A minimal model for cage breaking in active matter: three self-propelled disks in confinement

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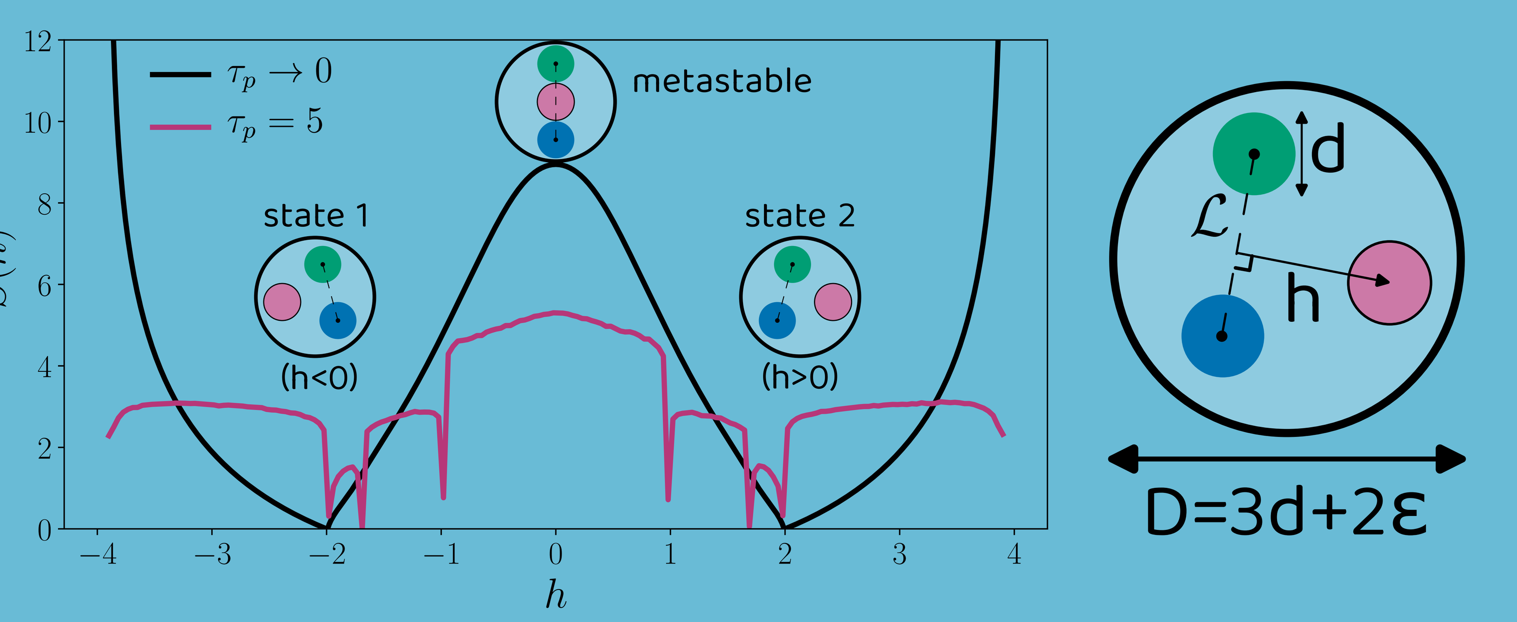
What is cage breaking, and how to model it?

Cage breaking (informally, swapping positions with your neighbors) is the elementary rearrangement event in dense, slowly-relaxing particle systems, from glasses to vibrated granular materials and biological collectives.



Eric Weeks and coauthors have developed a minimal model of cage breaking at thermal equilibrium: three distinguishable hard disks under circular confinement. The free energy landscape is analytically tractable:

