Large deviations and amorphous order in glassy systems

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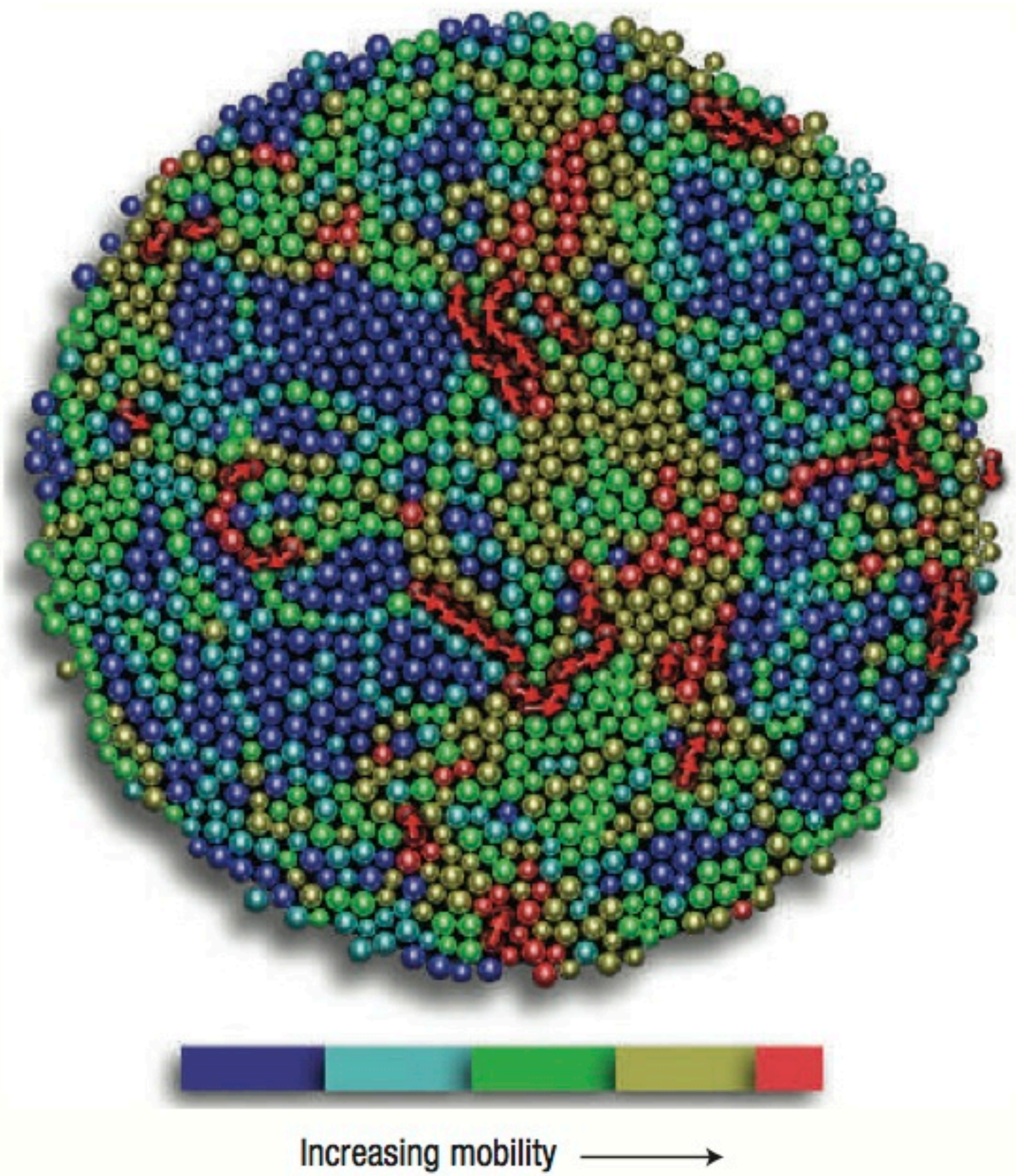
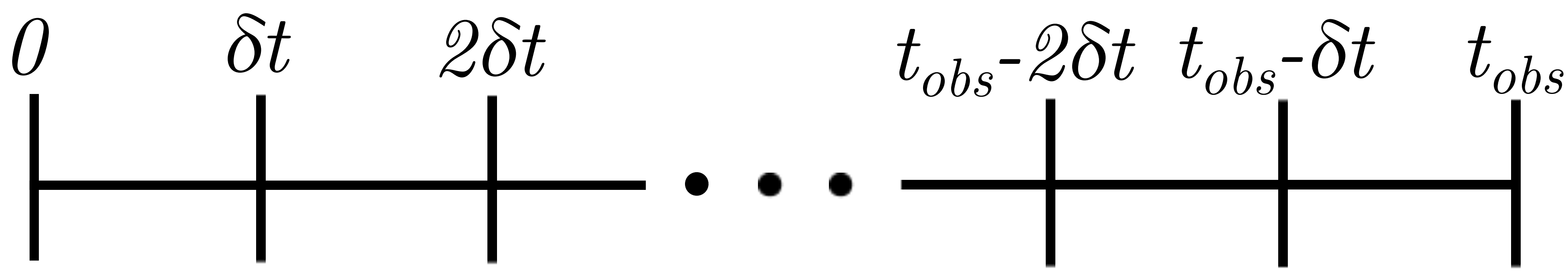
Outline

- There is something interesting about inactive configurations
- This ‘something’ is likely to do with their inherent structures
- The structure can be studied by pinning random particles & studying the behaviour of the remaining mobile particles

Keys, et. al Nat. Phys. 3, 260



Trajectories



Activity & the *s*-ensemble

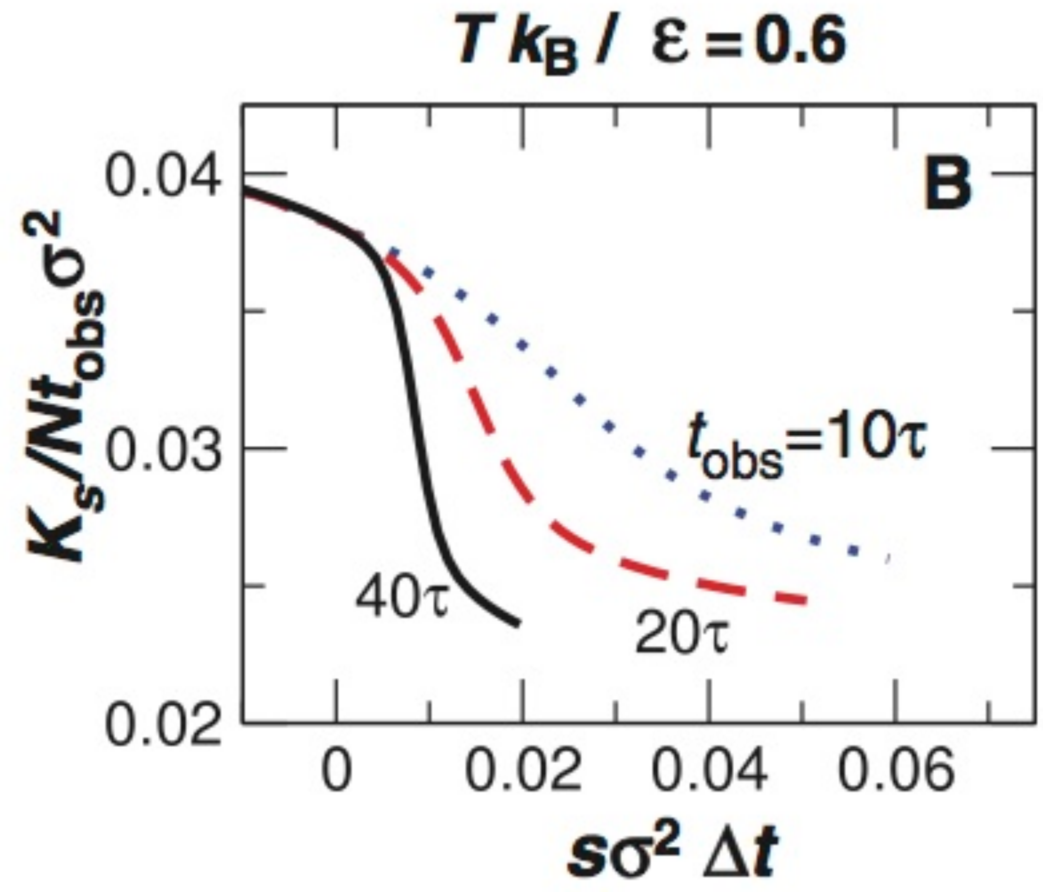
- Activity, K:

