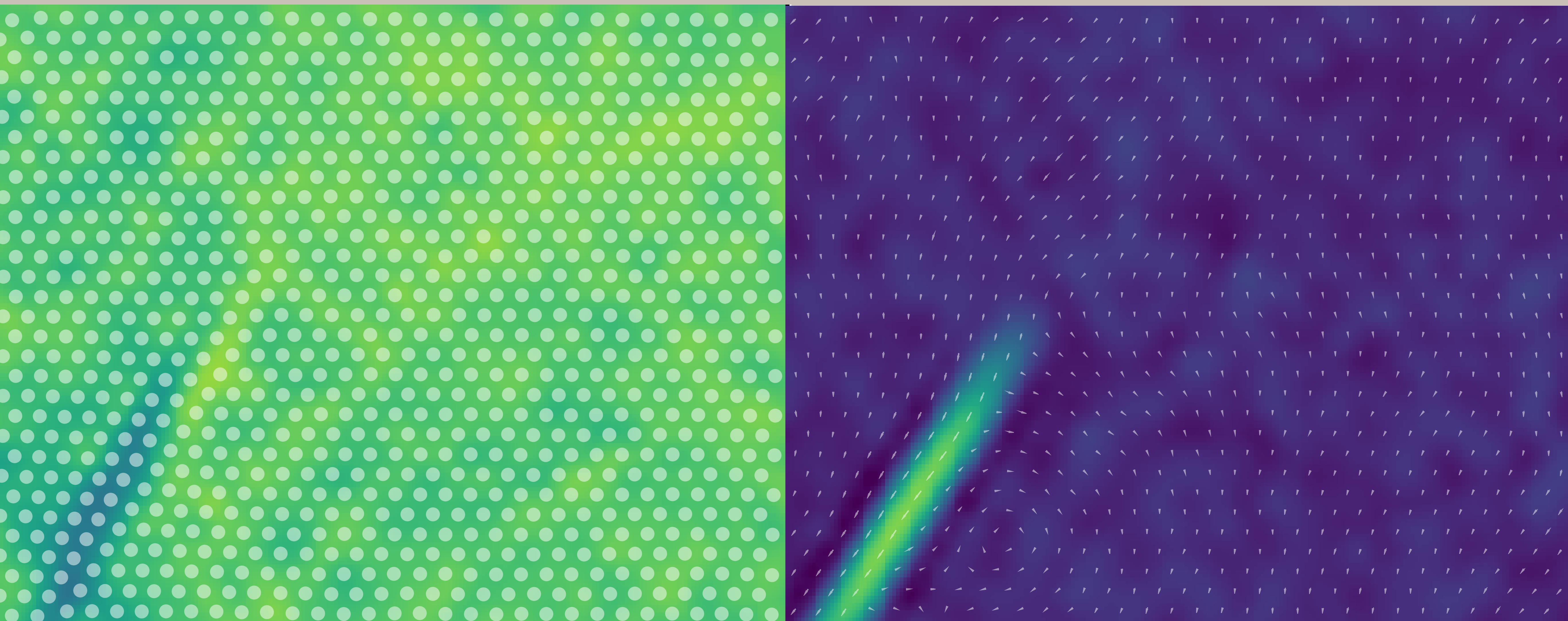
THE EQUILIBRIUM FIRST ORDER TRANSITION *UNDERLYING* IRREVERSIBLE DEFORMATION IN SOLIDS



Surajit Sengupta (TCIS, Hyderabad, India)

Collaborators: P. Nath (TCIS), S. Ganguly (HHU), J. Horbach (HHU), P. Sollich (Kings College), S. Karmakar (TCIS)