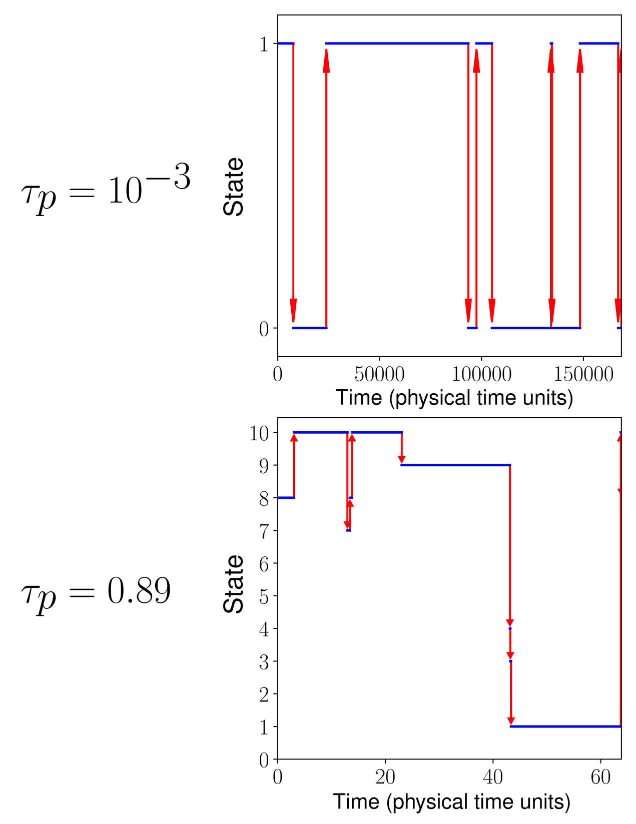
$$F = -TS(h) = -\log(n(h))$$ (Hard sphere U=0, set T=1)

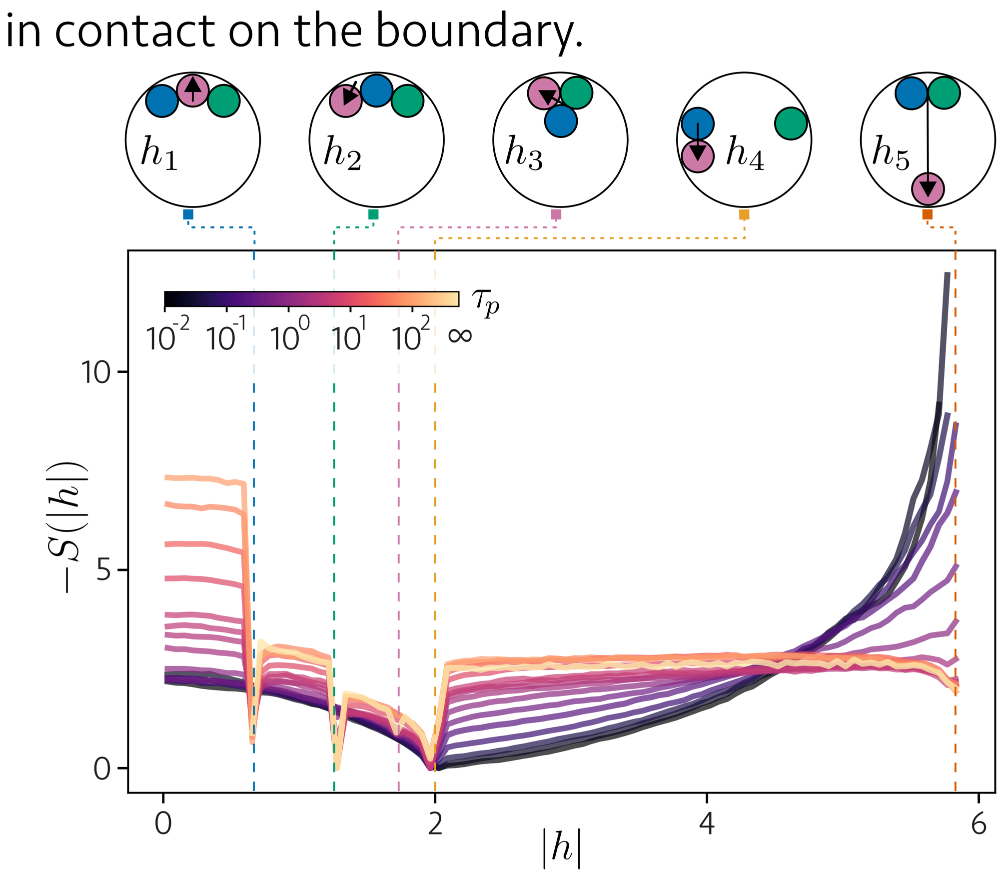
The geometry of available space for the disks in each configuration determines multiplicity of h values $n(h)$.

How does activity affect the dynamics?