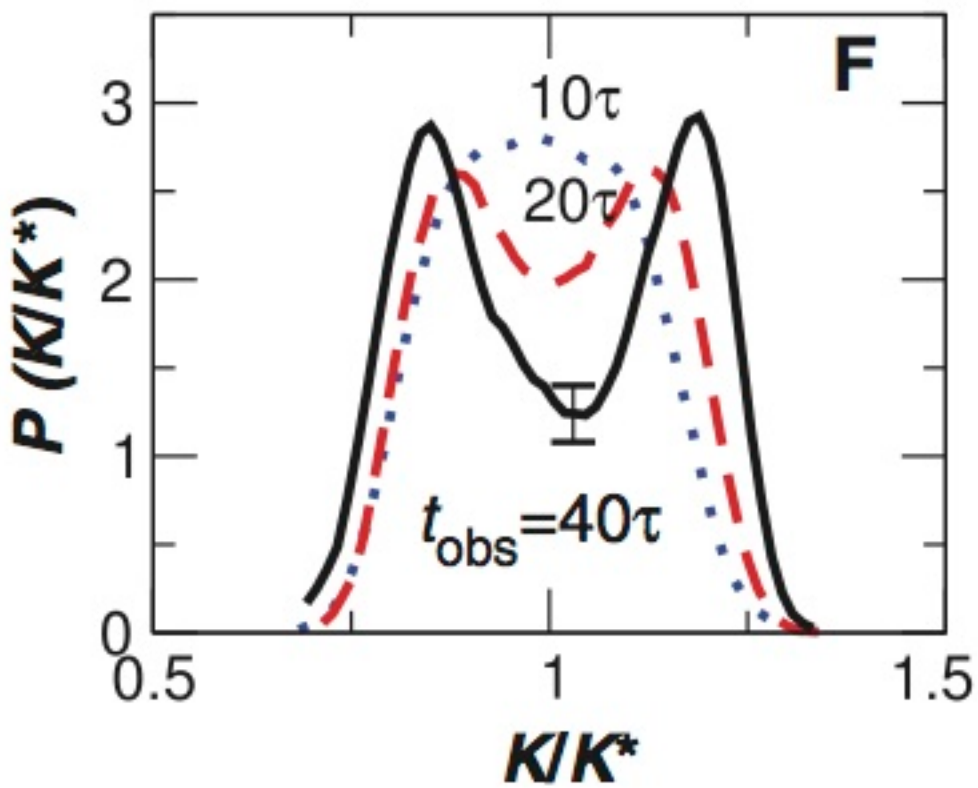
$$K[x(t)] = \delta t \sum_{t=0}^{t_{obs}} \sum_{i=0}^{N} |\vec{r}_i(t+\delta t) - \vec{r}_i(t)|^2$$

- Generate trajectories using shifting biased by:

$$\exp[-sK]$$

- Find active/inactive transition





Hedges, Jack, Garrahan, Chandler *Science 323*

Active vs inactive

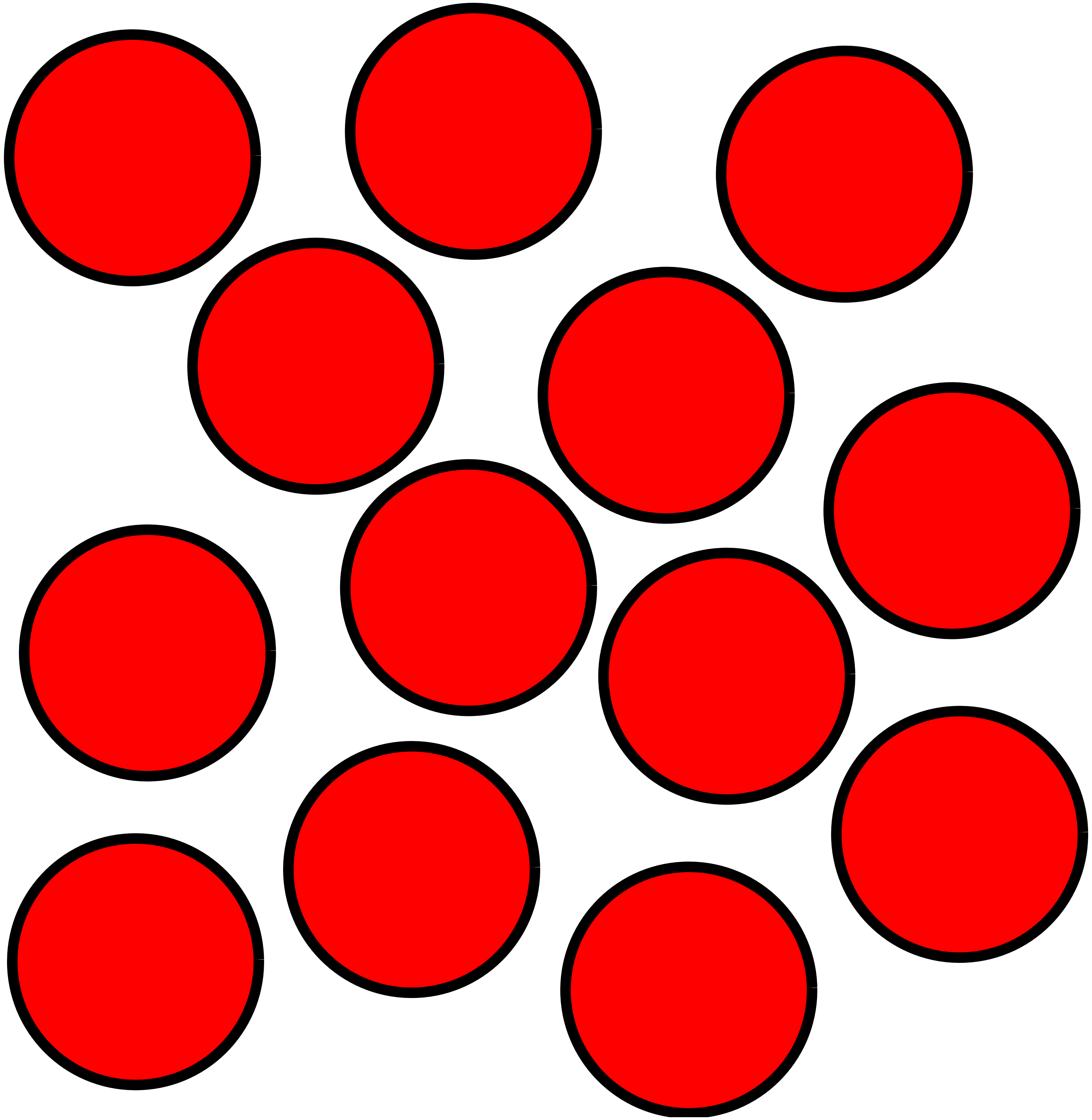
- Inactive configurations have lower average energy
- Can show that this is due to differences in inherent structure:

