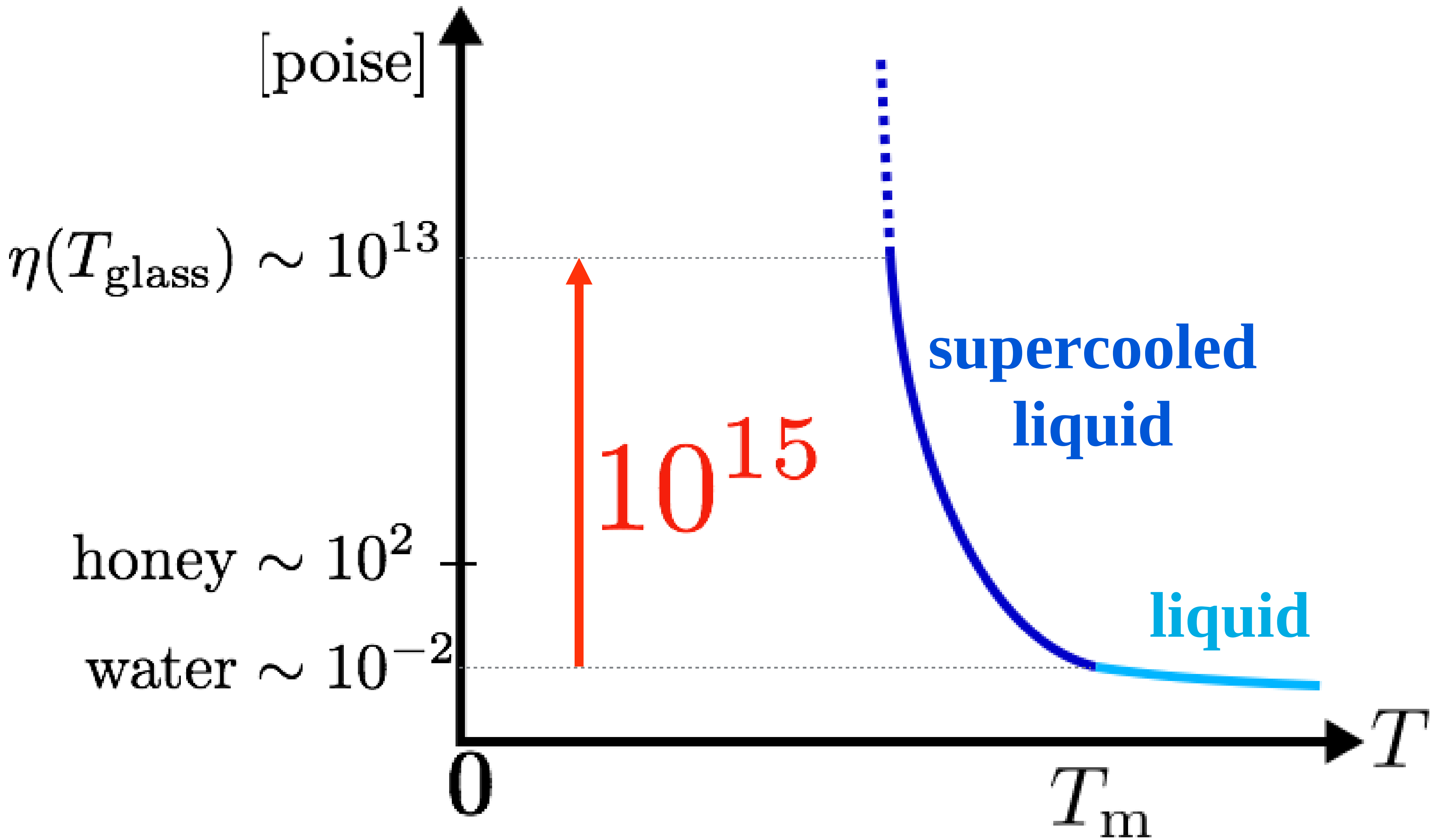

typical molecular liquids

Glass phenomenology

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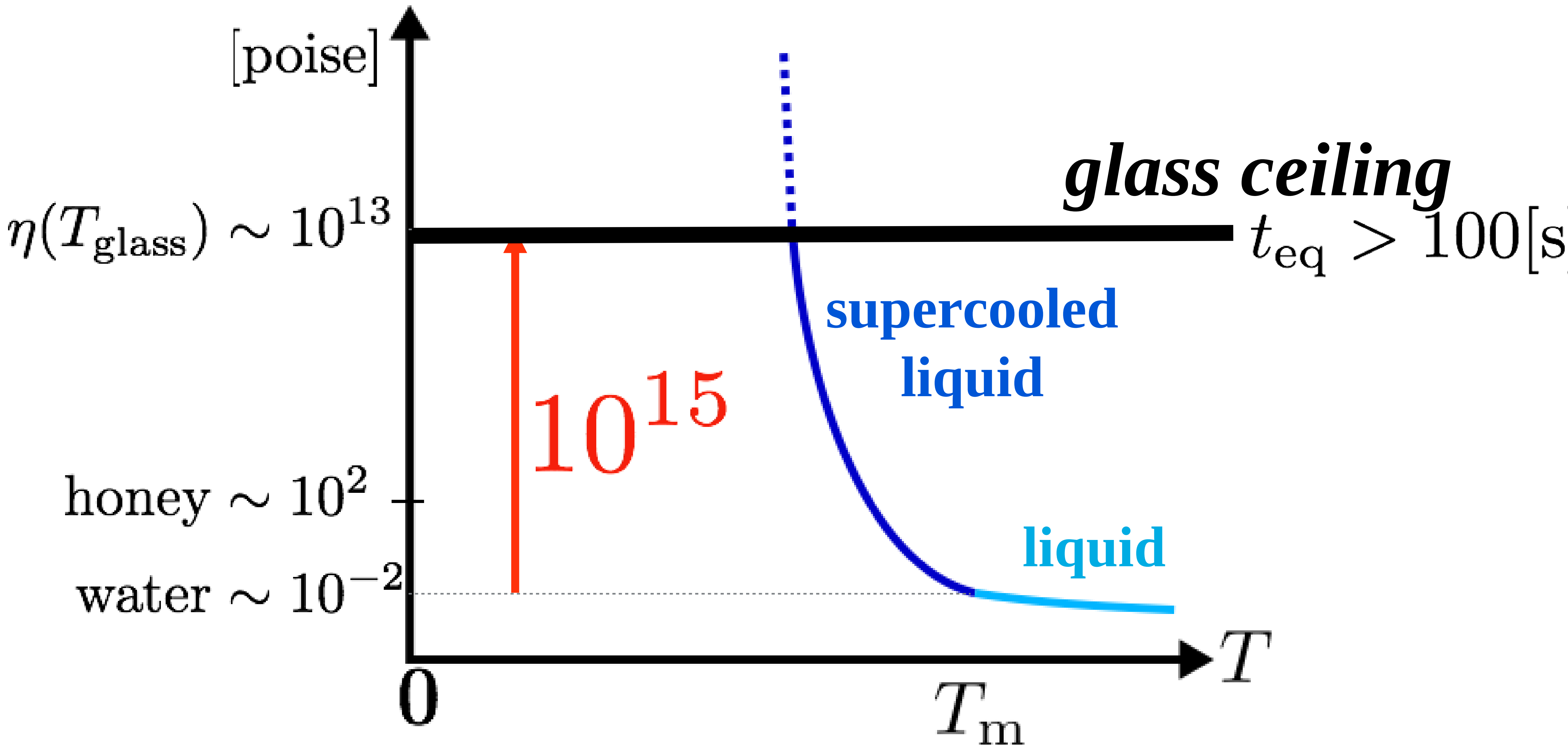
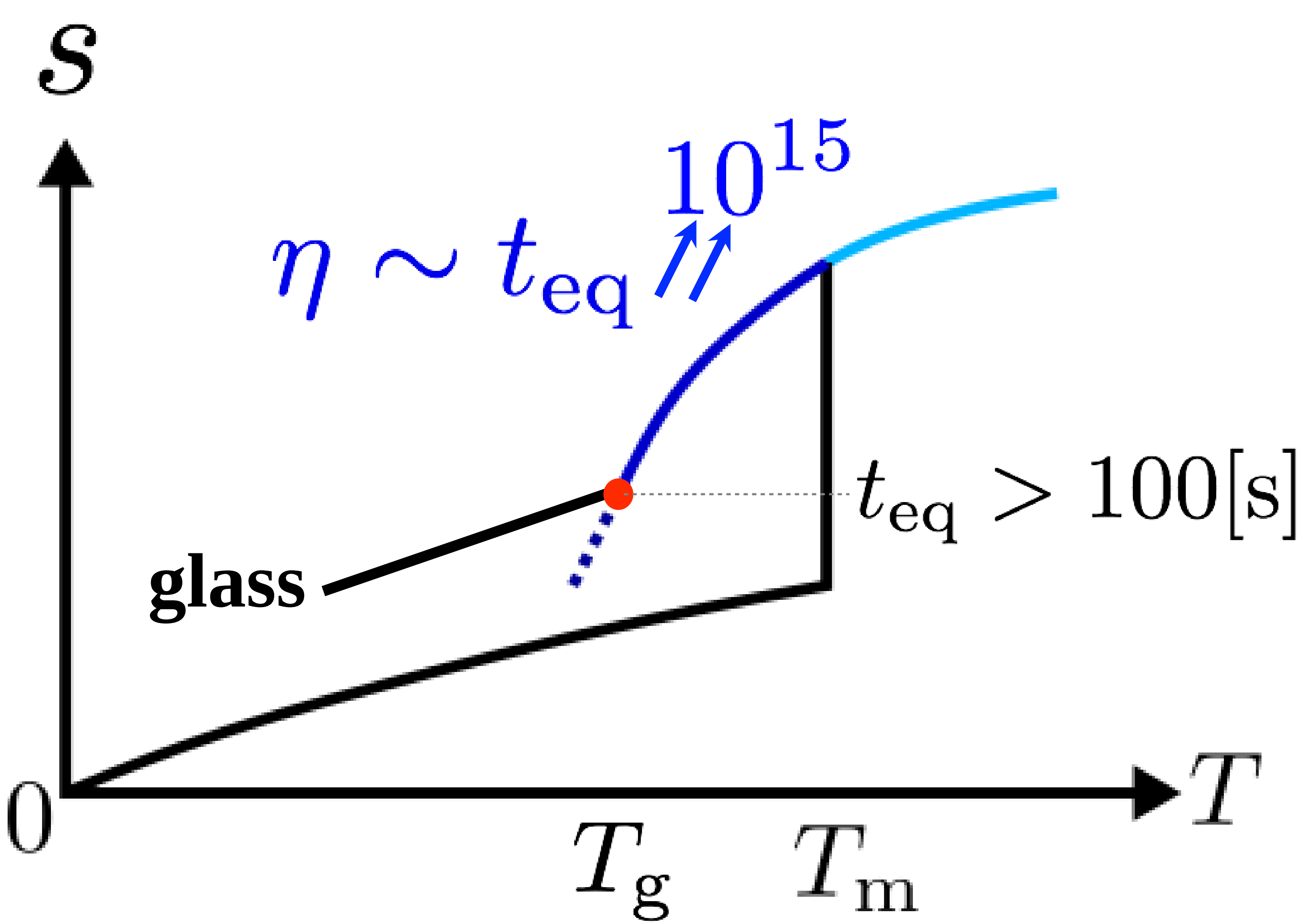
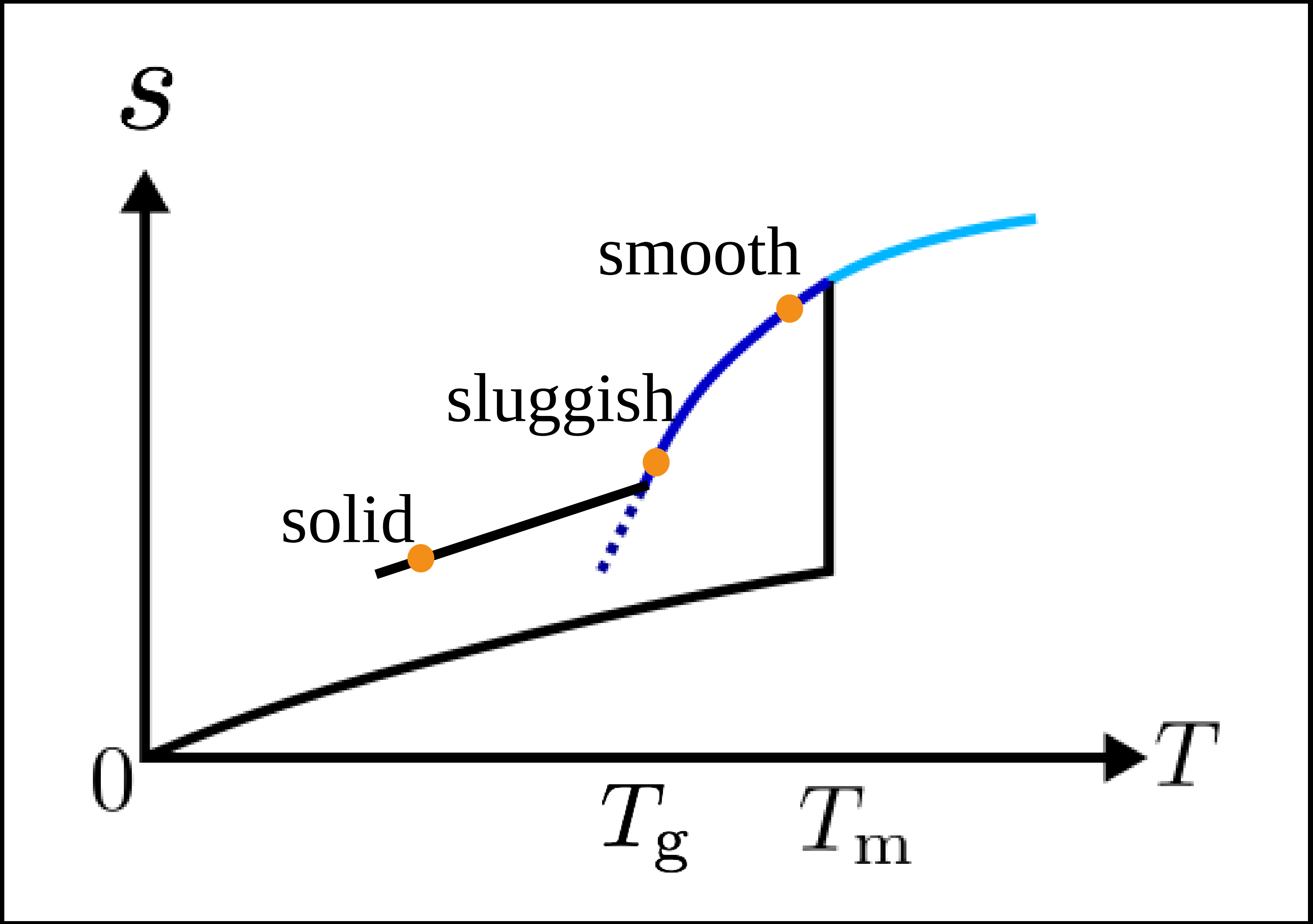


typical molecular liquids

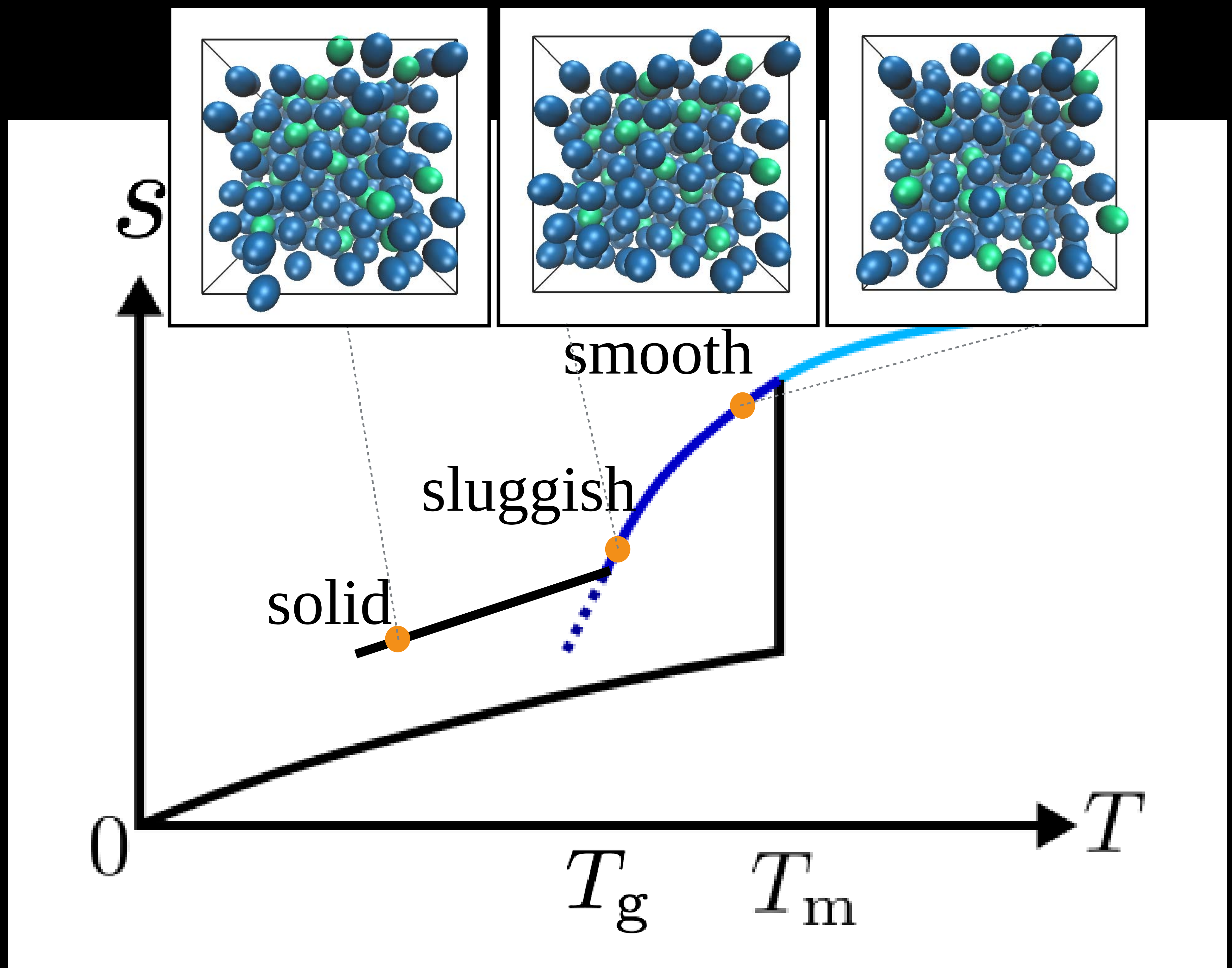
Glass phenomenology



Glass mystery?