Activity drives the system from two-state to multi-state

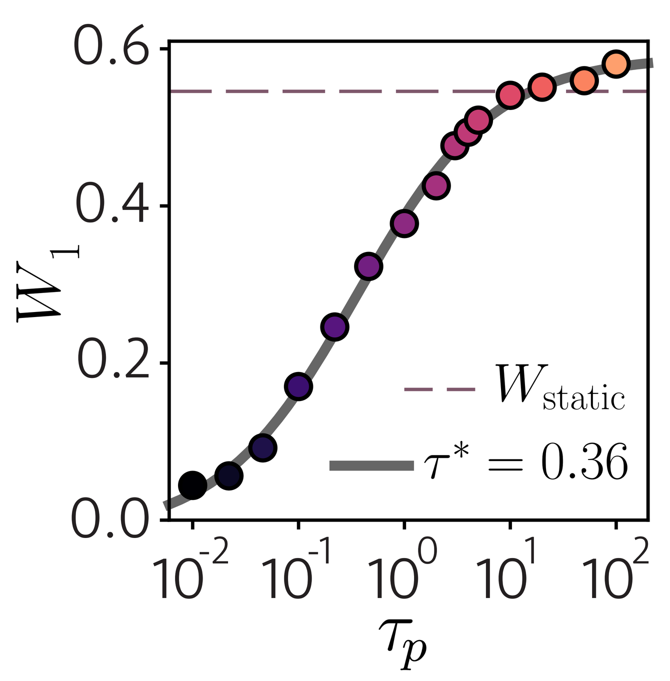
In analogy with the equilibrium case, we calculate the negative entropic landscape. As we increase activity, new dips appear, corresponding to configurations where disks are in contact on the boundary.





In 1D entropic landscape, high-persistence system **develops five metastable states**. In higher dimensions, more peaks emerge (see transition networks).

Quantifying Distance from Equilibrium



Wasserstein-1 distance between equilibrium and non-equilibrium landscapes:

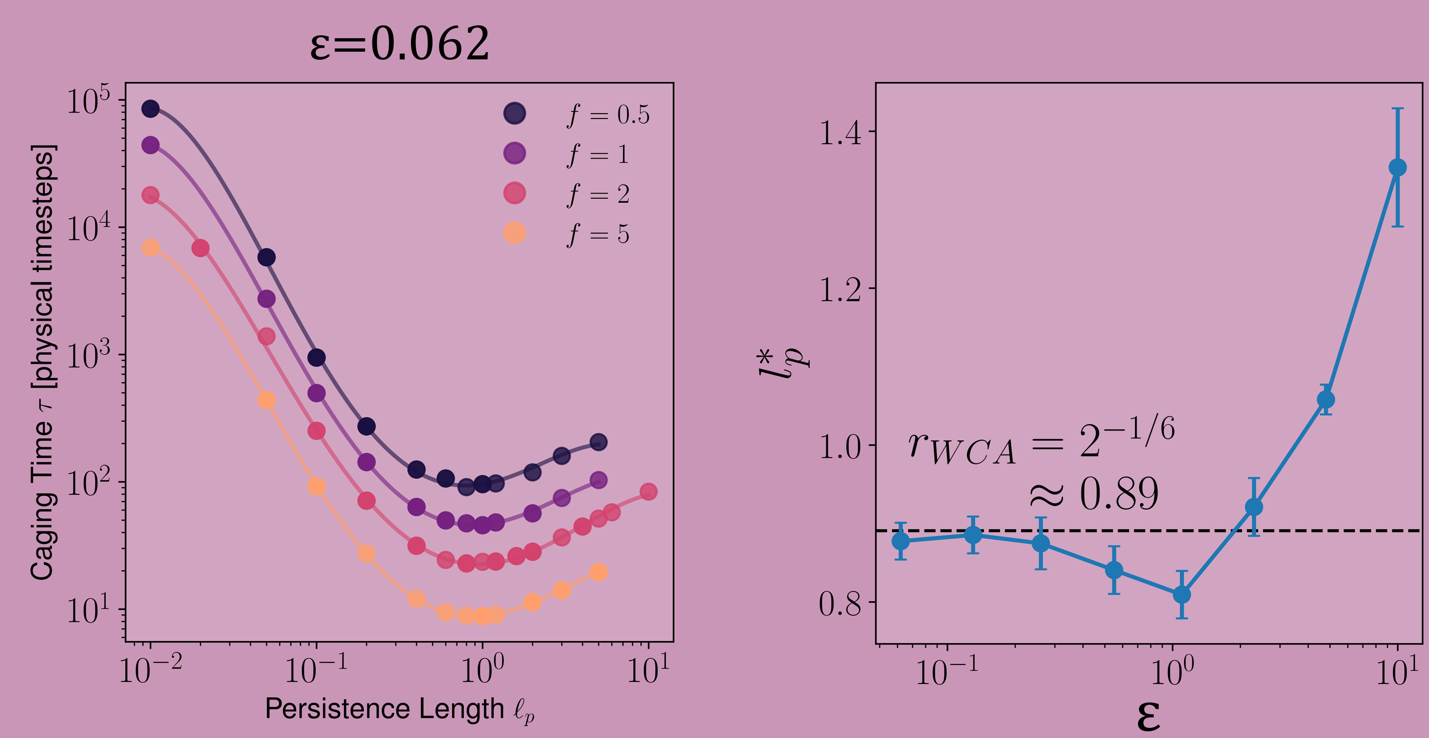
$$W_1(u,v) = \int_{-\infty}^{\infty} \left|U(|h|) - V(|h|)\right| d|h|$$