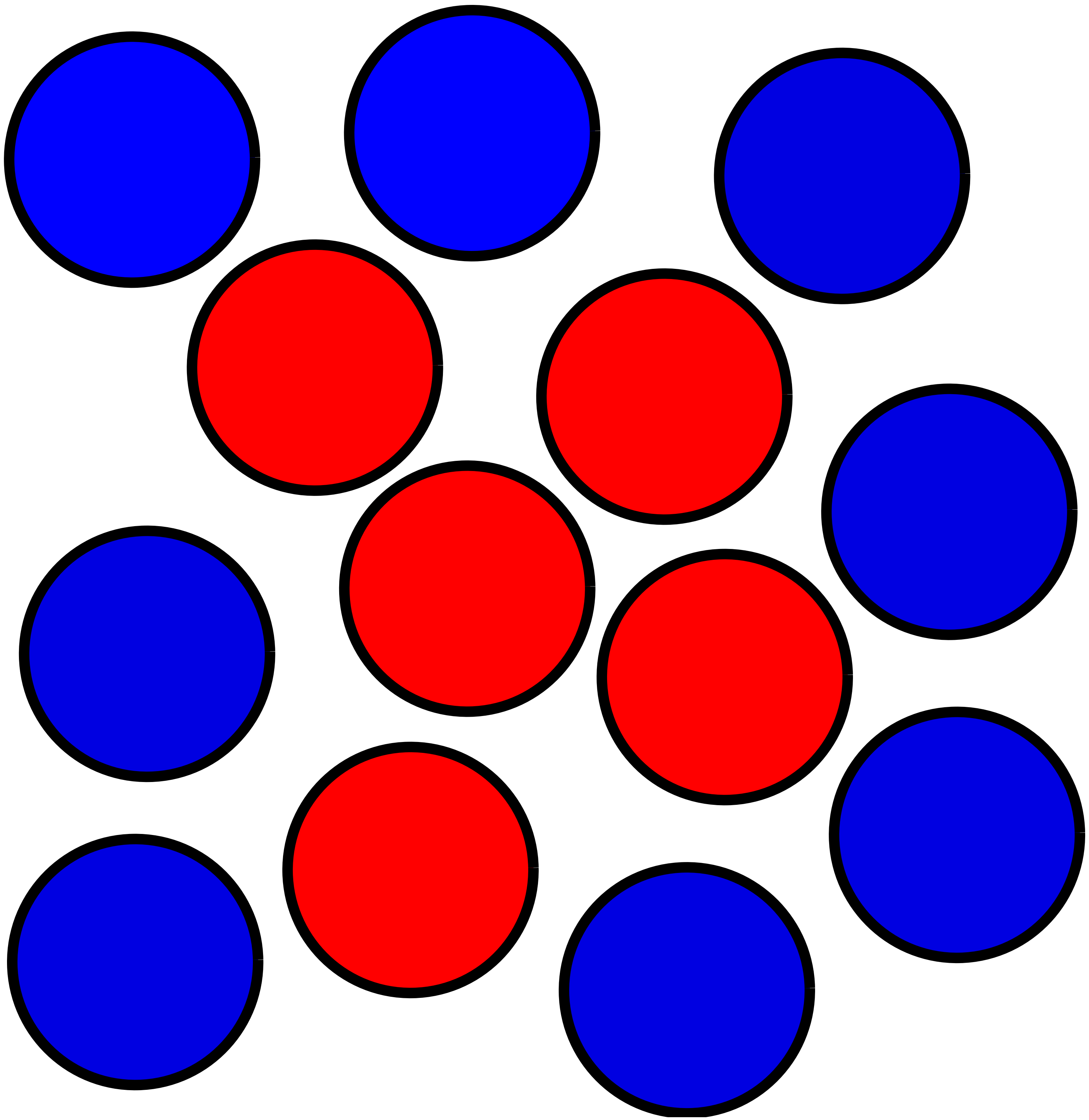
$$E_{tot} = E_{IS} + E_{vib}$$

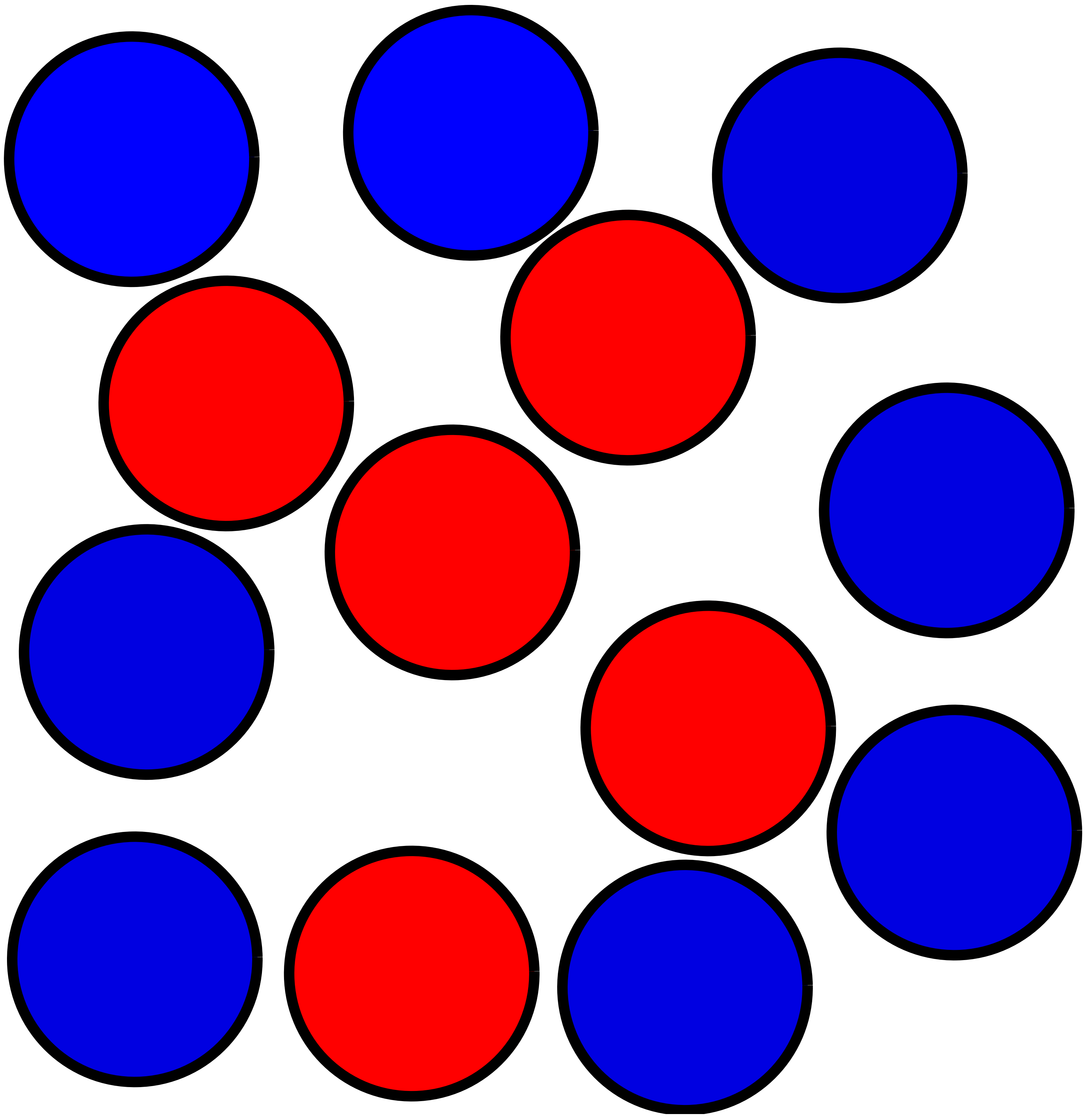
- Can this difference be quantified?

