Extreme spontaneous deformations of active crystals

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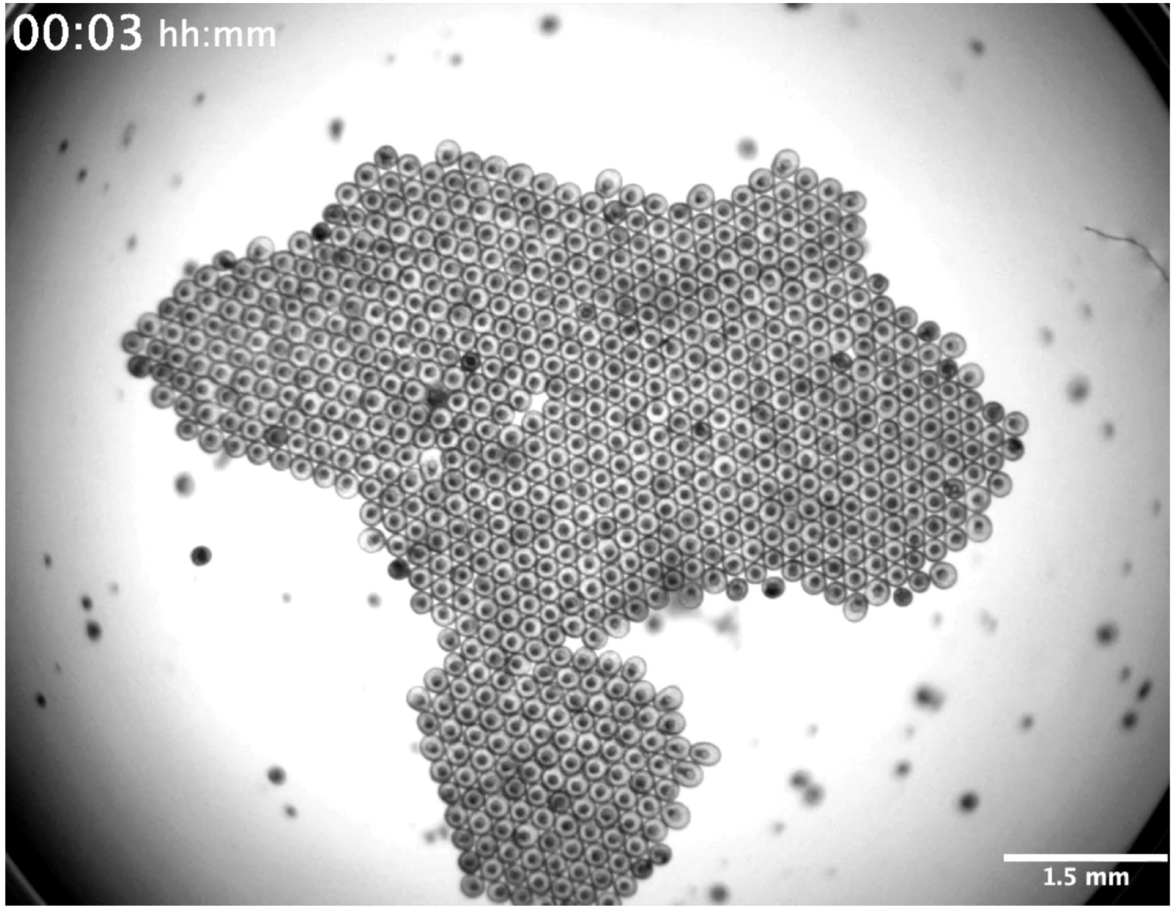
Introduction

- Unavoidably, people were going to look at 2D active crystals and how they melt…

- Two main reasons for this:
  - Fashion to look at anything-active
  - Fascination of theorists for KTHNY theory

- Also recent excitement about chiral active matter, odd elasticity, etc., with crystals found in experiments



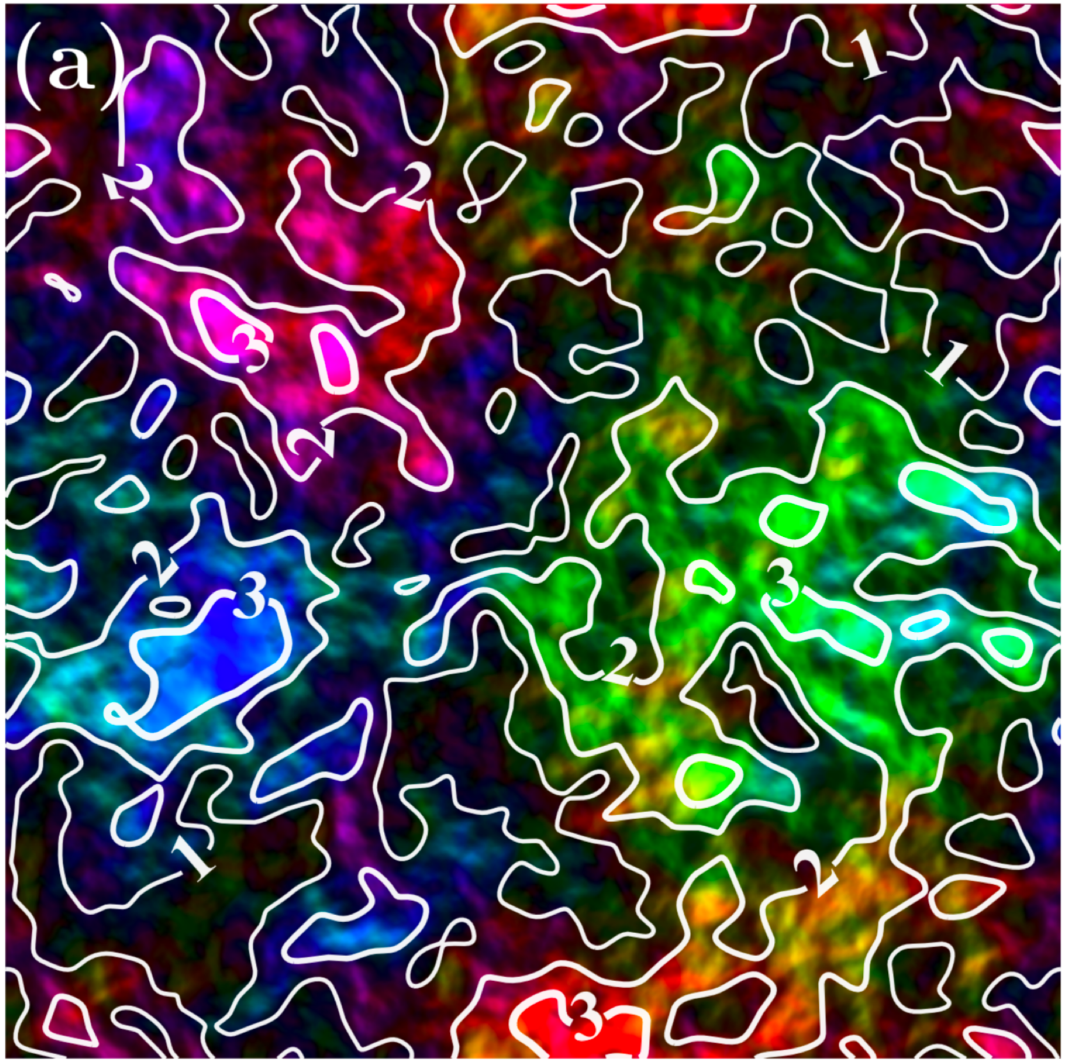
Crystal of spinning starfish embryos (Tan et al., Nature 607, 287 (2022)