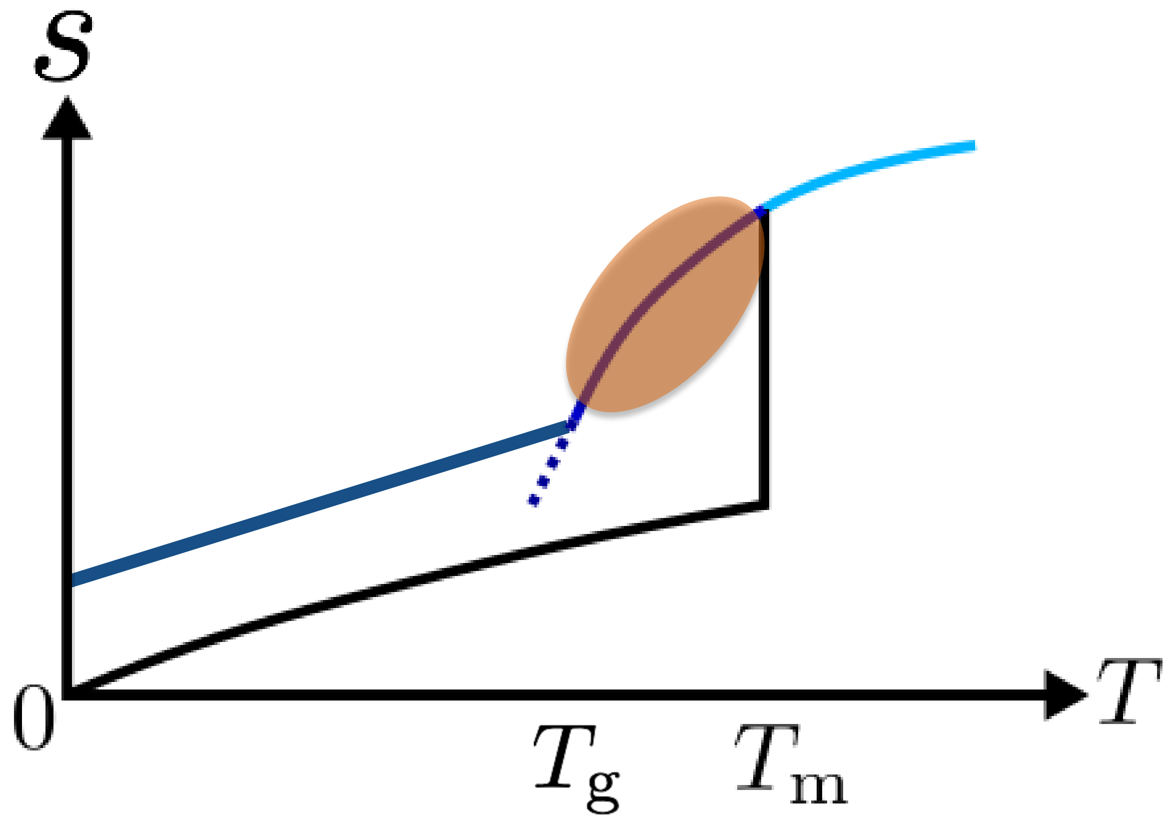


Glass mystery?



They all look the same, amorphous mess!

2 Amorphous order

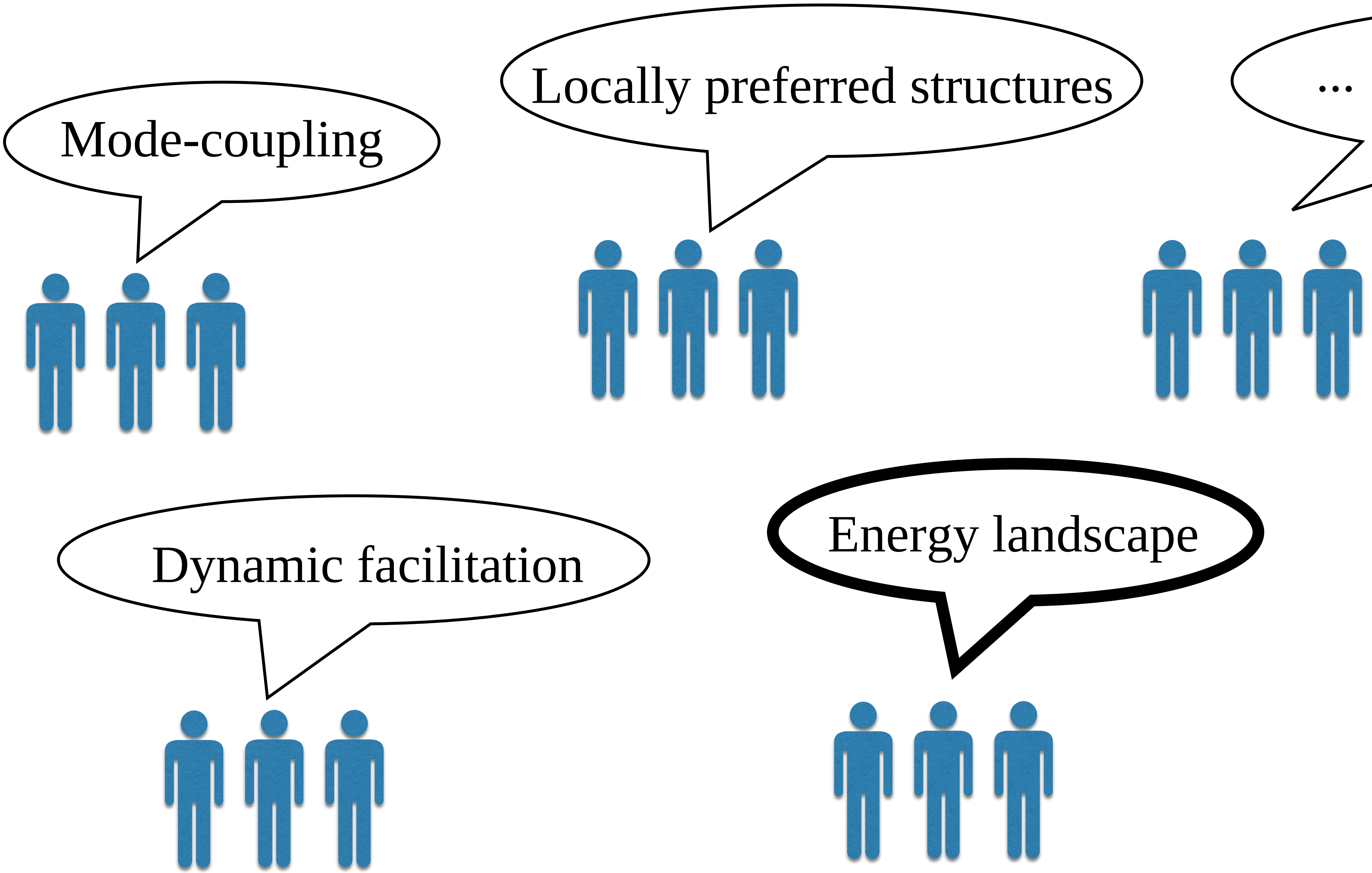


Glass slowdown

Dramatic slowdown without structural change:

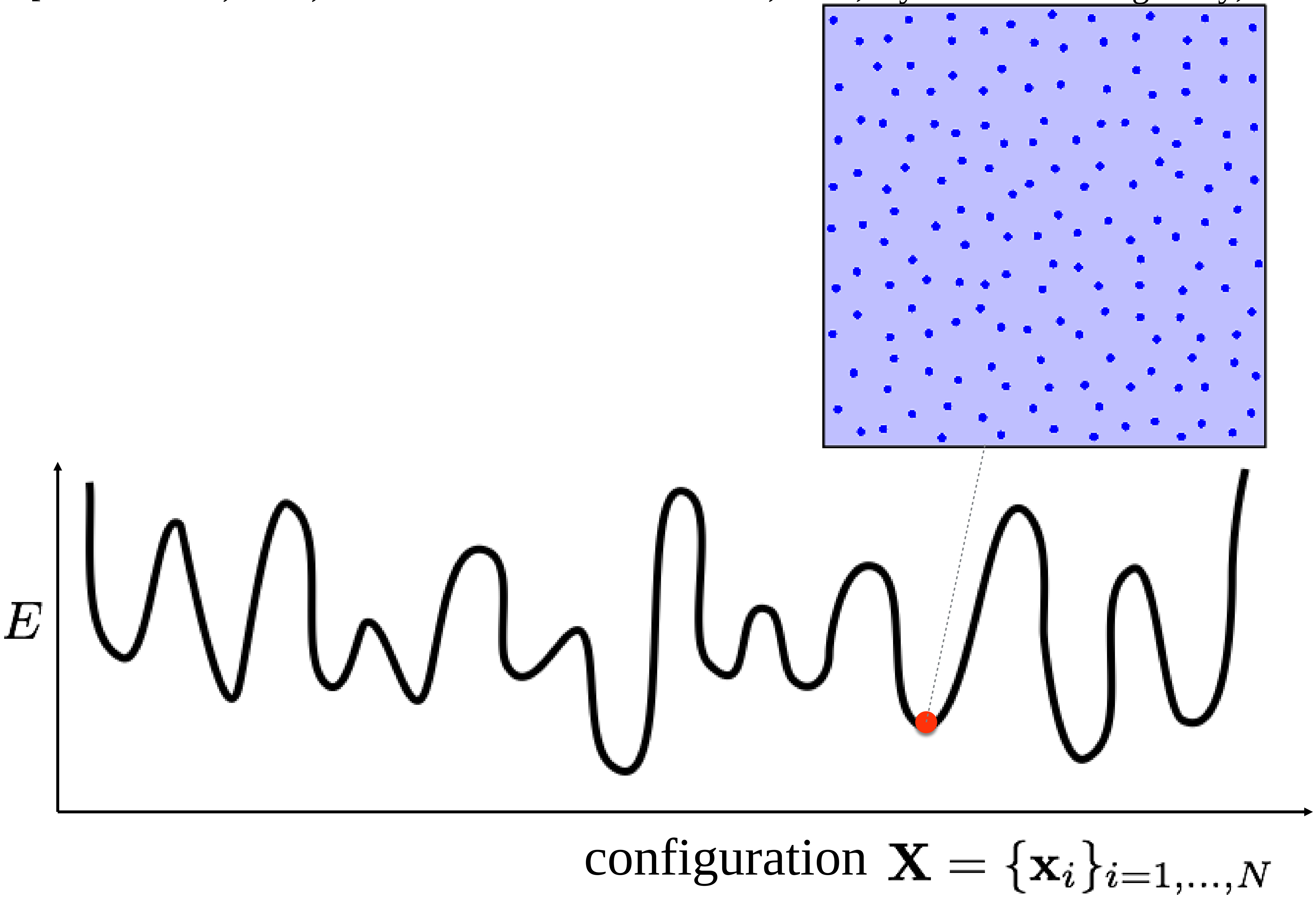
$\eta \nearrow 10^{15}$ while $\langle \rho(\mathbf{r}) \rho(\mathbf{0}) \rangle_T$ barely changes

Competing theories for slowdown



Energy landscape

[Adam-Gibbs, 1965; Random First-Order Transition, 1989; Dynamical Heterogeneity, ~2000]



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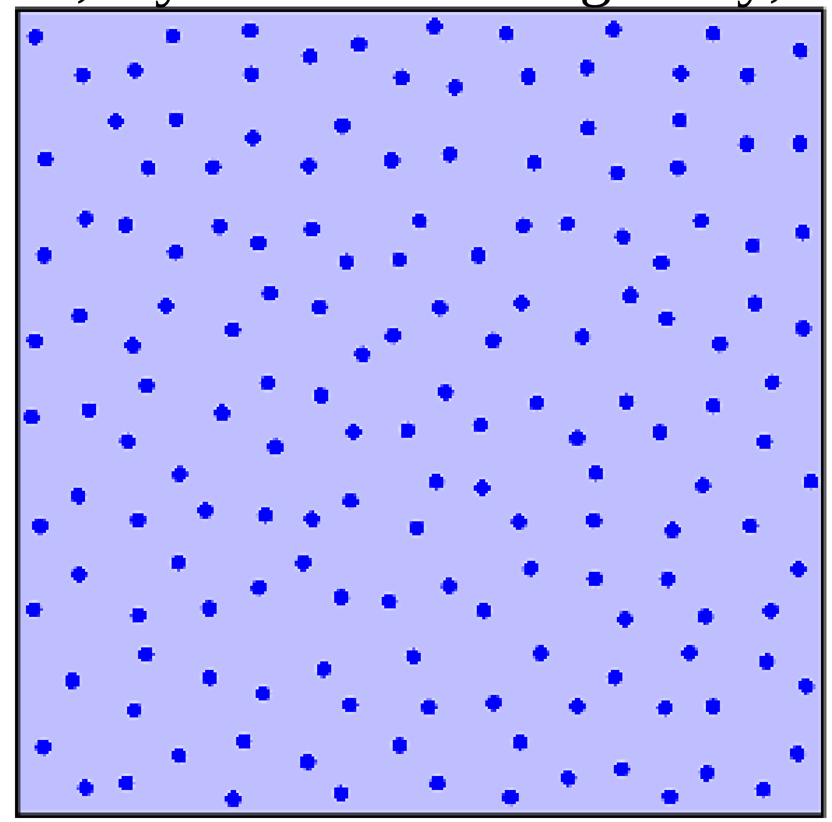
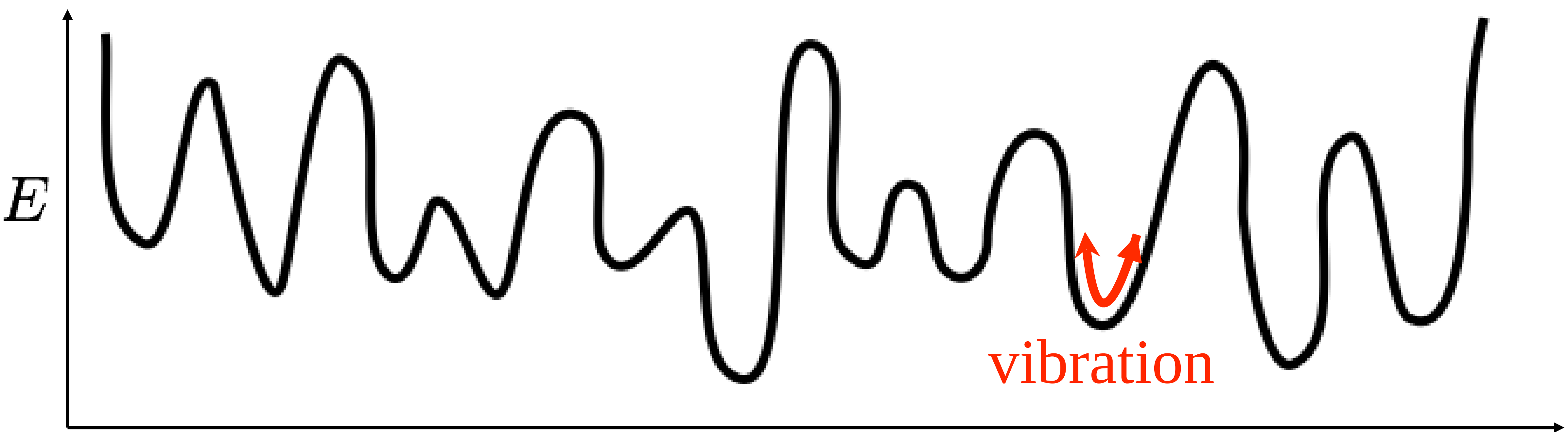
$$t \ll t_{\mathrm{eq}}$$





configuration $\mathbf{X} = \{\mathbf{x}_i\}_{i=1,\ldots,N}$

Energy landscape

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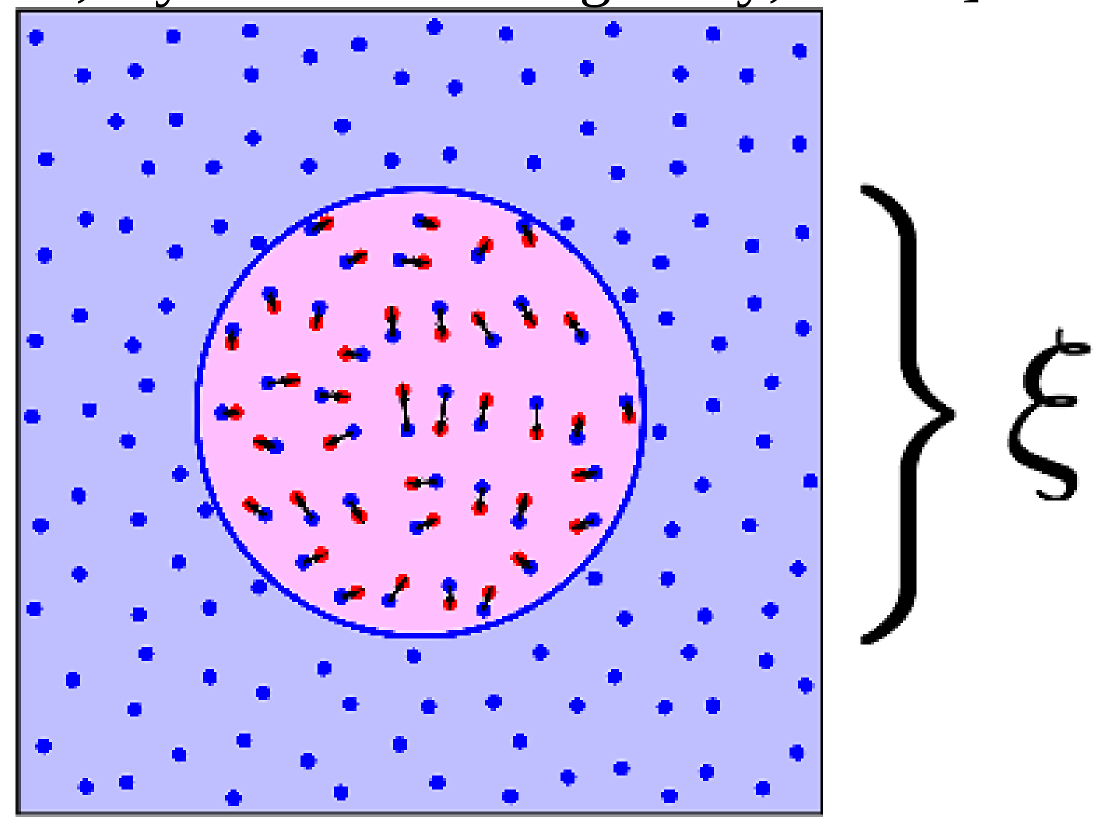
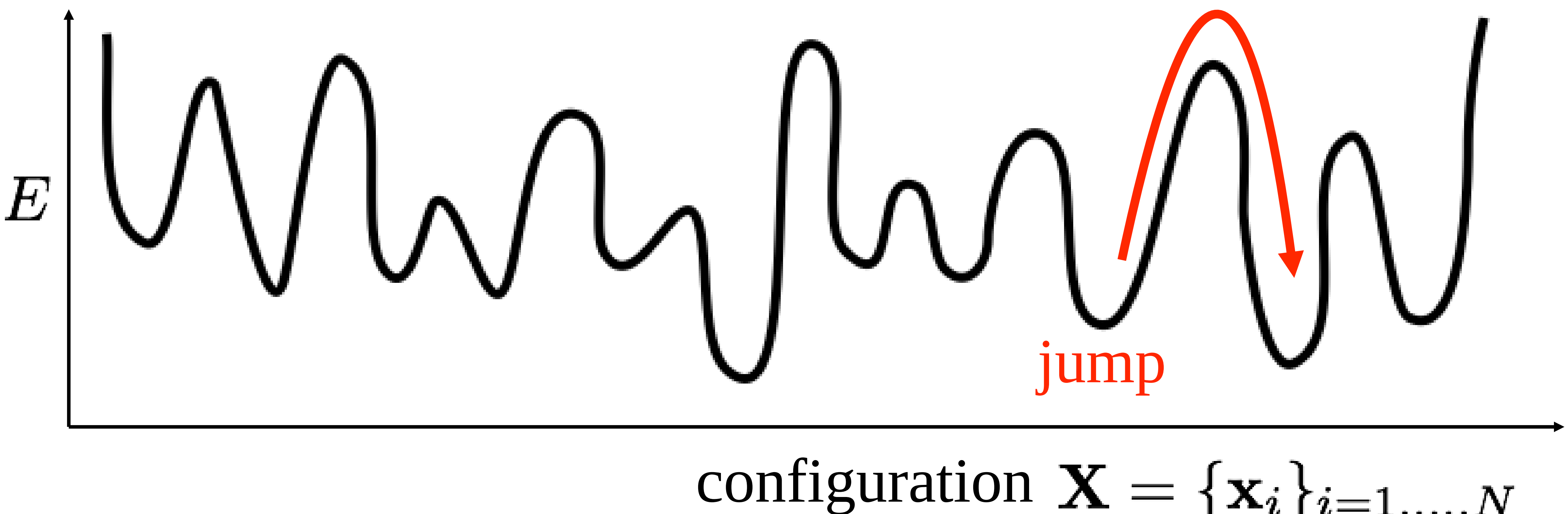
$$t \sim t_{\mathrm{eq}}$$