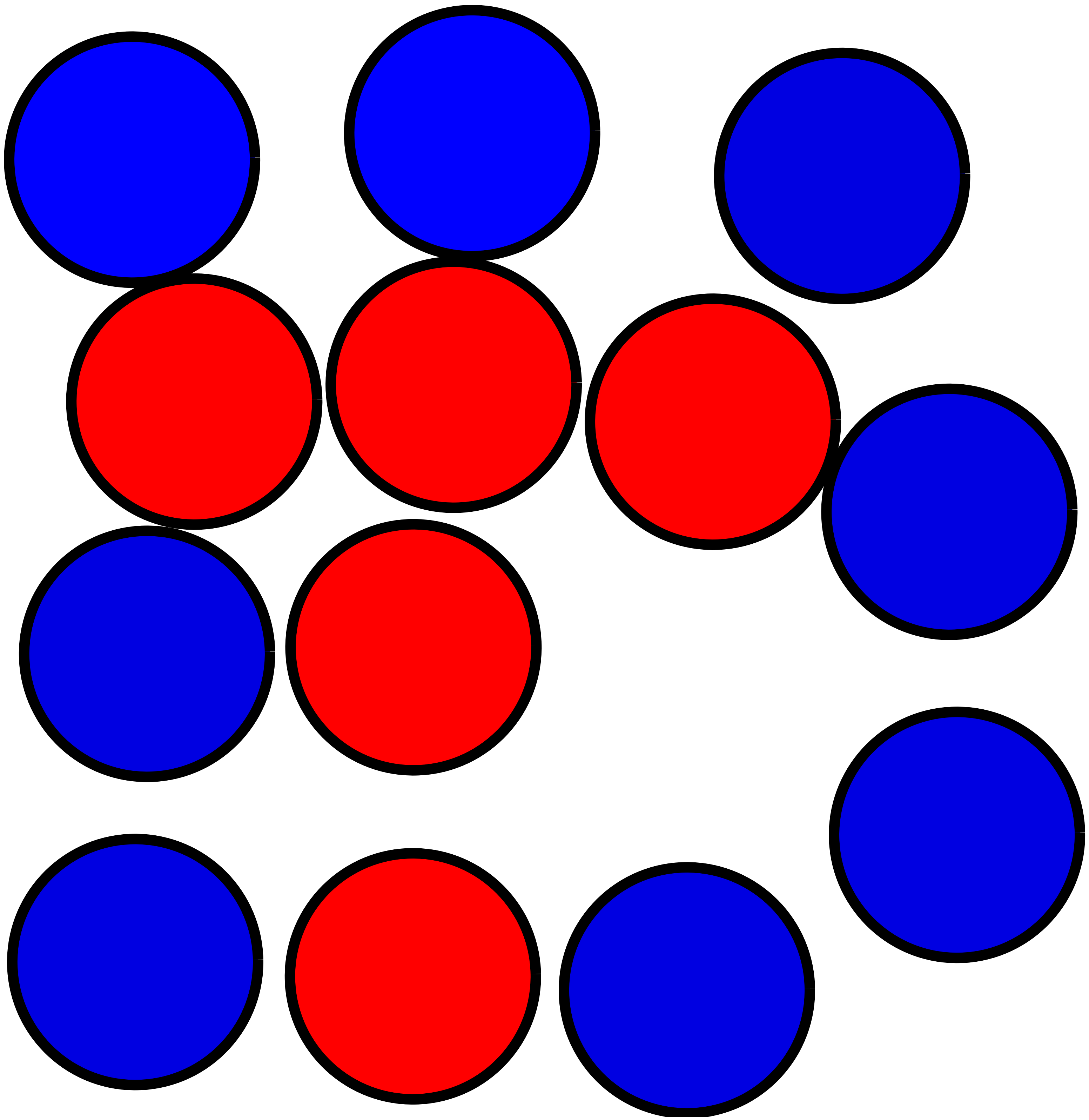
Measuring Amorphous order

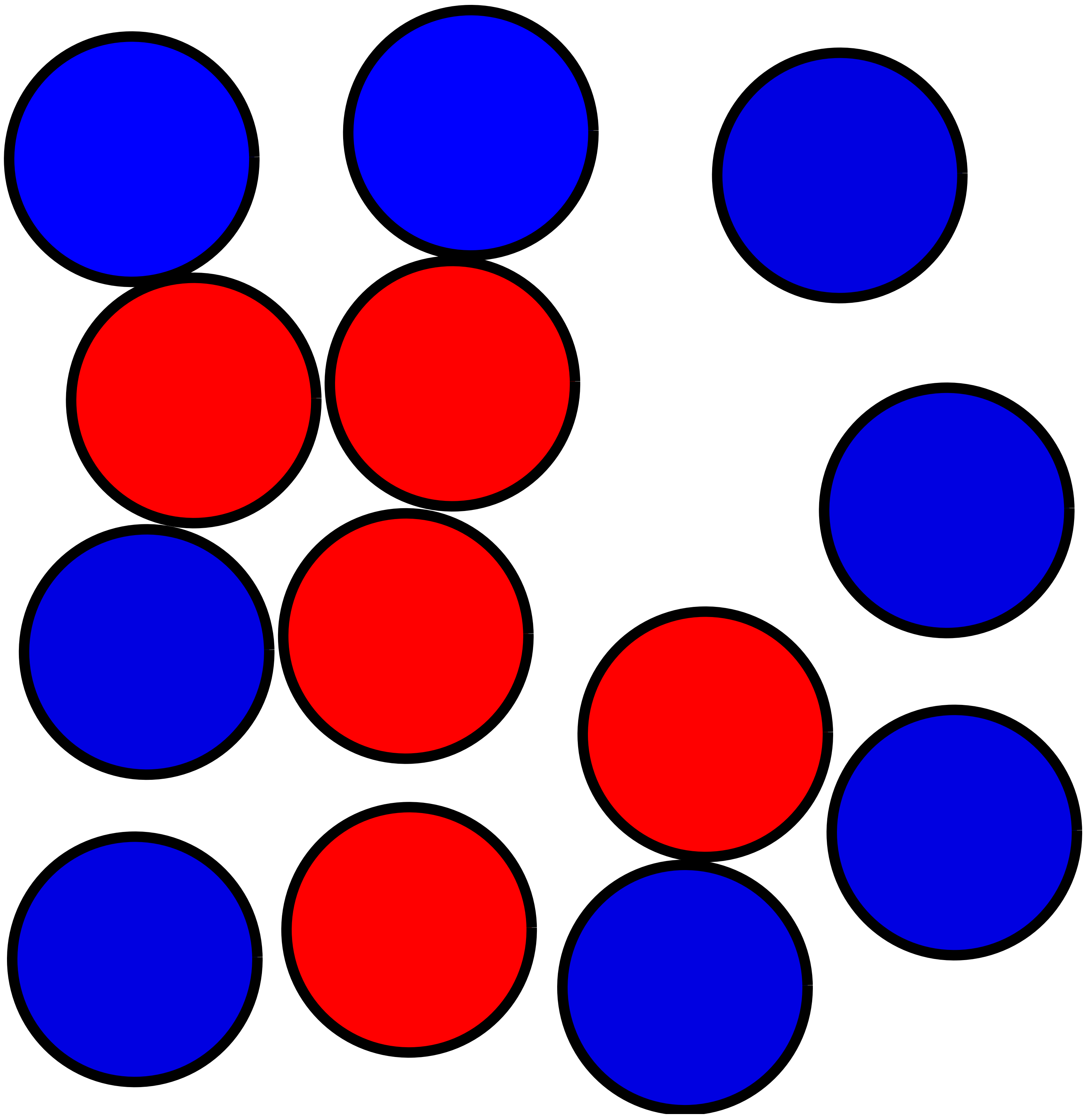
- Sounds like an oxymoron
- Measurable using point-to-set correlations