KTHNY: Kosterlitz-Thouless-Halperin-Nelson-Young

Introduction

- We consider a more general problem: stability, under their intrinsic fluctuations, of 2D crystals formed by interacting active particles
- previous works have considered this; in particular melting of crystals made of active particles such as active Brownian particles (ABP)
- Most concluded that KTHNY scenario holds or assumed it to be true…

Today we revisit this and show how and why 2D active crystals are very different from equilibrium ones



Deformation field of a large defect-less active crystal

Simple definition of ABPs: constant speed, motion along persistent intrinsic polarity θ, with $\dot{\theta}$ = white noise.

Outline

- Recall main results of KTHNY theory
- Numerical investigation of simple 2D active crystals
- Theoretical understanding
- Summary, remarks, perspectives

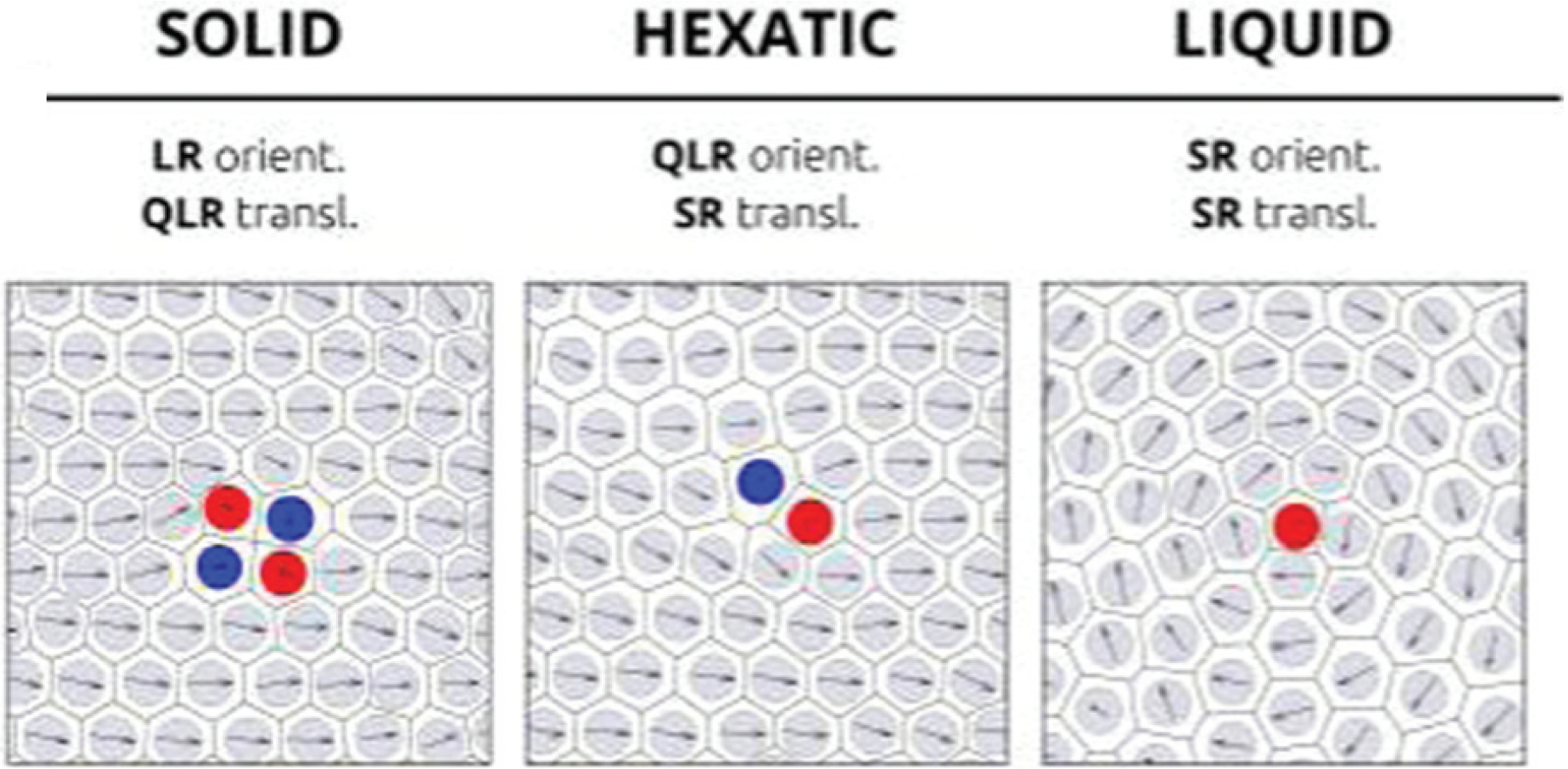
Main results of KTHNY theory

- 2D crystal:
  - QLR positional order and LR bond order.
  - Point defects [interstitials, vacancies] and bounded pairs of dislocations can be present nevertheless
- KTHNY: melting of 2D crystals, in equilibrium, *can* proceed in two steps:
  - LR: long range (finite asymptotic value)
  - QLR: quasi-long-range (algebraic decay to zero)
  - SR: short-range (exponential decay to zero)

- first, a continuous KT-like transition to a phase with SR positional order and QLR bond order (usually hexatic, i.e. 6-fold symmetry); driven by unbinding of pairs of dislocations, which move like a gas in the bond-quasi-ordered phase
- second, another KT transition where bond-order becomes short-range, leaving a fluid phase; driven by the unbinding of dislocations in free disclinations

Main results of KTHNY theory

Pictorially, for the triangular lattice case:



Schematics from Digregorio *et al.*, Soft Matter,**18**, 566 (2022)
(arrows are showing local hexatic order orientation)

Main results of KTHNY theory

- exponents & scaling laws characterizing each of these transitions are known, but were not observed really convincingly [difficult!]