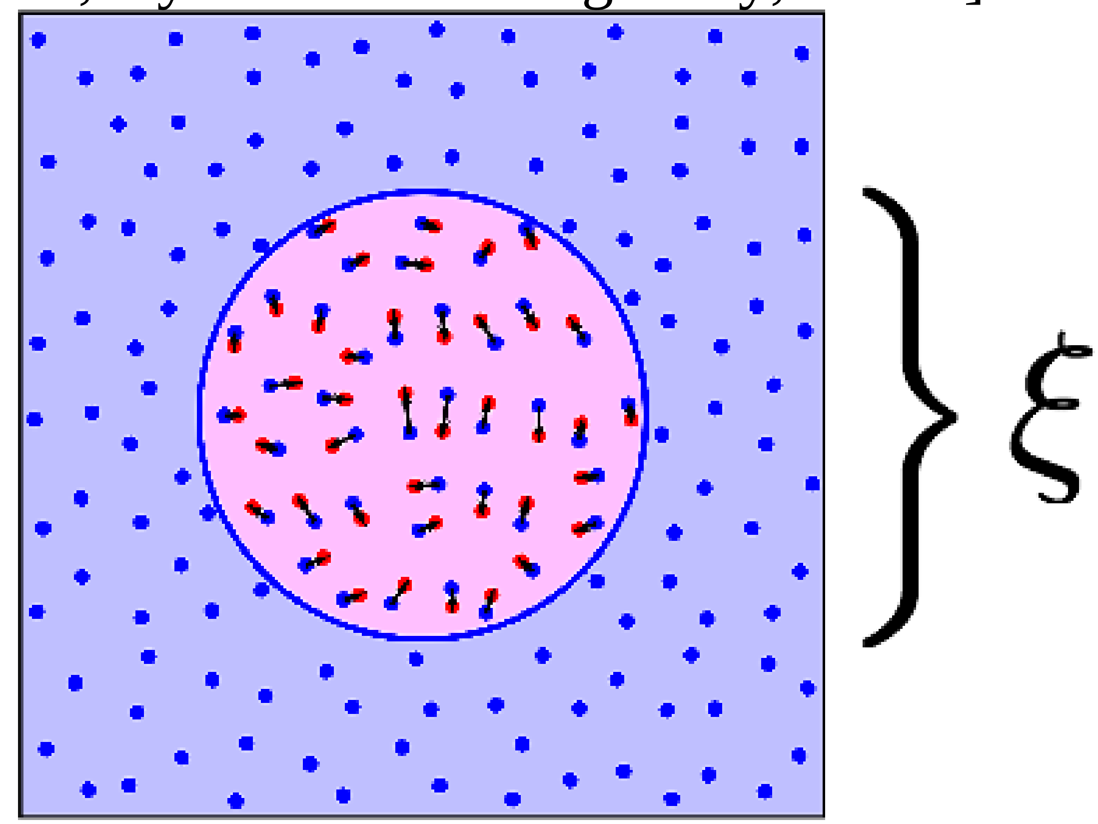
Energy landscape

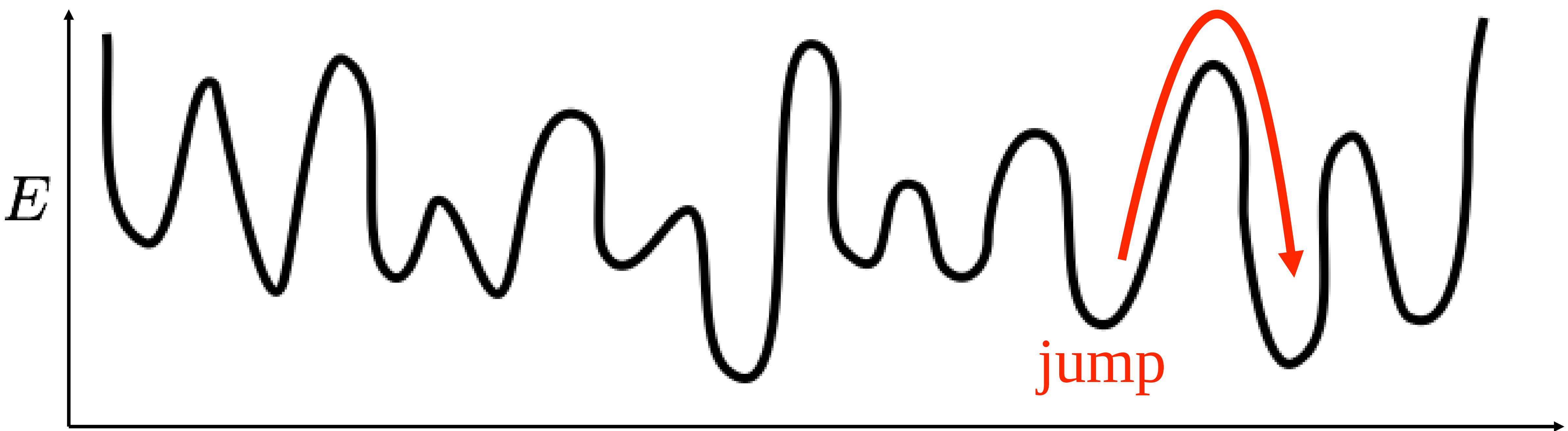
[Adam-Gibbs, 1965; Random First-Order Transition, 1989; Dynamical Heterogeneity, ~2000]

$$t \sim t_{\text{eq}}$$

$$\sim e^{\frac{E_{\text{act}}}{T}}$$

with $E_{\text{act}} \propto \xi^p$





configuration $\mathbf{X} = \{\mathbf{x}_i\}_{i=1,\ldots,N}$

Energy landscape

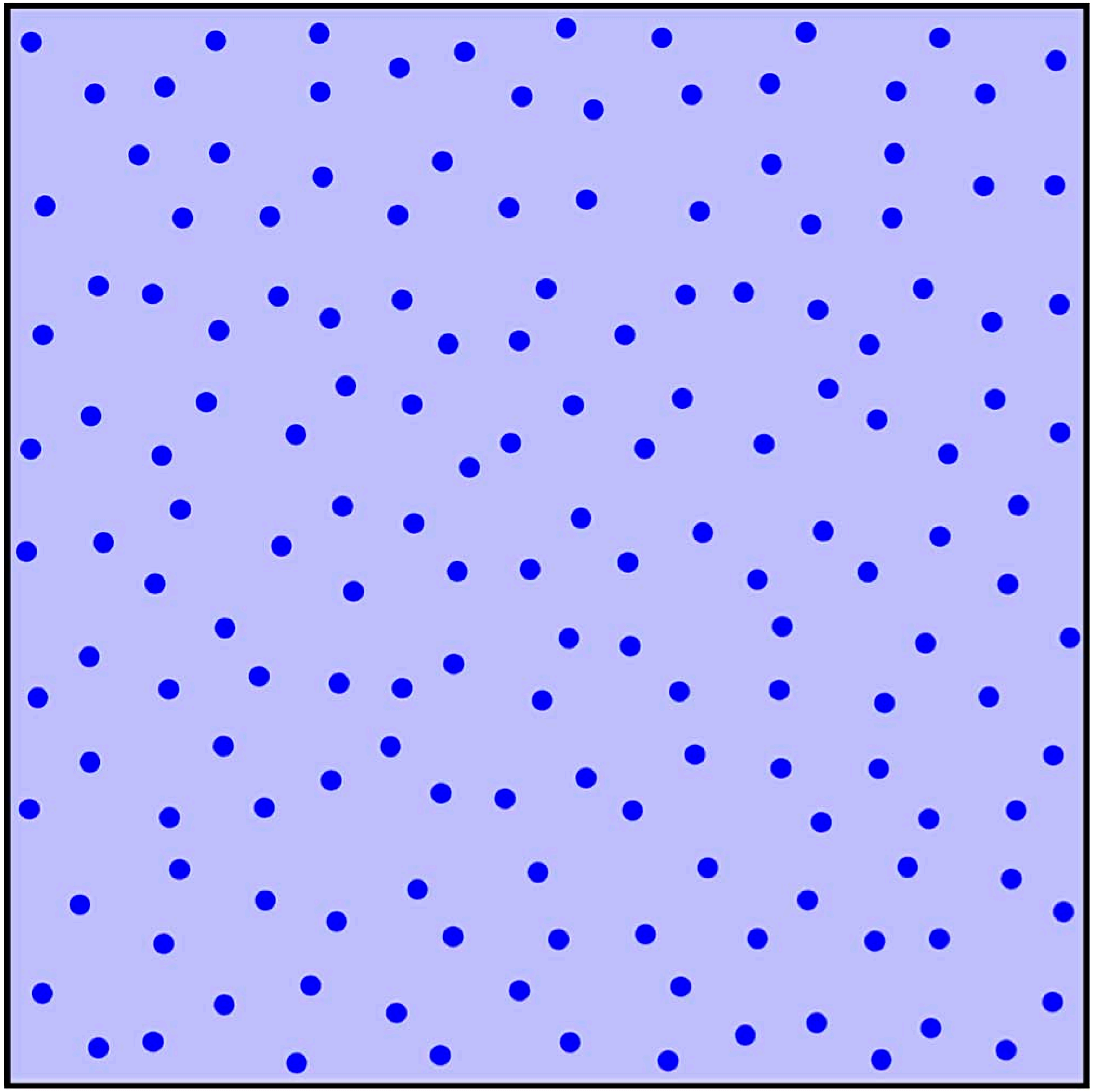
[Adam-Gibbs, 1965; Random First-Order Transition, 1989; Dynamical Heterogeneity, ~2000]

How do we make all this precise?

Point-to-set correlations!!!

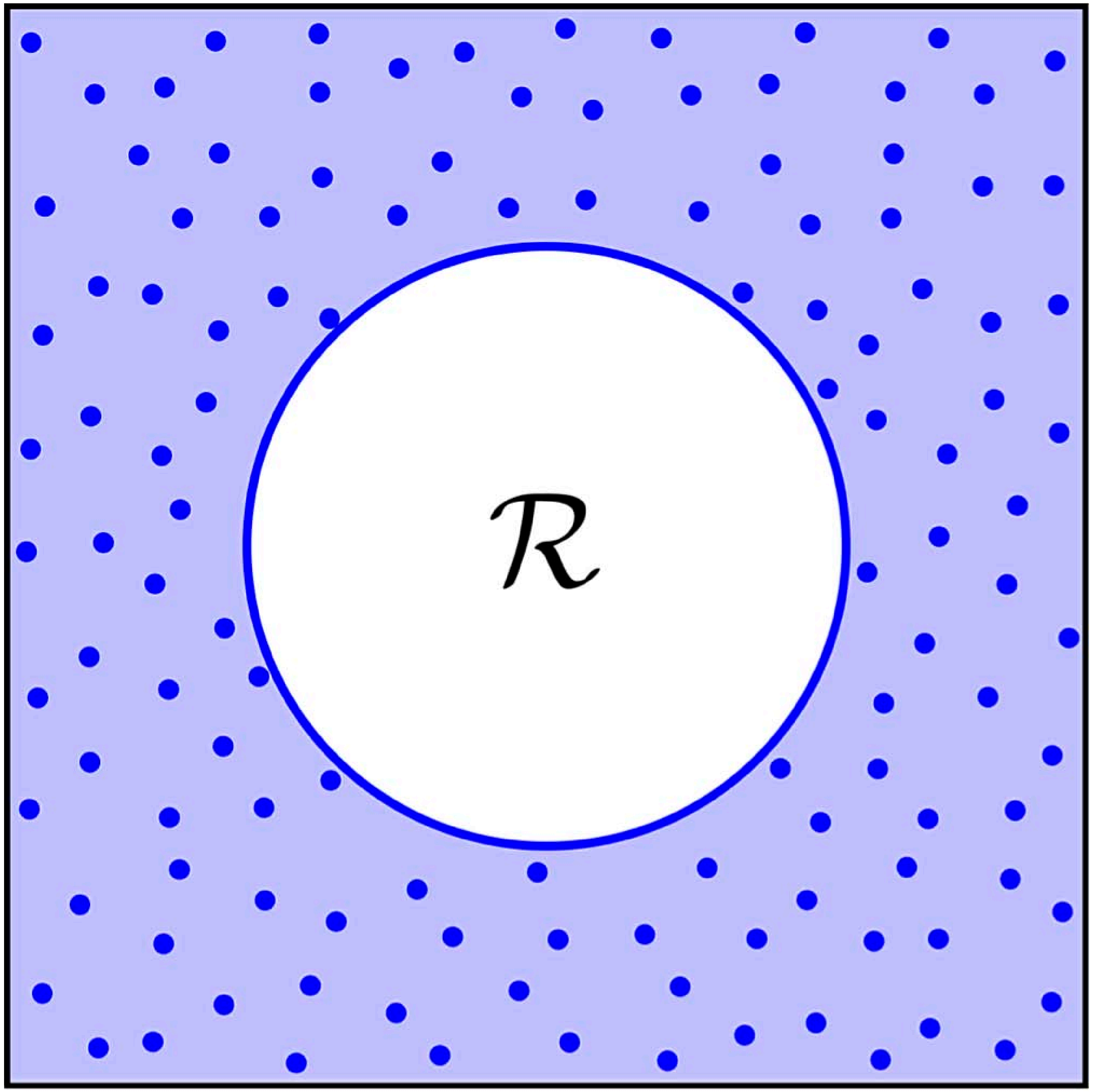
[Biroli-Bouchaud, 2004]
[Montanari-Semerjian, 2006]

Point-to-set correlations



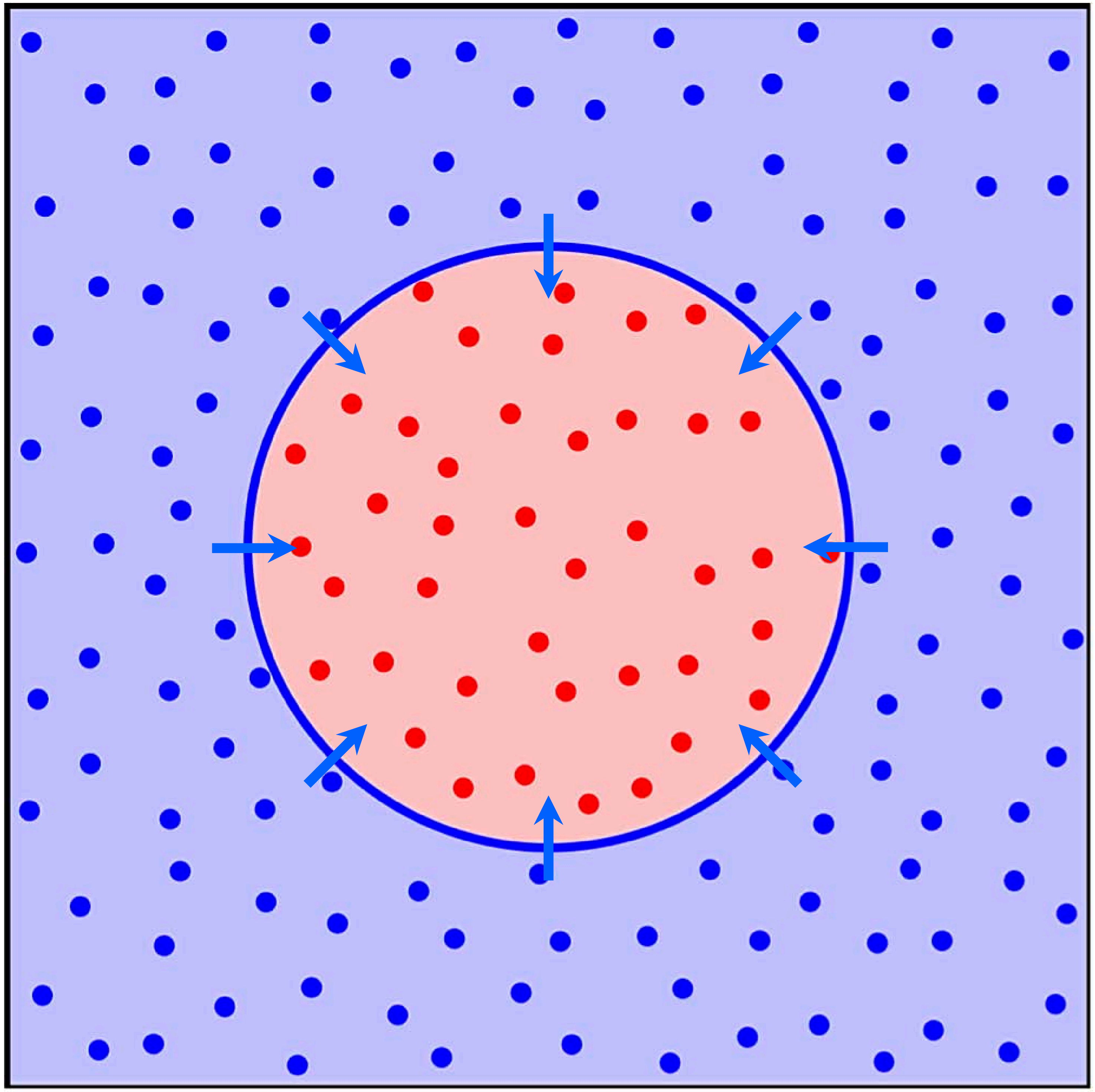
$$\mathbf{X}_1 = \{\mathbf{x}_i\}_{i=1,\ldots,N}$$