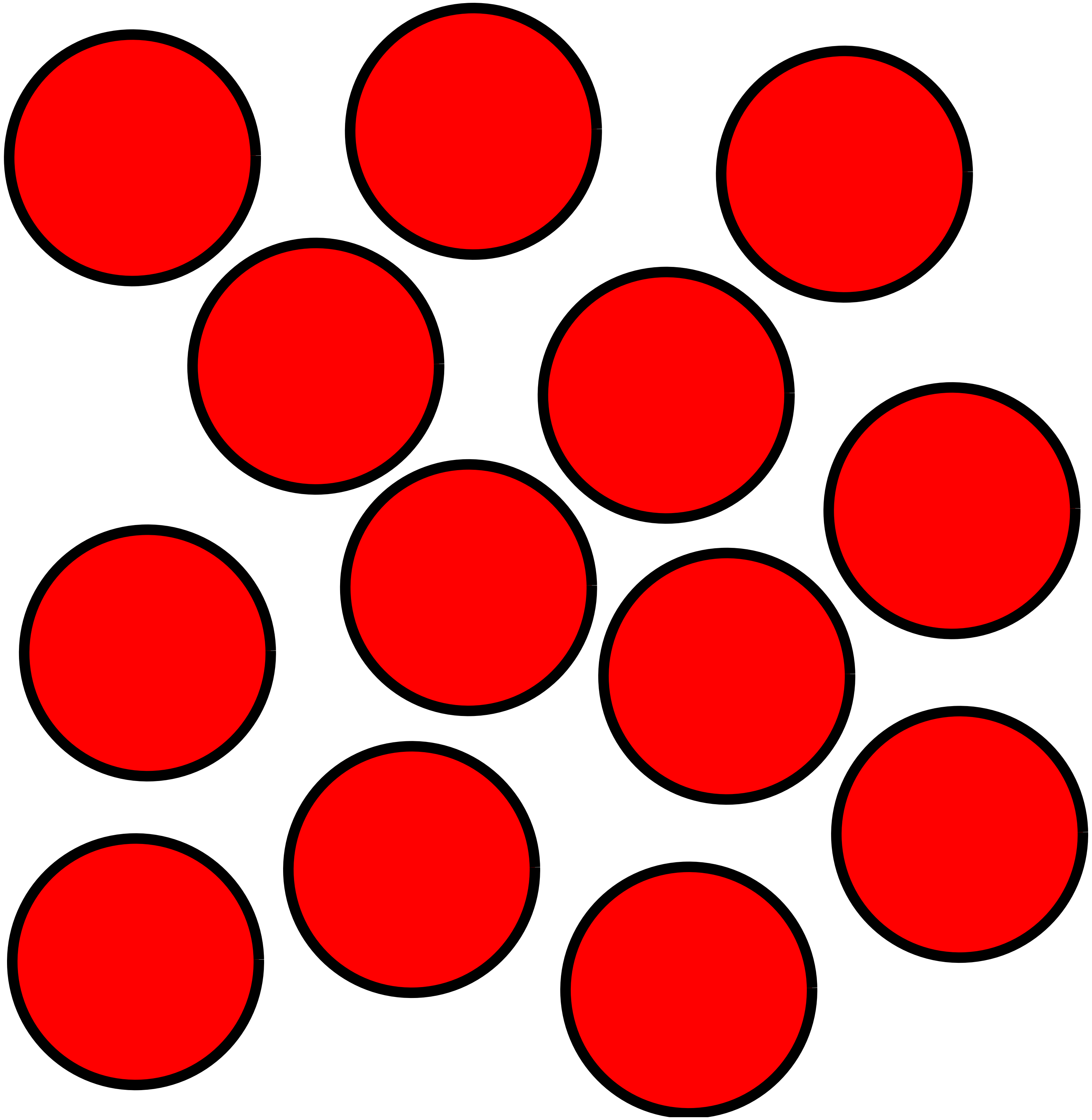


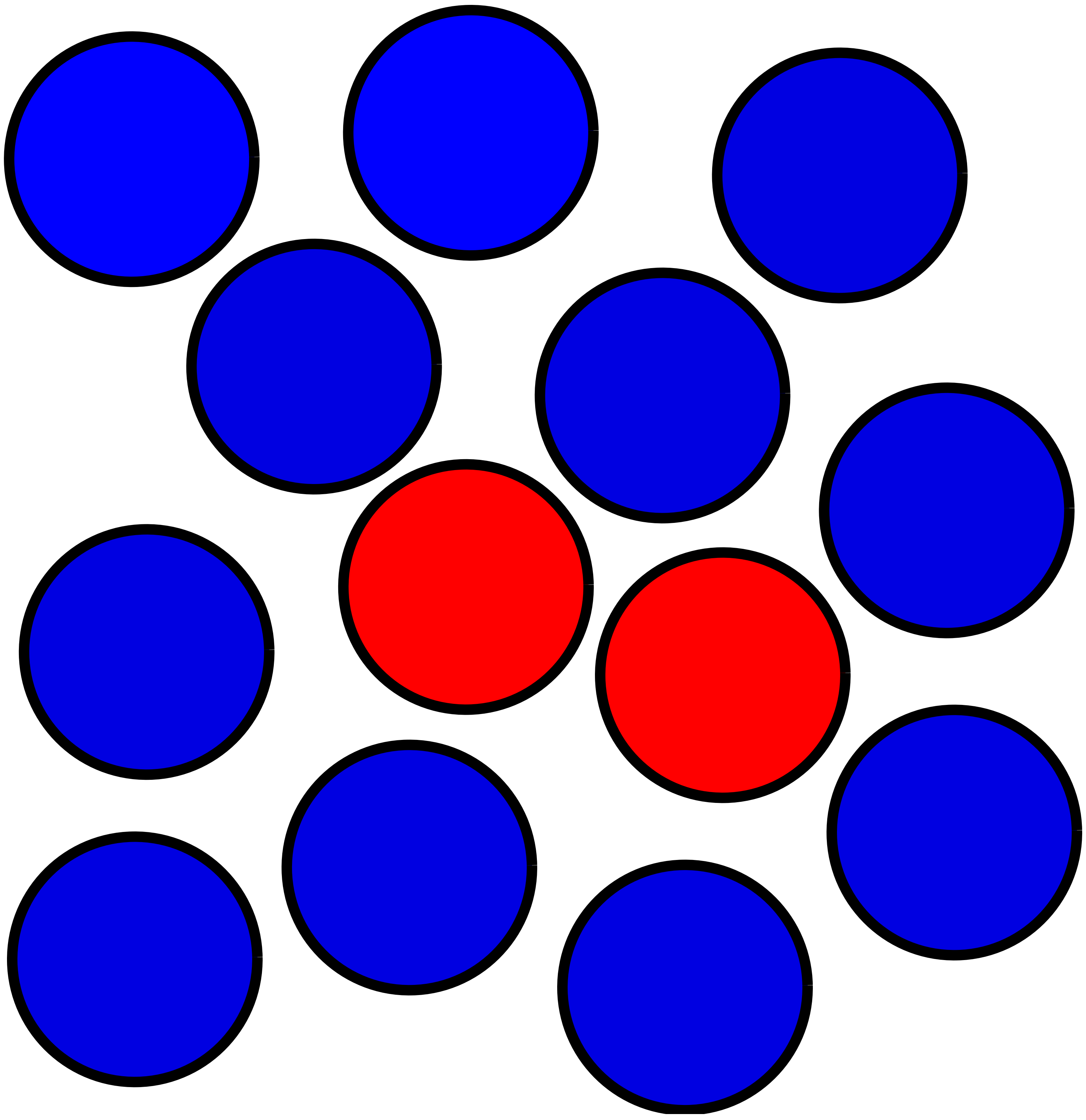


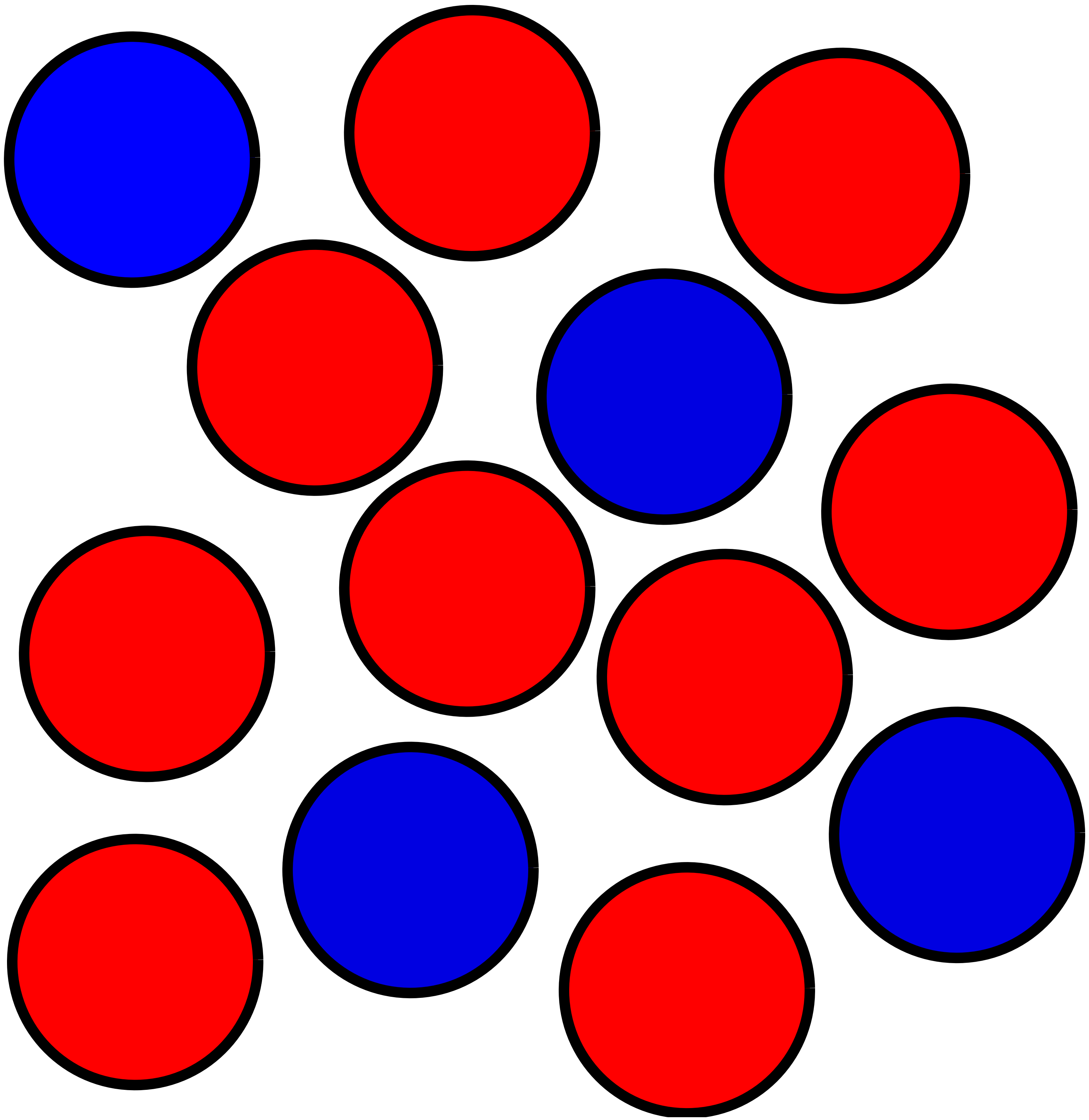












Pinning random particles

- Pin particles at random with probability f
- Run simulation
- Measure correlation functions
- Now have 2 types of average to worry about - configurational & over quenched disorder

