Statistical mechanics of the maximum-average submatrix problem

Vittorio Erba, Florent Krzakala, Rodrigo Pérez, and Lenka Zdeborová

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Swiss National Science Foundation

EPFL

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Given $N \times N$ matrix J of real numbers find $k \times k$ submatrix with **largest** sum of entries

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Given $N \times N$ matrix J of real numbers find $k \times k$ submatrix with **largest** sum of entries

Submatrix: intersection of k rows and columns, not necessarily adjacent

$$k = 4, N = 8$$

$$\begin{bmatrix}
J_{1,1} & J_{1,2} & J_{1,3} & J_{1,4} & J_{1,5} & J_{1,6} & J_{1,7} & J_{1,8} \\
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Maximum-average submatrix problem

Given $N \times N$ matrix J of real numbers find $k \times k$ submatrix with **largest** sum of entries

Submatrix: intersection of k rows and columns, not necessarily adjacent

Encoding: use two two N-dim $0/1$ vector σ, τ

$\sigma_i = 1$ iff i-th row chosen

$\tau_j = 1$ iff j-th column chosen

$$\text{Energy}(\sigma, \tau) = \sum_{i,j} J_{ij}\sigma_i \tau_j$$

Random + high dim setting:

J iid Gaussian, $N \to \infty$

$k = 4, N = 8$

$$\begin{array}{c|c}
\sigma \backslash \tau & \begin{array}{cccccccc} \downarrow & & \downarrow & \downarrow & & & \downarrow & \end{array} \\
\begin{array}{c} \\ \rightarrow \\ \rightarrow \\ \\ \\ \rightarrow \\ \\ \rightarrow \end{array} &
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Why is this model interesting

N matrix size
k submatrix size

1. Results for random Gaussian i.i.d. J, $N \to \infty$ and $k \ll N$ (small submatrices)

Missing: large submatrix regime $k \sim N$ + can we say more for $k \ll N$?

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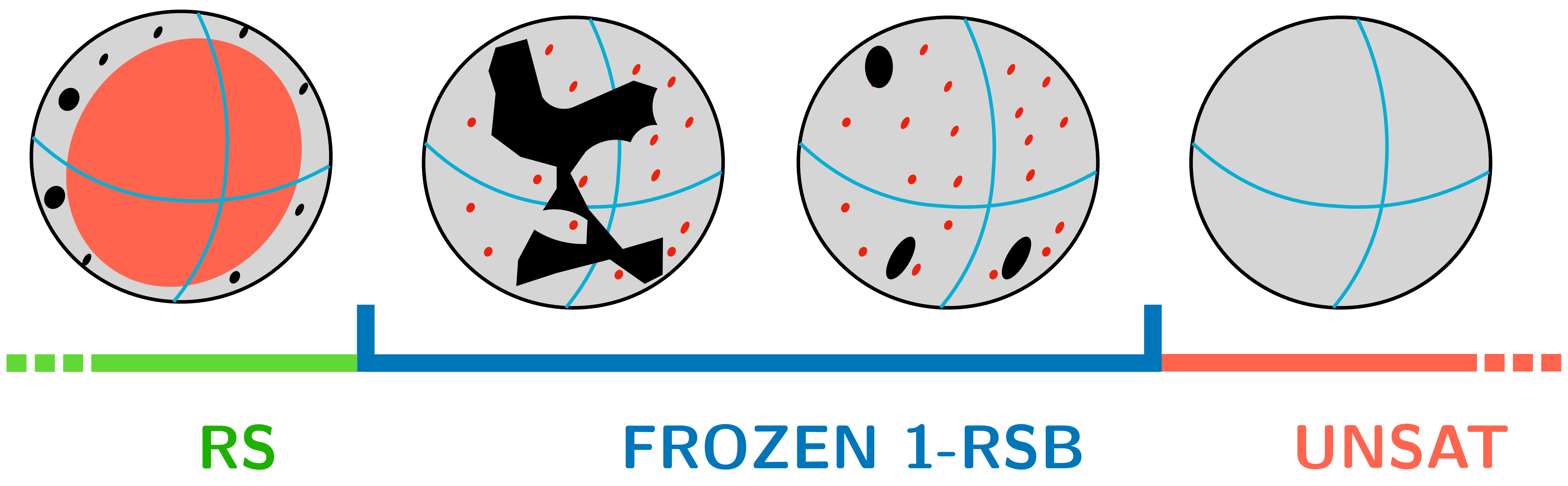
2. Unexpected link with rare cluster phenomenology of binary perceptron

Typical structure of energy level sets is clustered, but efficient algorithms work

Equilibrium vs

non-equilibrium vs

algorithmic properties?



Result: equilibrium phase diagram

N matrix size
k submatrix size
$m = k/N$

Symmetric case: $J = J^T$, same row/columns

Equilibrium/typical properties through

$$p(\sigma) \propto \exp \beta H(\sigma)$$

$$H(\sigma) = \frac{1}{2\sqrt{N}} \sum_{i<j} J_{ij} \sigma_i \sigma_j + h \sum_i \sigma_i$$

β: fix energy level

h: fix submatrix size

Variant of SK model computation ("classic" replicas)

- boolean spins + fixed magnetisation $m = k/N$
- small submatrix limit recovered for $m \to 0$
- rigorous [1]?

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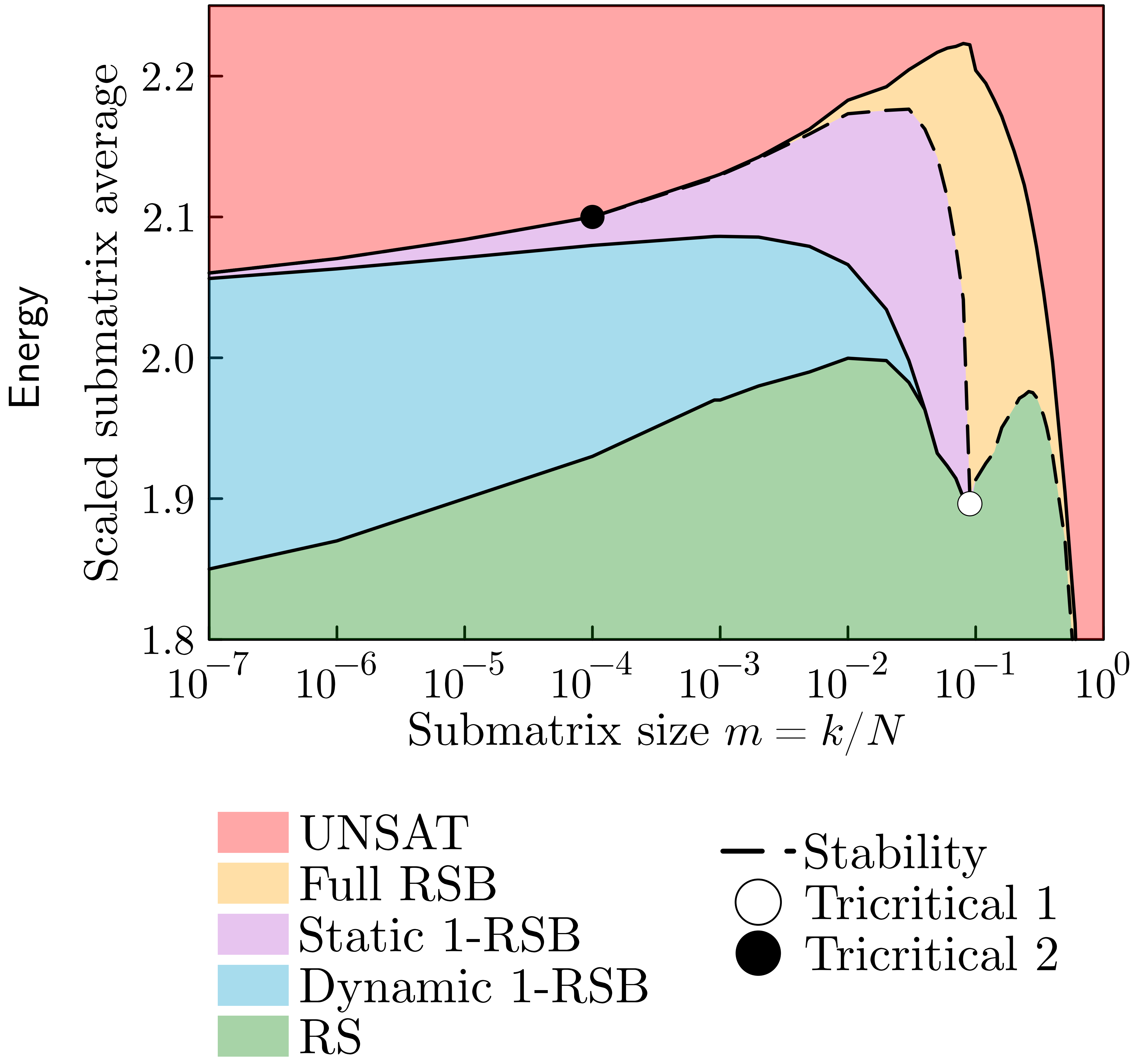

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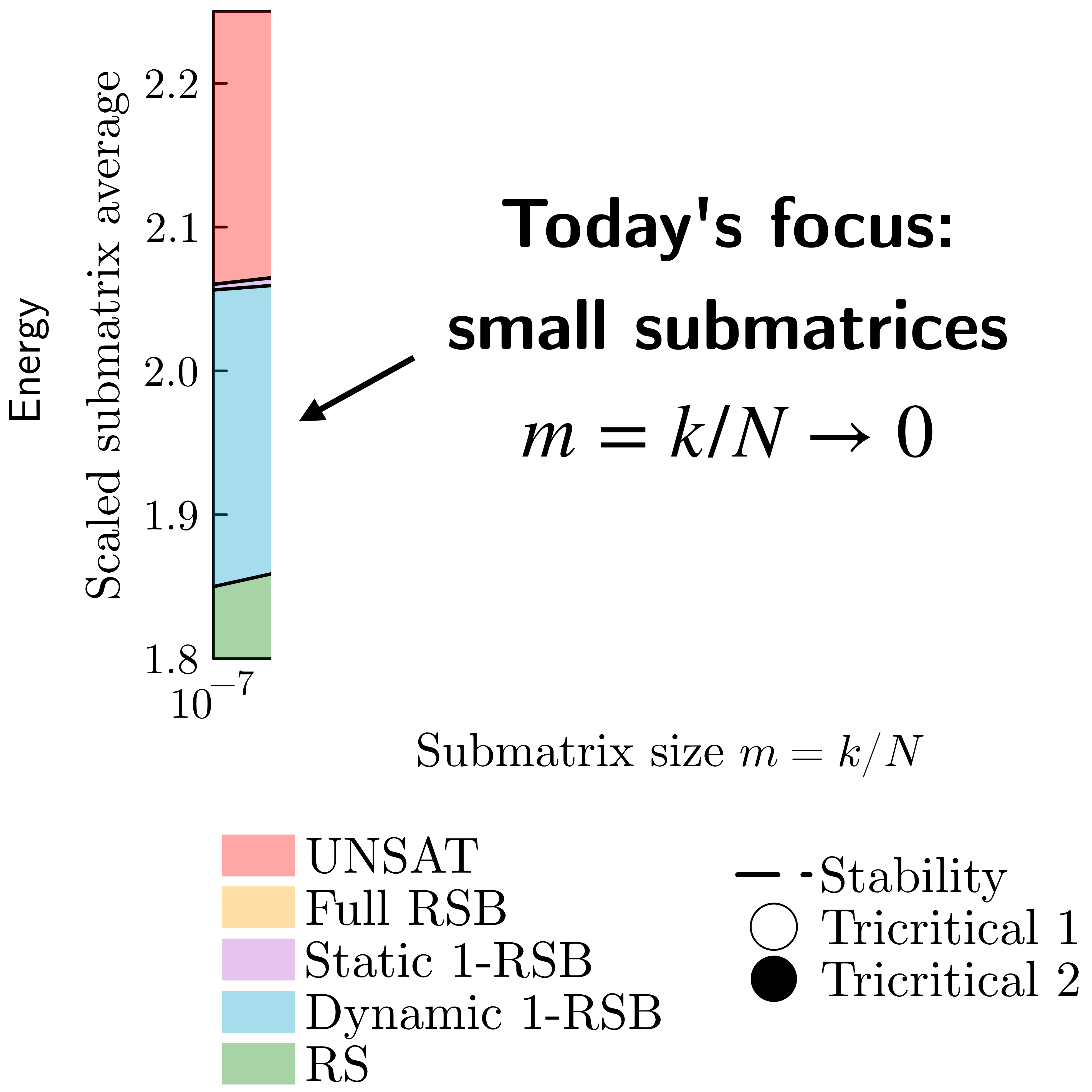

Today's focus: small submatrices
$m = k/N \to 0$

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A submatrix avg

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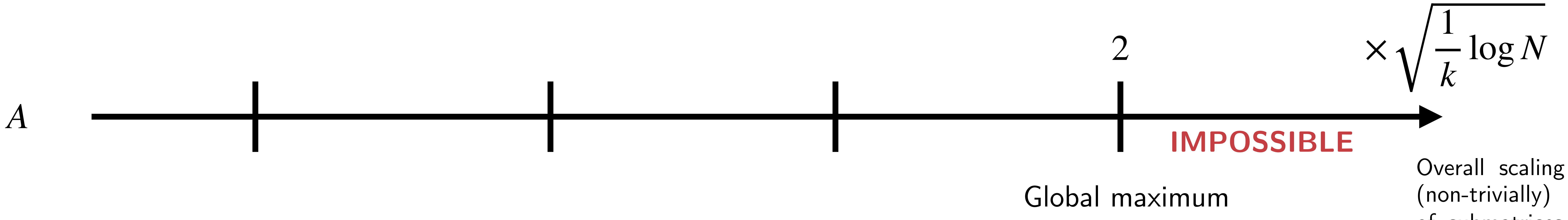

Overall scaling determined (non-trivially) by number of submatrices $\sim N^k$ and variance of submatrix-average A of $2k^{-2}$.

[1,3] The best possible submatrix-average equals the largest out of N^k independent Gaussians with variance $2k^{-2}$ (REM-like).

$$\begin{bmatrix}
J_{1,1} & J_{1,2} & J_{1,3} & J_{1,4} & J_{1,5} & J_{1,6} & J_{1,7} & J_{1,8} & J_{1,9} & J_{1,10} & J_{1,11} & J_{1,12} \\
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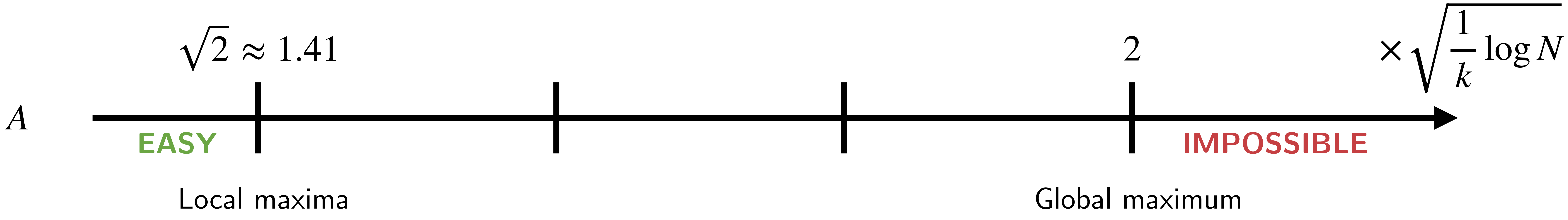
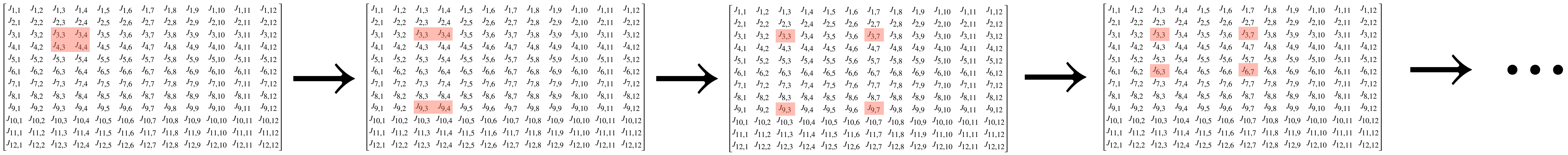
The phase diagram for small submatrices

N matrix size
k submatrix size
$m = k/N$
A submatrix avg



[1,2] Local maxima (stable among same-row or same-column) have lower submatrix-average than the best one, and can be found by an efficient iterative algorithm



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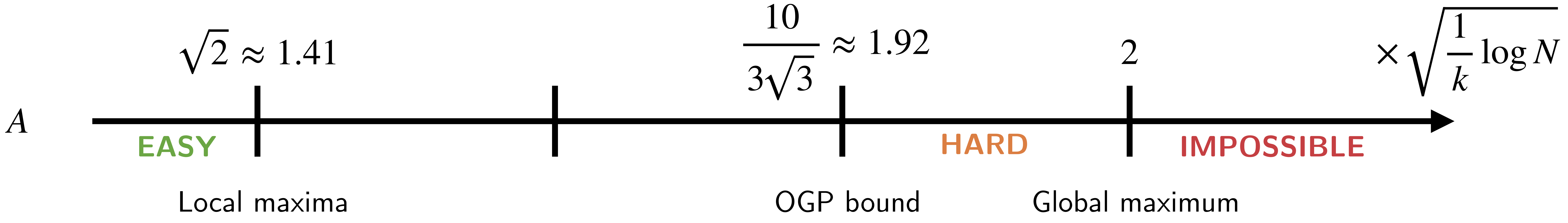

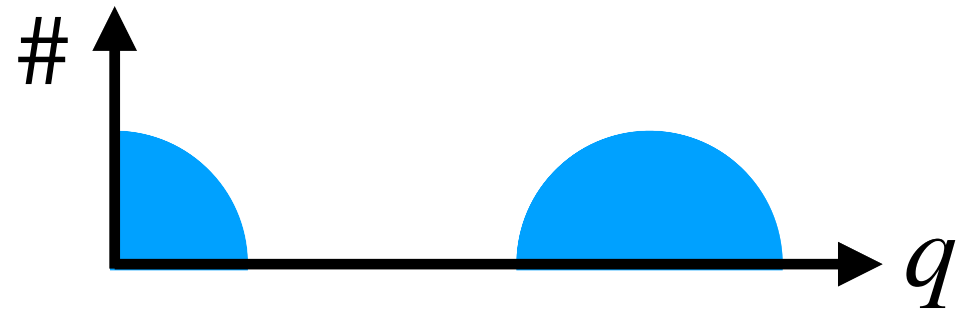

[2] Algorithmic hardness bound through Overlap Gap Property ⟶

Overlap Gap Property: w.h.p. on the disorder, each pair of submatrices with submatrix-average at this energy is either very close (large overlap q) or very far (zero overlap q). No intermediate distance can be observed.