- easier [and usually adopted] check of KTHNY: upper bounds that the theory sets on the decay exponents of correlations in the QLRO phases.

- In the crystal phase in particular, the two-point correlation function of positional order decays algebraically with an exponent η that increases continuously with temperature and $\eta < \eta_{max} \in \left[\frac{1}{4}, \frac{1}{3}\right]$

- remarks:
  - often the transitions are not continuous but discontinuous, with coexistence sub-regions
  - direct melting [from crystal to fluid] can also be observed

Main results of KTHNY theory

- KTHNY work essentially within linear elastic theory, plus energetic/entropic arguments about the nucleation and unbinding of dislocation pairs
- Spin wave fluctuations give

$$\eta = k_B T |\hat{\mathbf{G}}|^2 \frac{3\mu + \lambda}{4\pi\mu(2\mu + \lambda)}$$

- Melting occurs roughly when entropy and elastic energy for creating a dislocation are balanced

$$k_B T_m = \ell_0^2 \frac{\mu(\mu + \lambda)}{4\pi(2\mu + \lambda)}$$

- Combining the two equations yields (triangular lattice)

$$\eta = \frac{(\mu+\lambda)(3\mu+\lambda)}{3(2\mu+\lambda)^2} \leq \frac{1}{3}$$

- $|\mathbf{G}|$ is a reciprocal vector of lattice
- μ and λ are Lamé elastic constants
- ℓ_0 is the lattice spacing

Numerical study of crystals of ABPs

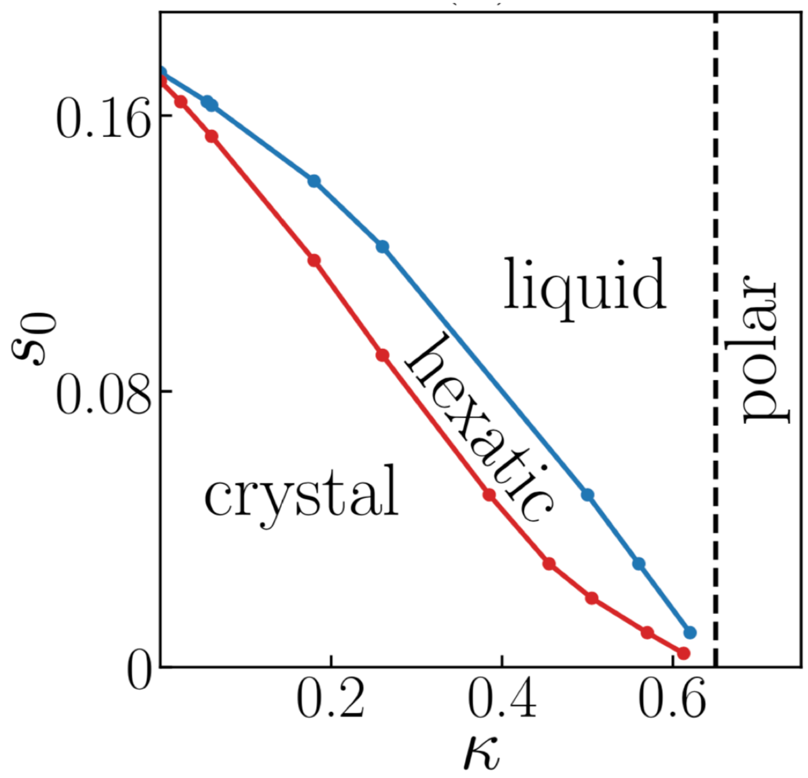
- interactions:
  mainly pair-wise repulsion
- most results obtained with weak local alignment of polarities

$$\dot{\mathbf{r}}_i = s_0\,\mathbf{e}(\theta_i) + \mu_r \sum_{j\sim i} (d_0 - r_{ij})\,\mathbf{e}_{ij}$$

$$\dot{\theta}_i = \kappa \sum_{j\sim i} \sin(\theta_j - \theta_i) + \sqrt{2D_r}\xi_i(t)$$

- s_0 is self-propulsion force / speed
- here harmonic potential
- D_r rotational diffusion
- κ term: ferromagnetic alignment
- ℓ_0 is the lattice spacing