Point-to-set correlations



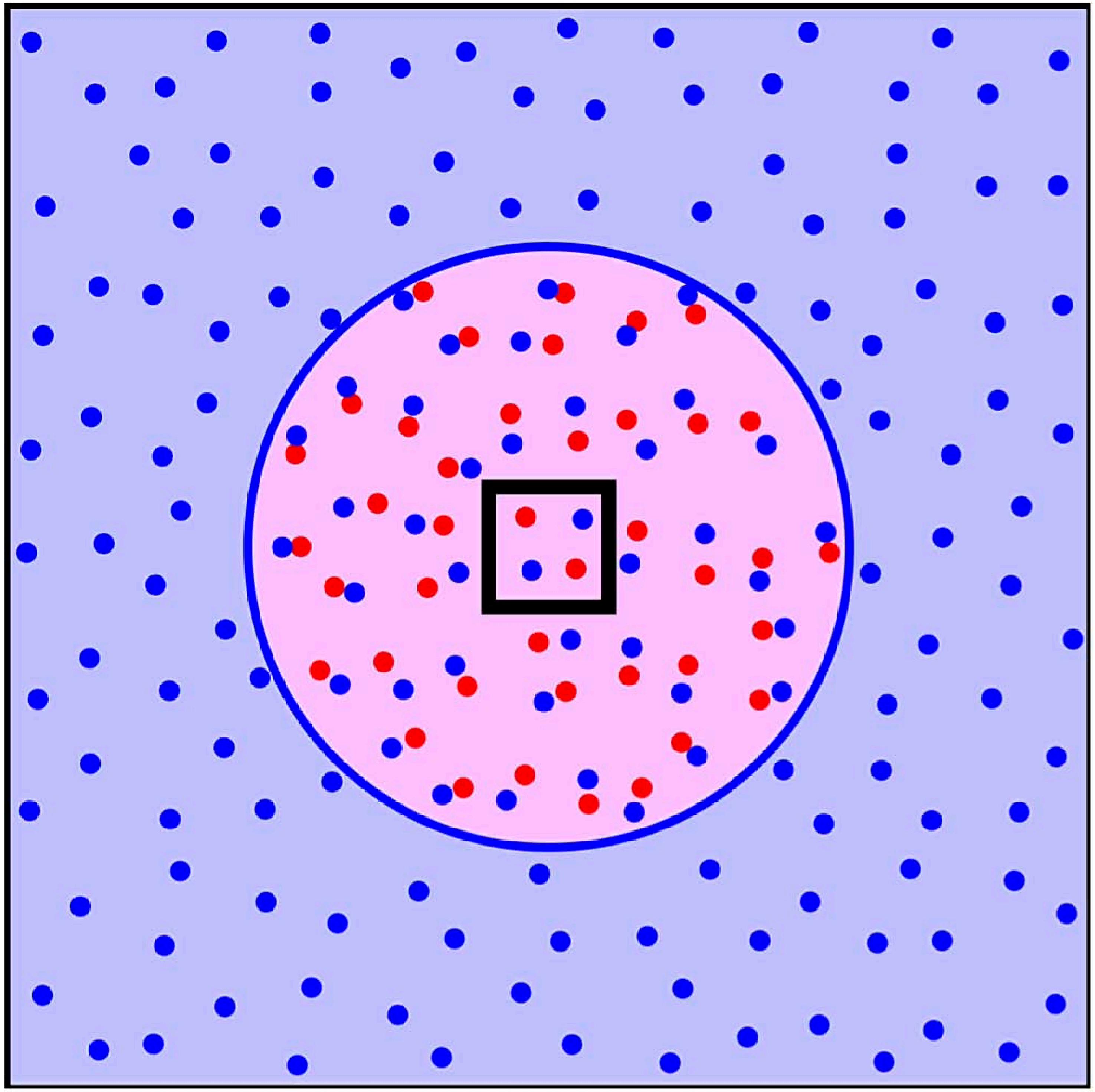
$\mathbf{X}_1^{\mathrm{out}}$

Point-to-set correlations



$$\mathbf{X}_2 = \mathbf{X}_1^{\mathrm{out}} + \mathbf{X}_2^{\mathrm{in}}$$

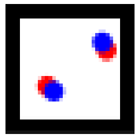
Point-to-set correlations

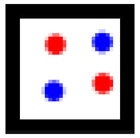


How similar $\mathbf{X}_1$ and $\mathbf{X}_2$?

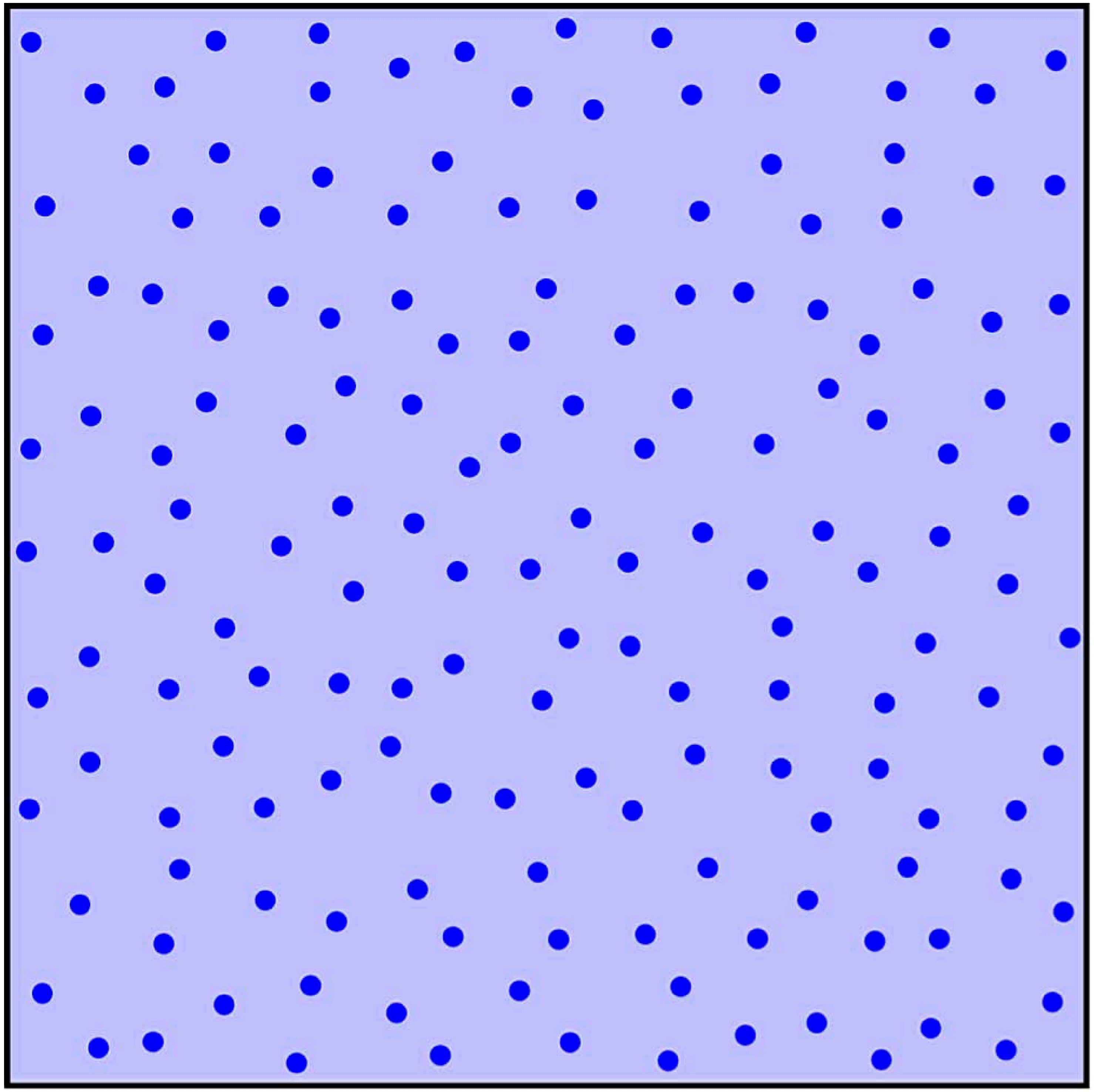
Overlap

$\hat{q}_{12}$


similar $q \sim 1$

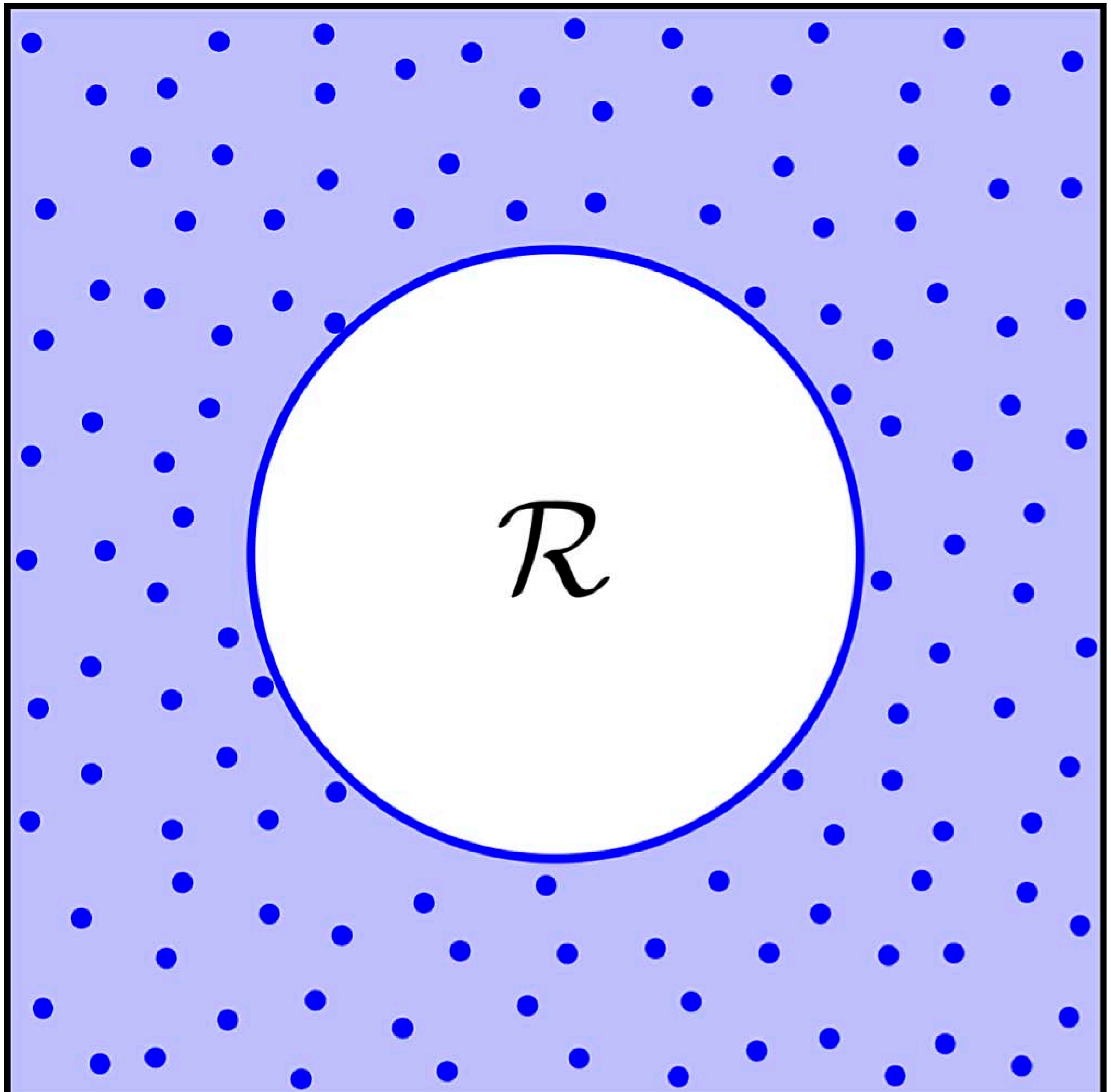

dissimilar $q \sim 0$

Point-to-set correlations



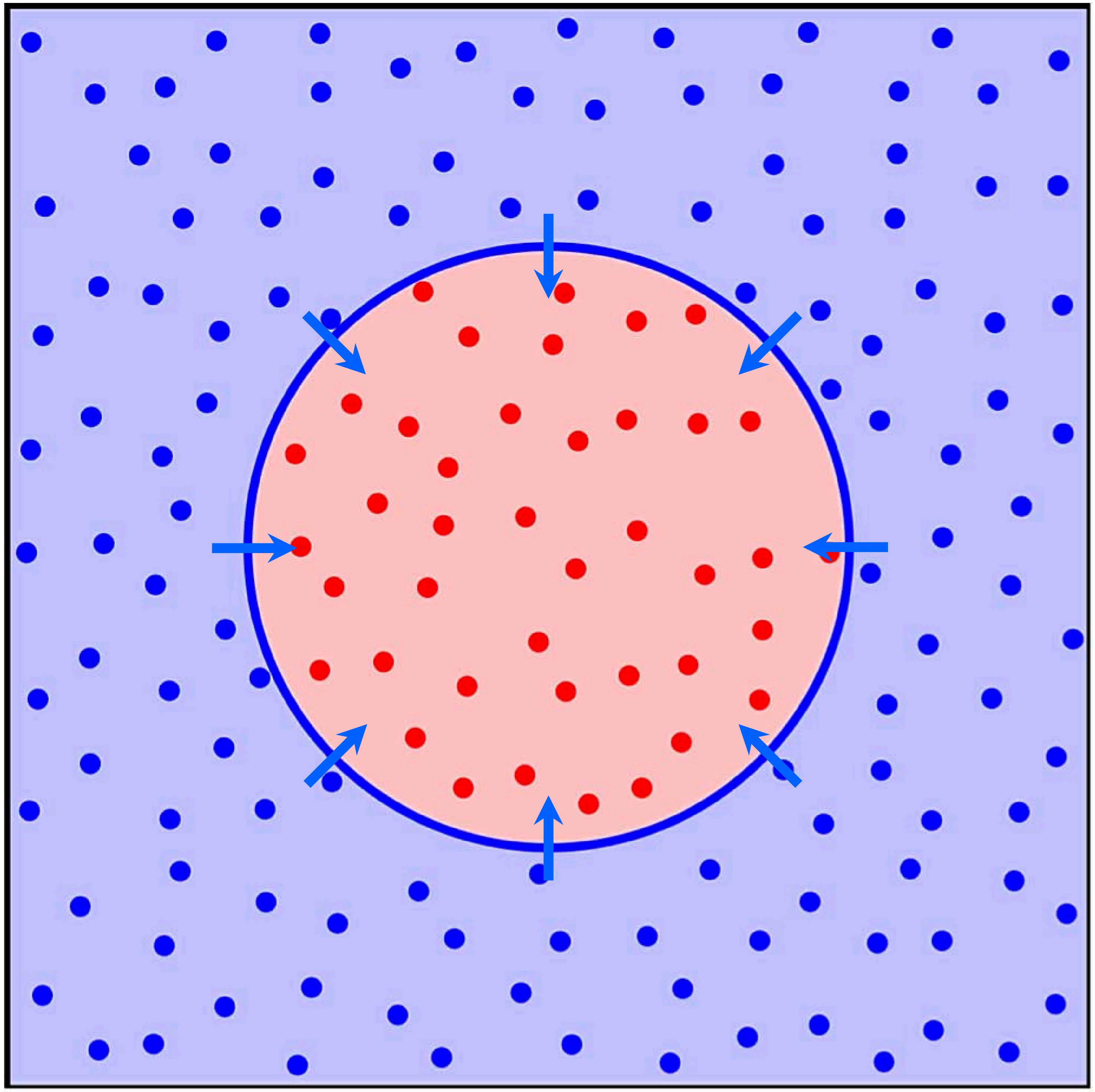
$$\mathbf{X}_1 = \{\mathbf{x}_i\}_{i=1,\ldots,N}$$