Gamarnik. "The overlap gap property: A topological barrier to optimizing over random structures." (2021)

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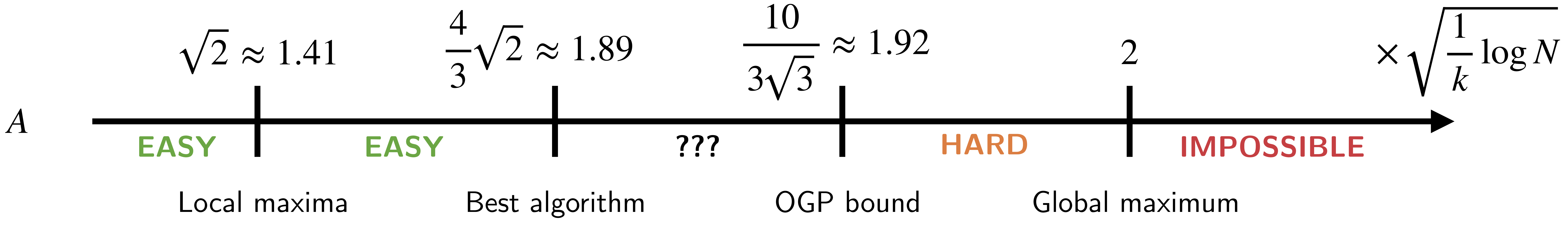
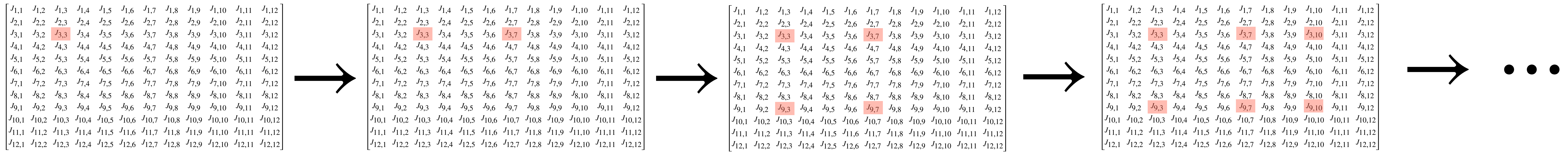


[2] Best efficient algorithm (greedy) performs better than typical local-maxima



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Results: weak clustering phase

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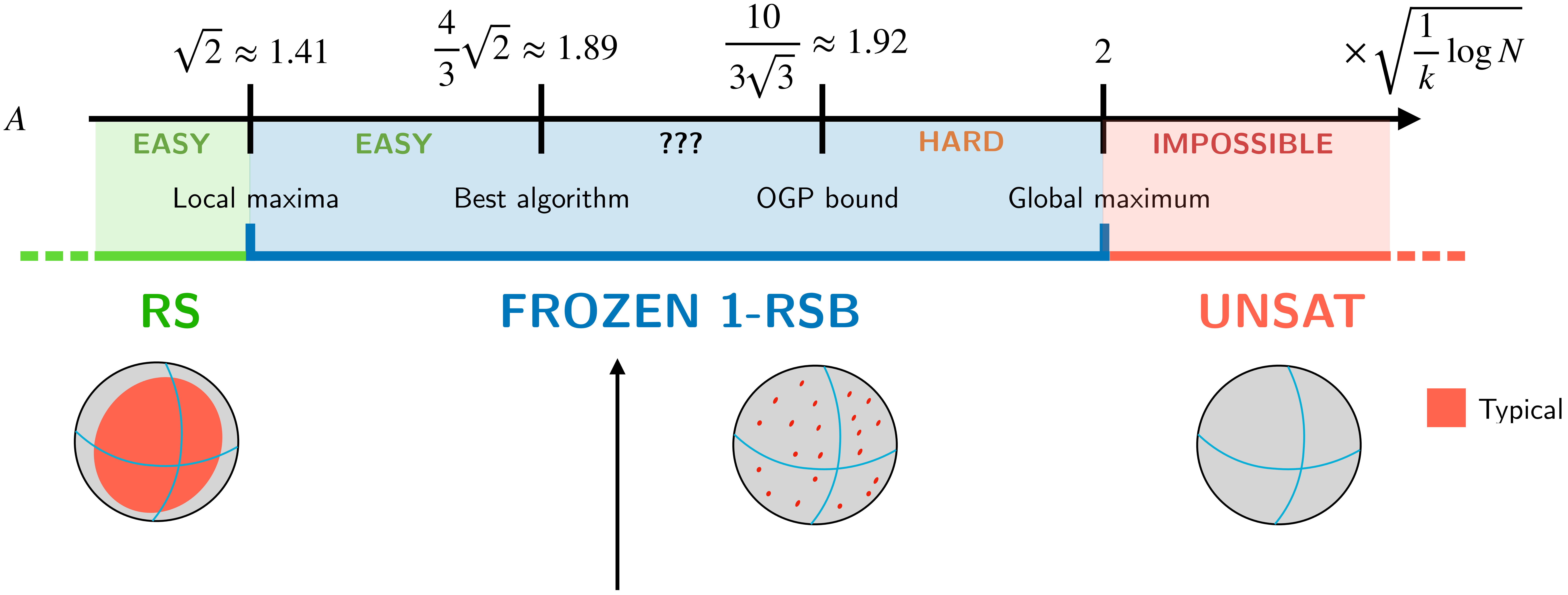

Clustering: exponential number of orthogonal clusters

Freezing: each cluster has zero entropy + internal overlap = 1

Algorithm working in frozen phase?

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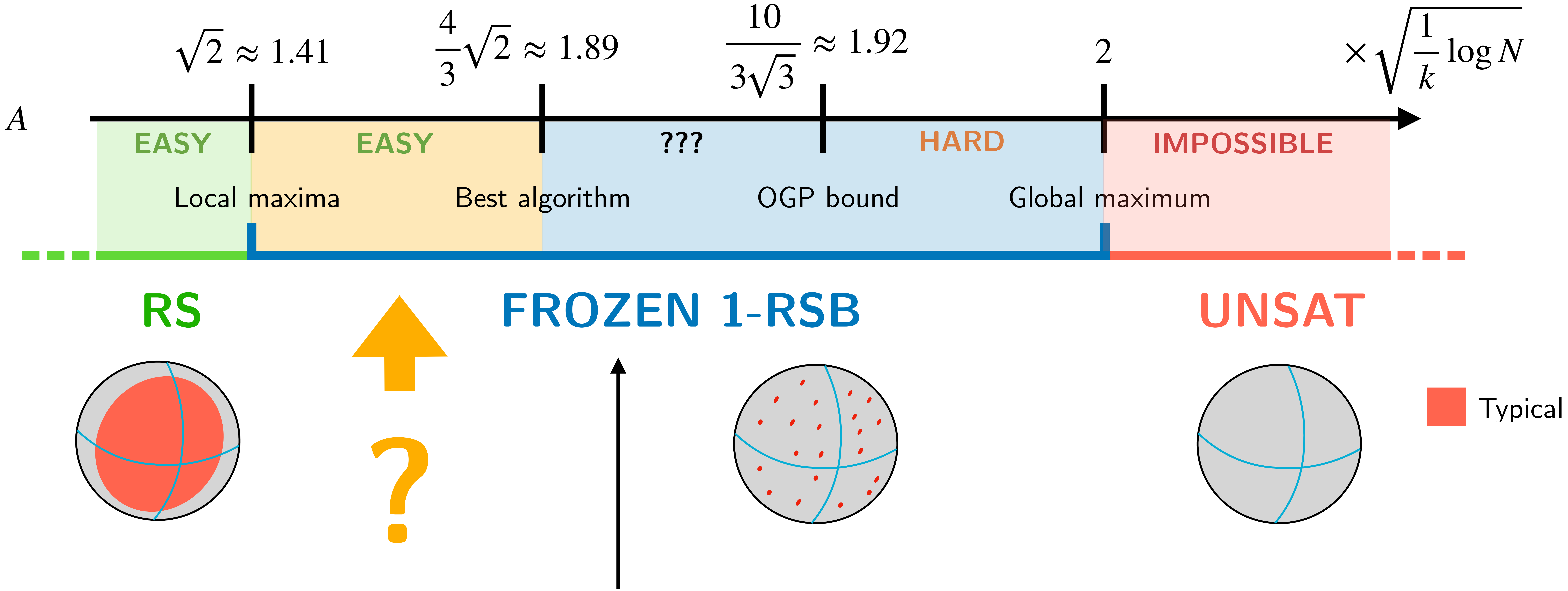

Clustering: exponential number of orthogonal clusters

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Atypical clusters?

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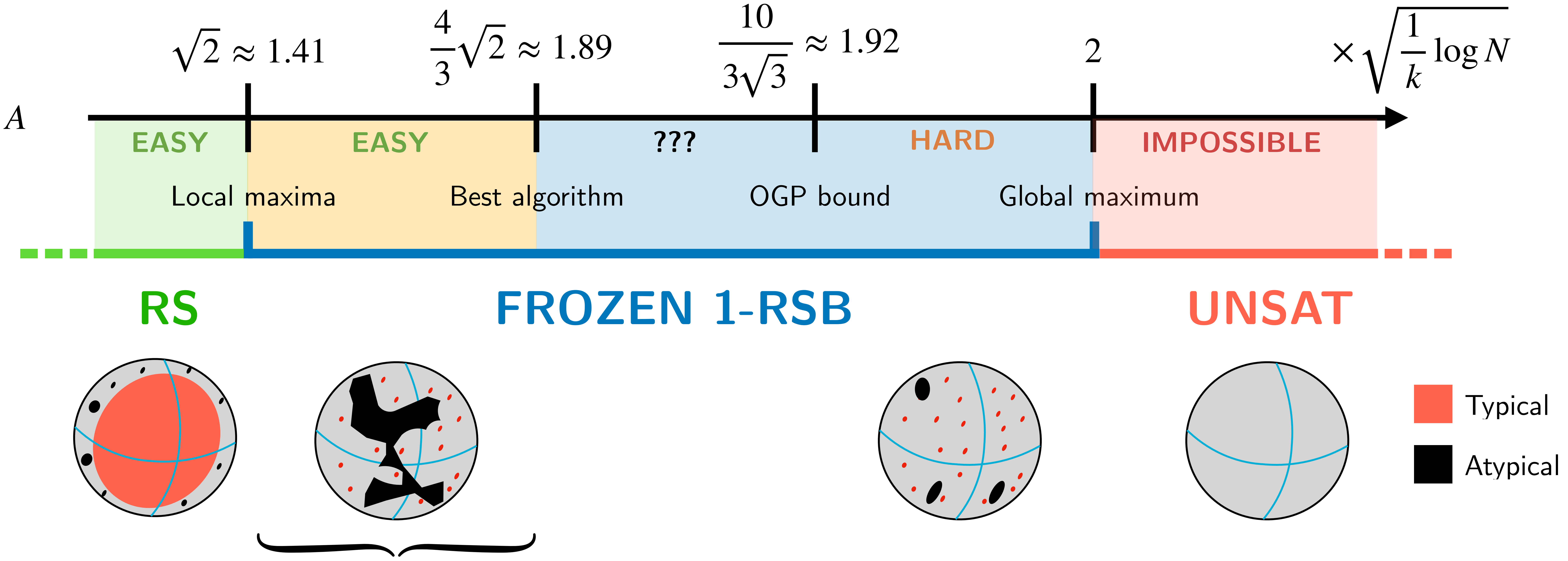
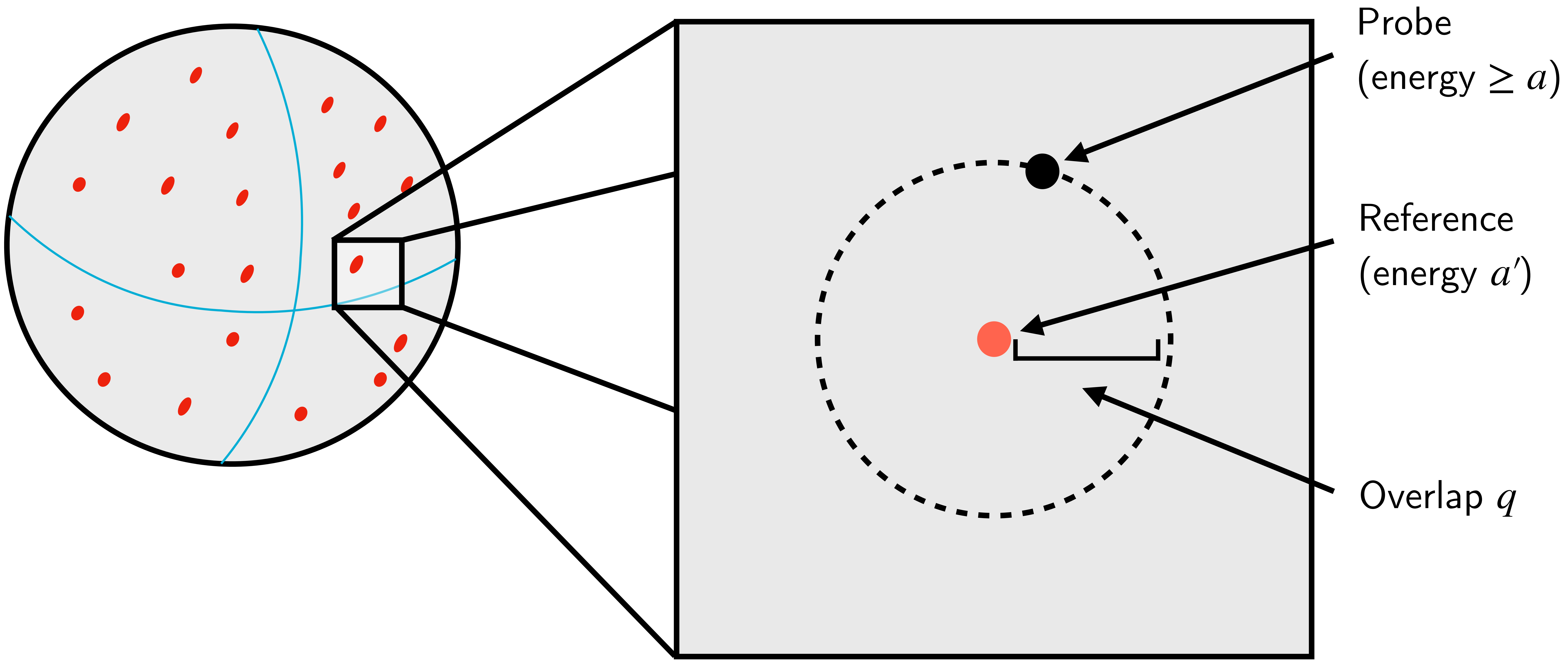


In binary perceptron: atypical clusters unfrozen + connected [1,2].

Is the same happening in this model? Need to look at non-equilibrium

[1] Baldassi et al. "Subdominant dense clusters allow for simple learning and high computational performance in neural networks with discrete synapses." (2015)
[2] Abbe, Li, Sly. "Binary perceptron: efficient algorithms can find solutions in a rare well-connected cluster." (2022)

Result: a first look at non-equilibrium properties



Franz-Parisi potential (For the curious: RS ansatz for probe, dynamical 1RSB ansatz for reference)

Entropy of probes (energy $\geq a$) at fixed overlap q with typical frozen states (energy a')

$\iff$ structure of super-level sets around typical frozen states

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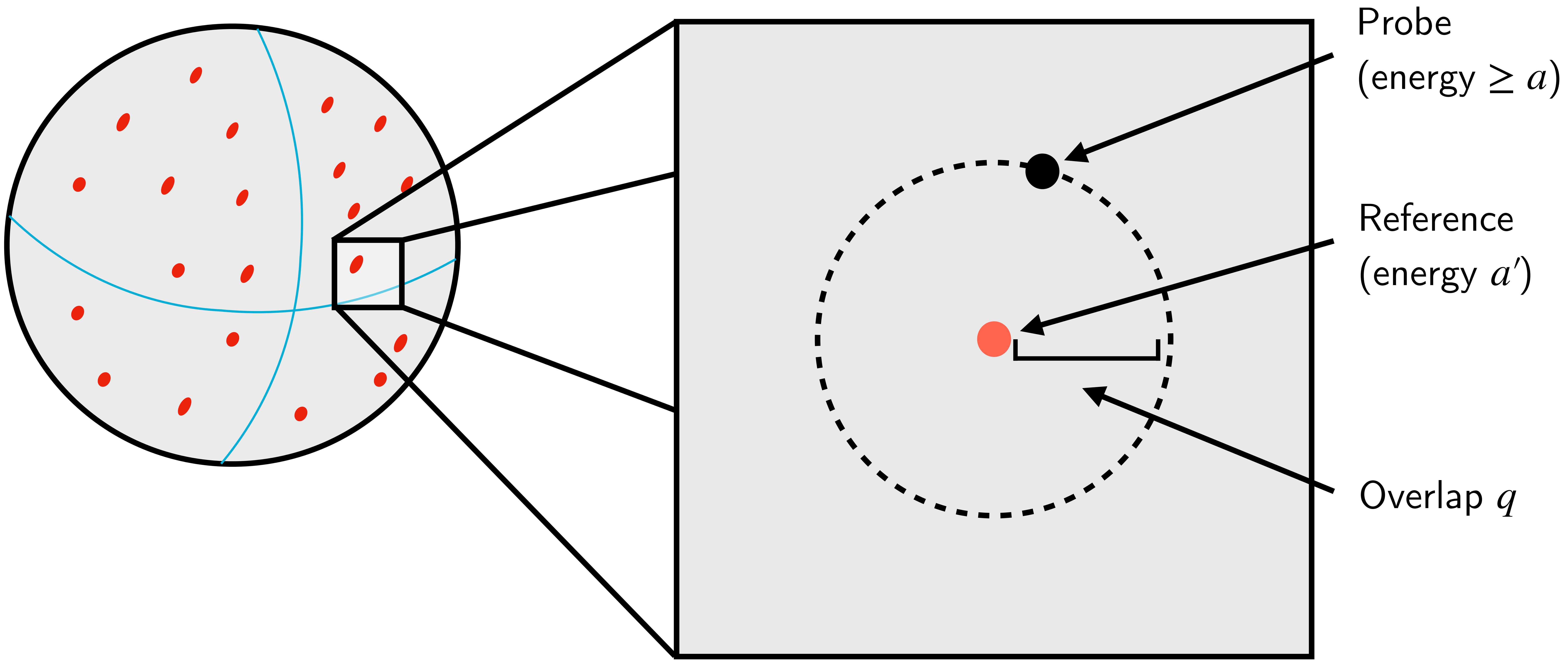

Only looks at surroundings of frozen clusters! Other atypical clusters could still exists!