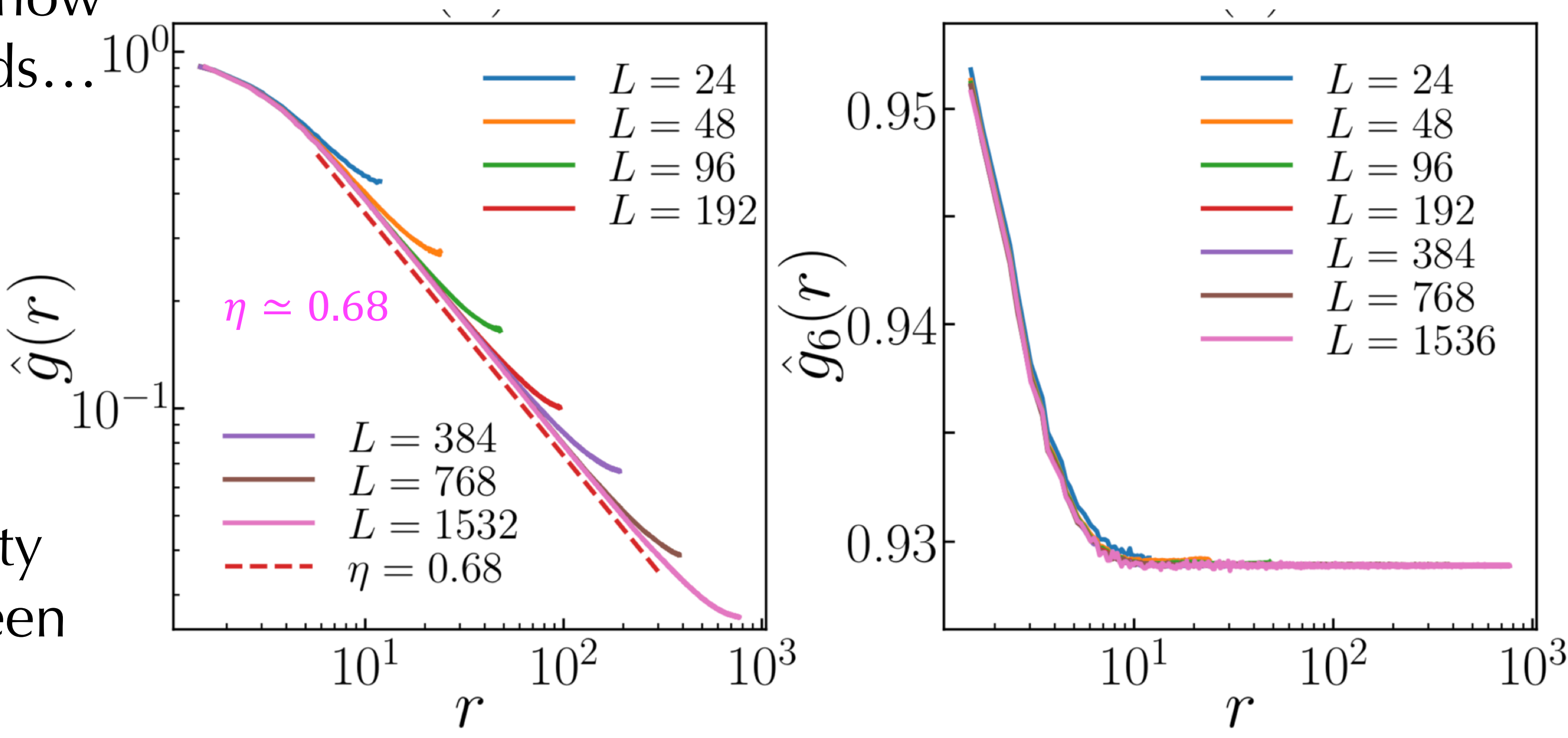
- use perfect triangular lattice as initial condition



Basic phase diagram in (κ, s_0) plane
(μ_r=1.5, $d_0 = D_r = 1$, $\ell_0 = \sqrt{3}/2$)

Numerical study of crystals of ABPs

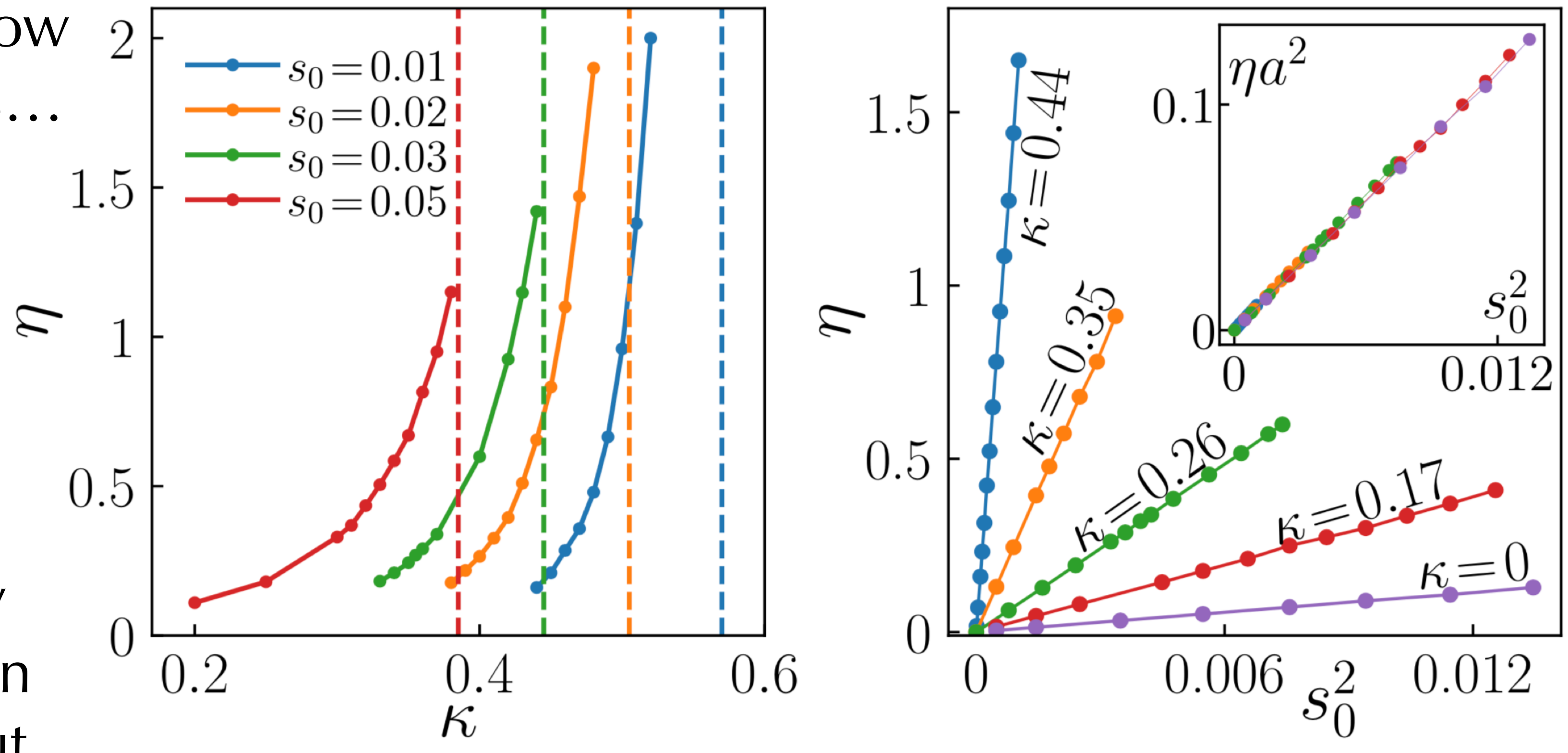
- phase diagram seems to show that KTHNY scenario holds…
- but $\eta > \frac{1}{3}$!!
- η can take very large values…
- $\eta \sim s_0^2$ indicates that polarity field $\mathbf{s} = s_0 \mathbf{e}(\theta)$ can be seen as effective space-time correlated noise