Point-to-set correlations



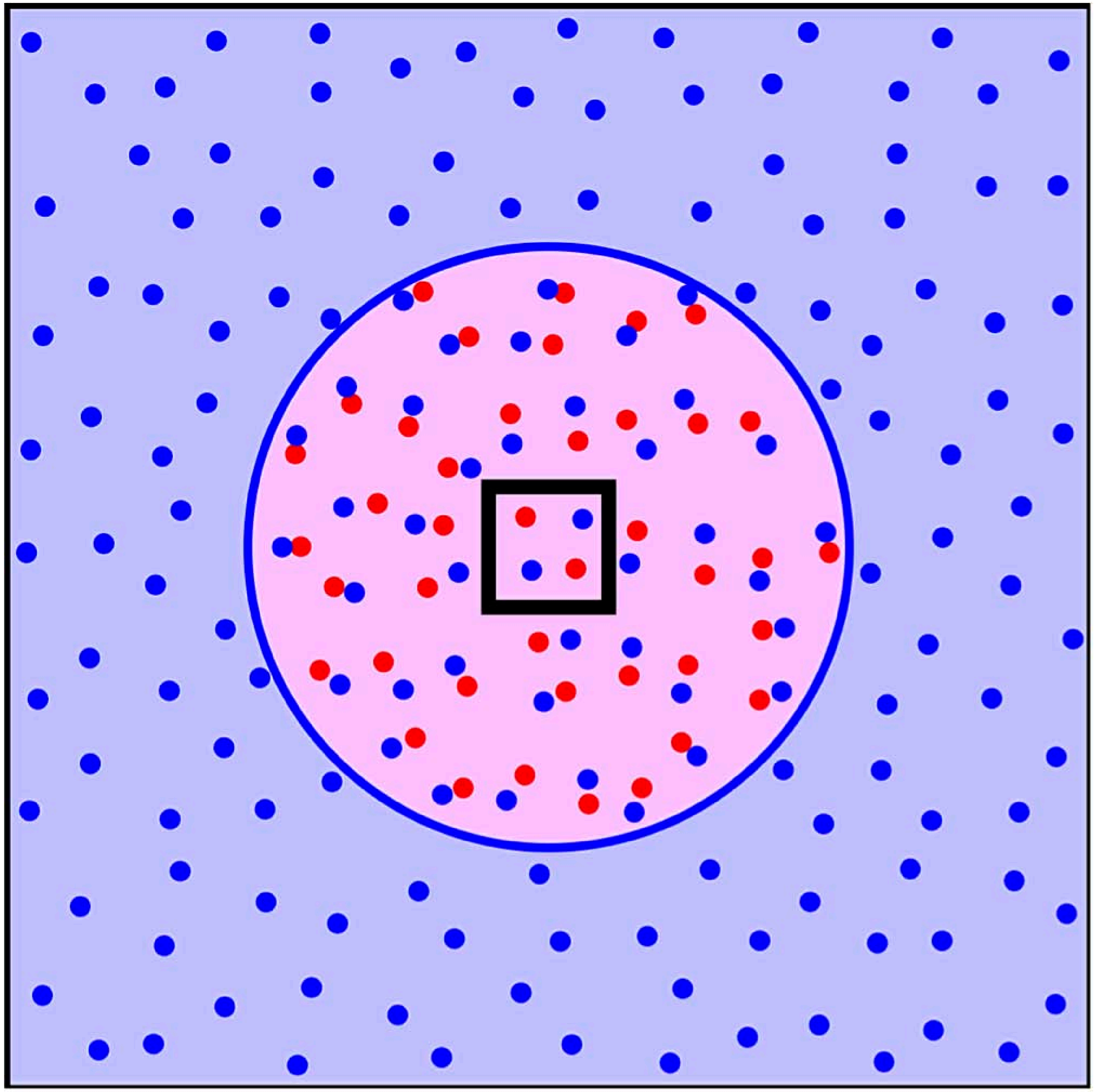
$\mathbf{X}_1^{\text{out}}$

Point-to-set correlations



$$\mathbf{X}_2 = \mathbf{X}_1^{\text{out}} + \mathbf{X}_2^{\text{in}}$$

Point-to-set correlations



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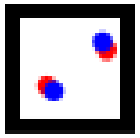
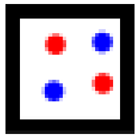
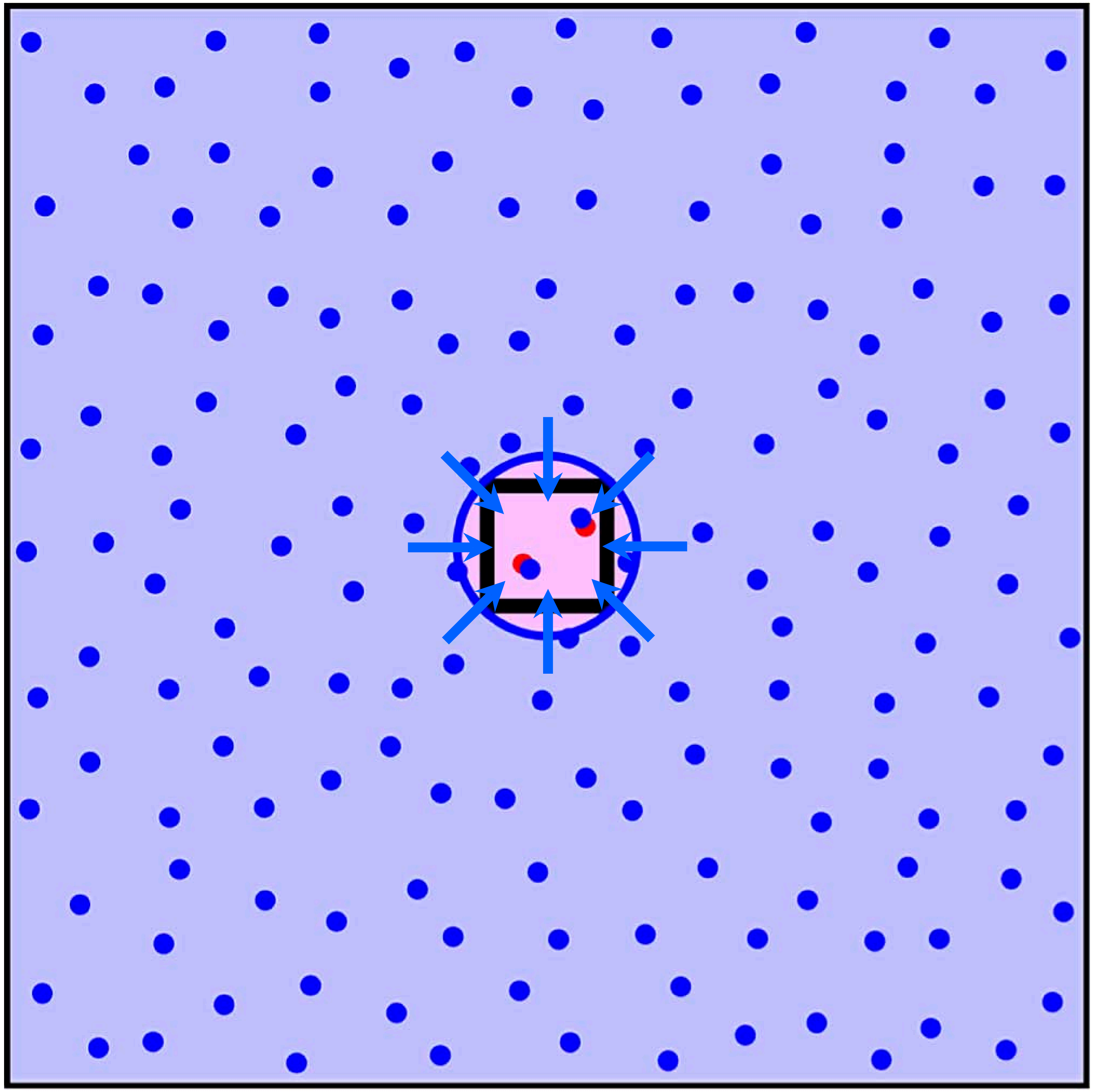