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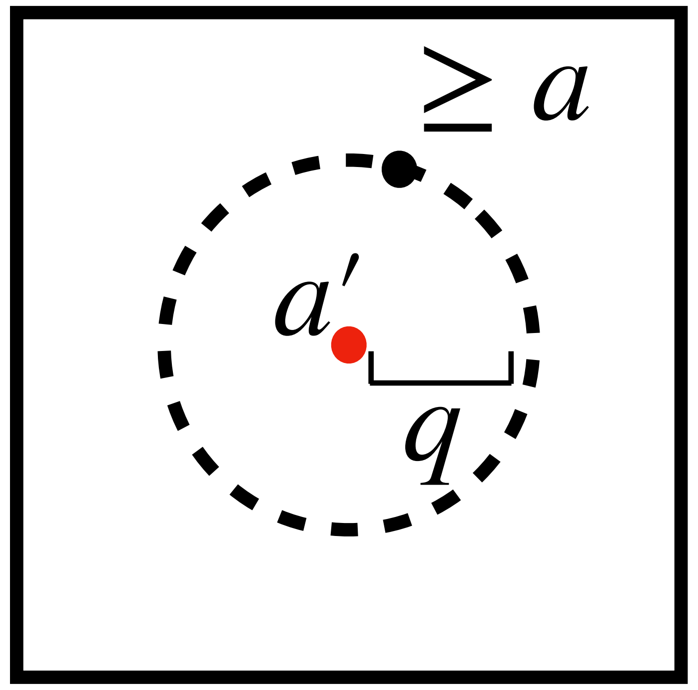
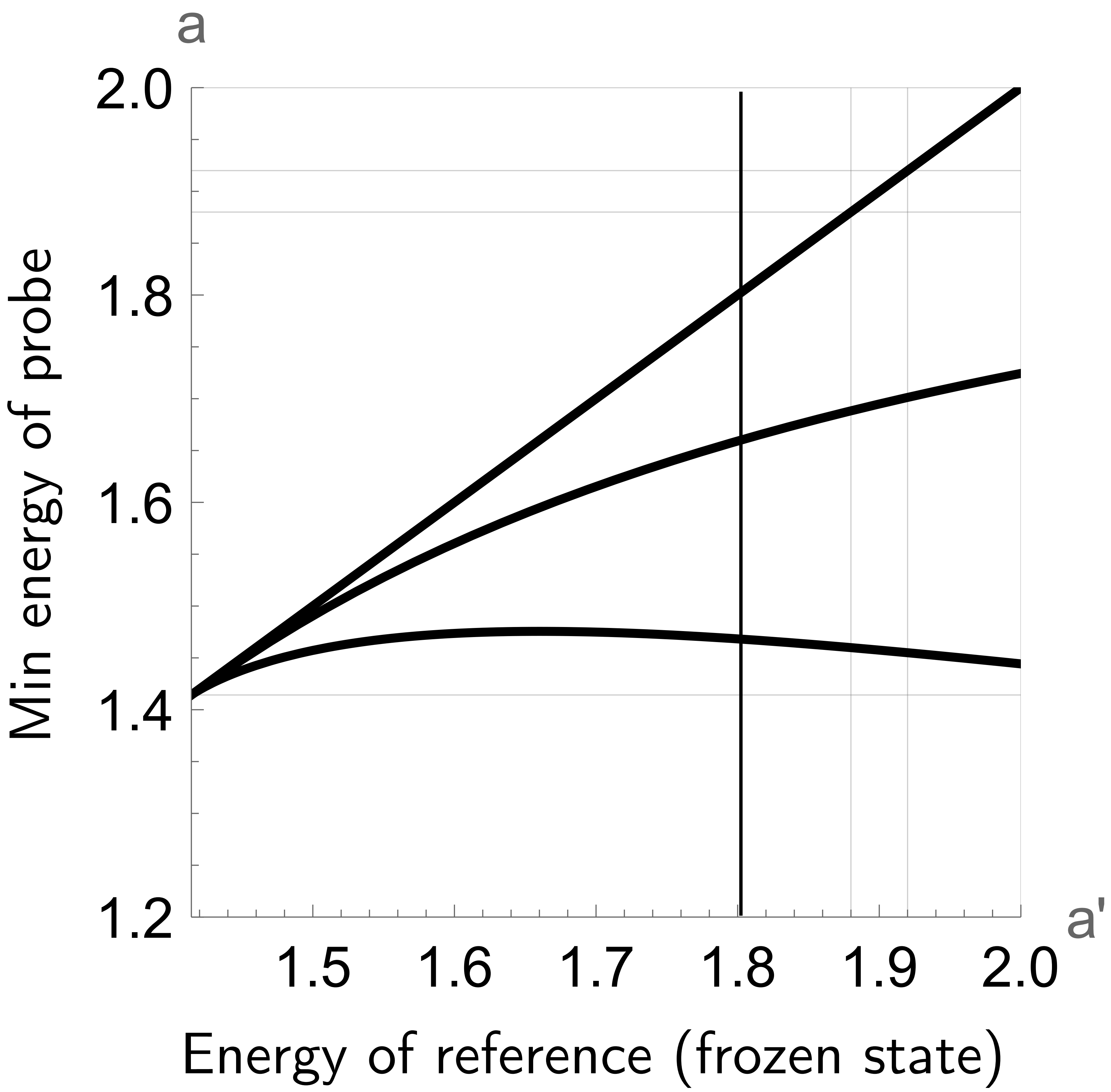
Result: Planted clusters in superlevel sets



Fix one typical frozen state (energy a'). Compute entropy of probes at all energies $\geq a$ and at fixed overlap $q \implies$ planted cluster



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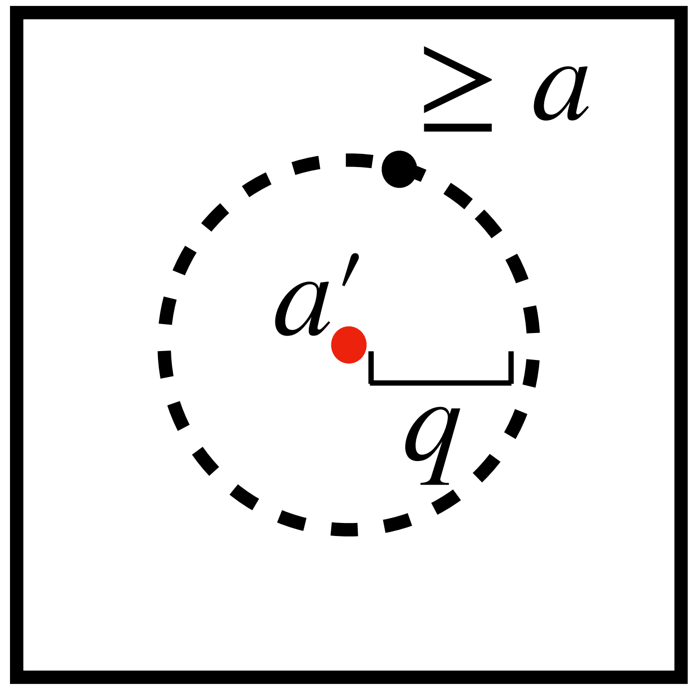

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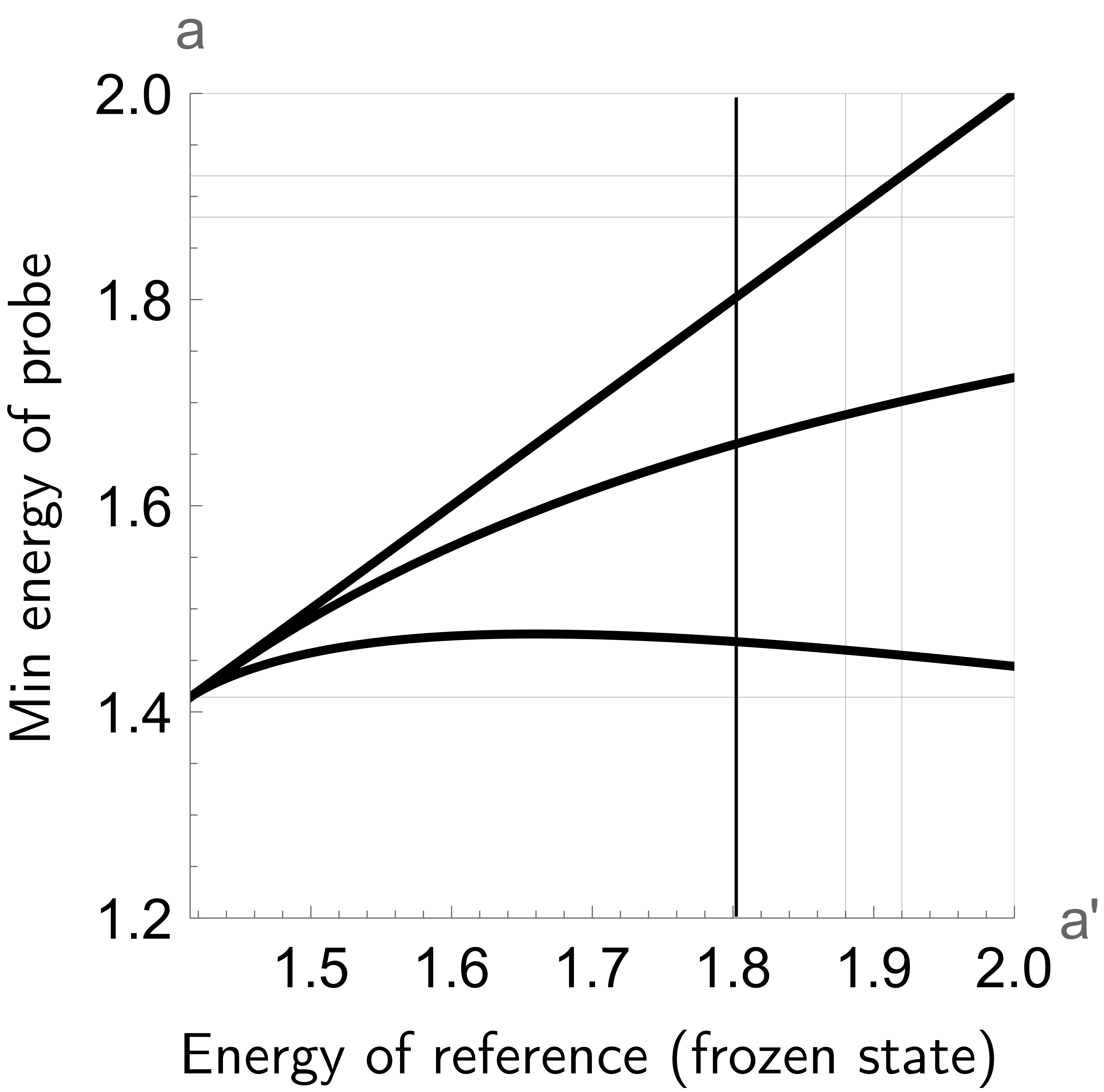

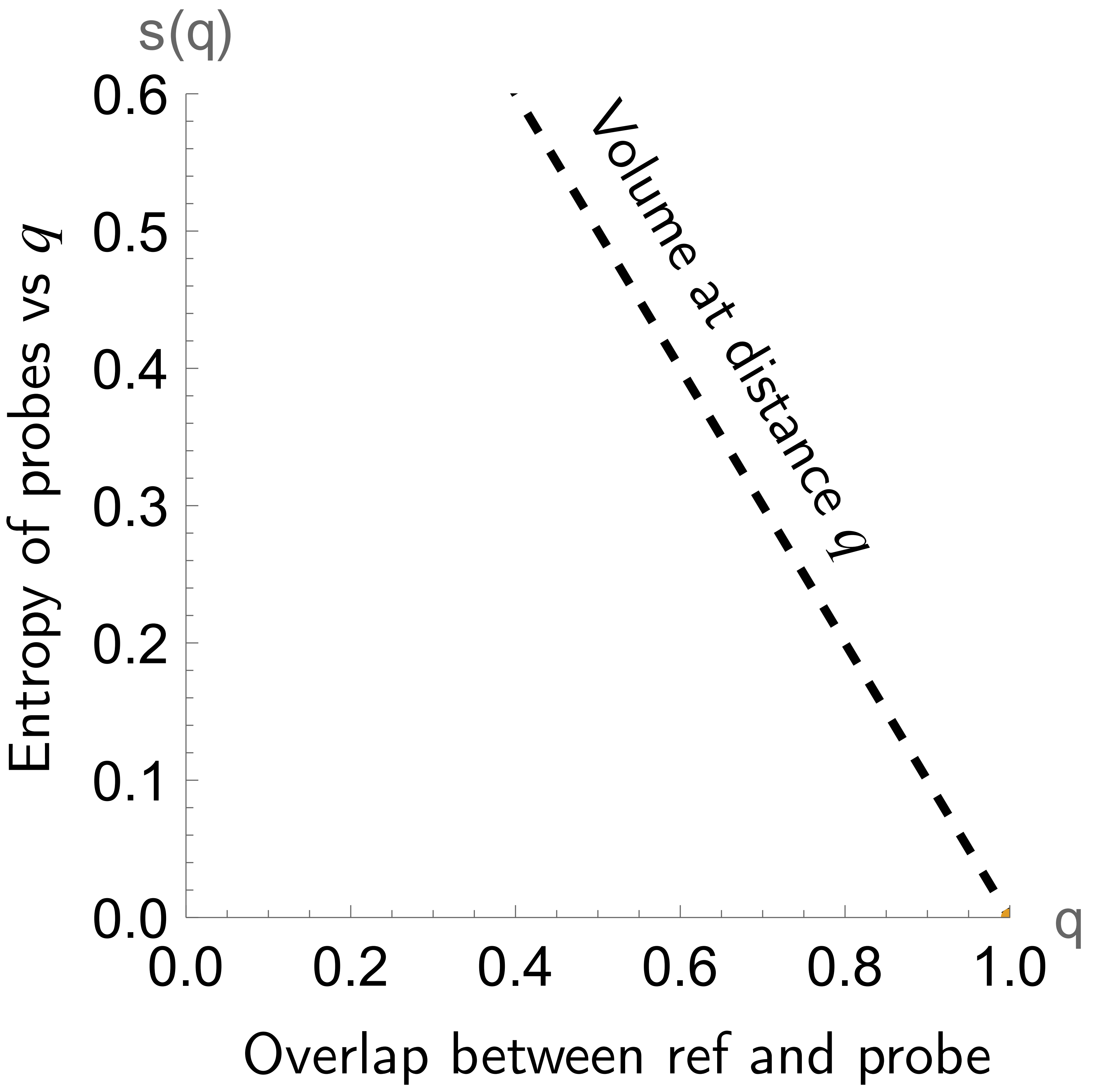

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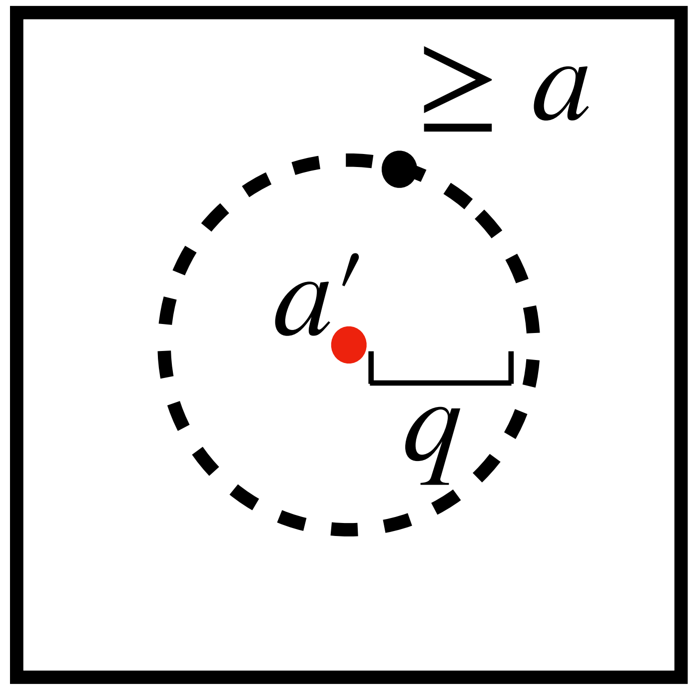