Decay of two-point correlation functions in crystal phase
Left: positional order. Right: bond (hexatic order)

Numerical study of crystals of ABPs

- phase diagram seems to show that KTHNY scenario holds…
- but $\eta > \frac{1}{3}$!!
- η can take very large values…
- $\eta \sim s_0^2$ indicates that polarity field $\mathbf{s} = s_0\mathbf{e}(\theta)$ can be seen as effective temperature, but with space-time correlations



Variation of η with parameters (crystal phase)
Note that $\eta \sim s_0^2$ with slope increasing with κ (right panel)

Theoretical understanding

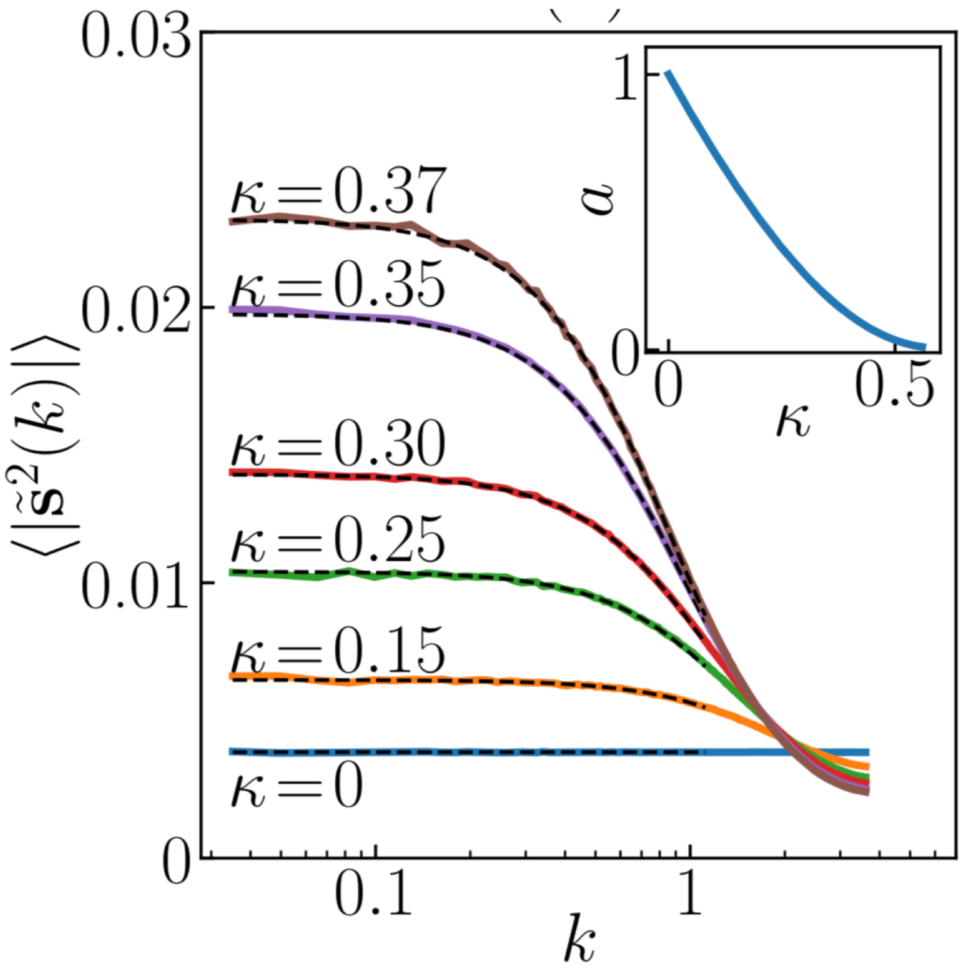
- Spatial power spectra of **s** confirm increase of effective large-scale temperature T_S with κ
- but only on large scales…
  two-temperature picture?
- Within linear elastic theory, displacement field **u** obeys

$$\partial_t \mathbf{u} = (\lambda + \mu)\nabla(\nabla \cdot \mathbf{u}) + \mu \nabla^2 \mathbf{u} + \mathbf{s}$$

- In equilibrium **s** is noise; here **s** obeys

$$\partial_t \mathbf{s} = -a\mathbf{s} + b\nabla^2 \mathbf{s} + \boldsymbol{\sigma}$$

with $\boldsymbol{\sigma}$ white noise of variance $s_0^2 D_r \rho$



Spatial spectra of ***s*** *at various κ values*

- ***u*** *is displacement from perfect crystal positions*
- *a and b > 0, b due to alignment*