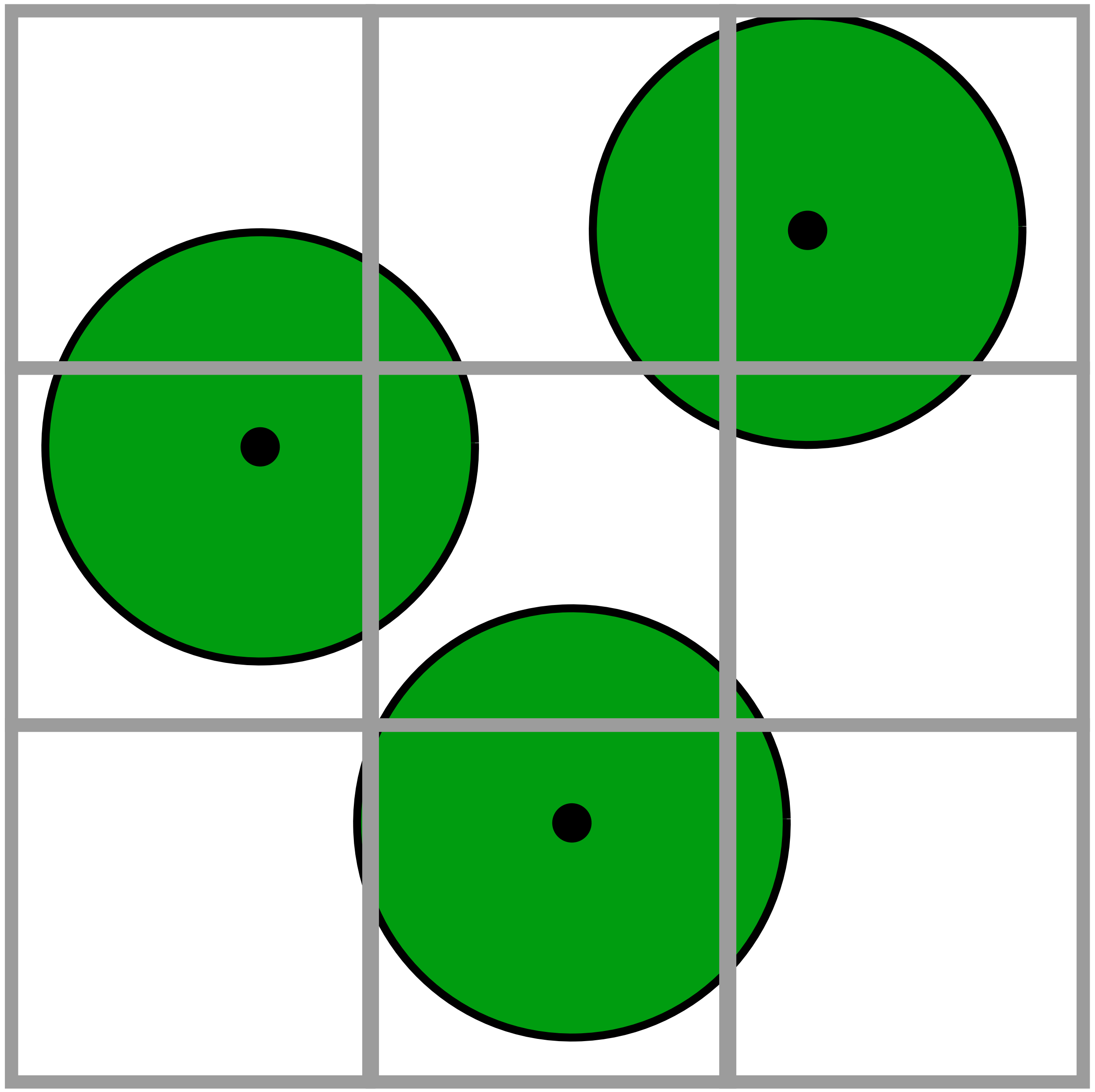
System Details

- Kob-Anderson Liquid (80:20 Lennard-Jones mixture)

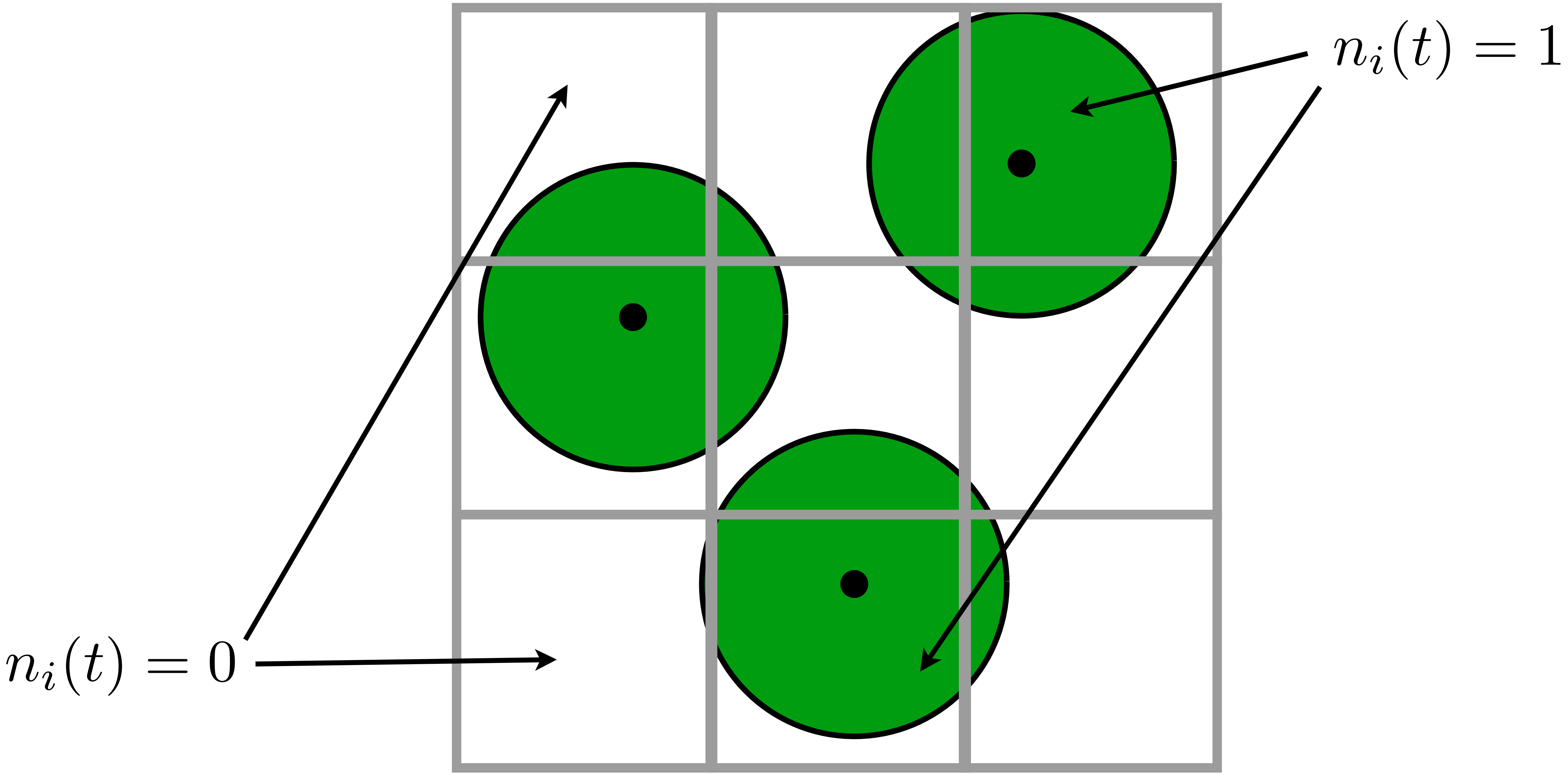
$$V(r_{ij}) = \frac{\epsilon_{ij}}{2}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

- Well studied as model glass former
- Measure collective overlap, $q_c(t)$

Cells



Cells



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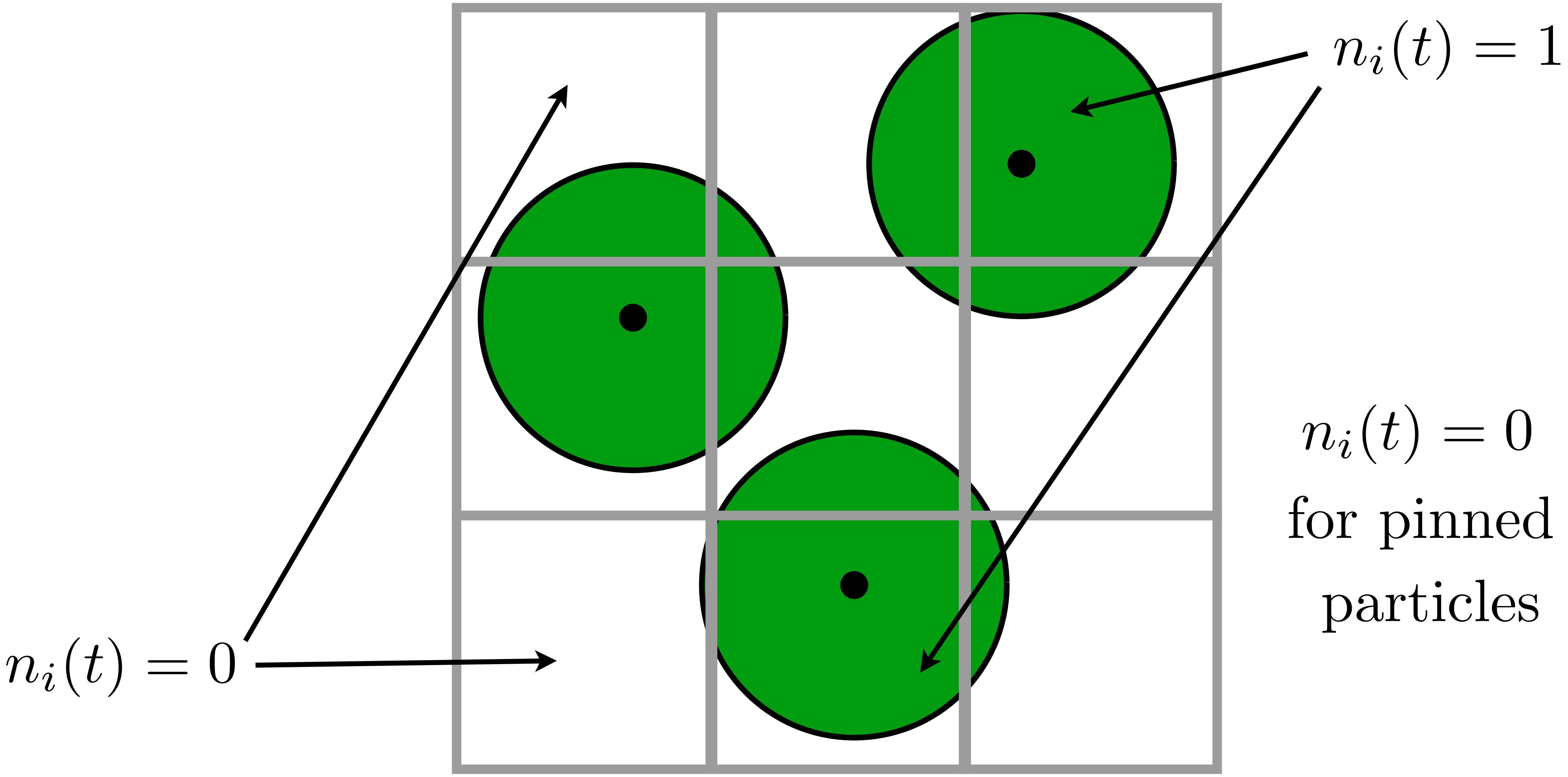