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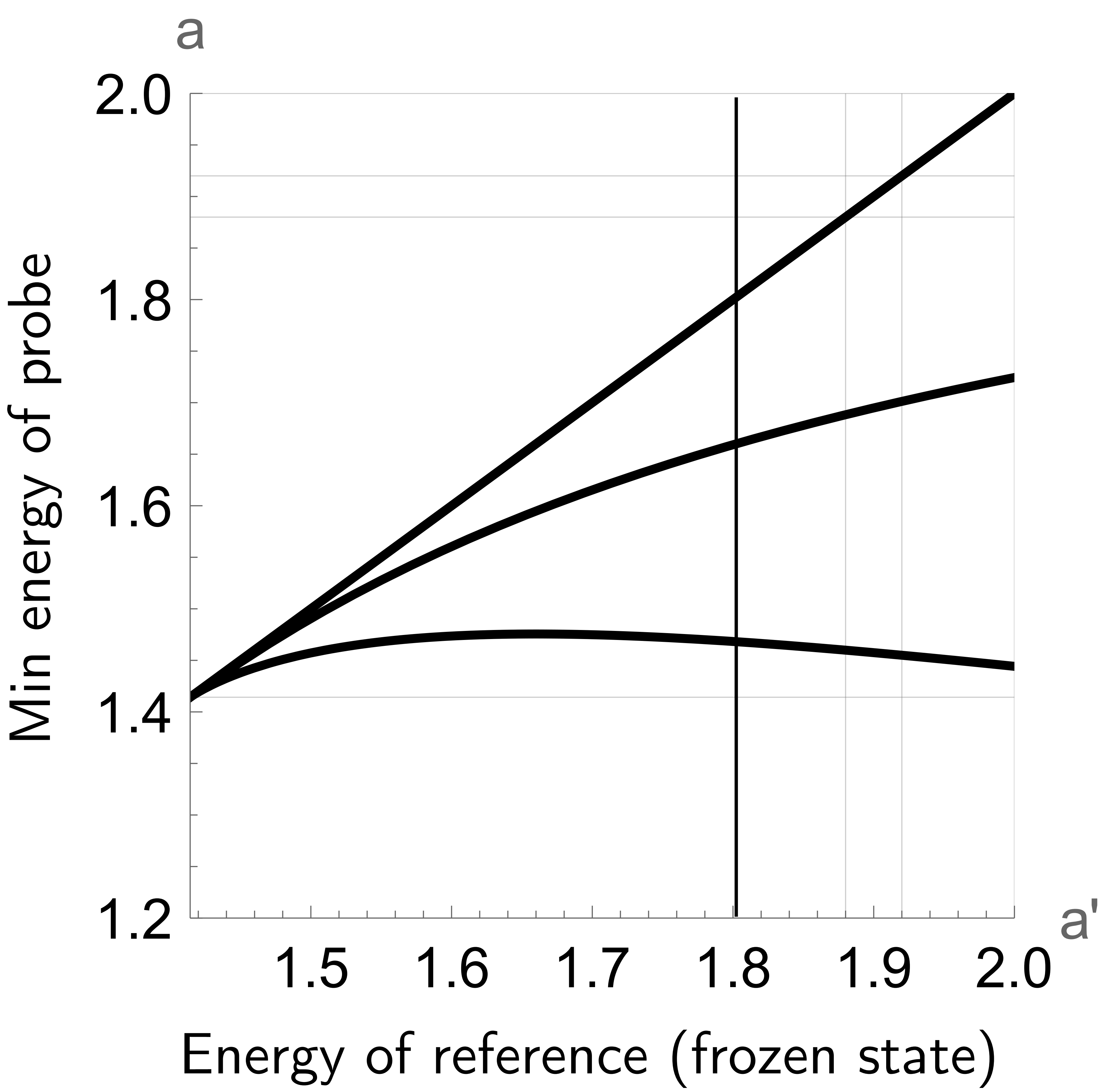

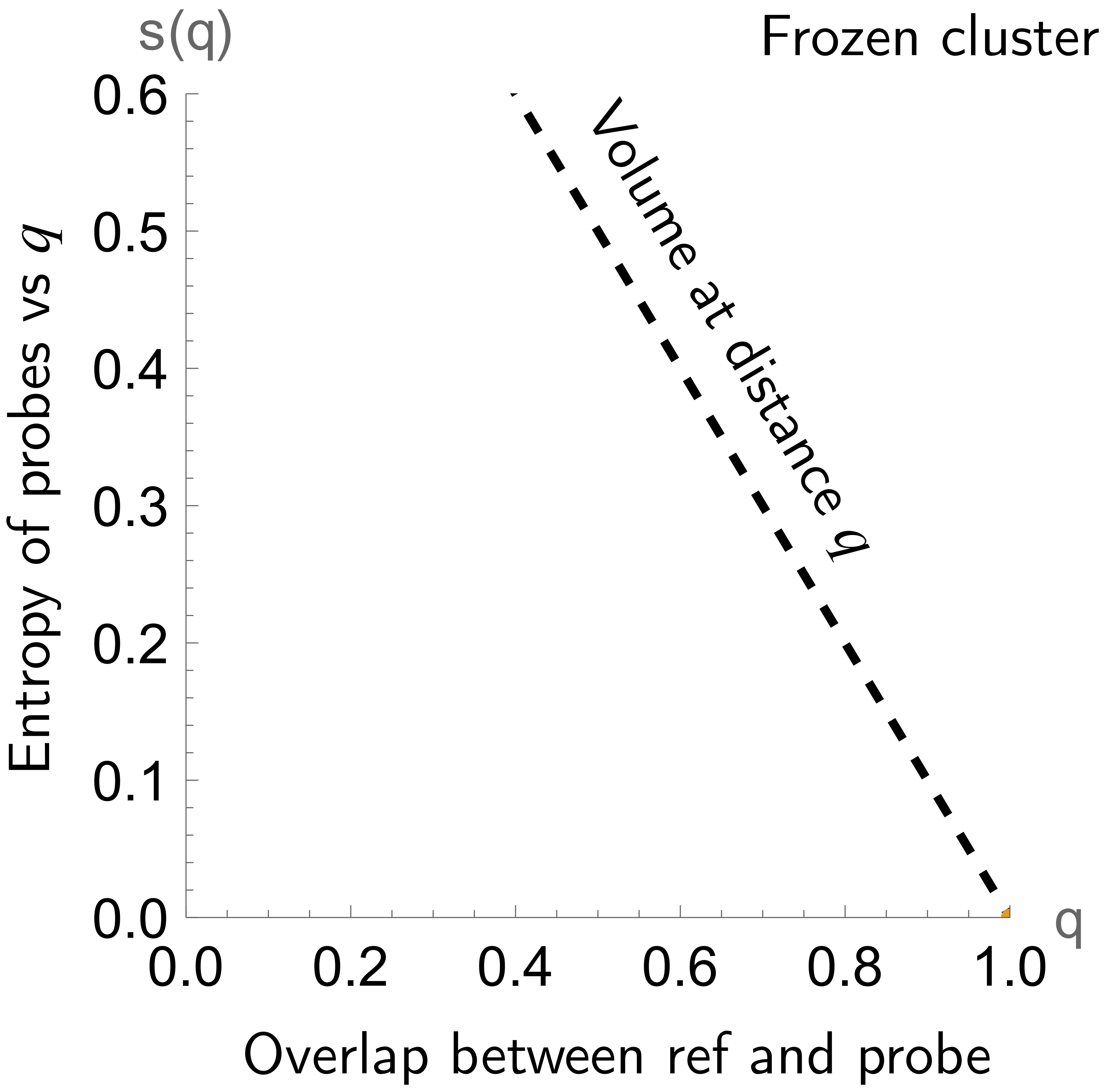

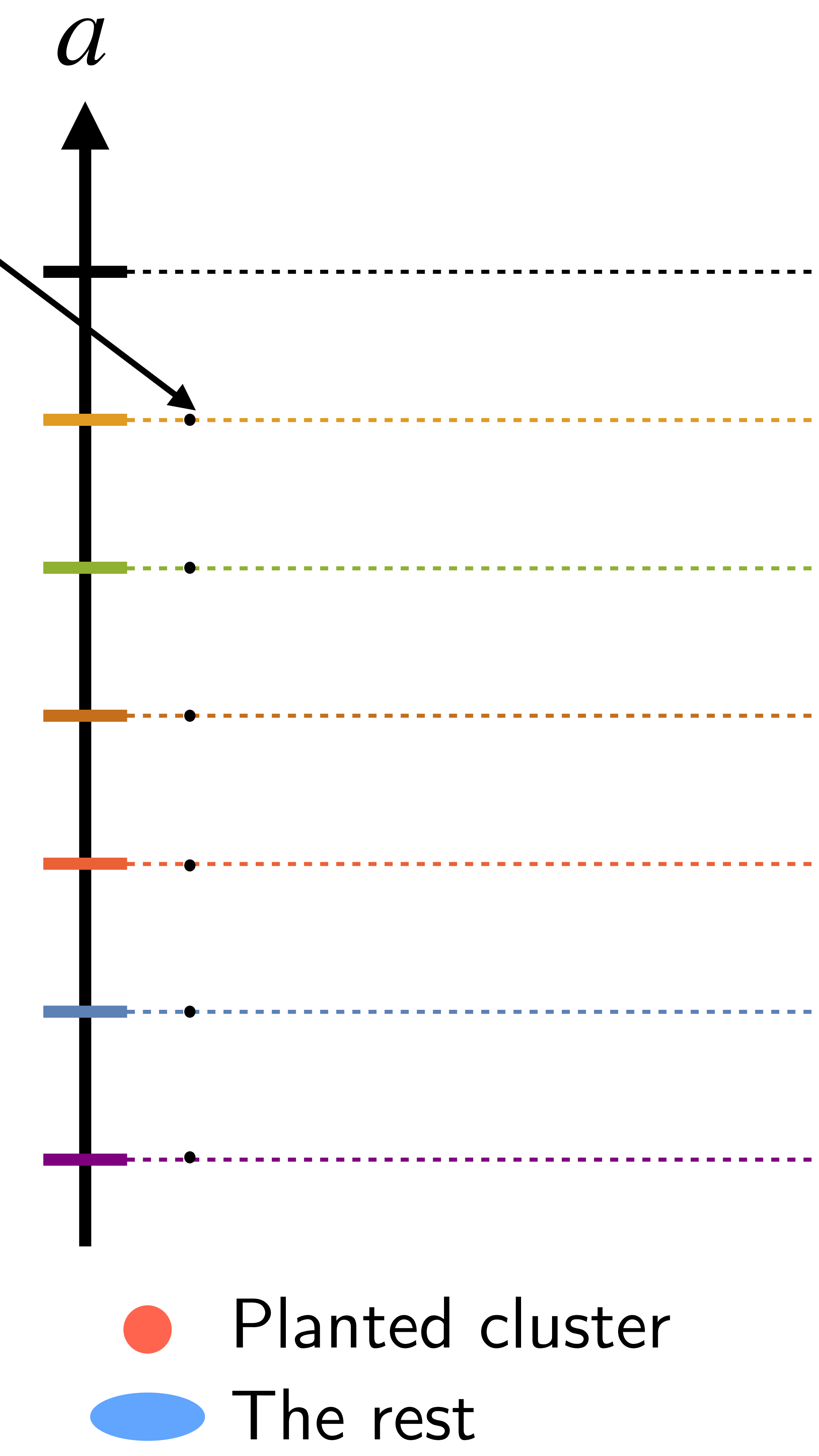

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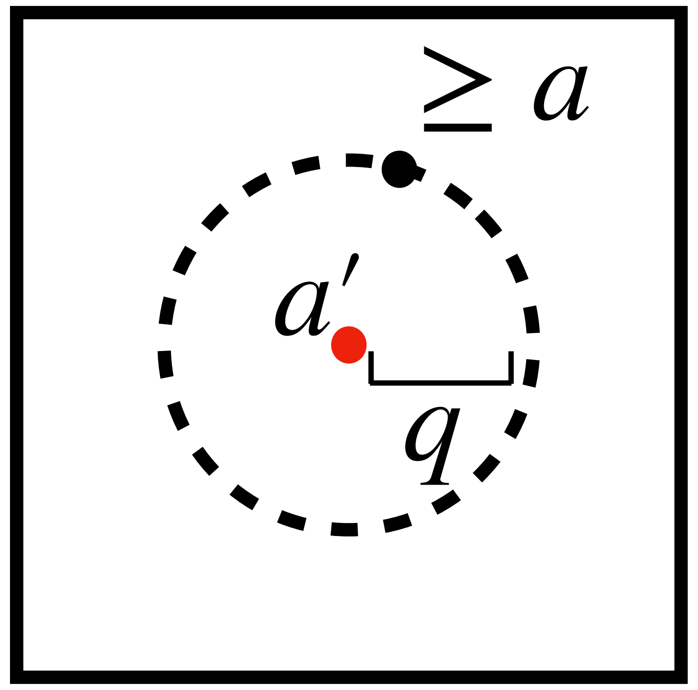

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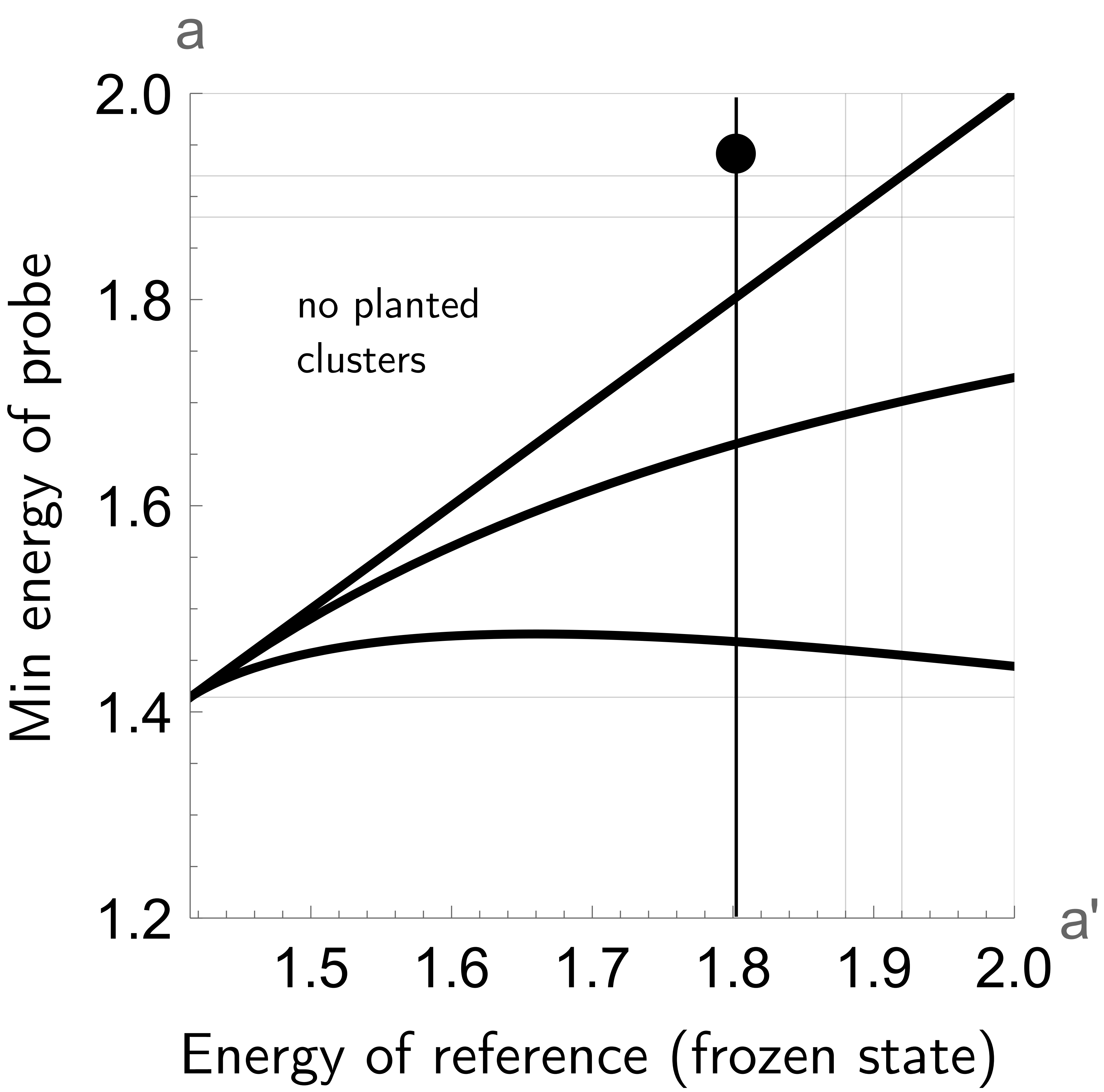