for probability distributions u, v with CDFs U, V.

The data follow a sigmoid function of persistence time, whose inflection point marks the **transition between near- and far-from-equilibrium behavior**.

Optimal cage breaking at intermediate persistence

We find that cage breaking is **optimized** when the persistence length matches the particle radius (intrinsic length scale of the WCA potential).

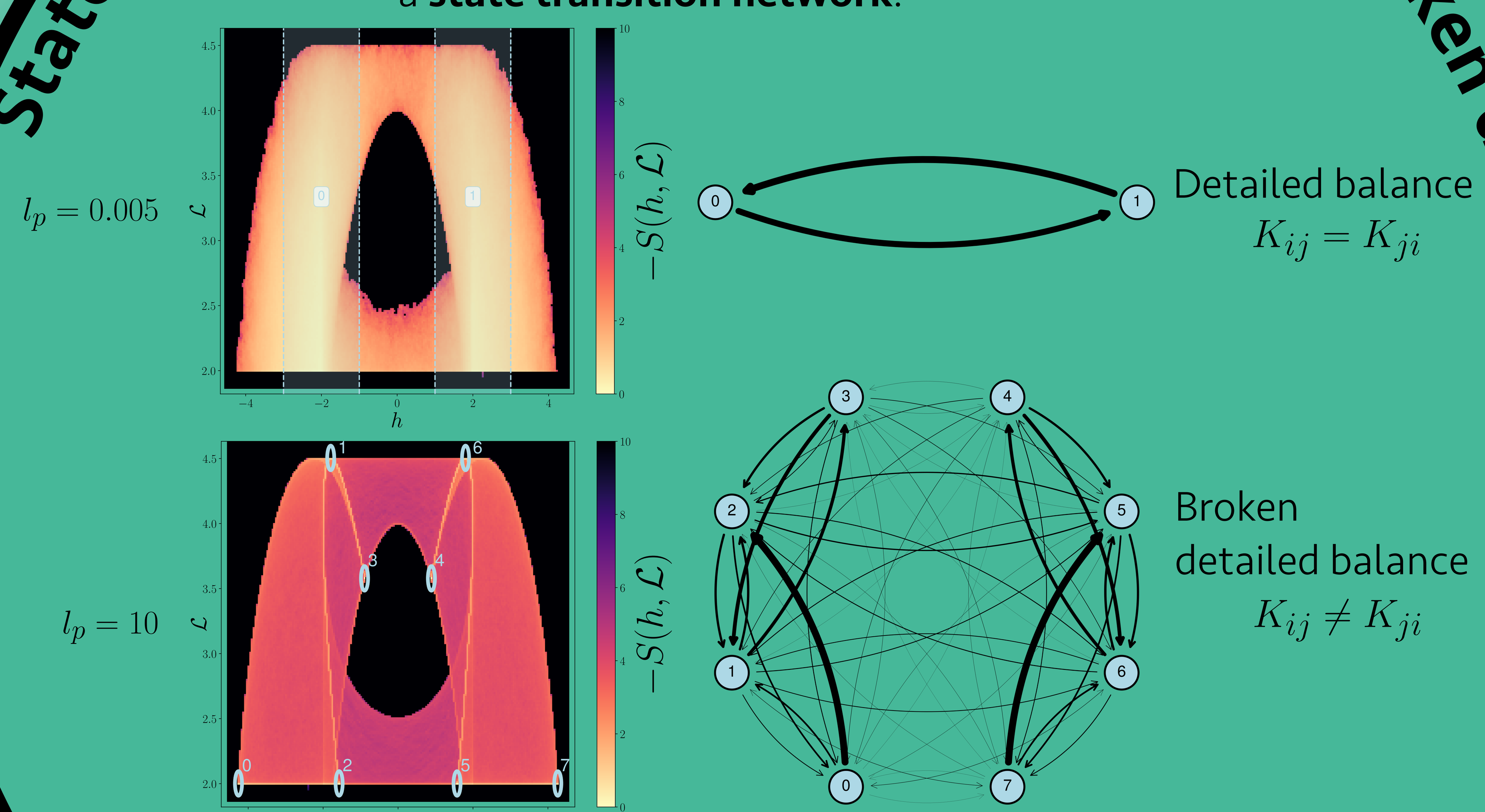


Our results support previous work in bulk active glassy systems showing that **intermediate persistence optimizes transport in dense systems** [3]. However, the optimal length scale in these systems was set by the cage length, as opposed to the particle radius as we observe.

Our system has significantly lower packing fractions ($\phi \leq 0.33$) than bulk systems near the glass transition ($\phi \sim 0.58$). It is plausible that there is a transition to the bulk behavior as particle number density increases.

State transition network for cage breaking & broken detailed balance

We extend the entropic landscape to two dimensions by tracking the length of the triangle spanned by the disk centers $\mathcal{L}$. From the peaks of this 2D distribution, we construct a **state transition network**.