The overlap

$$q_c(t) = \frac{1}{A}\left[\frac{\frac{1}{M}\sum_i \langle n_i(t) n_i(0)\rangle}{\frac{1}{M}\sum_i \langle n_i(t)\rangle} - \frac{N}{M}\right]$$

$$A = 1 - \frac{N}{M}$$

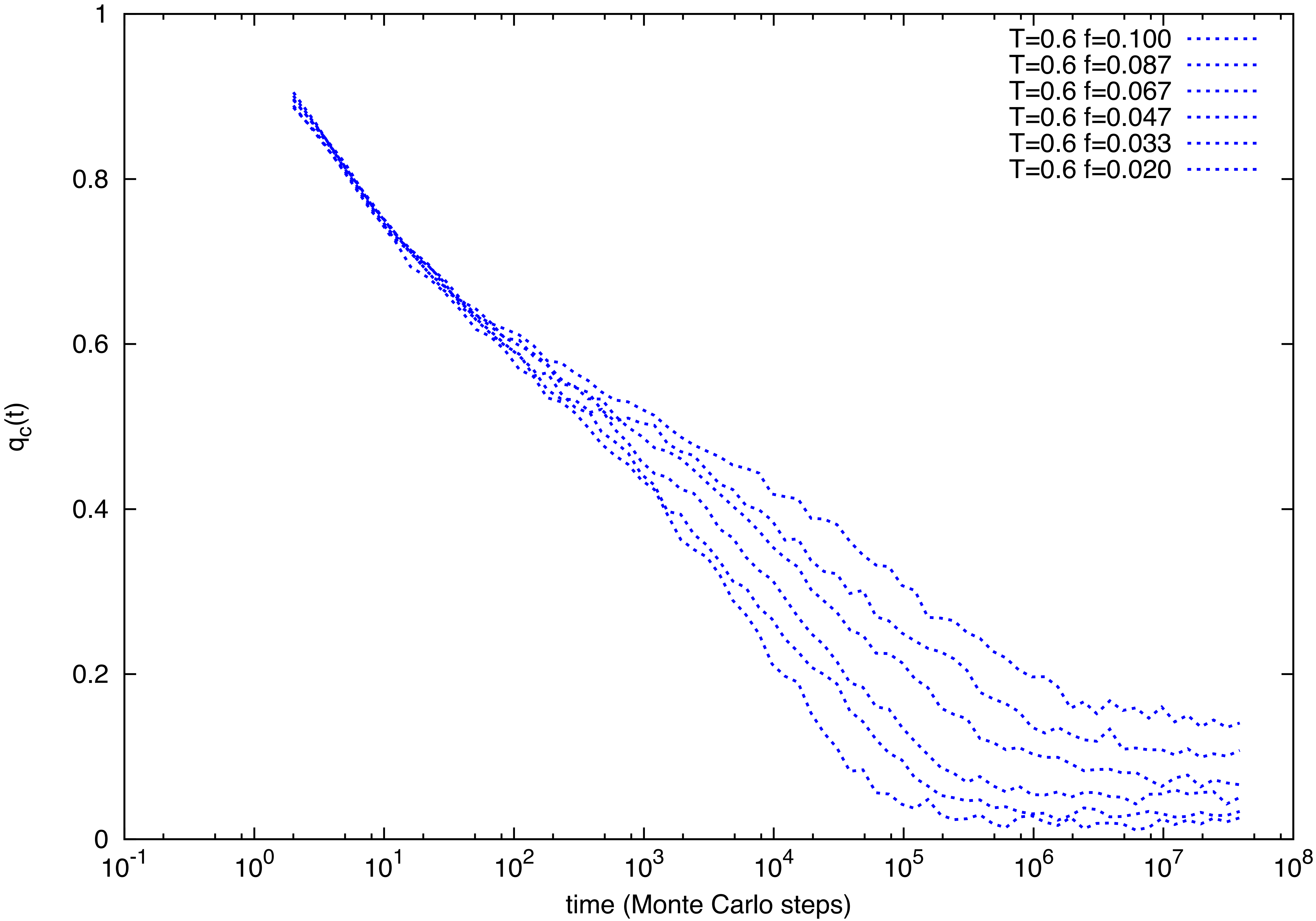
Expectations

$$\langle n_i(t) n_i(0) \rangle \to \langle n_i(t) \rangle \langle n_i(0) \rangle$$

$$\frac{\frac{1}{M}\sum_i \langle n_i(t) \rangle \langle n_i(0) \rangle}{\frac{1}{M}\sum_i \langle n_i(t) \rangle} = \frac{1}{M}\sum_i \langle n_i(t) \rangle = \frac{N}{M}$$

$$q_c(t) \to 0 \text{ for } f = 0$$

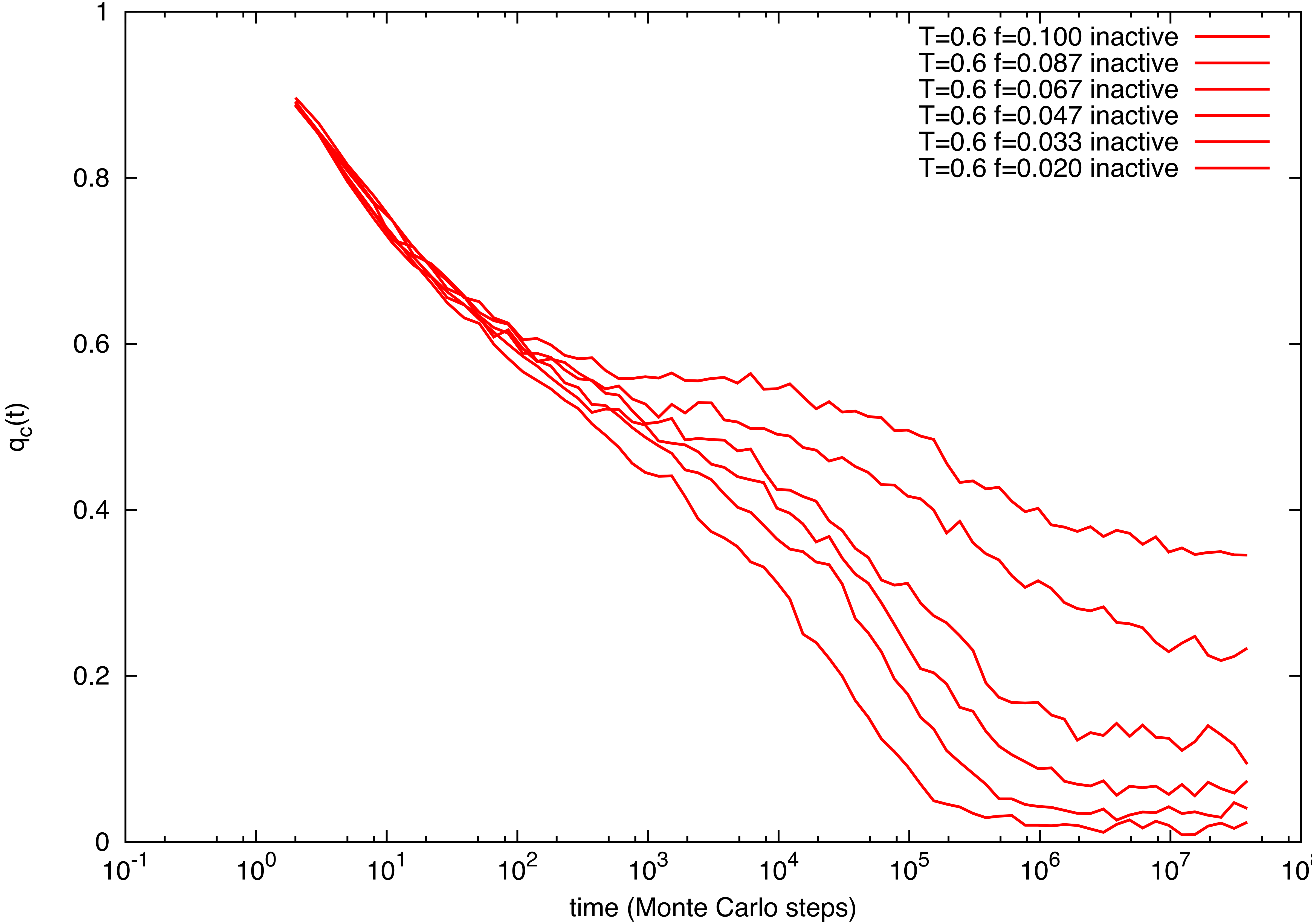
$$q_c(t) \to q_c^{\infty} \text{ for } f > 0$$