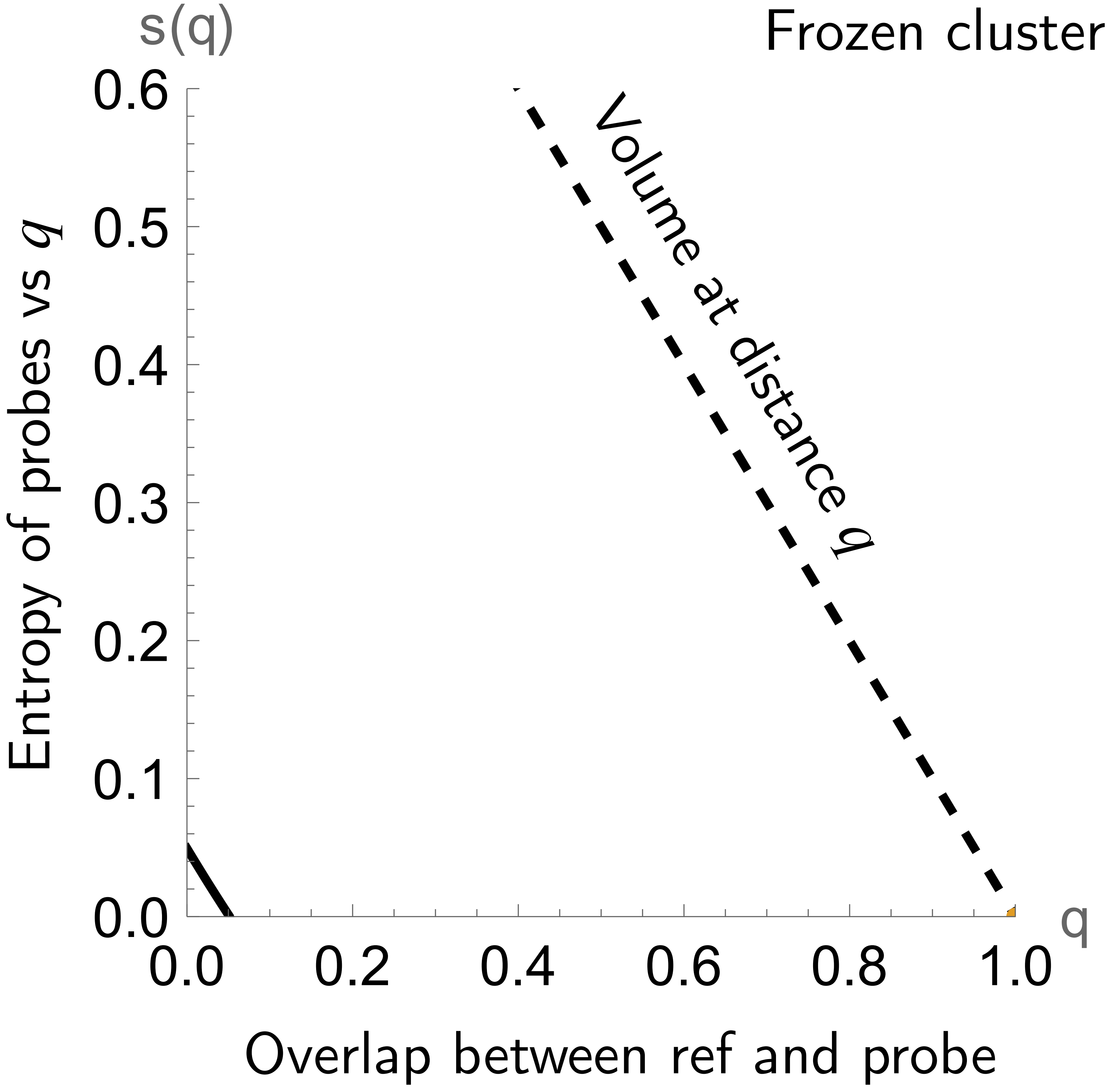

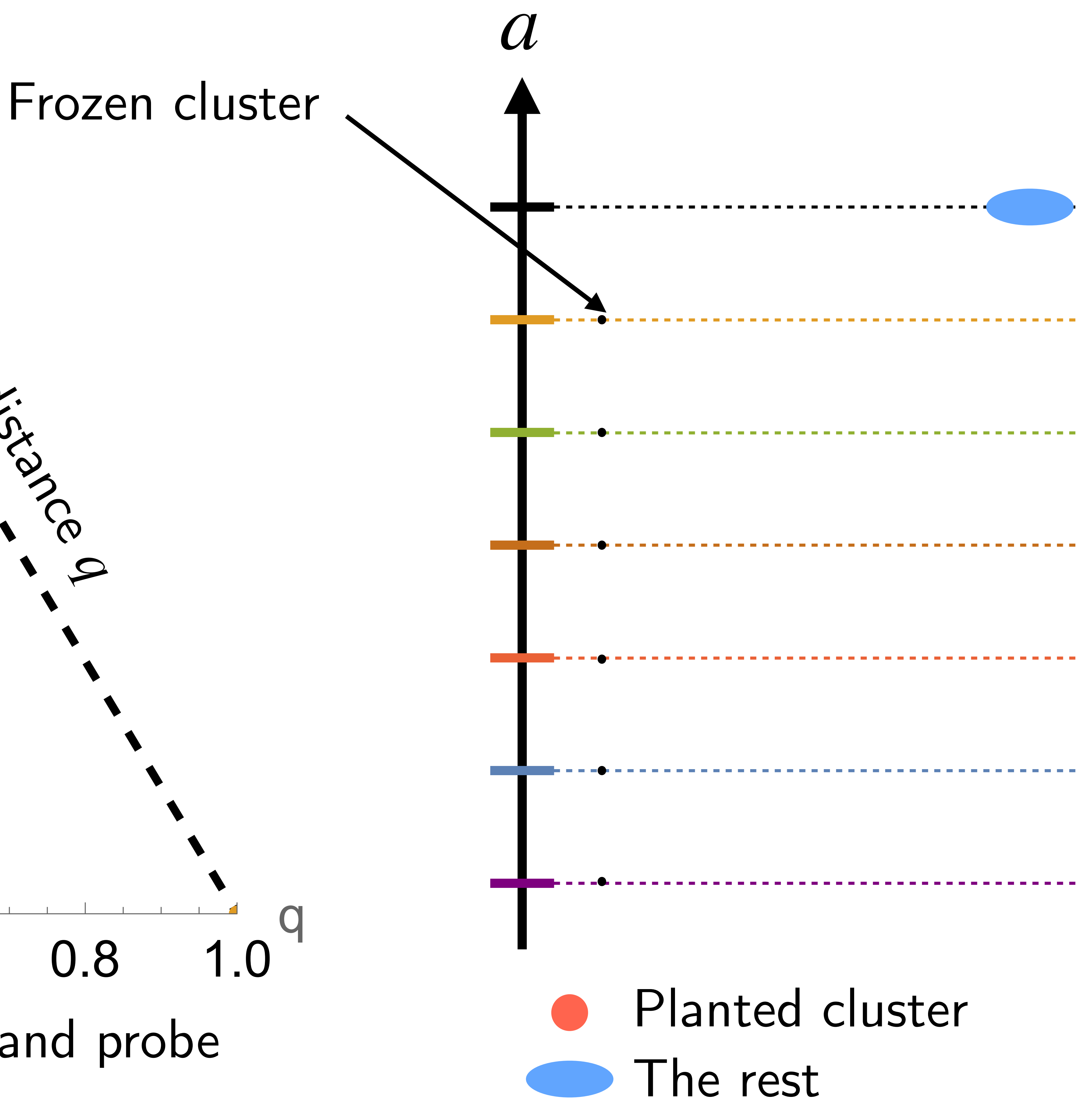

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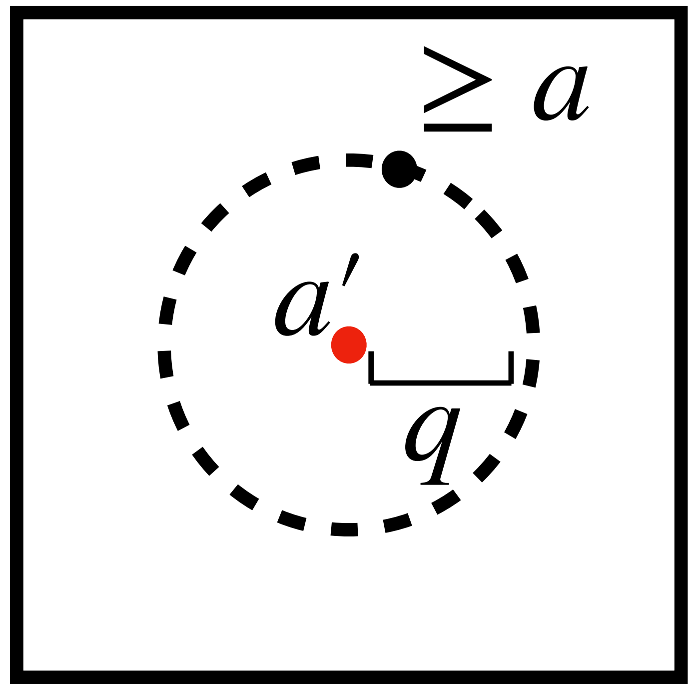

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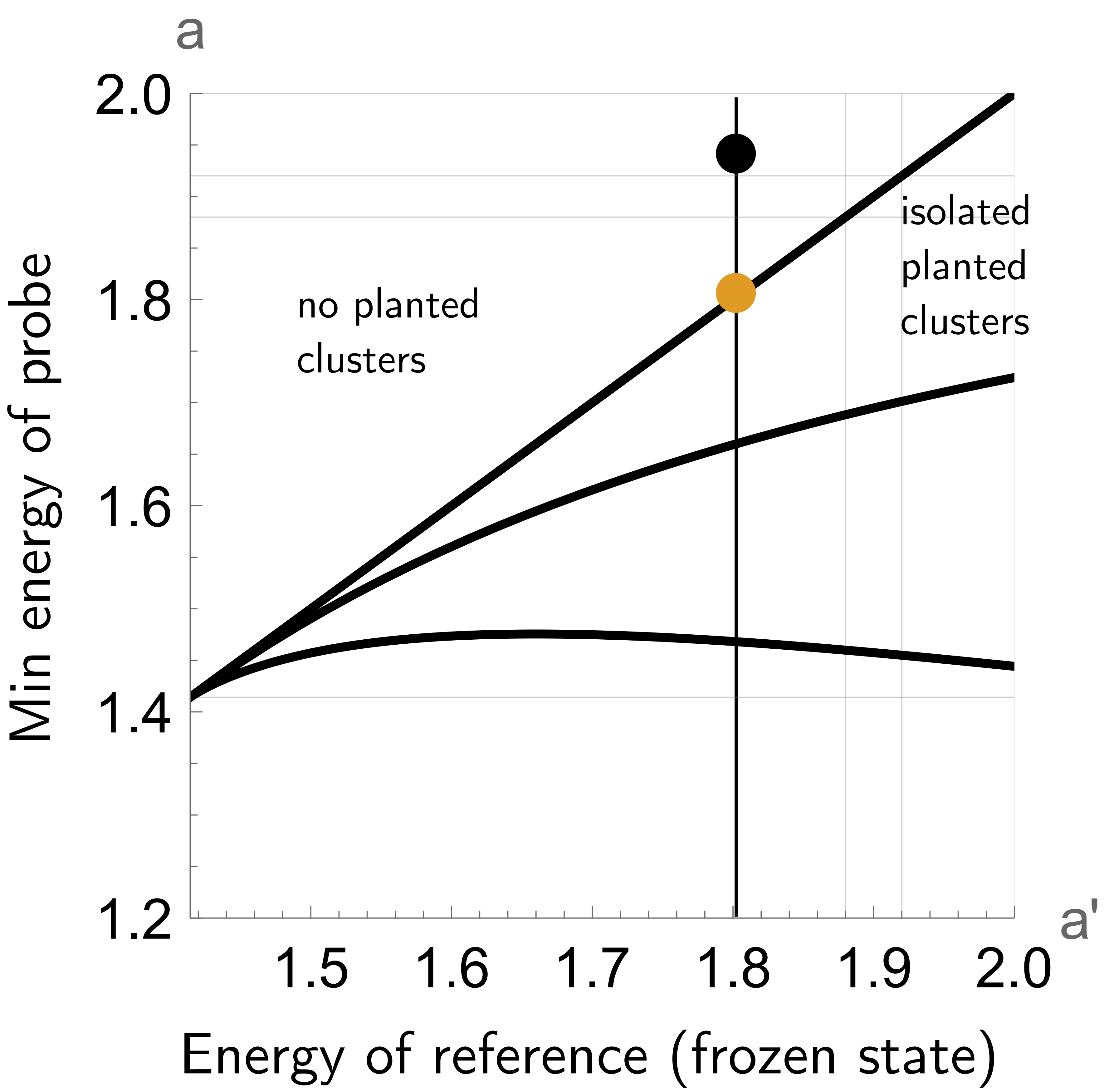
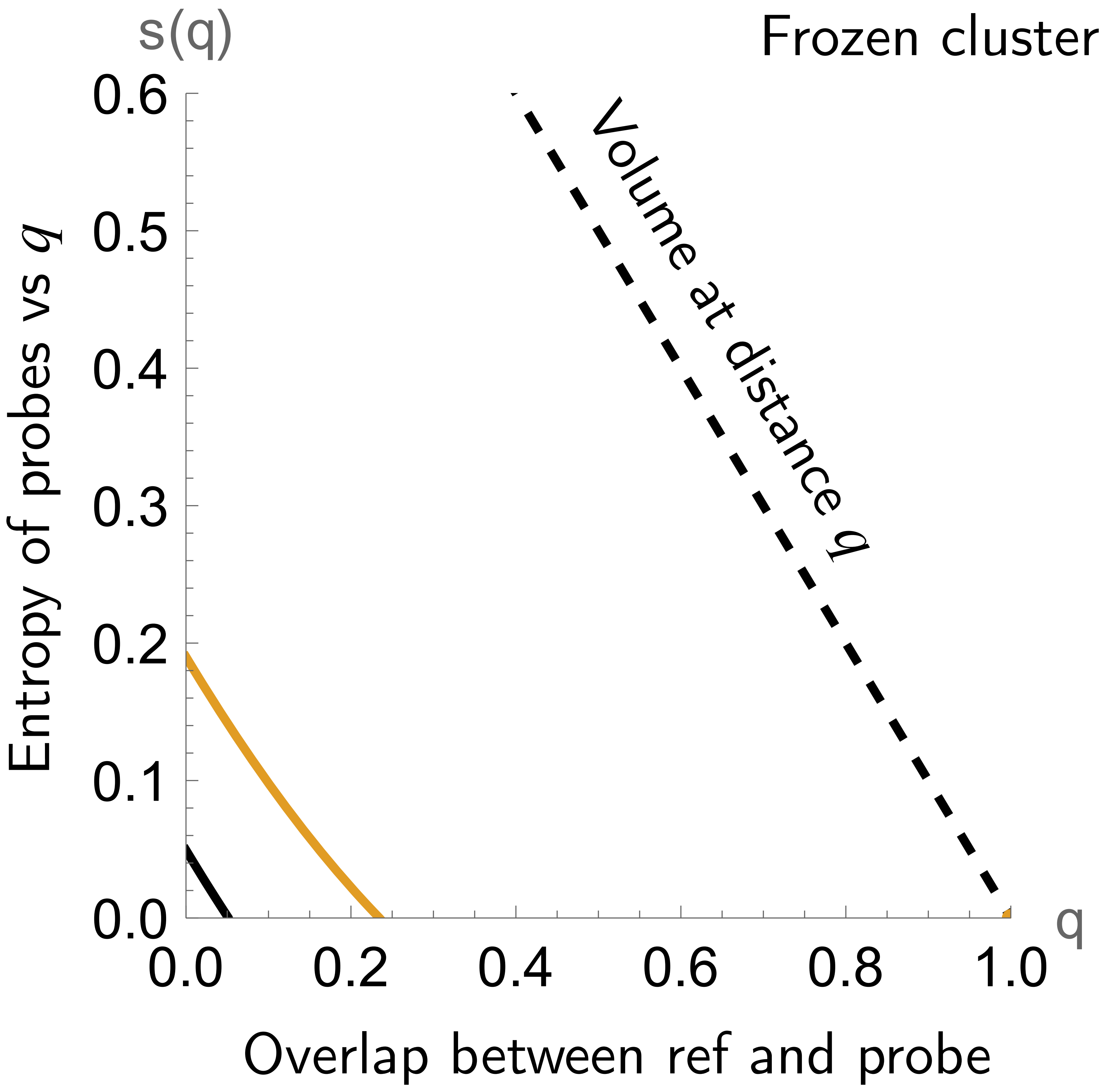
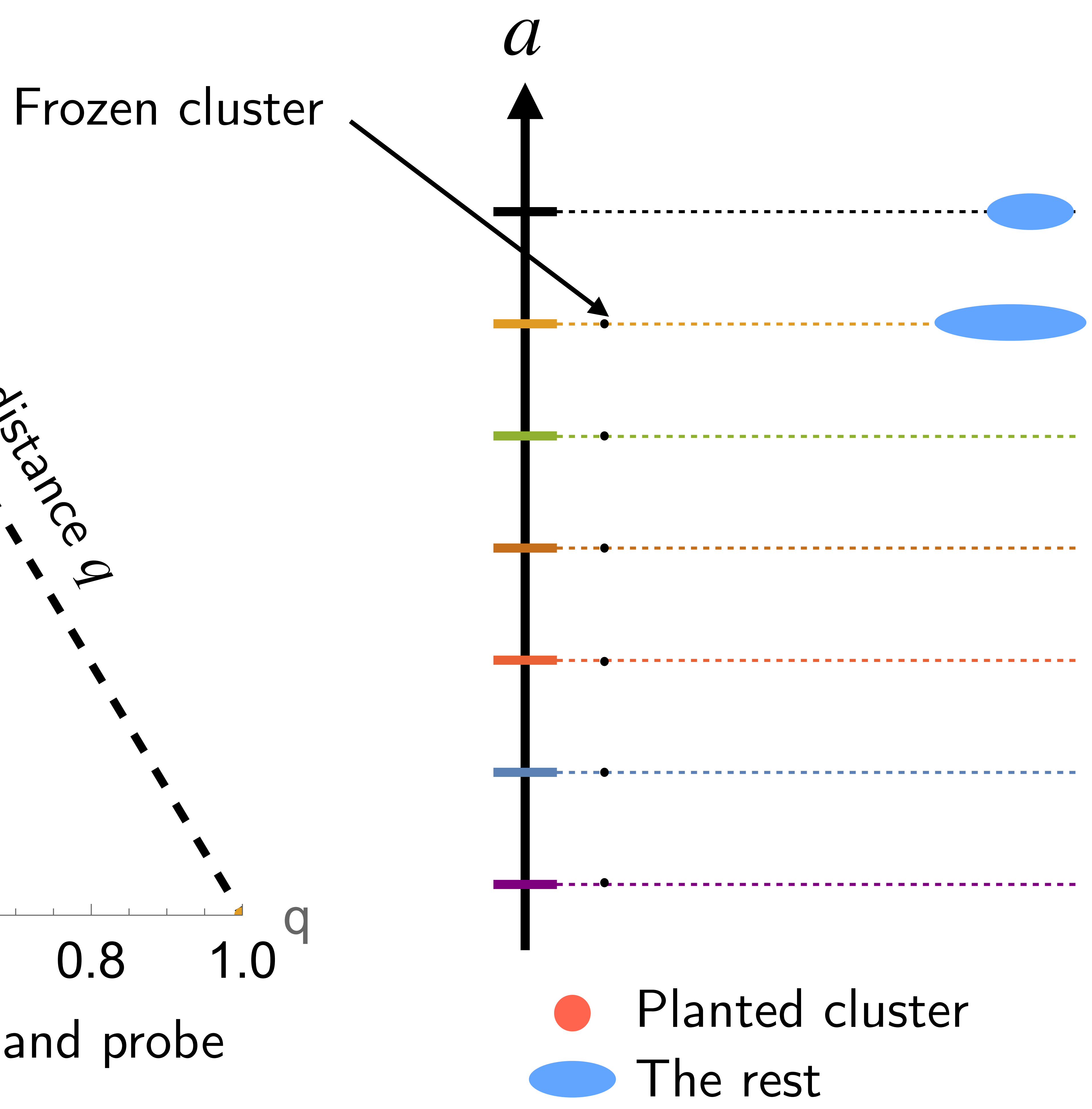
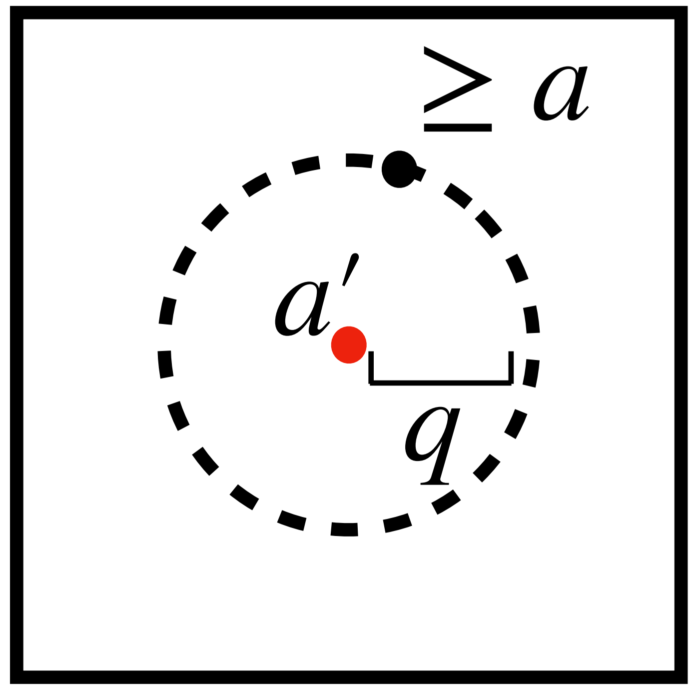