ICTS *CQDISCOR-2017*

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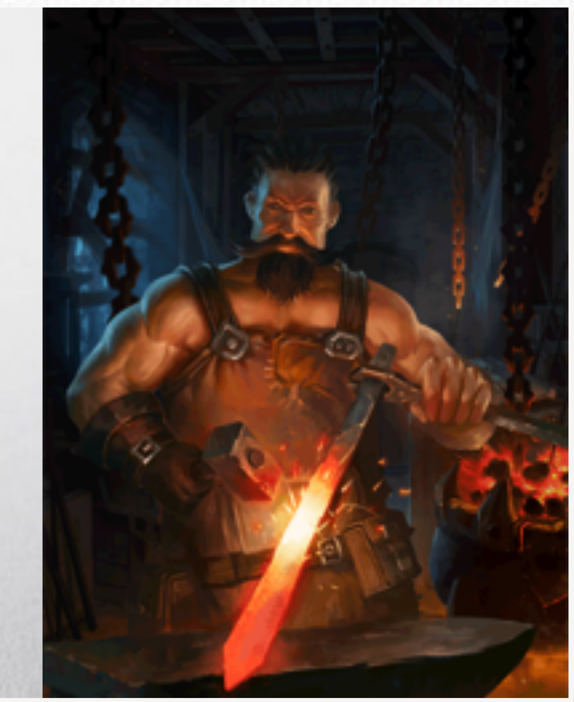

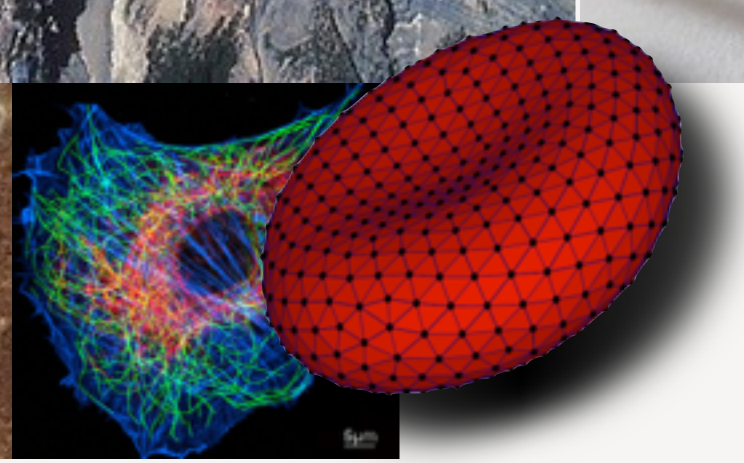

MOTIVATION

"The extension of a piece of metal [is] in a sense more complicated than the working of a pocket watch and to hope to derive information about its mechanism from two or three data derived from measurement during the tensile test [is] perhaps as optimistic as would be an attempt to learn about the working of a pocket watch by determining its compressive strength. "

–Orowan (1944)

"…plasticity is a 'many-body' problem and poses huge statistical challenges in that what is sought are suitable averages over the entire distribution of dislocations as they traverse a disordered medium. "

–Rob Phillips (2004)