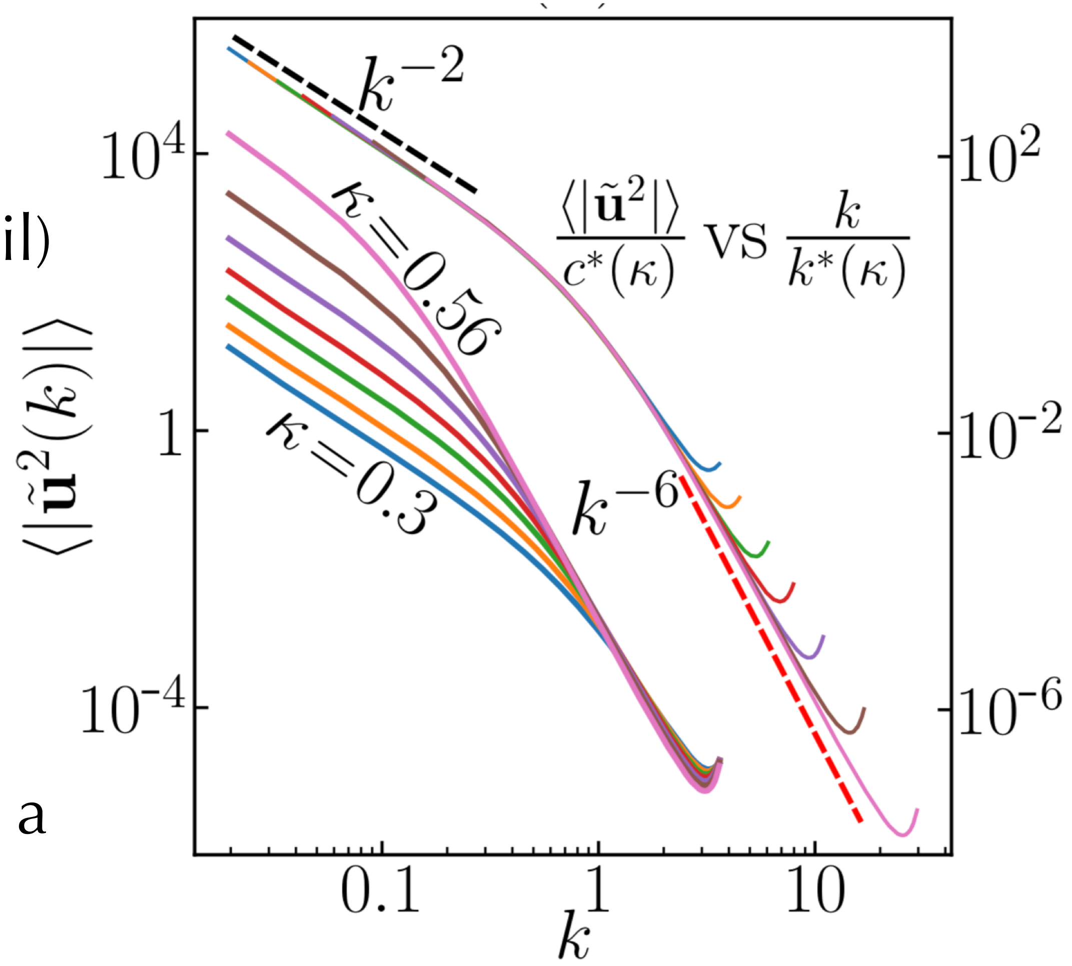
Theoretical understanding

- Spatial power spectra of **u** can be calculated; good agreement with numerics (included k^{-6} tail)
- small-k limit:

$$\lim_{k\to 0}\langle|\tilde{\mathbf{u}}(k)|^2\rangle = \frac{\rho(\lambda+3\mu)}{\mu(\lambda+2\mu)}\frac{s_0^2 D_r}{2a^2k^2}$$

yields effective $T_S = \frac{1}{2}s_0^2 D_r/a^2$

- rescaling wavenumbers by $k^*(\kappa)$ and spectra by a coefficient $c^*(\kappa)$ yields an excellent collapse



*Spatial spectra of **u** at various κ values and collapse using κ-varying coefficients*

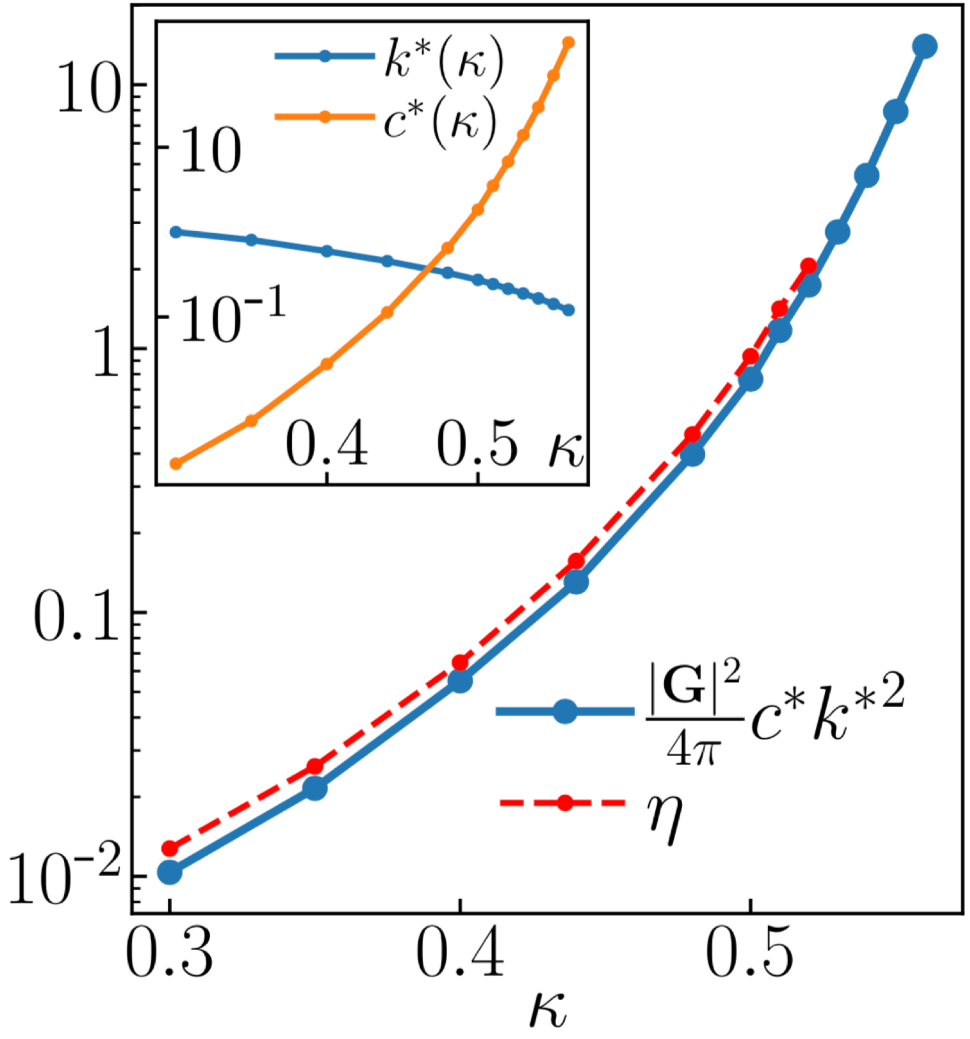
Theoretical understanding

- The product $c^*(\kappa)k^{*2}(\kappa)$ provides an estimate of the prefactor of $1/k^2$ scaling region of **u** spectra
- Using spinwave expression for η yields

$$\eta = \frac{1}{4\pi}|\hat{\mathbf{G}}|^2 c^* k^{*2}$$

- Agreement with direct estimates and extrapolation to very high values where direct measures cannot be performed