Result: Planted clusters in superlevel sets



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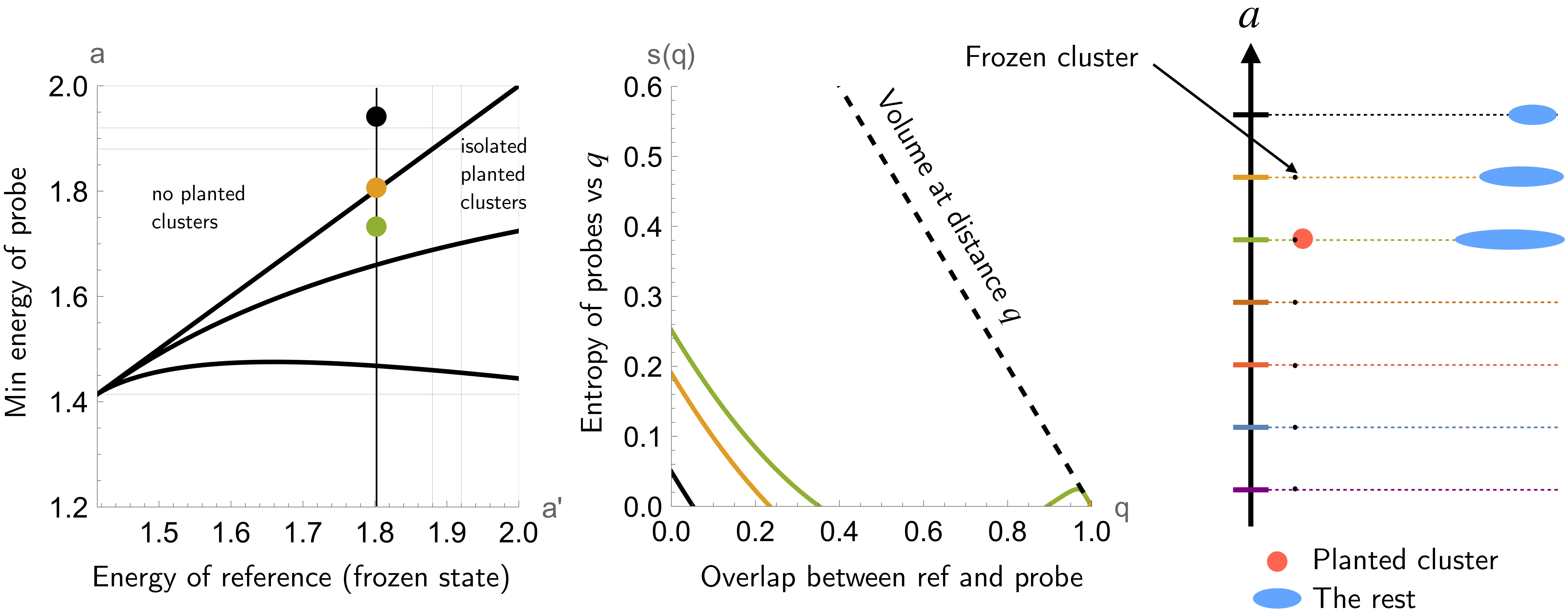

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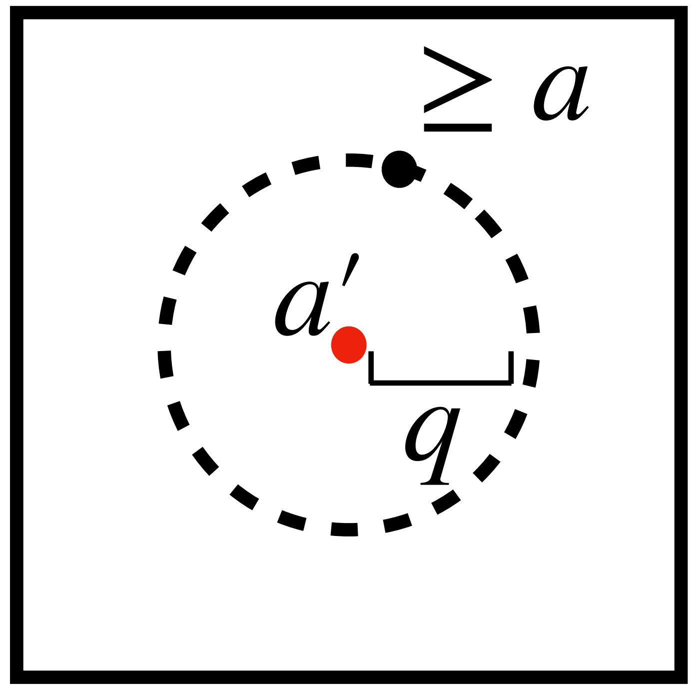

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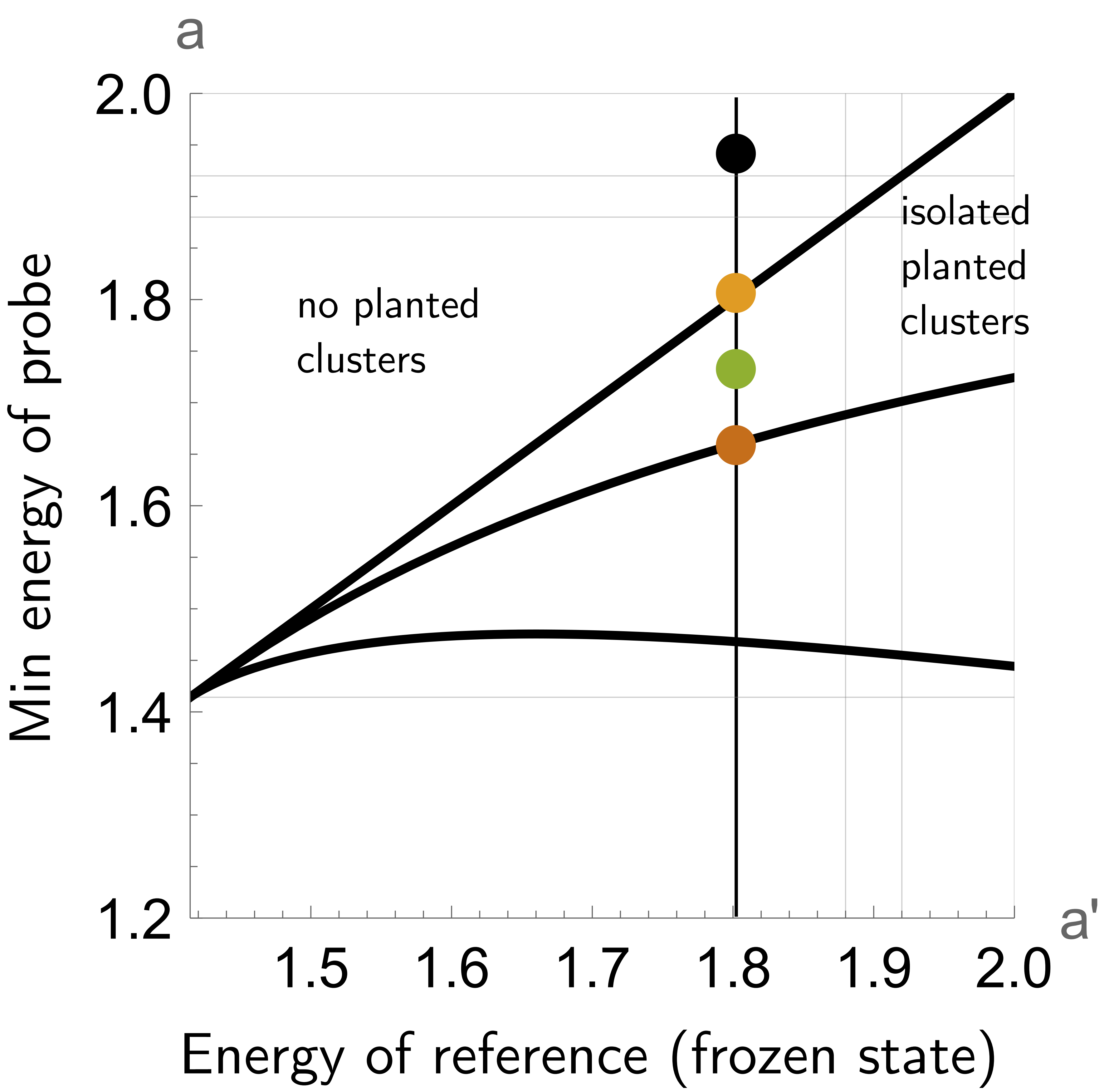

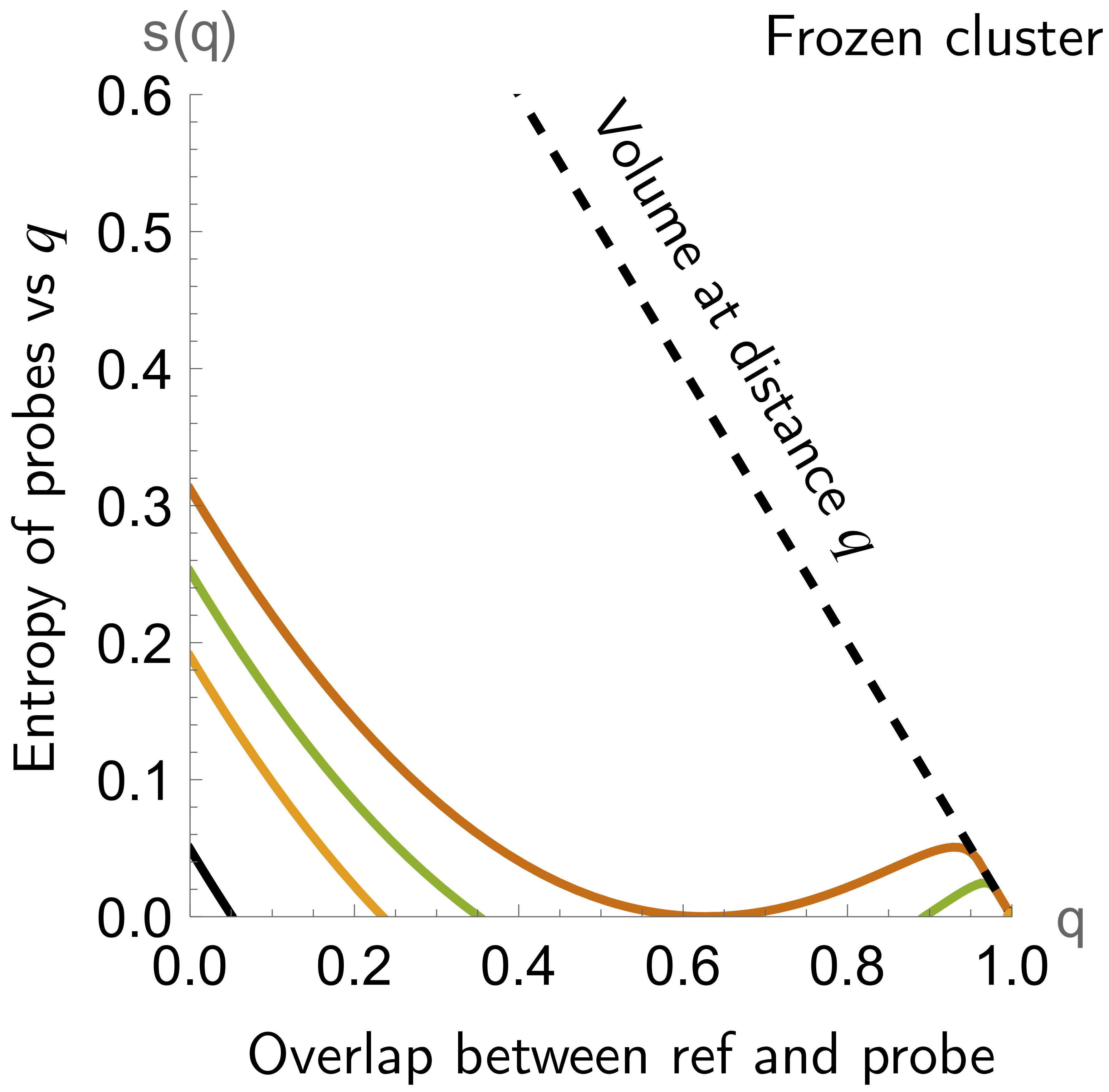

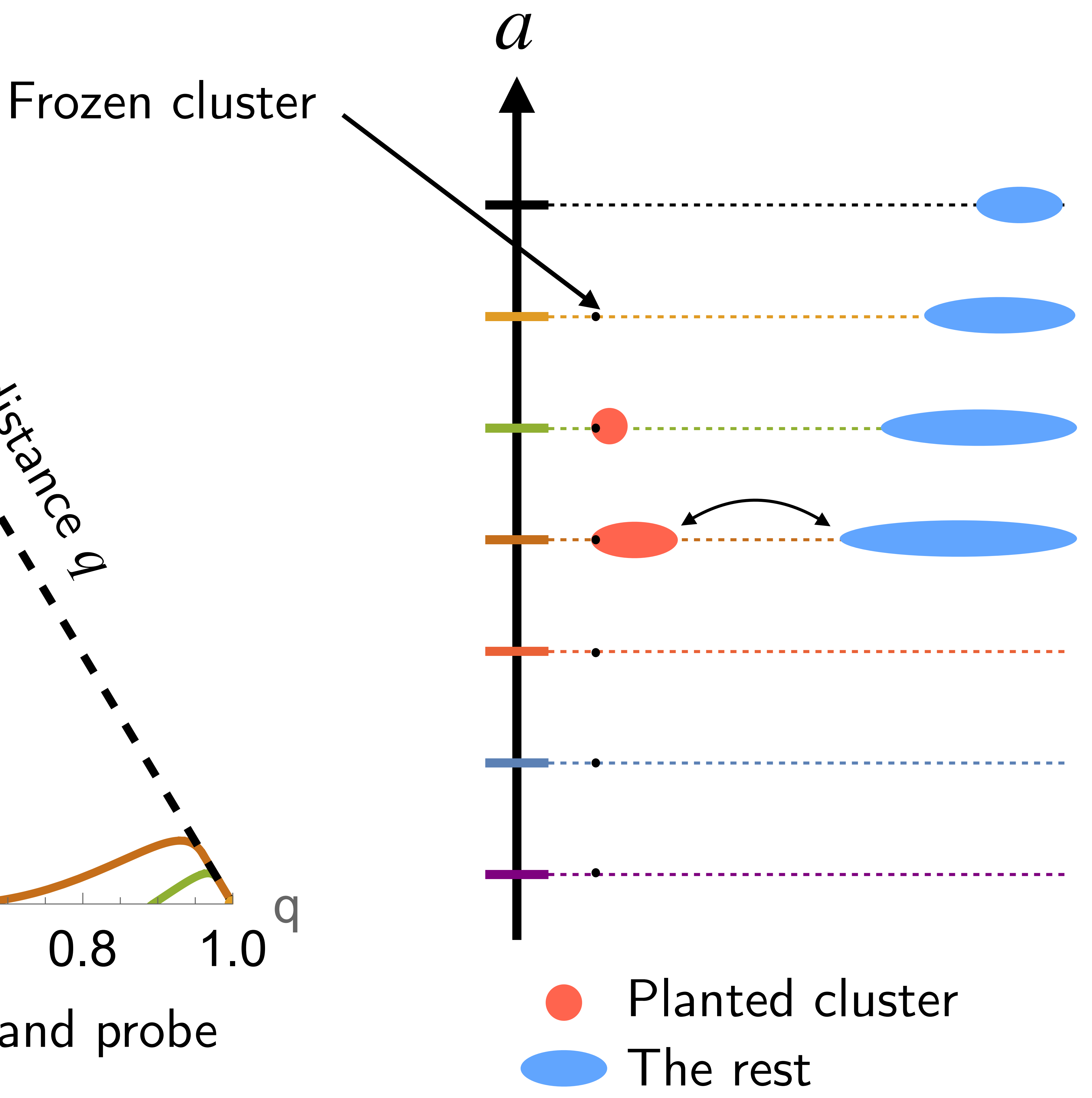

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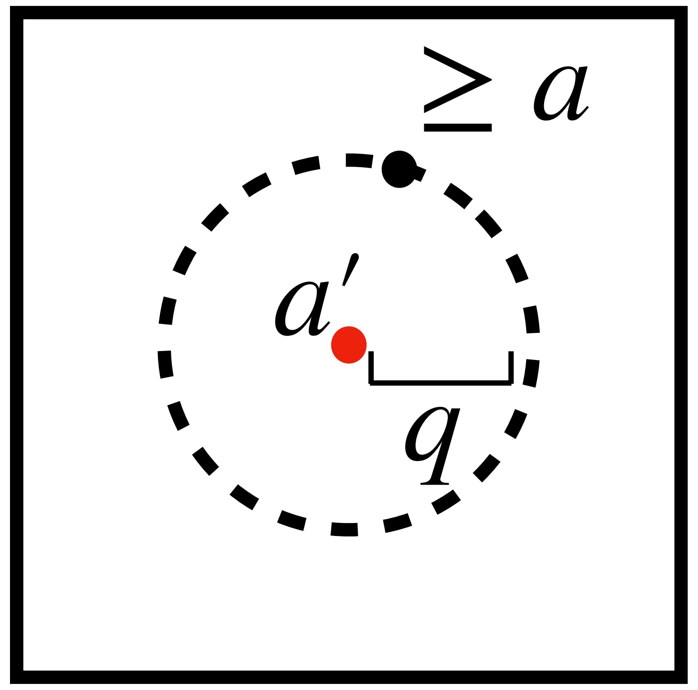