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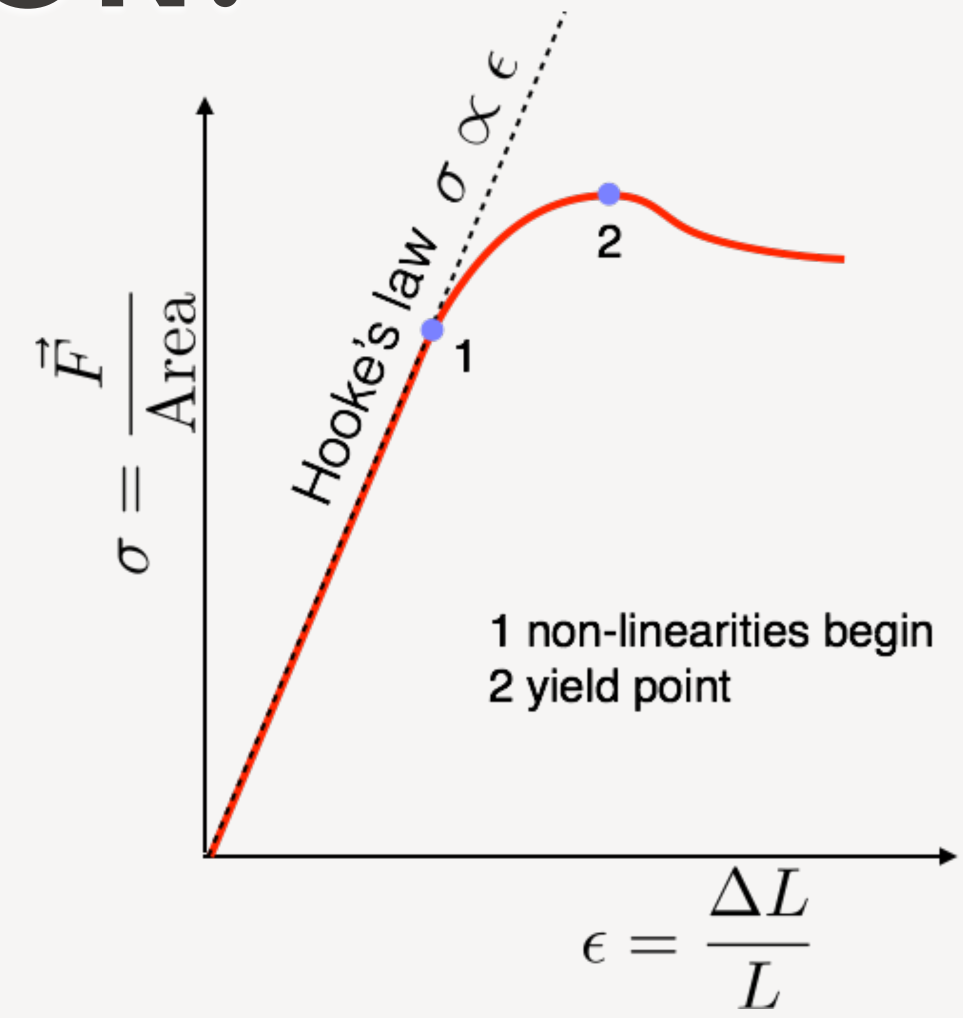
MOTIVATION:



- "Yield point" usually associated with stress drop in constant strain rate experiments.
- Not well defined. Not fully understood even in crystals.
- Is yielding a dynamical phase transition ?

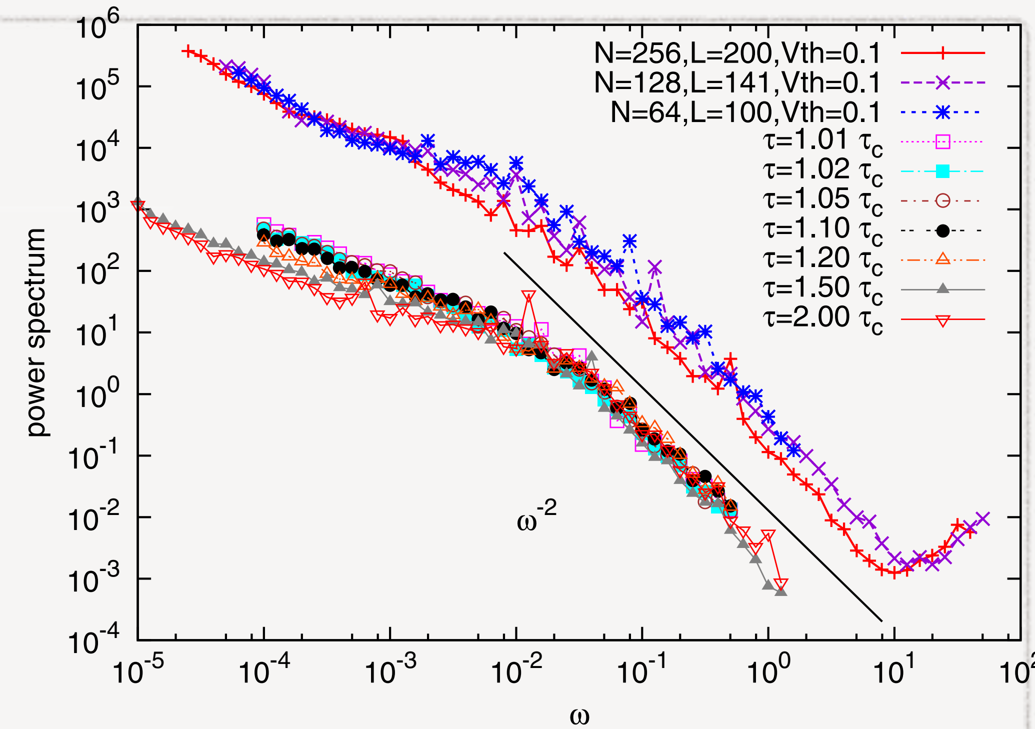
A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