(displacements beyond lattice spacing, Bragg peak ill-defined)



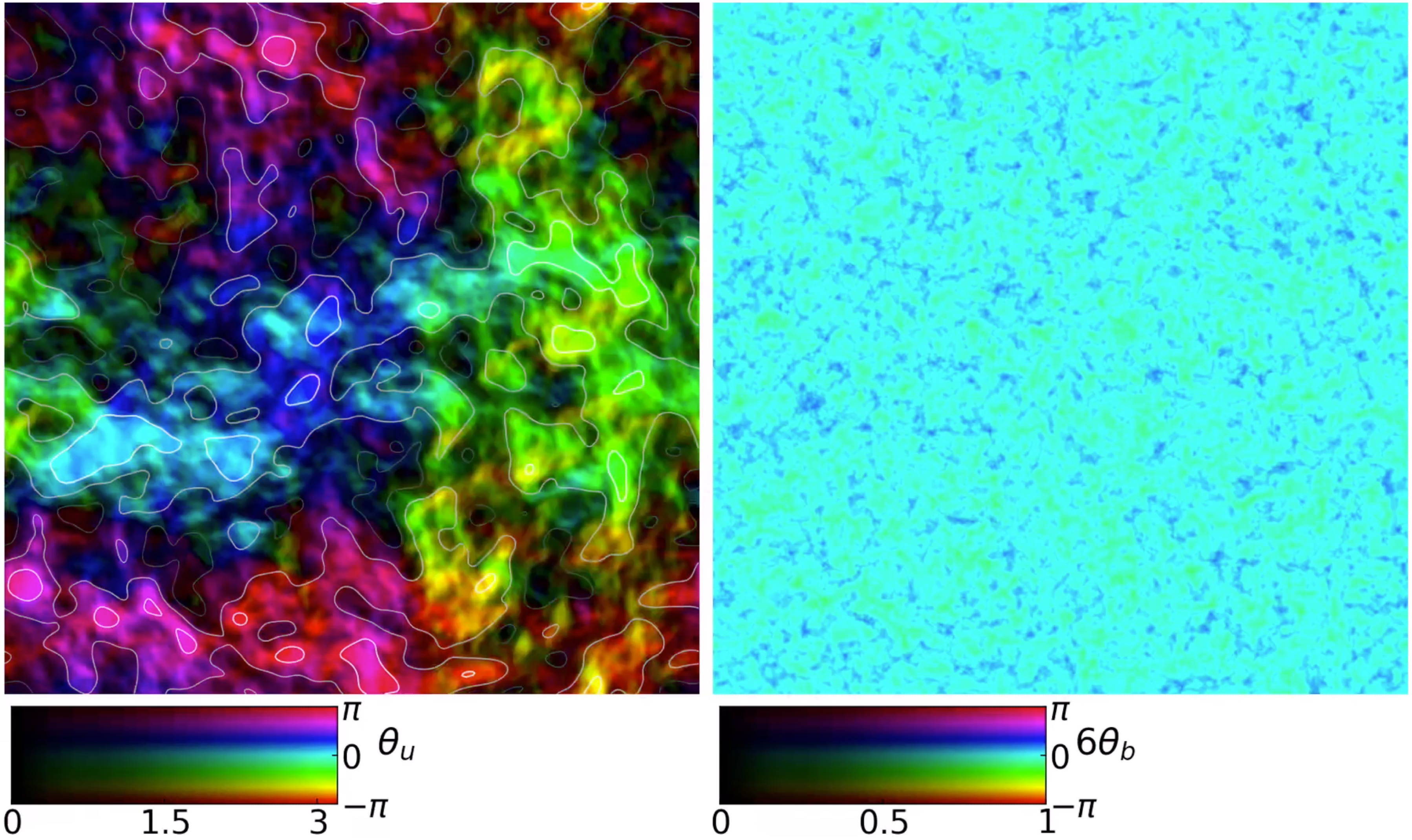
Decay exponent η from direct measures and using κ-varying coefficients

Theoretical understanding

Movie of large crystal in strong deformation regime

- system of size 1536x1536
- (indirect) value of decay exponent η =14 !!
- Maximum |**u**| larger than 3 lattice spacings
- Perfect crystal order without defects

*Displacement field **u** (left) and hexatic order field (right)*
(color is orientation, intensity is magnitude)