similar $q \sim 1$

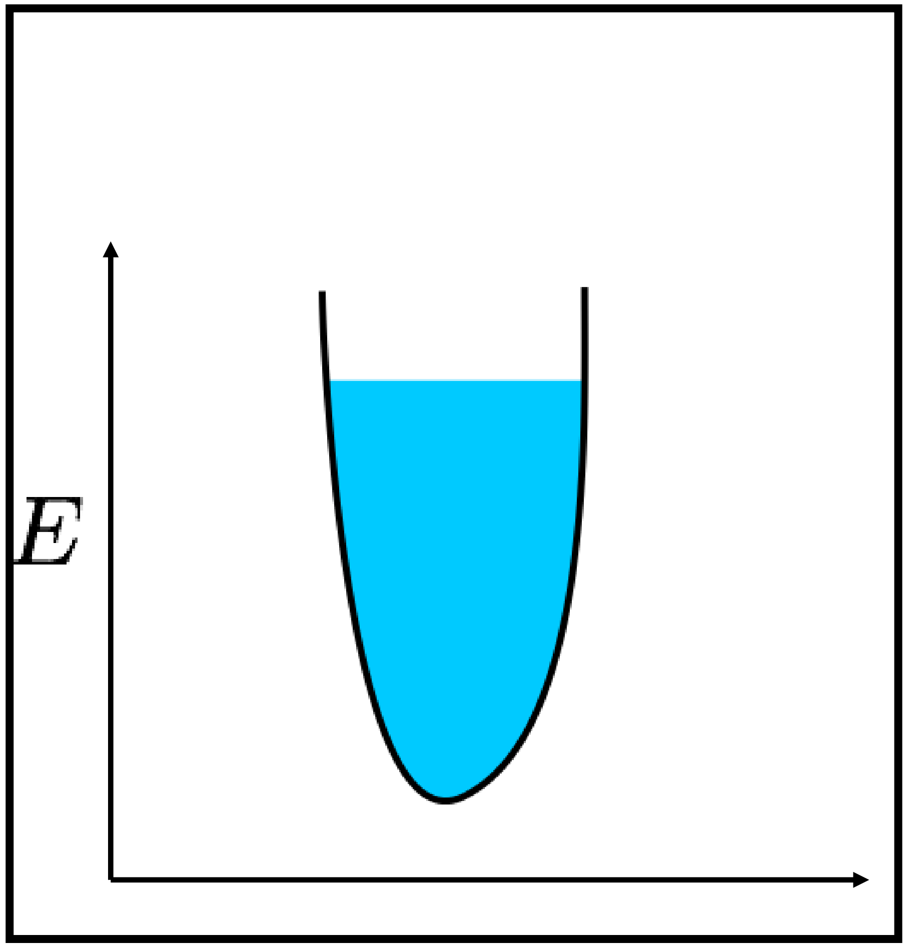


dissimilar $q \sim 0$

Local free-energy landscape



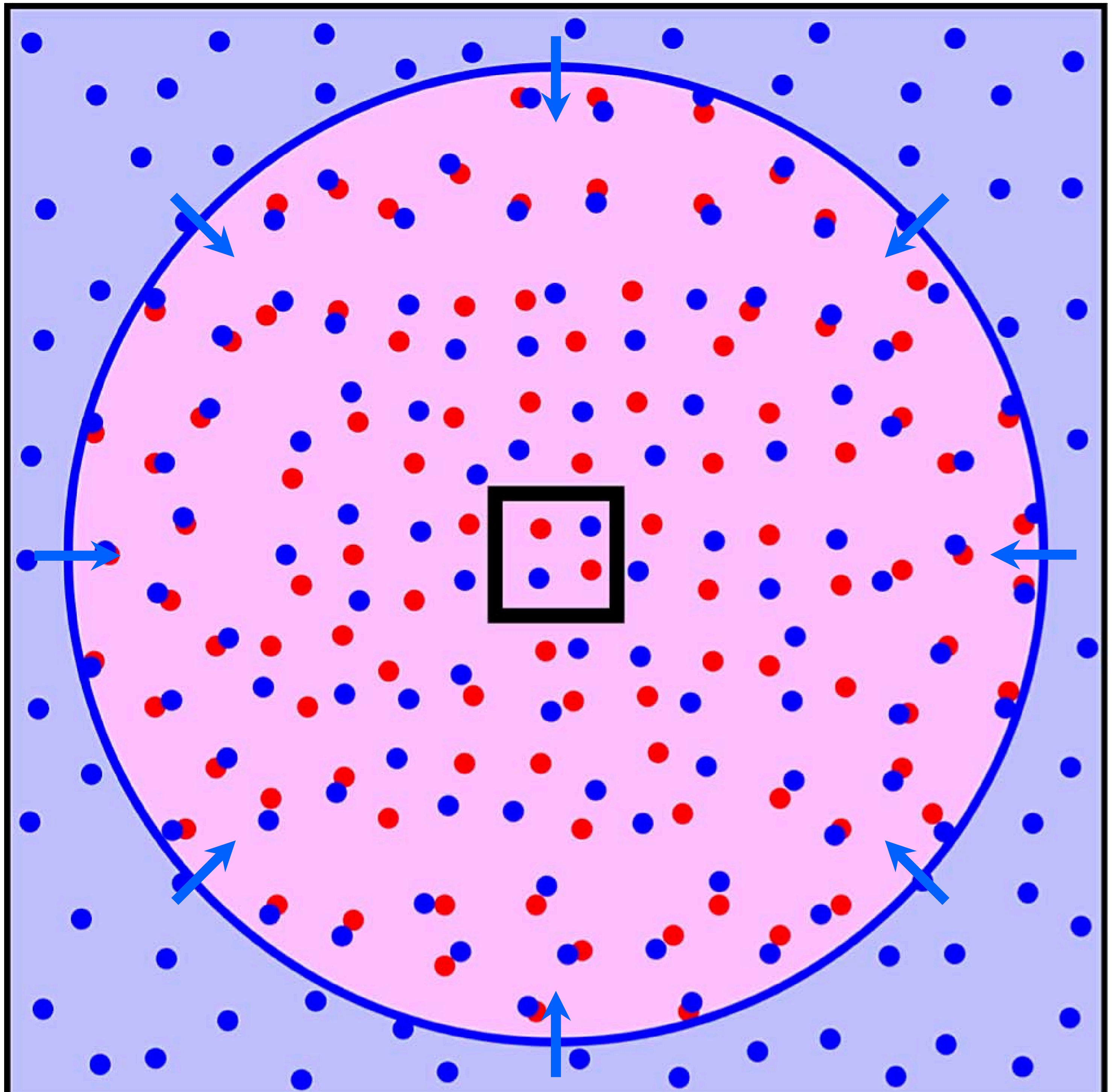
$\mathcal{R}$ small



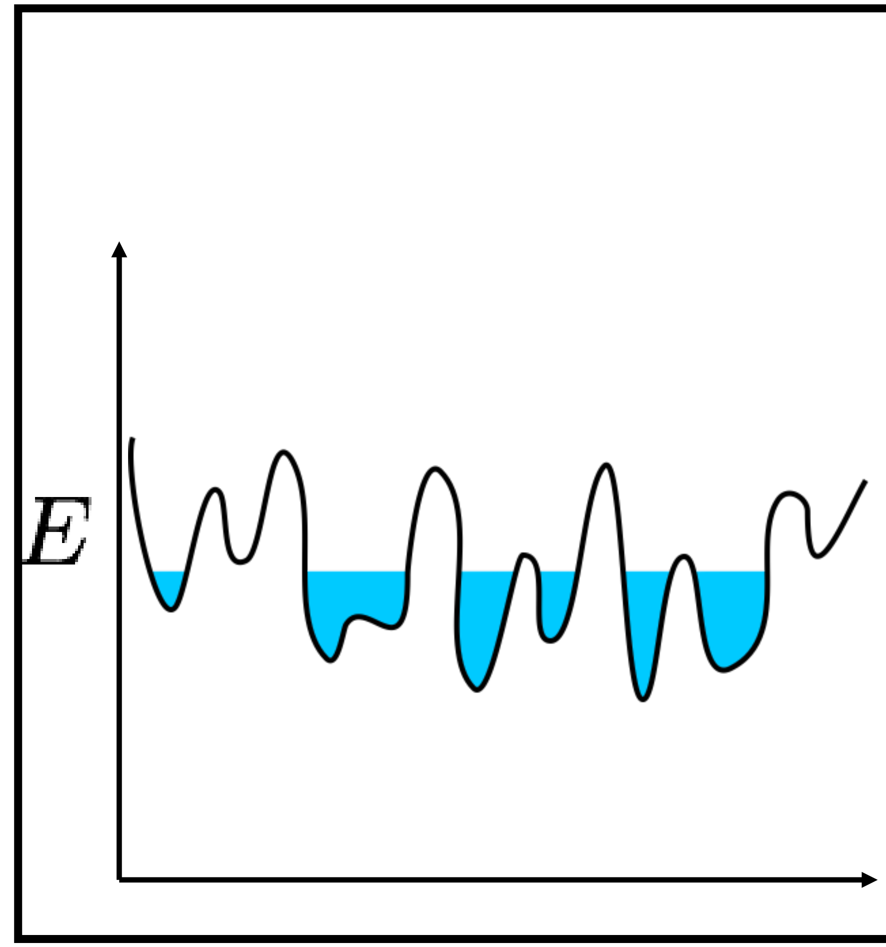
Overlap: High

$$\hat{q}_{12} \sim 1$$

Local free-energy landscape



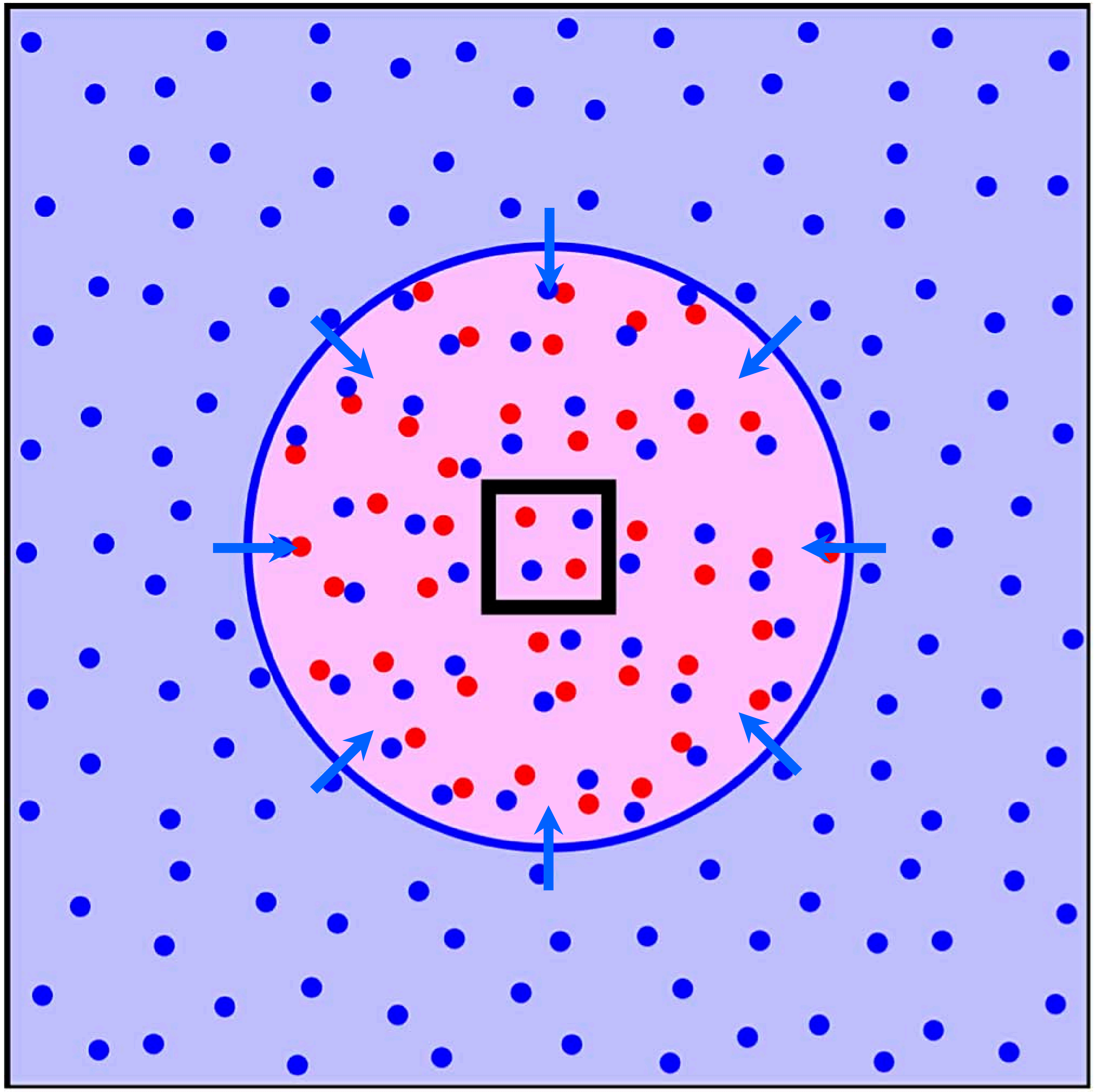
$\mathcal{R}$ big

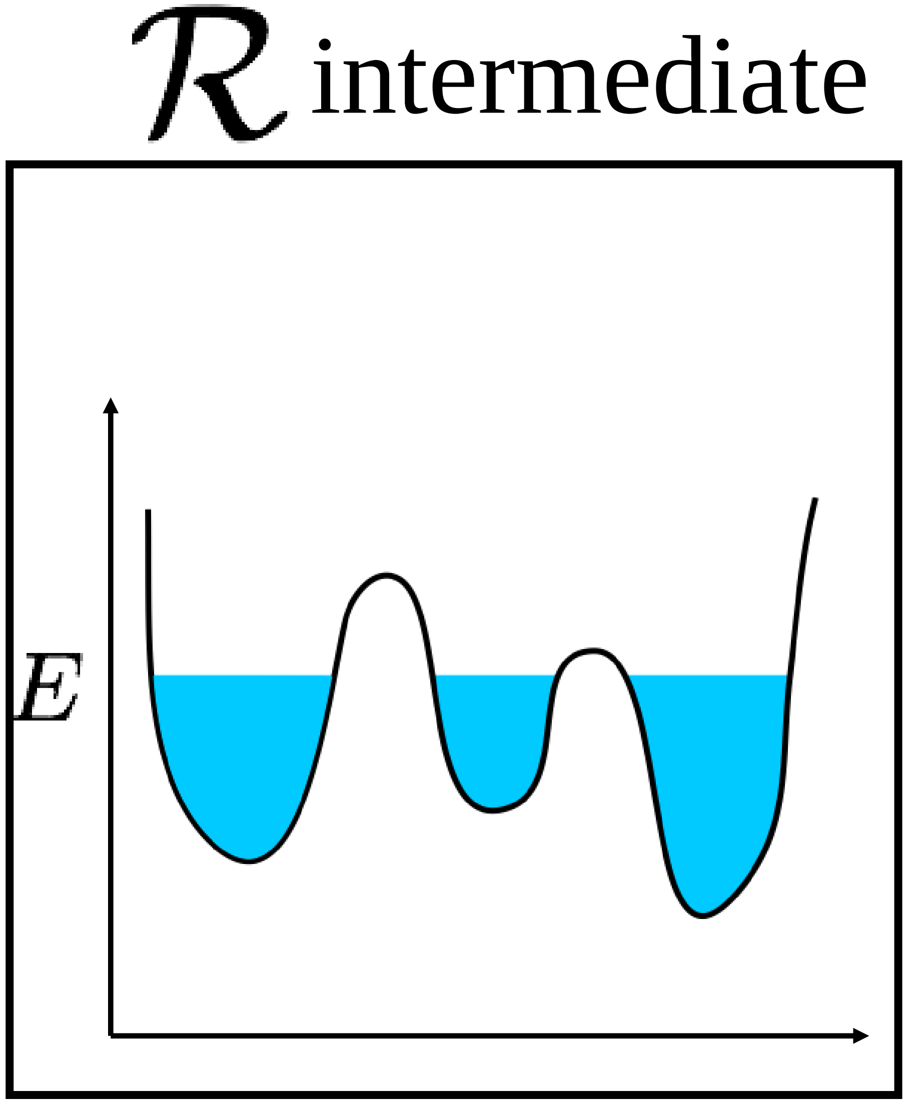


Overlap: Low

$$\hat{q}_{12} \sim 0$$

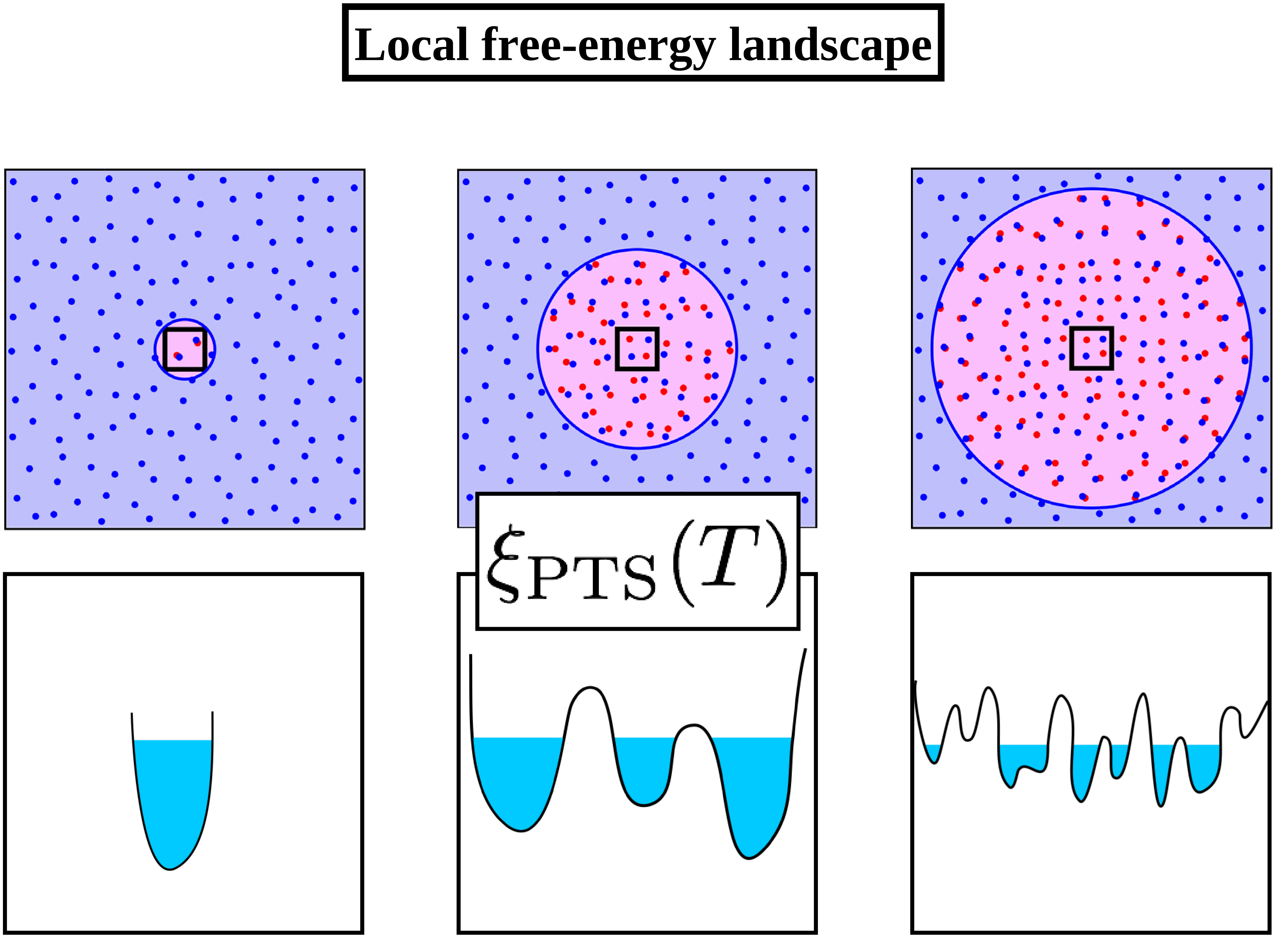
Local free-energy landscape



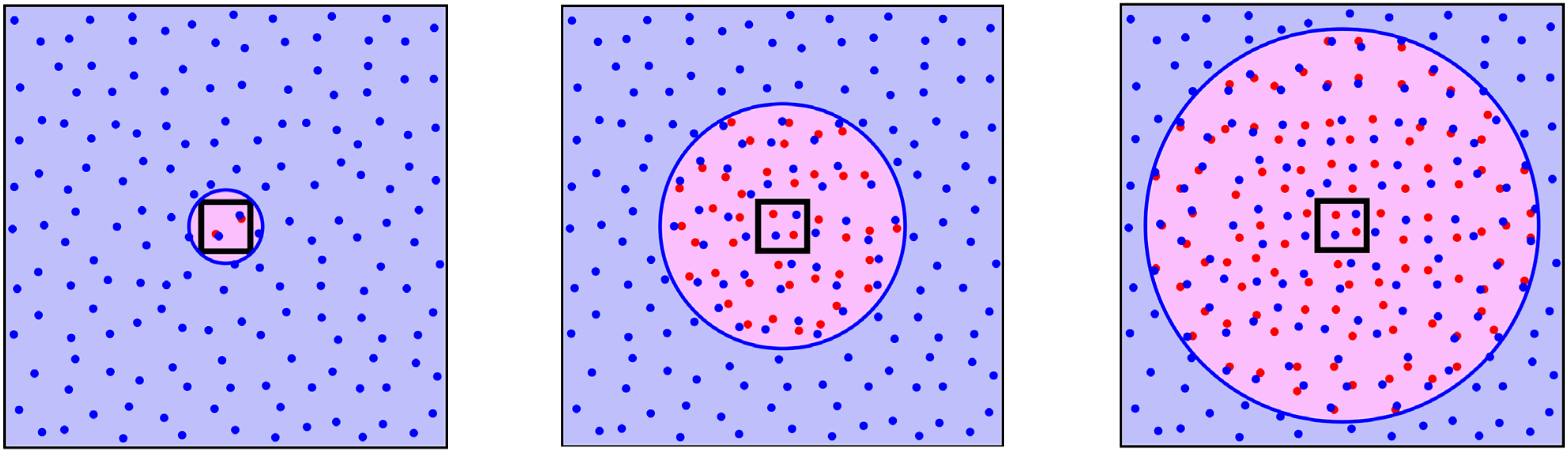


Overlap: Medium

$\hat{q}_{12} \sim 0.5$


Local free-energy landscape
$\xi_{\rm PTS}(T)$

Local free-energy landscape



Is this real?

Can we "see" it?

→ **Simulations!**

Measuring point-to-set

No reliable measurements for a decade...

2 obstacles:

glassy slowdown $t_{\mathrm{eq}} \sim e^{\xi^p}$ → long computational time

confining cavity → even slower...

Measuring point-to-set

Parallel-tempering

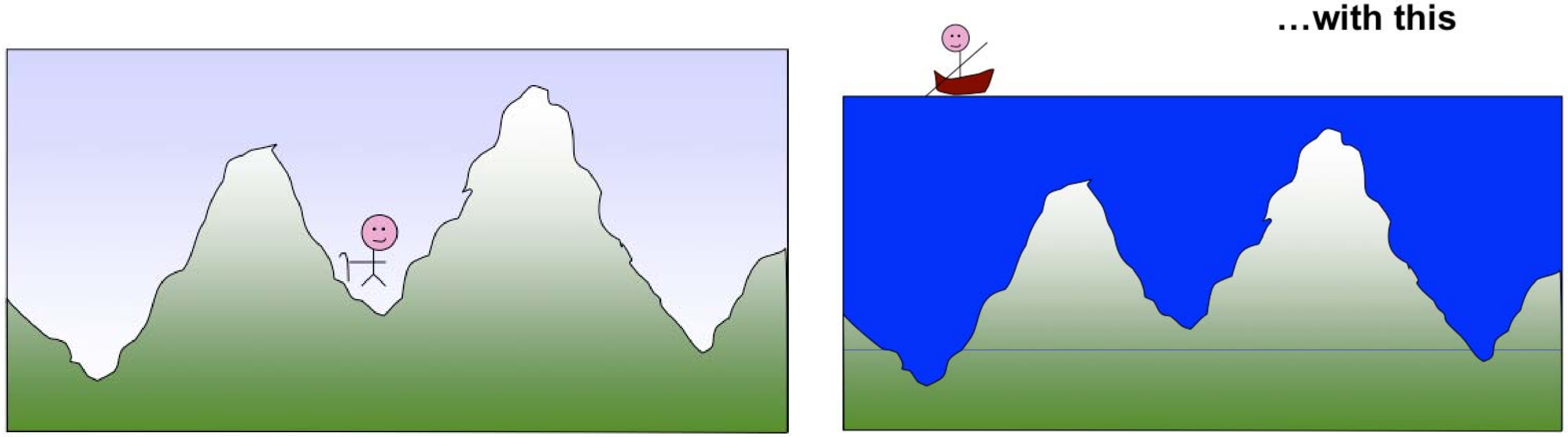


Figure credit: Daan Frenkel

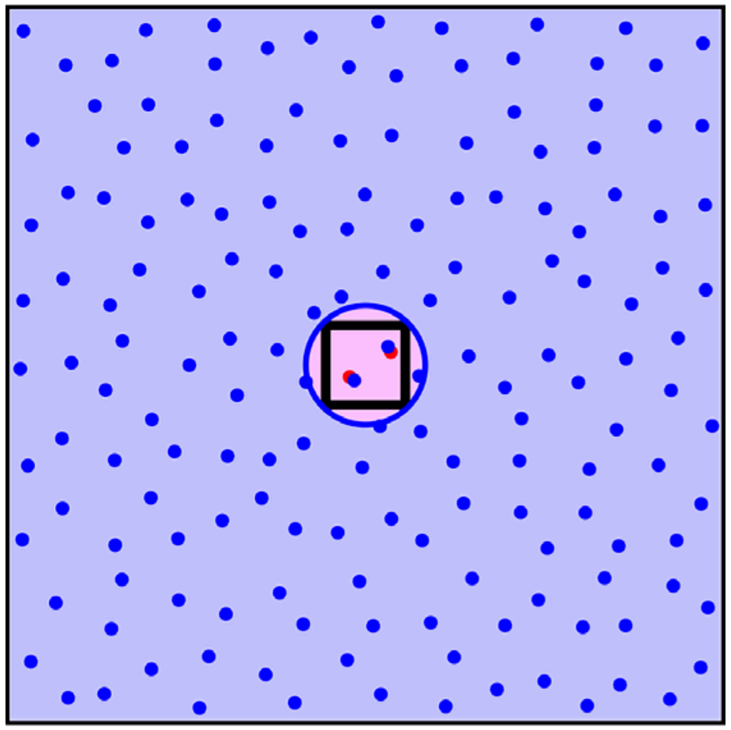
2 obstacles:

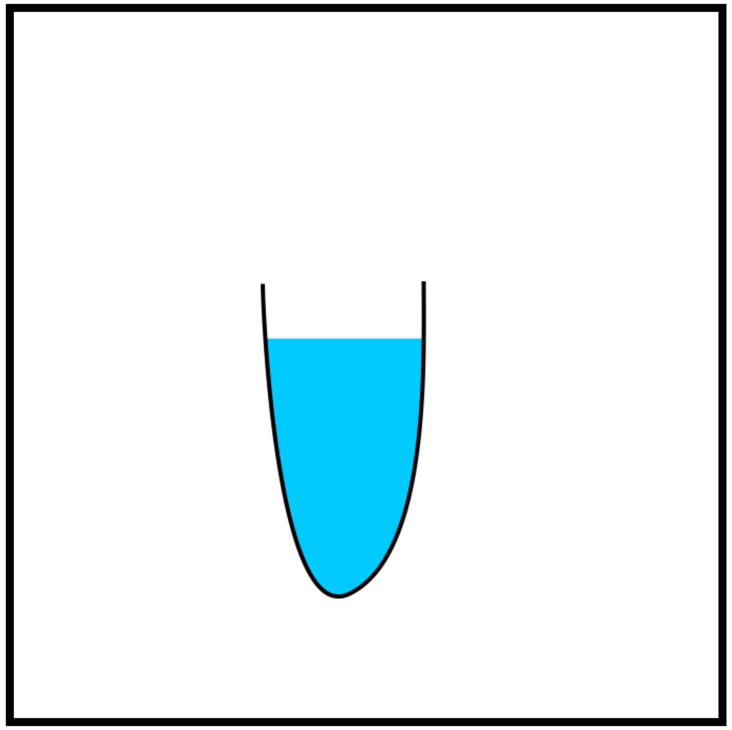
glassy slowdown $t_{\mathrm{eq}} \sim e^{\xi^p}$ → long computational time

confining cavity → even slower...

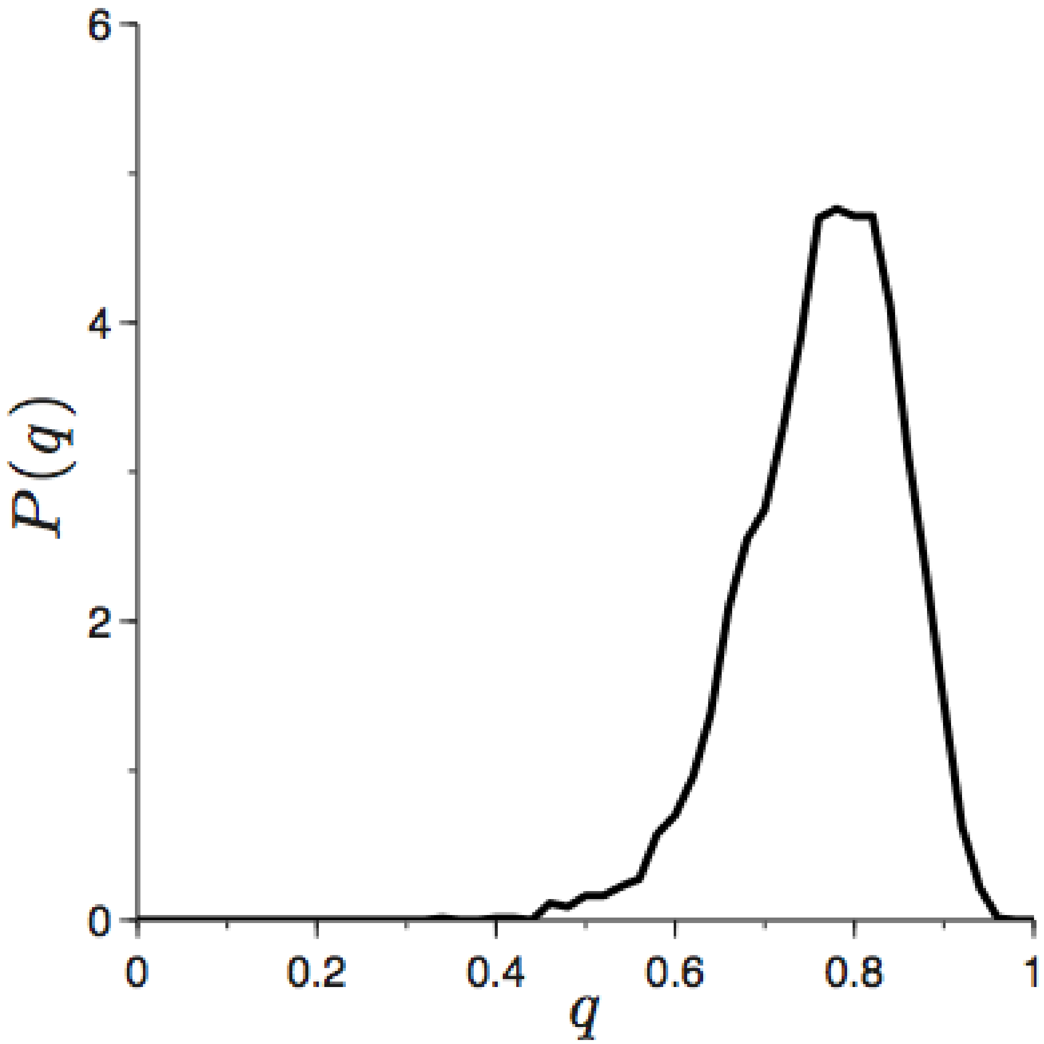
[Berthier-Charbonneau-Yaida, J. Chem. Phys. (2016)]

Seeing landscape





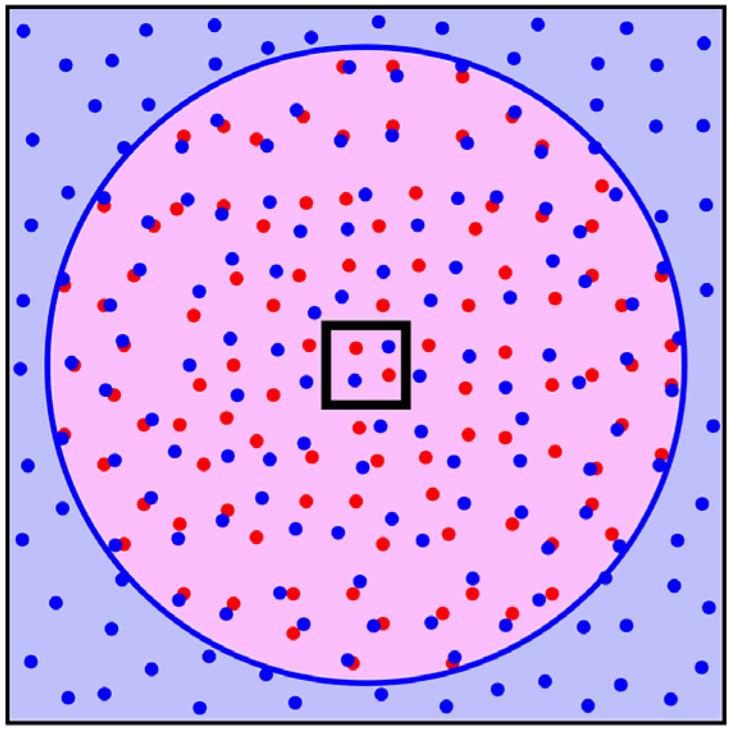
Binary Lennard-Jones liquid (Kob-Andersen @ $T = 0.51$)