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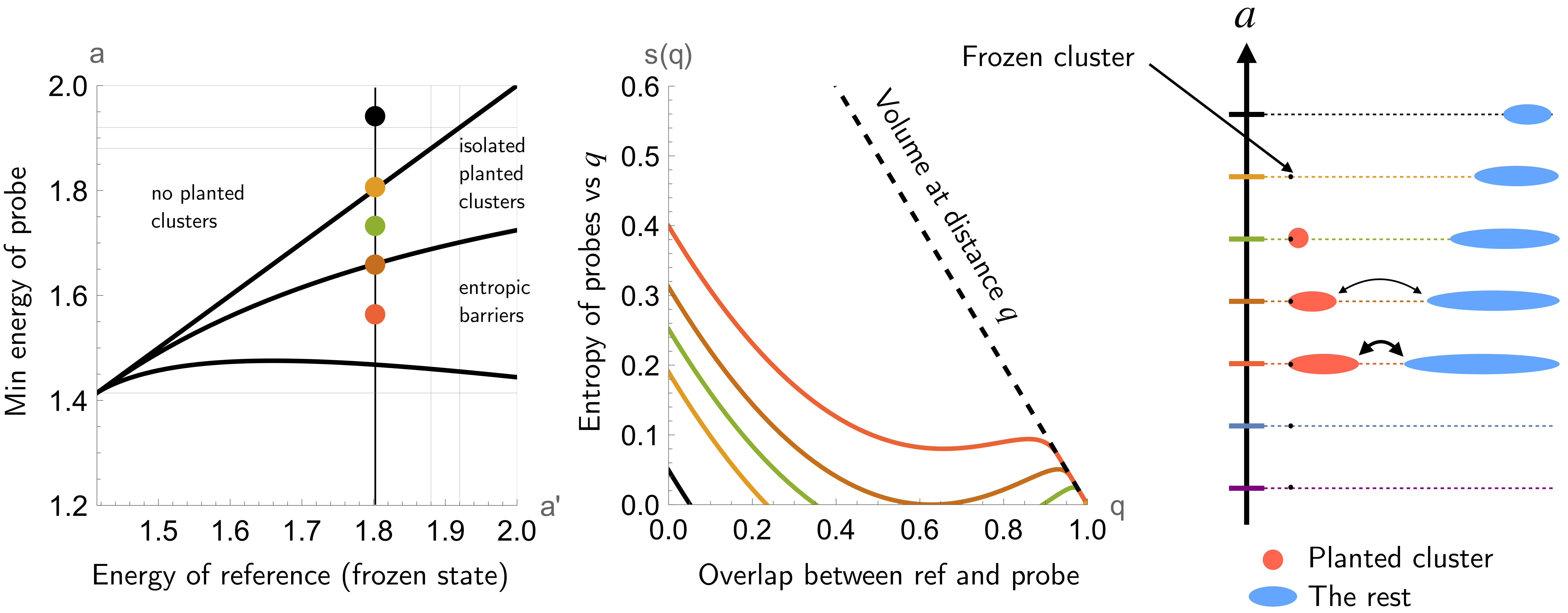

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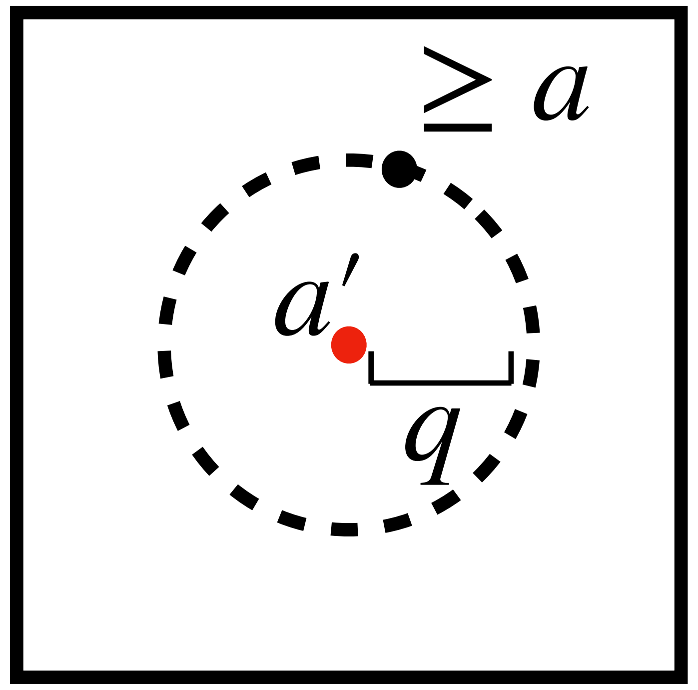

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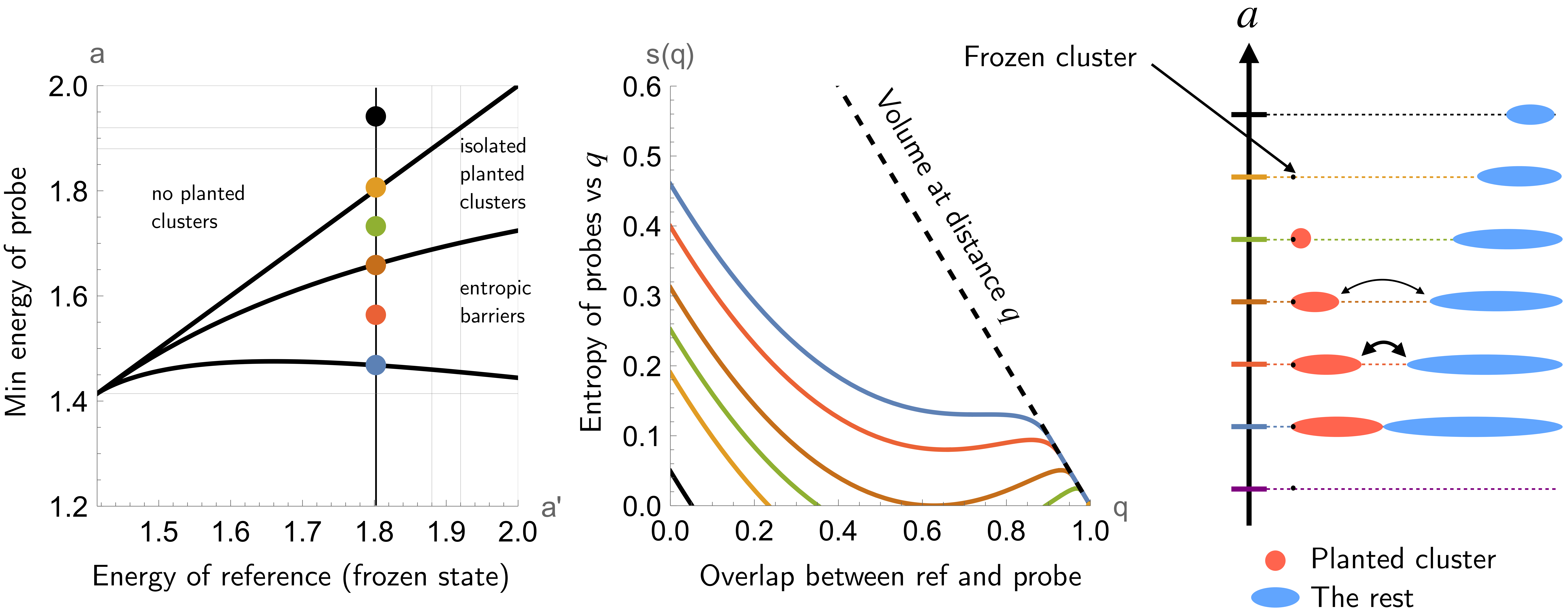

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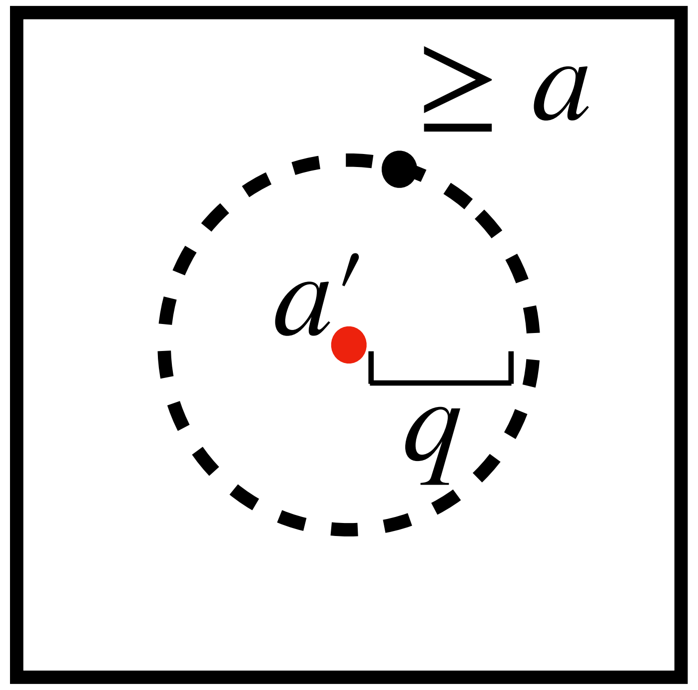

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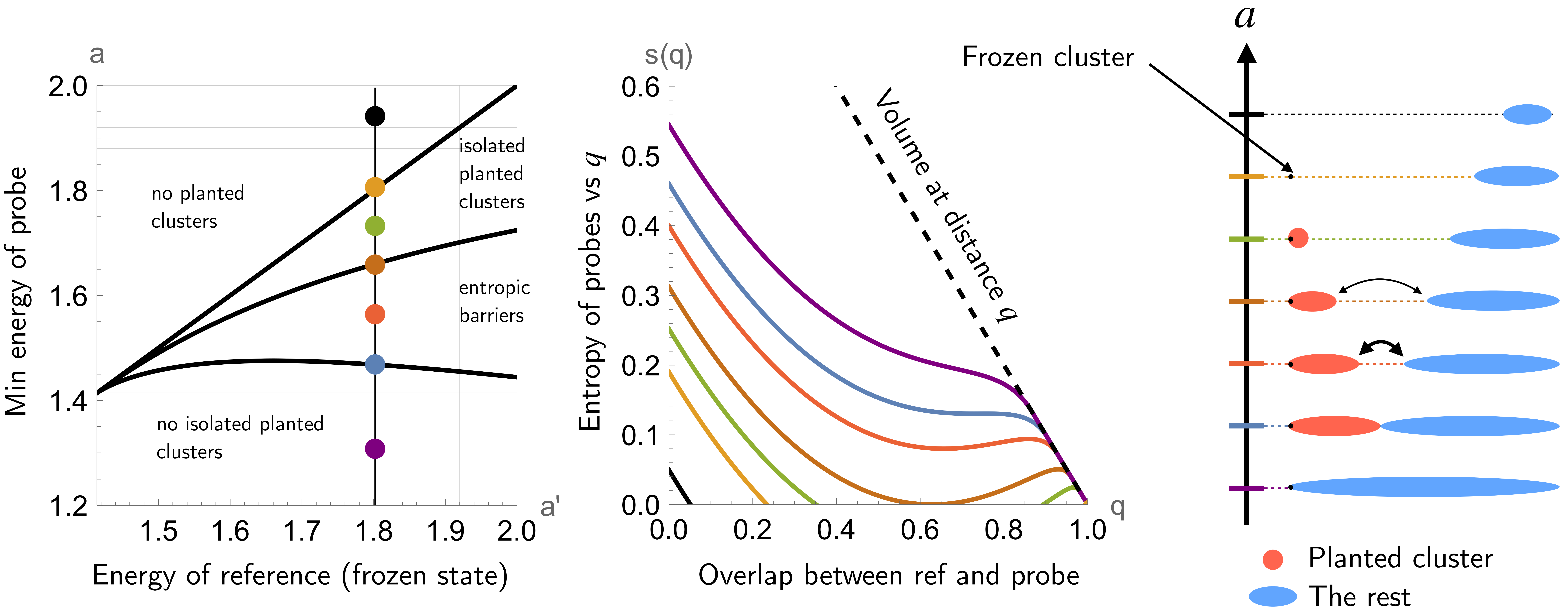
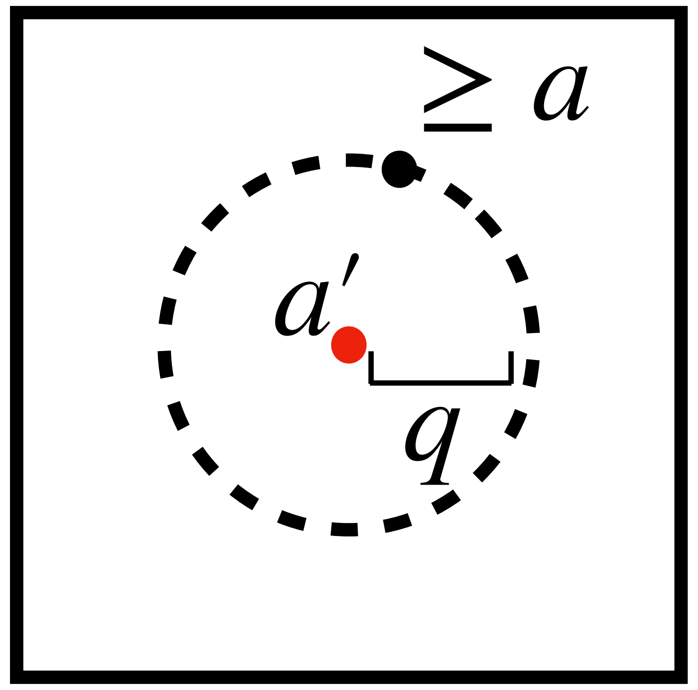
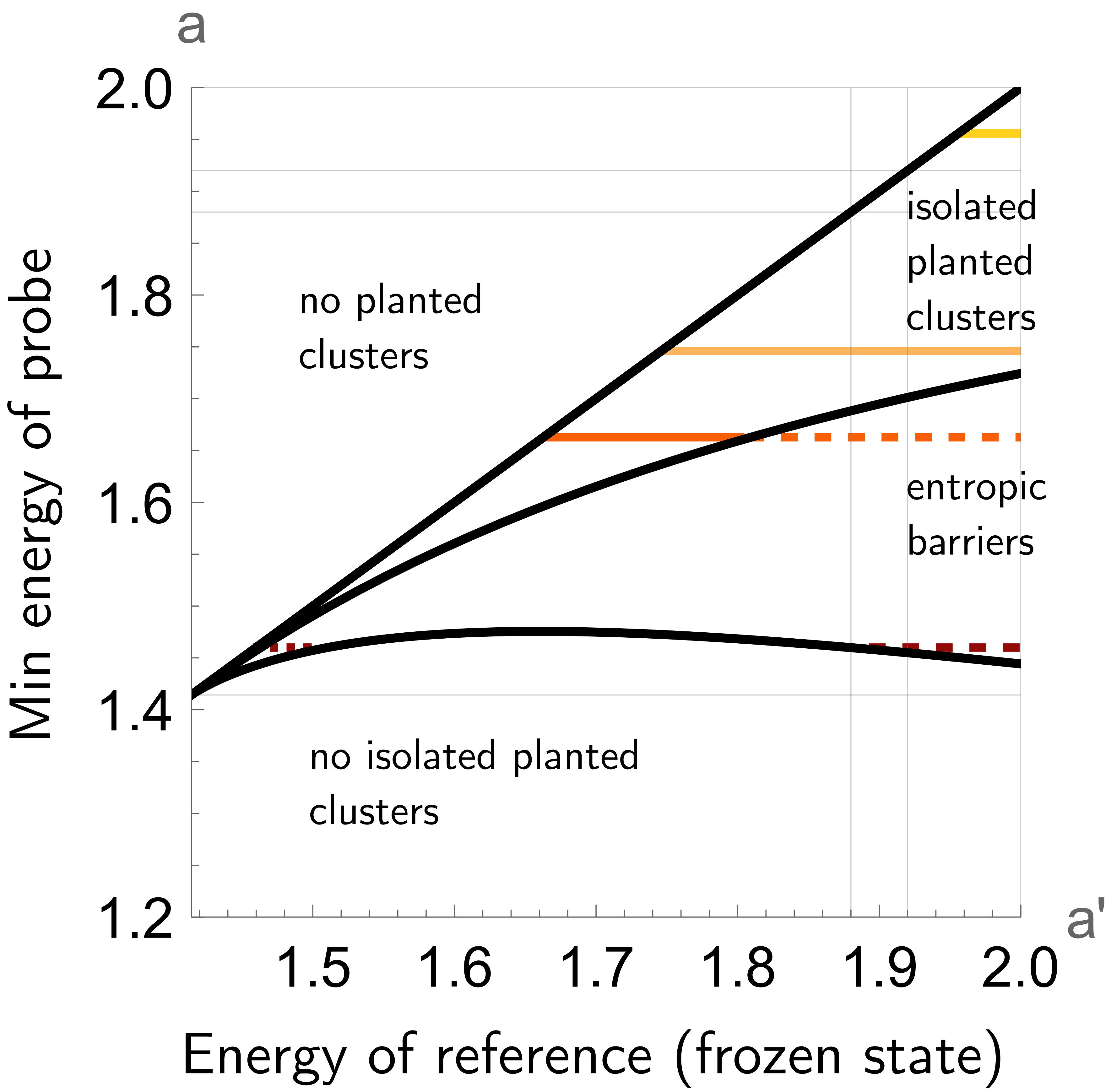


Result: Complexity vs Entropy



Fix energy super-level of probes (energy $\geq a$)

How many planted clusters are there in the super-level, and how large?