Theoretical understanding

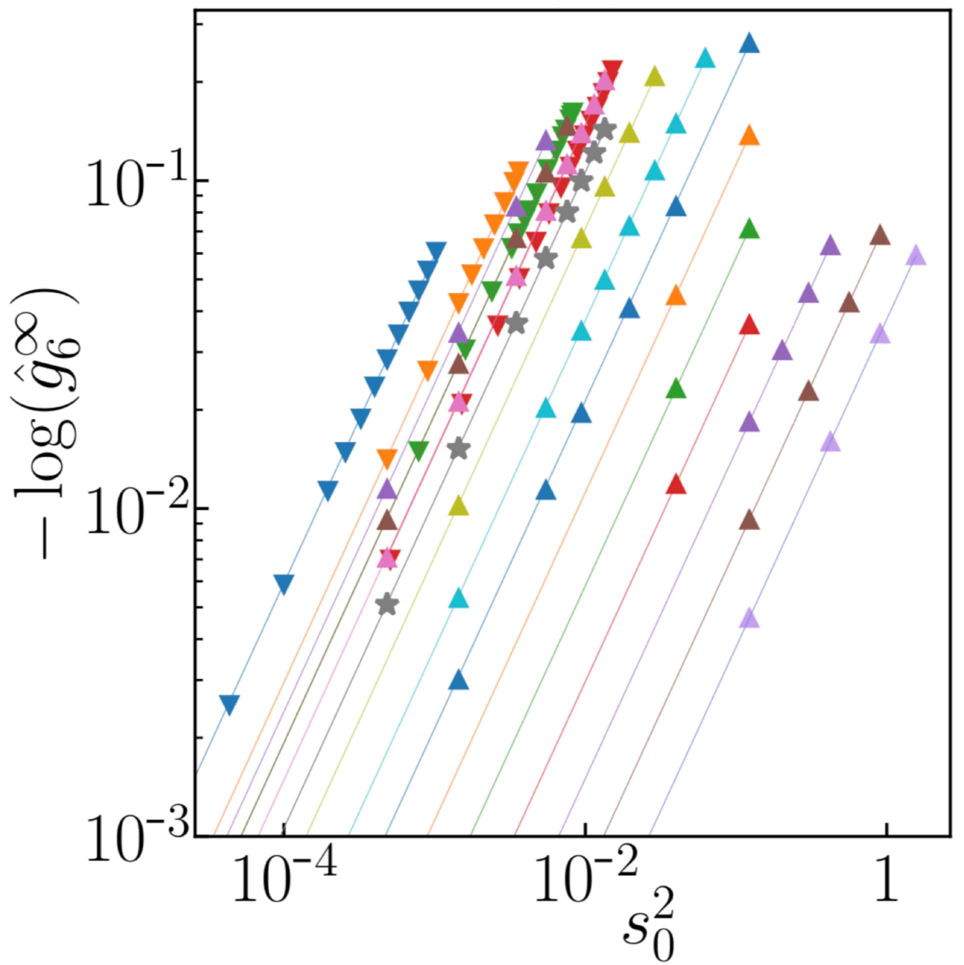
Let's now turn to the LR bond order

- Equilibrium predicts that

$$\hat{g}_6^{\infty} = \lim_{L,r\to\infty} \hat{g}_6(r)$$

decreases exponentially with T

- We do observe that $-\log(\hat{g}_6^{\infty}) \sim s_0^2$
- This suggests the existence of a "bond-order (effective) temperature" $T_6 = t_6(\kappa, D_r) s_0^2$
- To be meaningful, T_6 must be adjusted to coincide with T_S in the equilibrium $D_r \to \infty$ limit



Variation of asymptotic bond-order value with s_0^2 at various κ and D_r values (all straight lines have slope 1)

Theoretical understanding

- Since $T_S = \frac{D_r}{2a^2} s_0^2$ we define

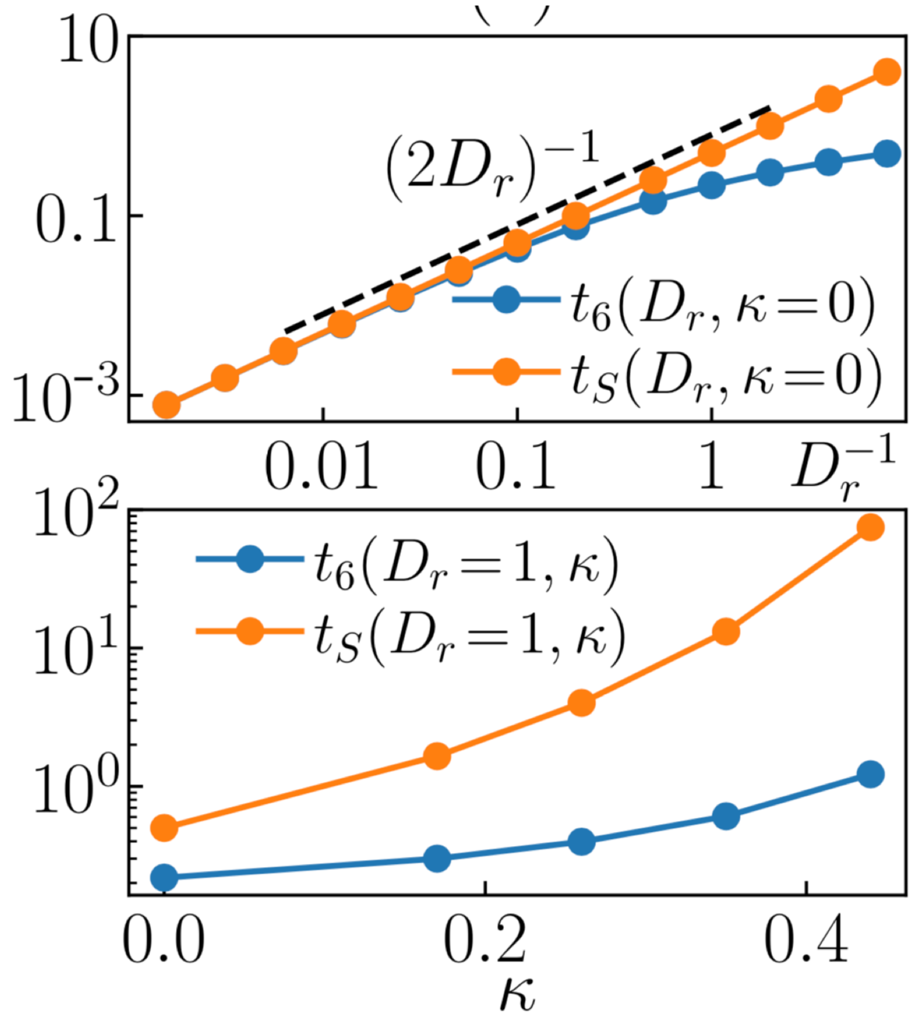
$$t_S(D_r,\kappa) = T_S/s_0^2 = D_r/2a^2$$

and adjust t_S and t_6 so that they coincide in equilibrium

- divergence of t_S and t_6 as κ increases, but also with D_r even for κ=0

- bond temperature t_6 lower than elastic temperature t_S

➢ *wild deformations without unbinding dislocations*



Variation of reduced temperatures t_S and t_6 with κ and D_r

Summary, remarks, perspectives

- Active crystals can sustain strong spontaneous deformations without melting
- KTHNY bounds do not apply: melting can occur at arbitrarily large values of η, but also, probably, for $\eta<1/4$
- Two-temperature picture: local fluctuations stay weak while large-scale elastic deformations occur
- Alignment not crucial; key ingredient is (time-) persistence of fluctuations
- Similar results obtained in systems without alignment, with chirality, for passive crystals in active bath, even for XY model with time-correlated noise
- Key open problem is whether melting transition remains KT-like

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