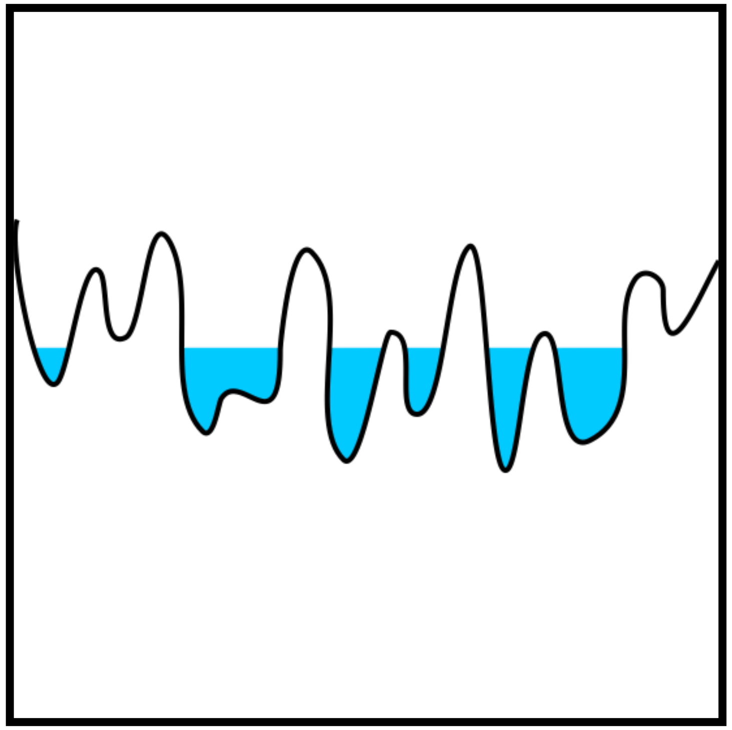


$$\mathcal{R} \ll \xi_{\mathrm{PTS}}$$

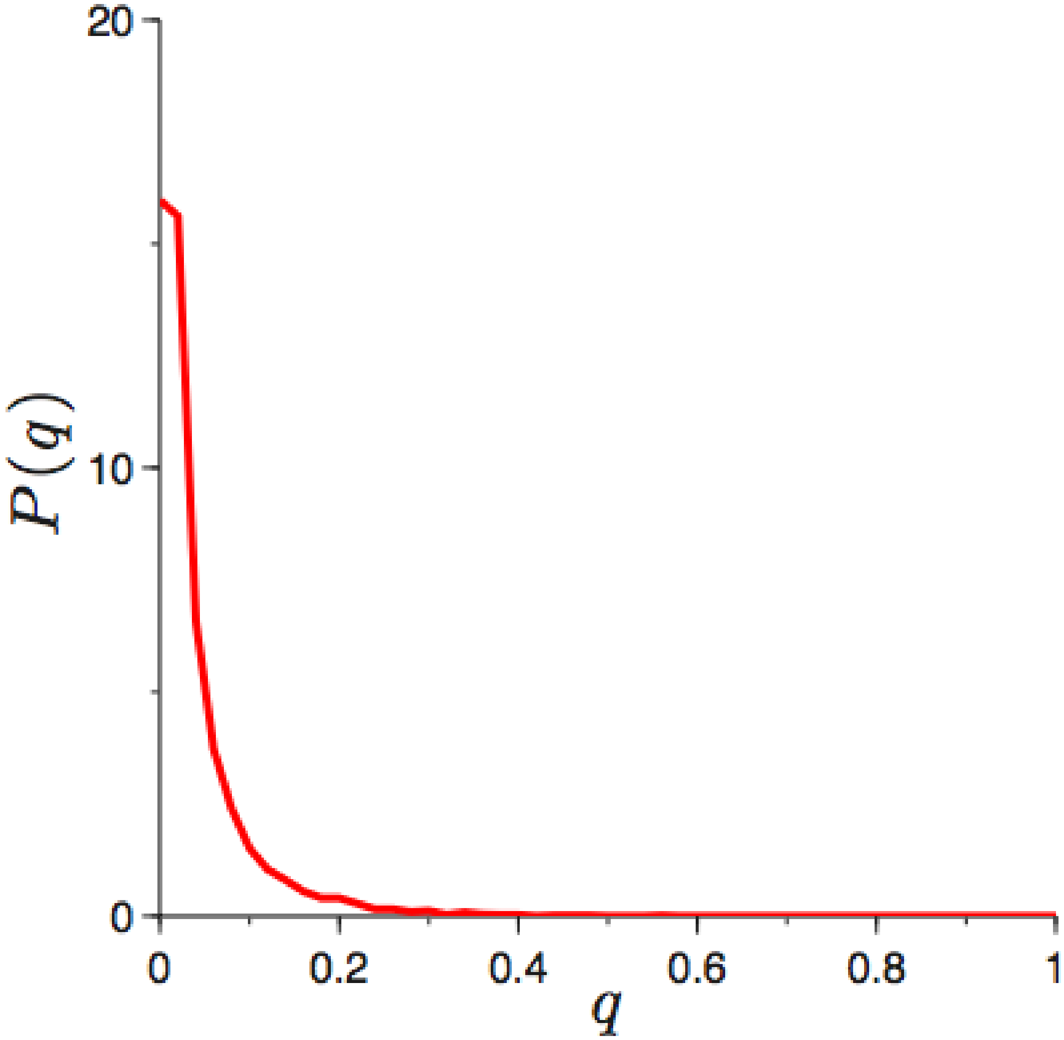
[Berthier-Charbonneau-Yaida, J. Chem. Phys. (2016)]

Seeing landscape





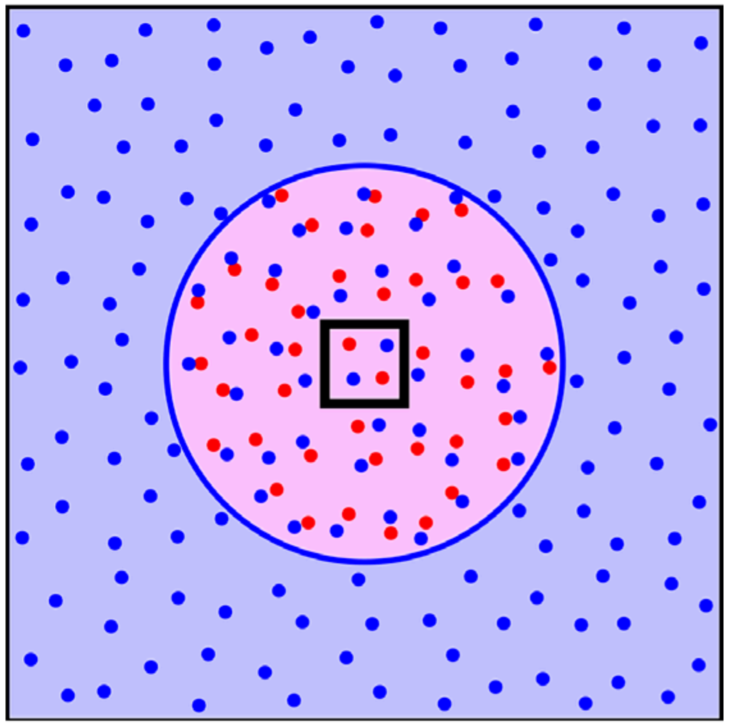
Binary Lennard-Jones liquid **(Kob-Andersen @ $T = 0.51$)**

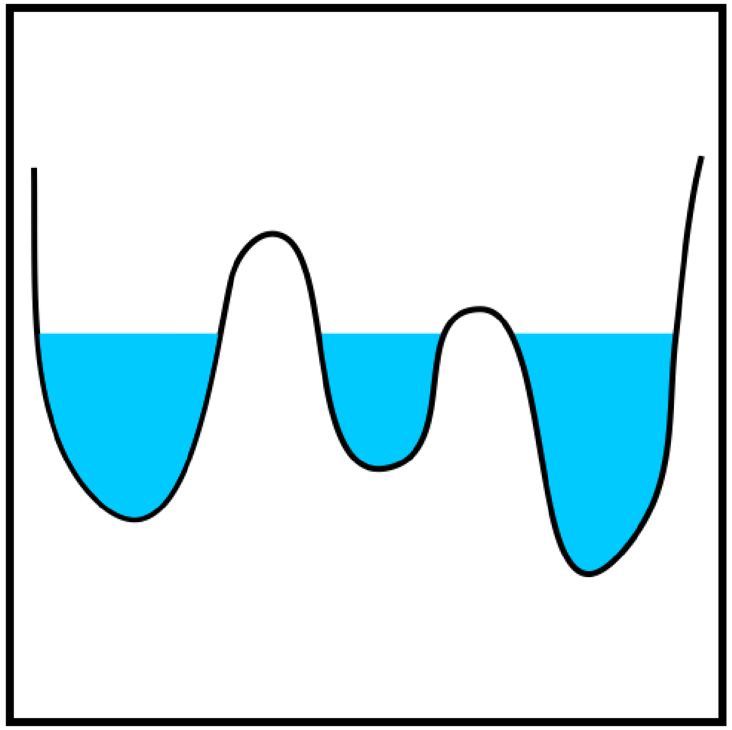


$$\mathcal{R} \gg \xi_{\text{PTS}}$$

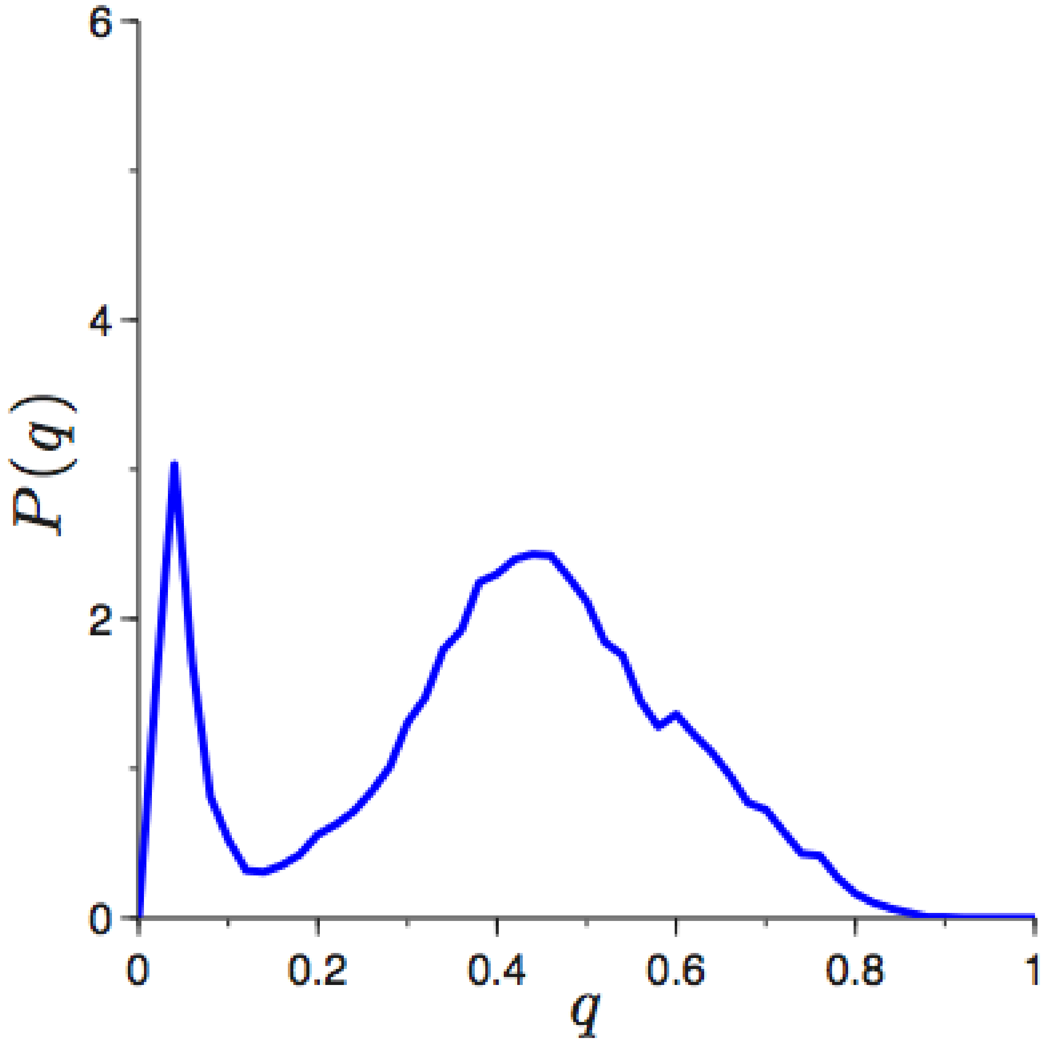
[Berthier-Charbonneau-Yaida, J. Chem. Phys. (2016)]

Seeing landscape





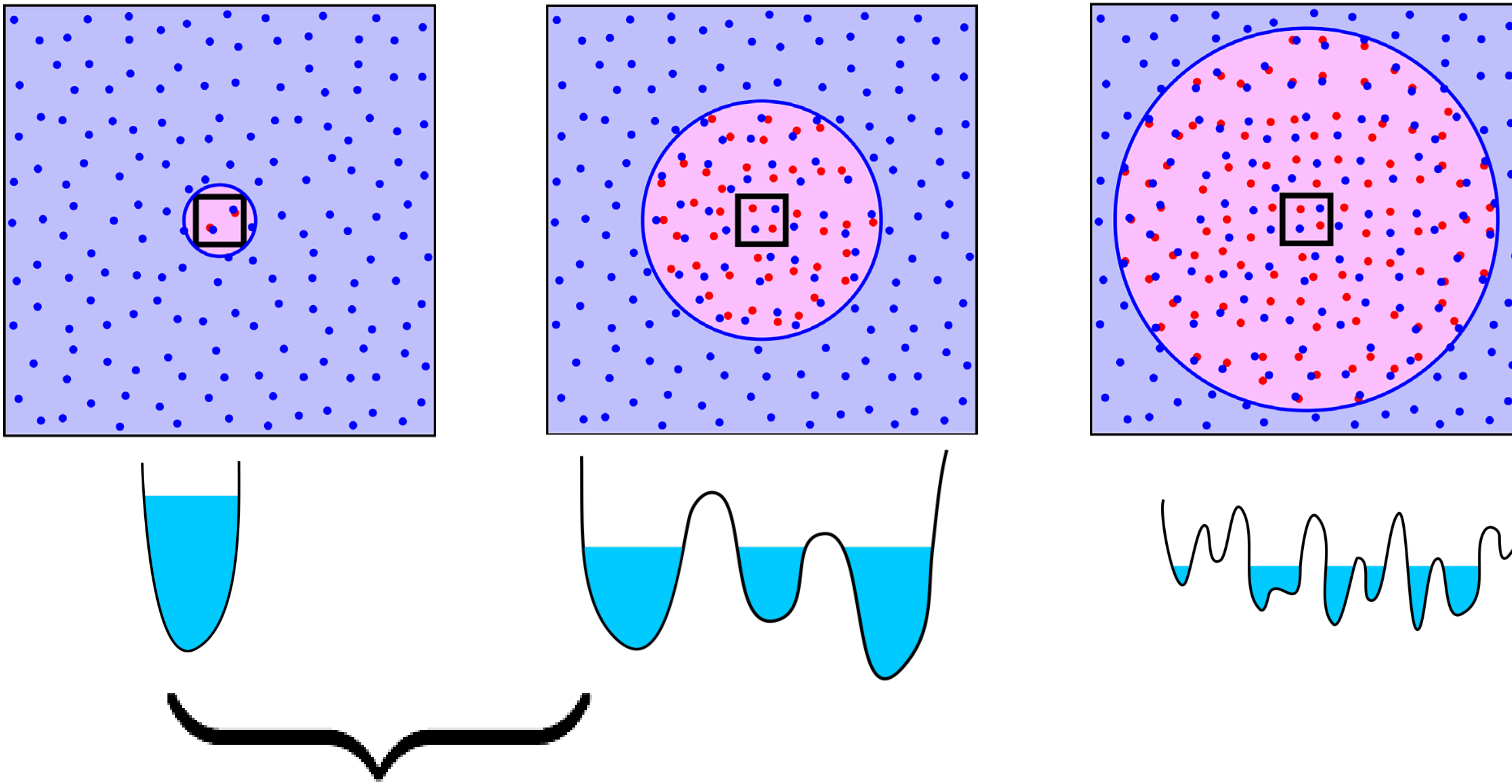
Binary Lennard-Jones liquid **(Kob-Andersen @ $T = 0.51$)**



$$\mathcal{R} \sim \xi_{\mathrm{PTS}}$$

[Berthier-Charbonneau-Yaida, J. Chem. Phys. (2016)]

Seeing landscape

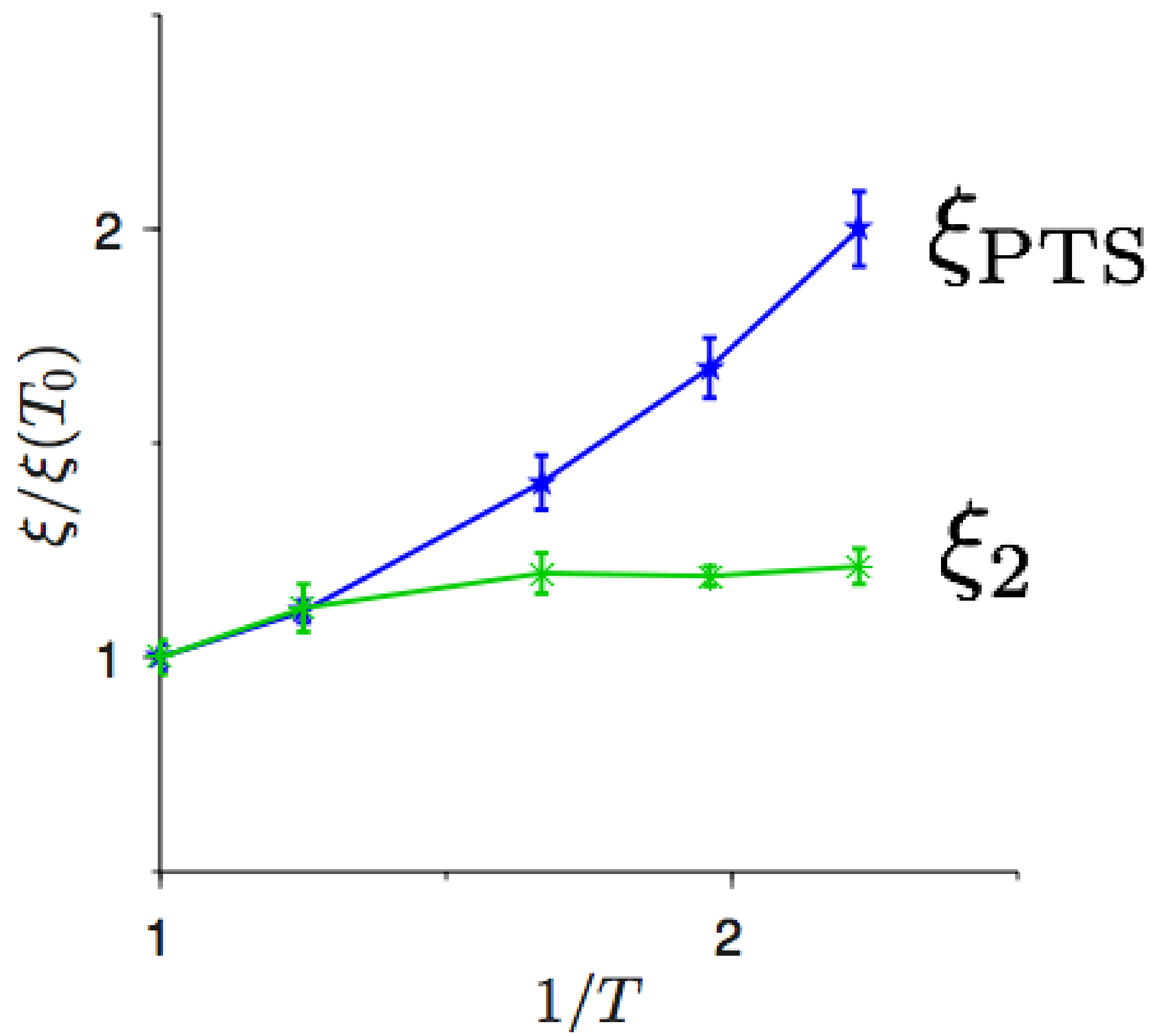


$\mathcal{R} \lesssim \xi_{\mathrm{PTS}}$ governed by **“amorphous order”**

[Berthier-Charbonneau-Yaida, J. Chem. Phys. (2016)]

Defining glassiness

Rarefaction of metastable states → $\dfrac{\xi_{\rm PTS}}{\xi_2} \nearrow$ → **defines glassiness!**