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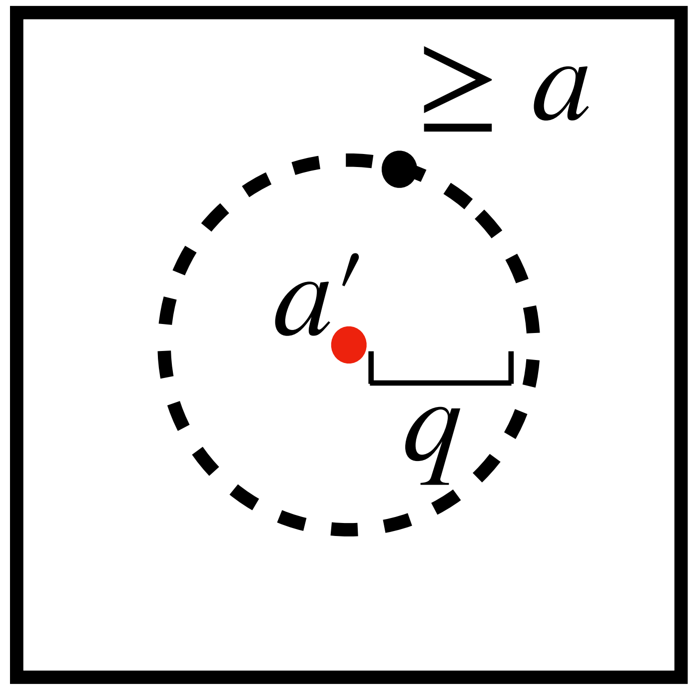

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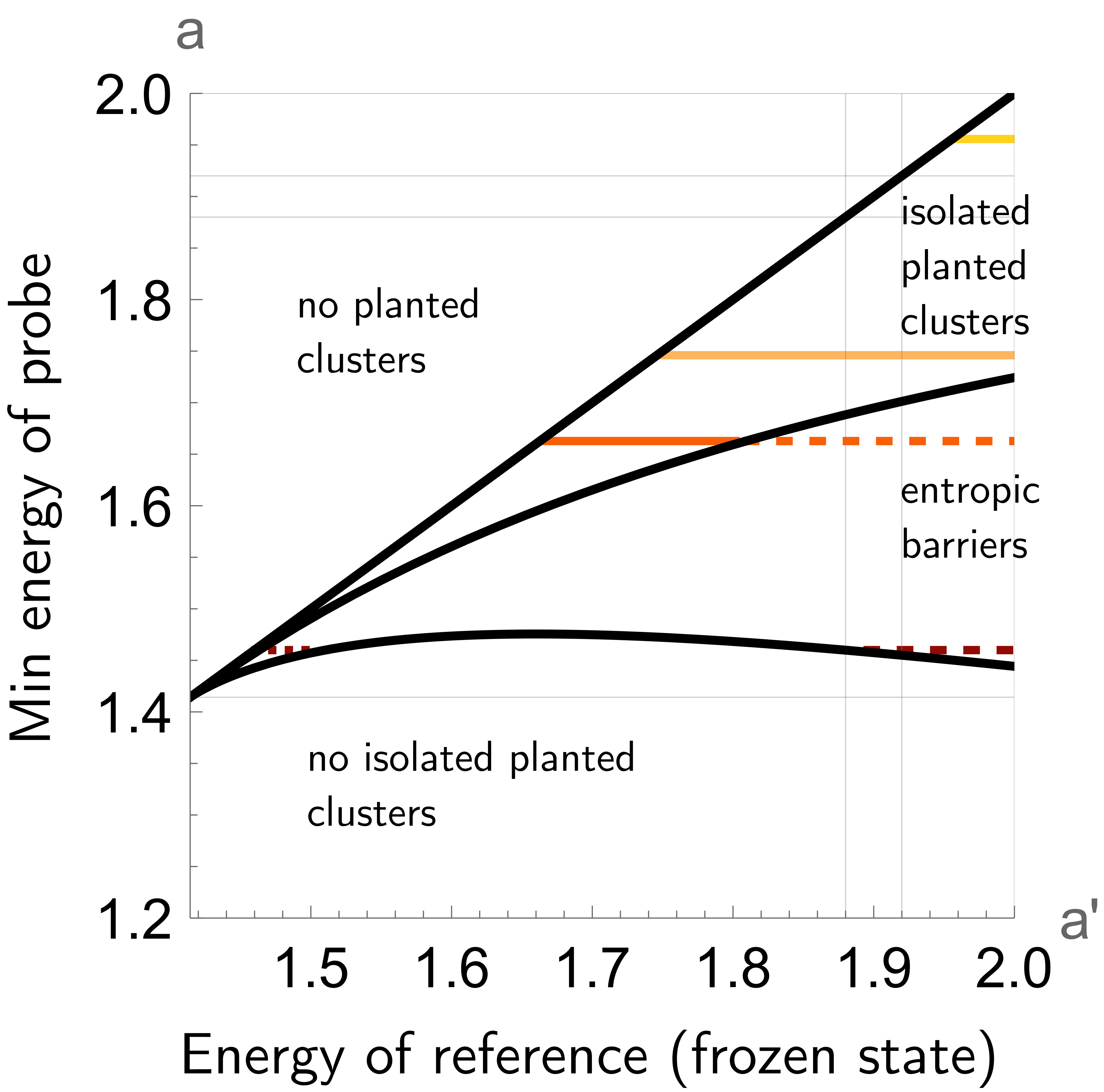
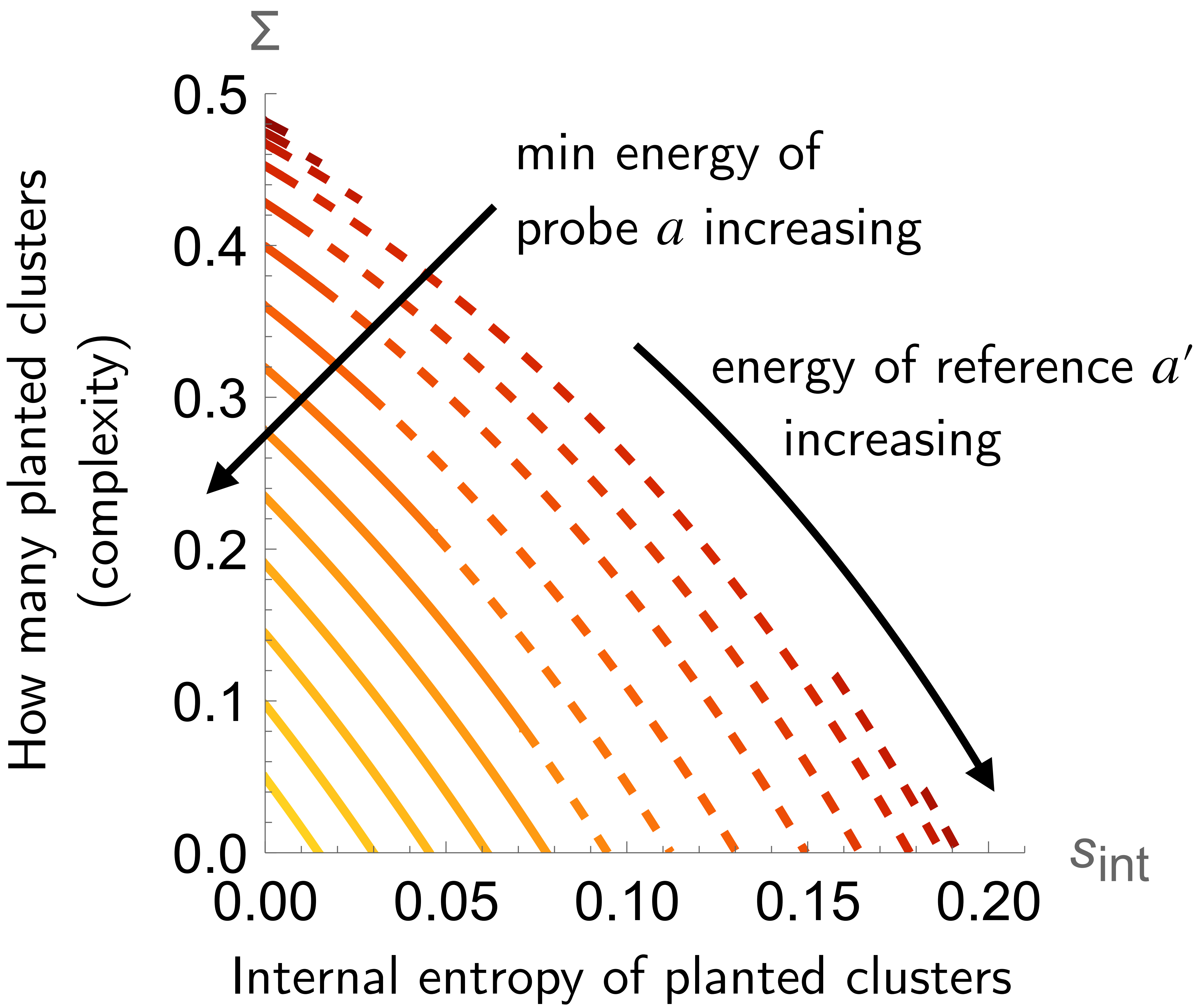
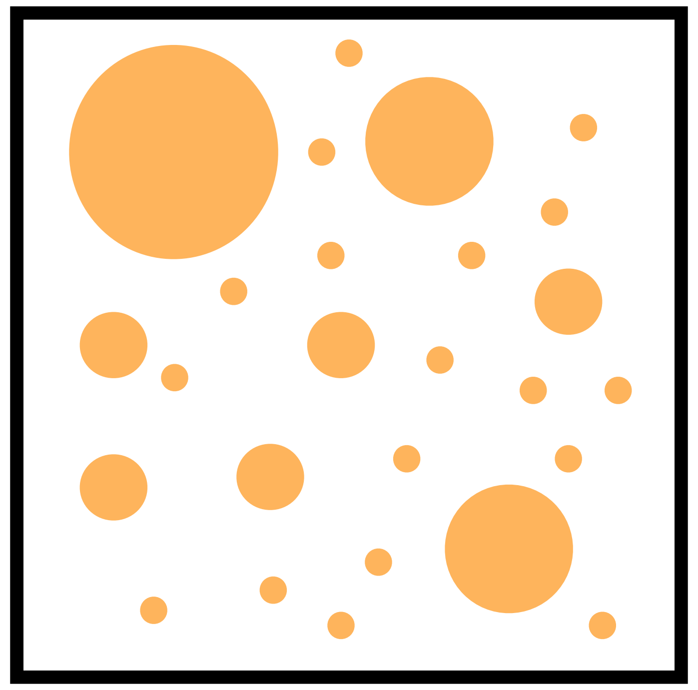
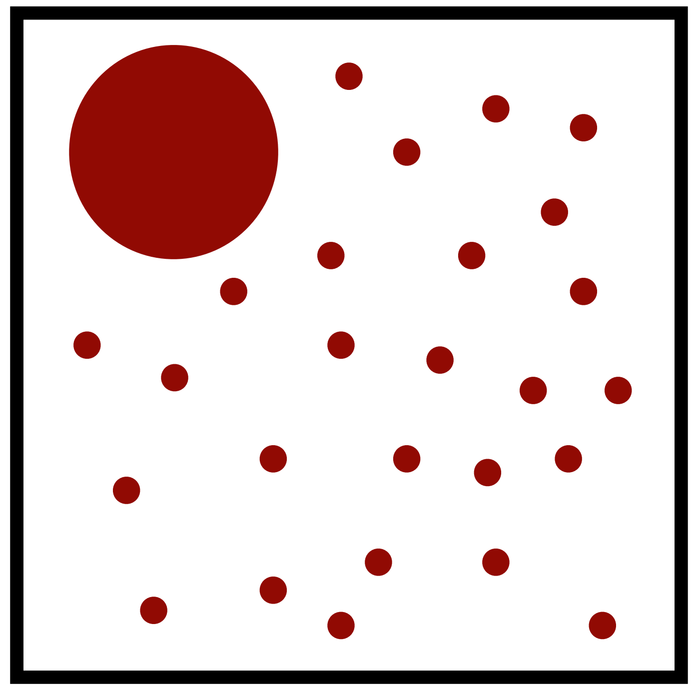




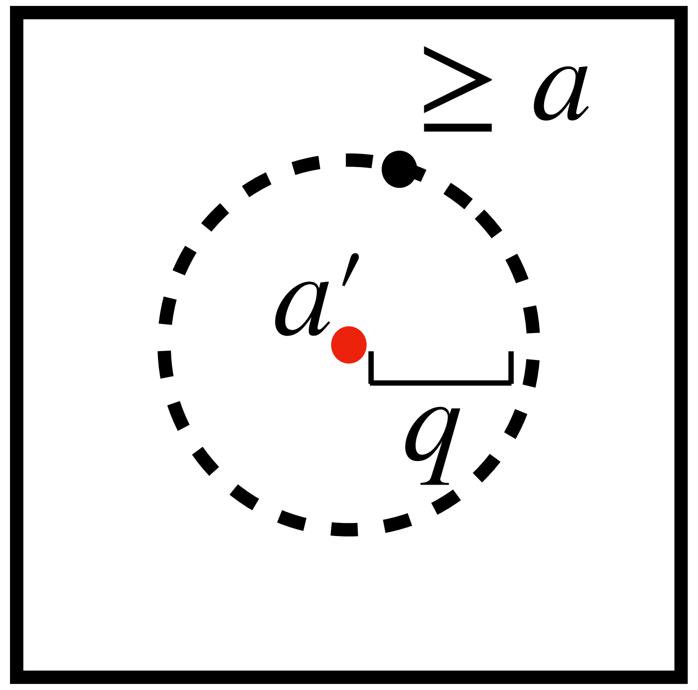
a close to global max

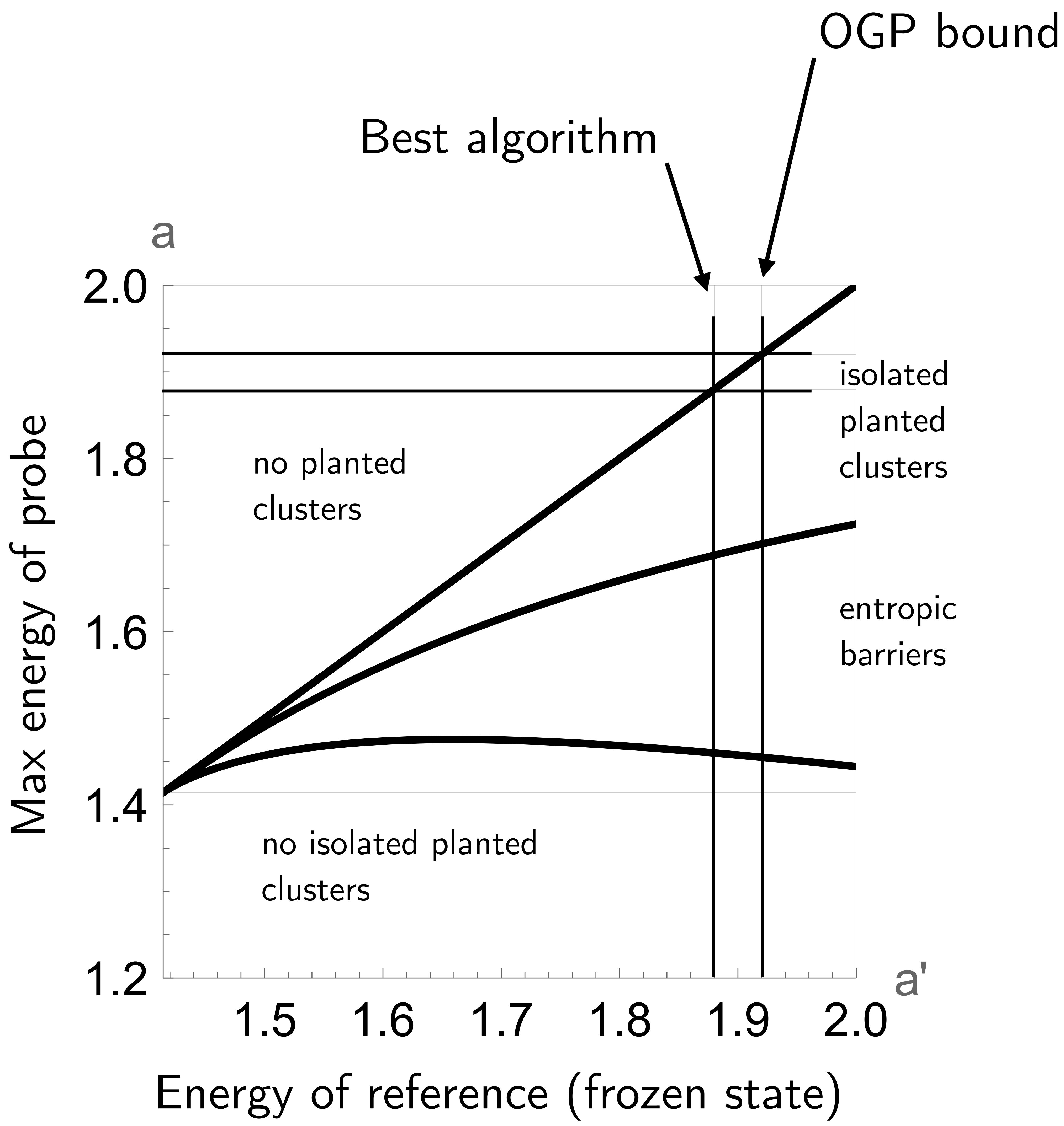


a close to freezing



A first look at non-equilibrium properties





There seems to be **no correlation** between planted clusters and algorithmic/OGP thresholds!

We learn structural informations on level sets + that planted clusters are not responsible for algorithmic properties

Only looks at surroundings of frozen clusters! Other atypical clusters could still exists

Results and open questions

N matrix size
k submatrix size
$m = k/N$

Characterised phase diagram in large ($0 < m < 1$) and small ($m \to 0$) submatrix regimes

Found frozen 1-RSB phase where efficient algorithms provably work for $m \to 0$

Studied planted clusters around frozen configurations for $m \to 0$
Found no link with algorithmic properties

Technical: very simple and explicit formulas (SP equations solved) for $m \to 0$!!

Thank you!

Paper on arXiv:2303.05237