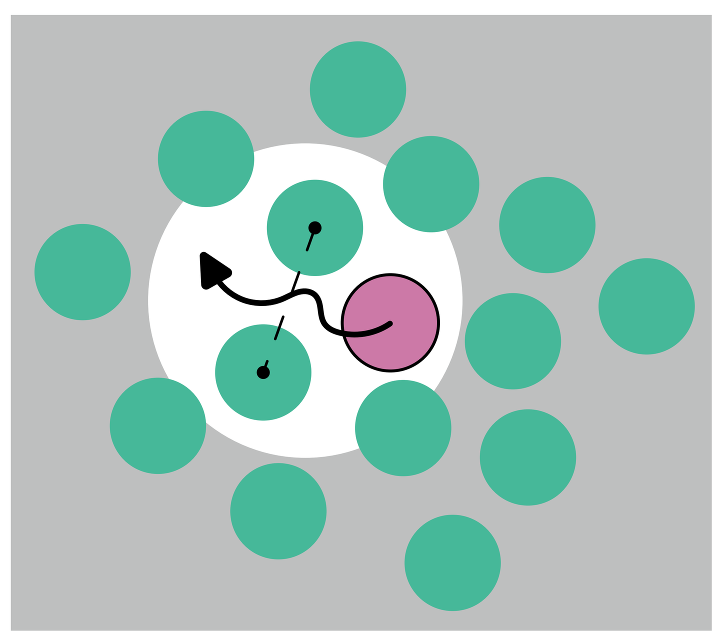


The state transition network for highly persistent systems **breaks detailed balance**, meaning that there is a net flux of transitions in the phase space of the system states.

Thus, directed motion biases transitions between particle arrangements - a possible control parameter for particle systems?

Conclusion/Outlook

Activity induces disks to collect on the boundary, biasing their exploration of space and producing emergent metastable states in the entropic landscape. We capture state transitions on this landscape via a Markov state model, and find that these transitions break detailed balance.



How this can be used to steer dynamics in robotic particles, and the effect of other nonequilibrium forces such as nonreciprocity, are near-term focuses of ours.

References

1. G. L. Hunter and E. R. Weeks, "Free-energy landscape for cage breaking of three hard disks", *Physical Review E* 85, 1–10 (2012).

2. X. Du and E. R. Weeks, "Energy barriers, entropy barriers, and non-Arrhenius behavior in a minimal glassy model", *Physical Review E* 93, 1–9 (2016).

3. V.E. Debets, X.M. De Wit, and L.M. Janssen, "Cage length controls the nonmonotonic dynamics of active glassy matter", *Physical Review Letters* 127(27) (2021).