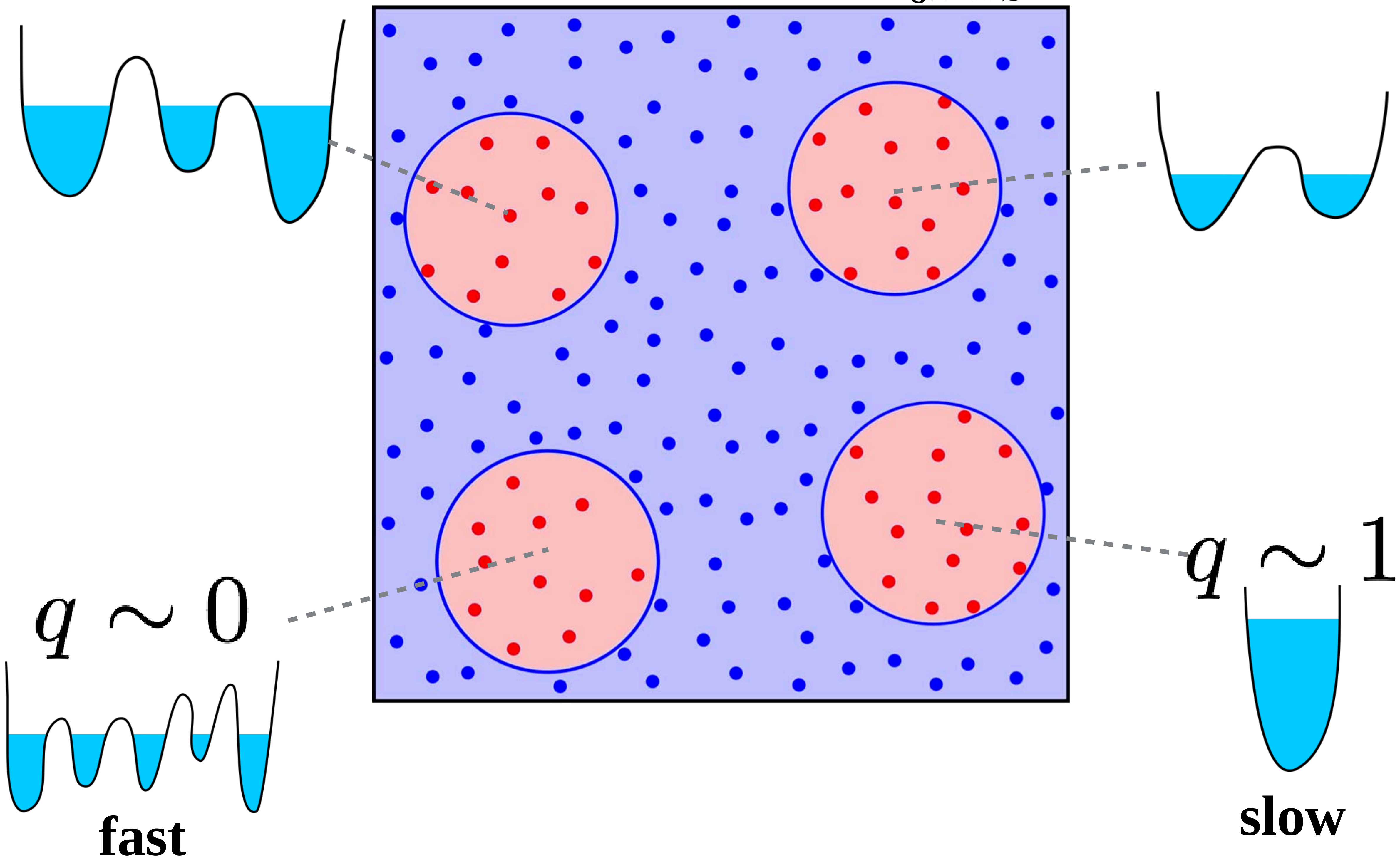


as $\eta \nearrow\nearrow$

[Yaida-Berthier-Charbonneau-Tarjus, Phys. Rev. E (2016)]

Statics and dynamics

Probe with $\mathcal{R} = \xi_{\mathrm{PTS}}$



[Hocky *et al.*, PRL (2014)]

[Charbonneau-Dyer-Lee-Yaida, JSTAT (2016)]

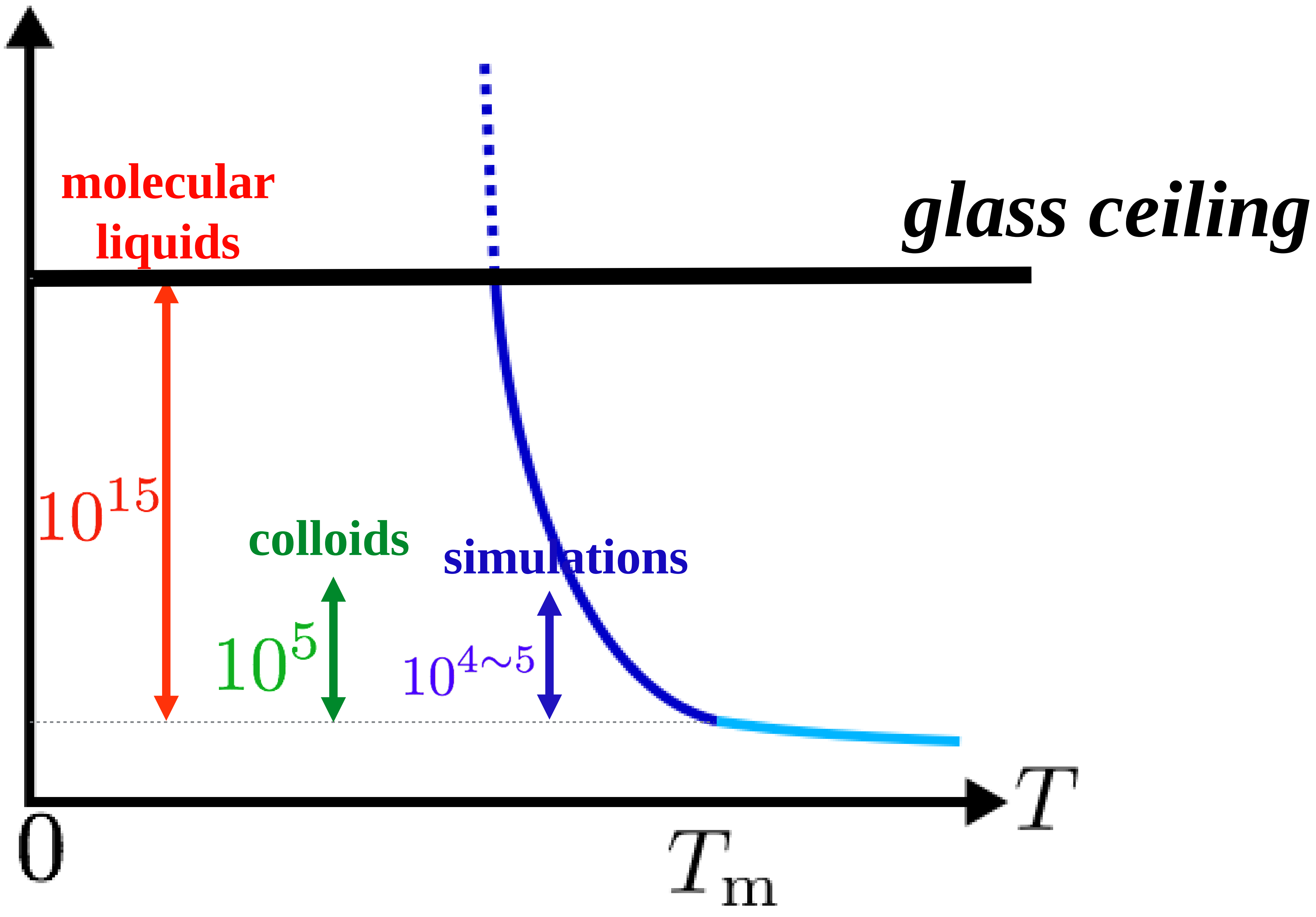
Rarefaction of metastable states in a complex landscape

↓ point-to-set correlations

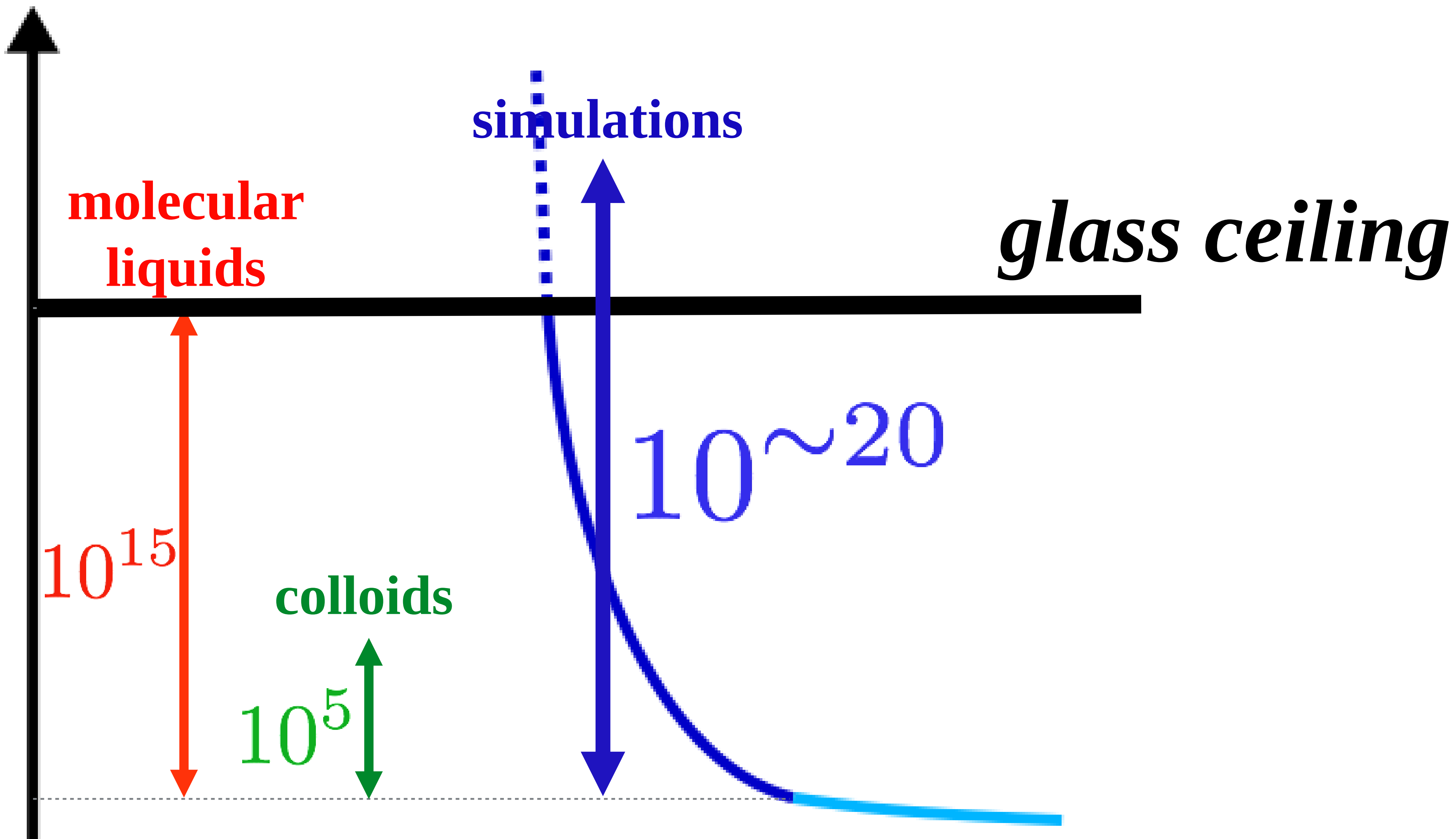
Dramatic slowdown of glassy systems

3 Beyond the glass ceiling

Breaking the glass ceiling

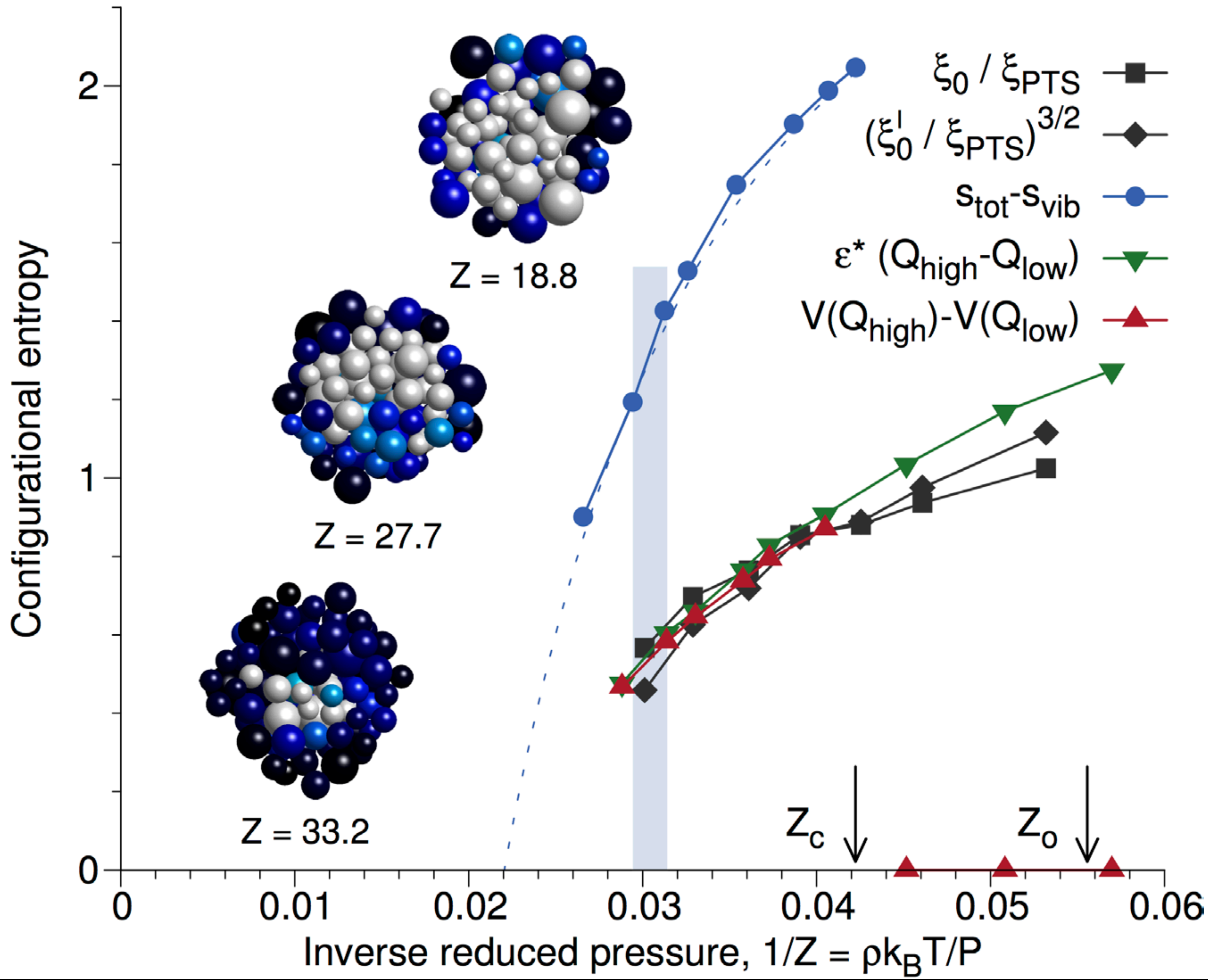


Breaking the glass ceiling



Tuning both algorithm AND system WHILE also retaining glassy physics

Breaking the glass ceiling



Rarefaction of metastable states **keeps driving** glassy slowdown

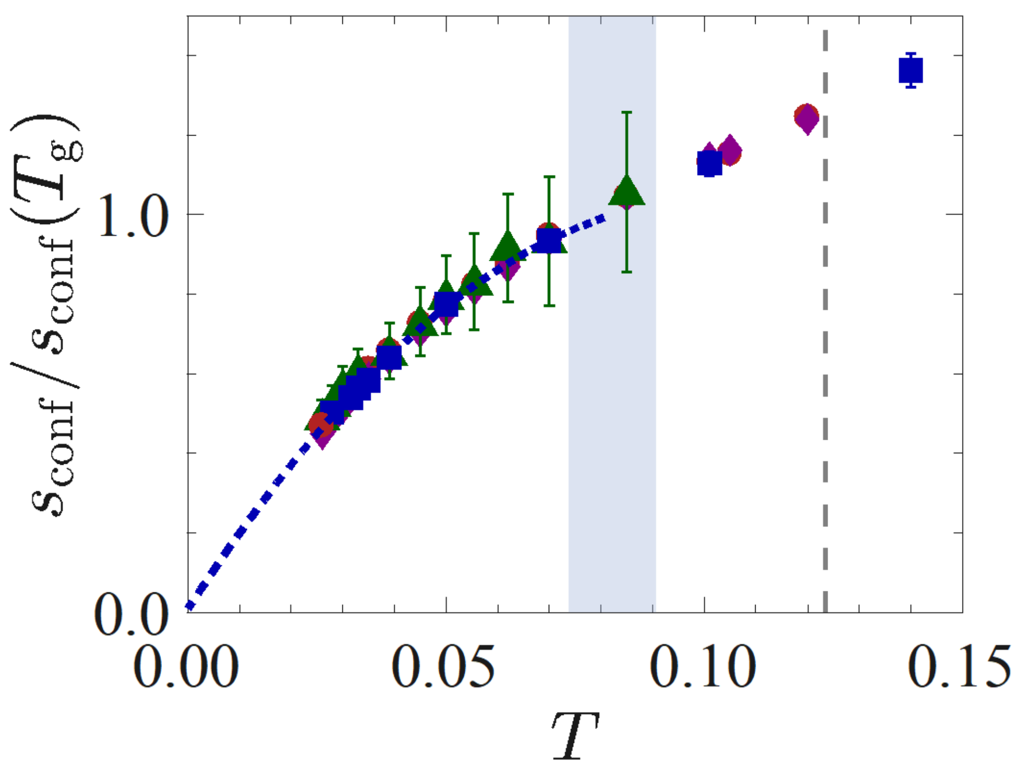
[Berthier-Charbonneau-Coslovich-Ninarello-Ozawa-Yaida, PNAS (2017)]

Breaking the glass ceiling

Difference between glassy liquids in

$$d = 2 \text{ and } d \geq 3$$

- [Flenner-Szamel, Nat. Comm. (2015)]
- [Vivek-Kelleher-Chaikin-Weeks, PNAS (2017)]
- [Illing-Fritschi-Kaiser-Klix-Maret-Keim, PNAS (2017)]



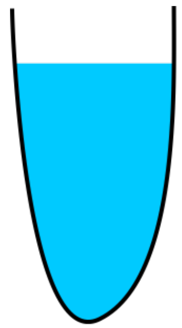
$$T_{\rm K} = 0 \text{ in } d = 2$$

[Berthier-Charbonneau-Ninarello-Ozawa-Yaida, arXiv:1805.09035]

Summary

Glassy slowdown is cool and puzzling

Point-to-set correlations capture **amorphous order** determined by surroundings for $\mathcal{R} \lesssim \xi_{\mathrm{PTS}}$



Rarefaction of metastable states drives $\frac{\xi_{\mathrm{PTS}}}{\xi_2} \nearrow$ & $\eta \nearrow\nearrow$

Local amorphous order is a good predictor of local dynamics

Point-to-set correlation length **universal**ly grows

Recently tested **beyond the glass ceiling**