T=0.6 f=0.100
T=0.6 f=0.087
T=0.6 f=0.067
T=0.6 f=0.047
T=0.6 f=0.033
T=0.6 f=0.020
$q_c(t)$
time (Monte Carlo steps)
0
0.2
0.4
0.6
0.8
1
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
10^{8}

Configurations from inactive trajectories

- Not interested in melting of inactive configuration
- Freeze fraction f of particles in inactive configuration
- Allow all others to return to equilibrium
- Only now start to measure $q_c(t)$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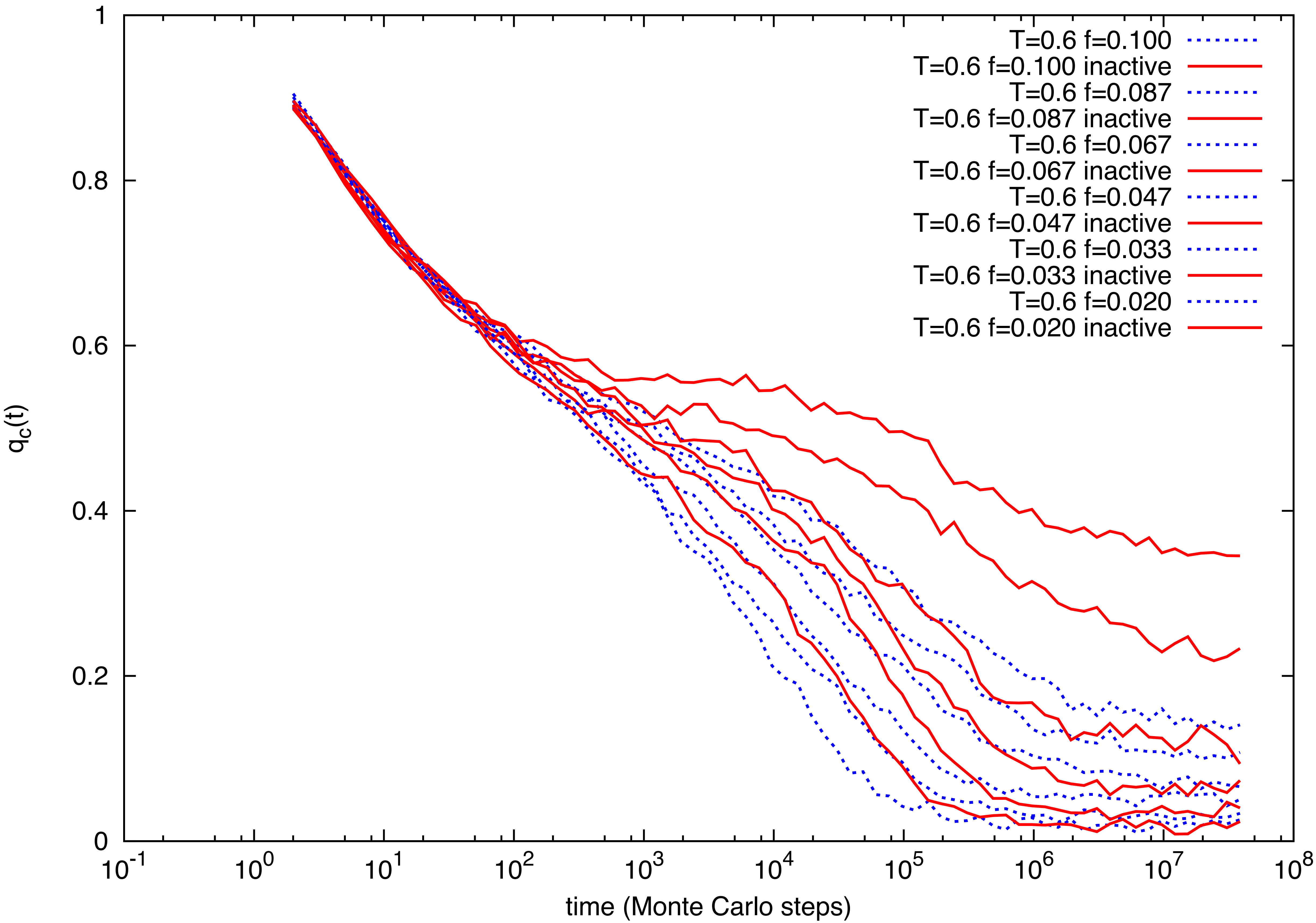

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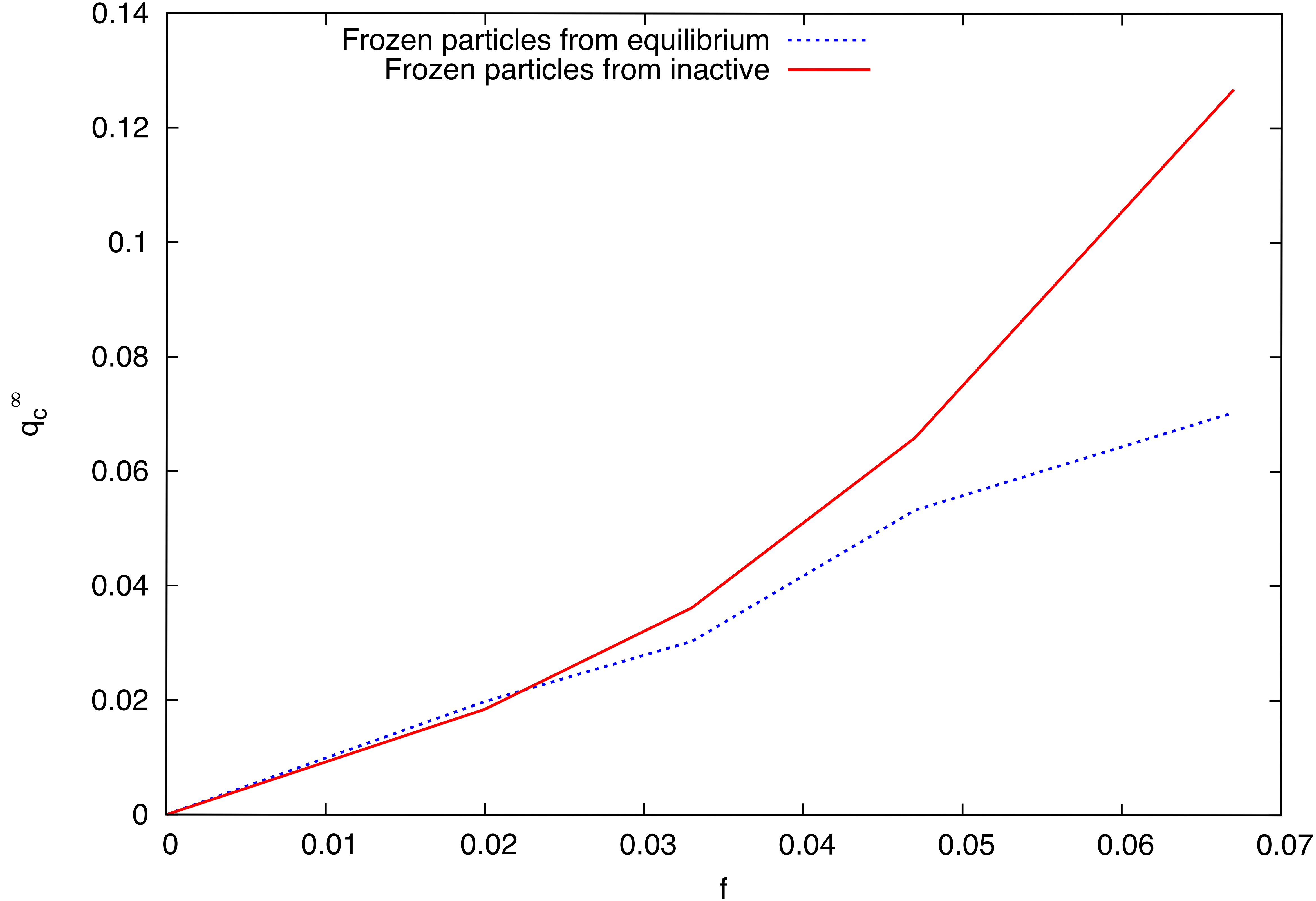
10^{8}



Frozen particles from equilibrium
Frozen particles from inactive
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
f

Conclusions

- There is something interesting about the structure of inactive configurations
- We can measure this using point-to-set correlations (pinning particles)
- We don't have to pin very many particles for this difference to be apparent - this is pretty surprising!