EPL, **101** (2013) 36003
doi: 10.1209/0295-5075/101/36003

Determination of the universality class of crystal plasticity

G. TSEKENIS, J. T. UHL, N. GOLDENFELD and K. A. DAHMEN

= mean field *interface depinning* transition



Crackling noise

NATURE | VOL 410 | 8 MARCH 2001 | www.nature.com

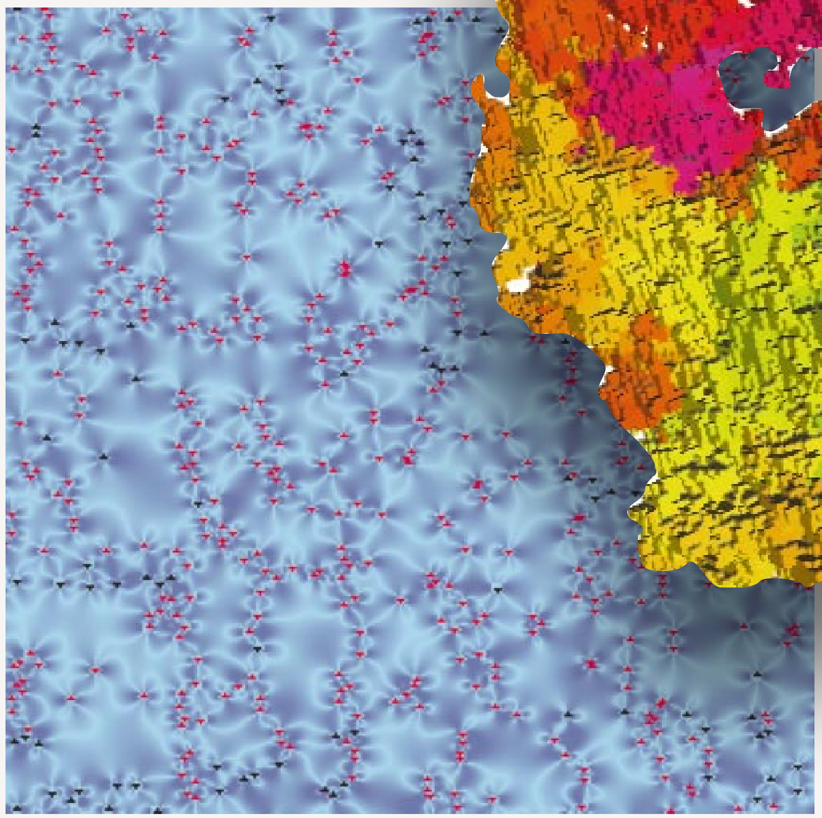
James P. Sethna*, Karin A. Dahmen† & Christopher R. Myers‡

*Laboratory of Atomic and Solid State Physics, Clark Hall, Cornell University, Ithaca, New York 14853-2501, USA (sethna@lassp.cornell.edu)
†Department of Physics, 1110 West Green Street, University of Illinois at Urbana-Champaign, Illinois 61801-3080, USA (dahmen@physics.uiuc.edu)
‡Cornell Theory Center, Frank H. T. Rhodes Hall, Cornell University, Ithaca, New York 14853-3801, USA (myers@tc.cornell.edu)

Intermittent dislocation flow in viscoplastic deformation

M.-Carmen Miguel*†, Alessandro Vespignani*, Stefano Zapperi‡, Jérôme Weiss§ & Jean-Robert Grasso‖

NATURE | VOL 410 | 5 APRIL 2001 | www.nature.com



yield point = critical point

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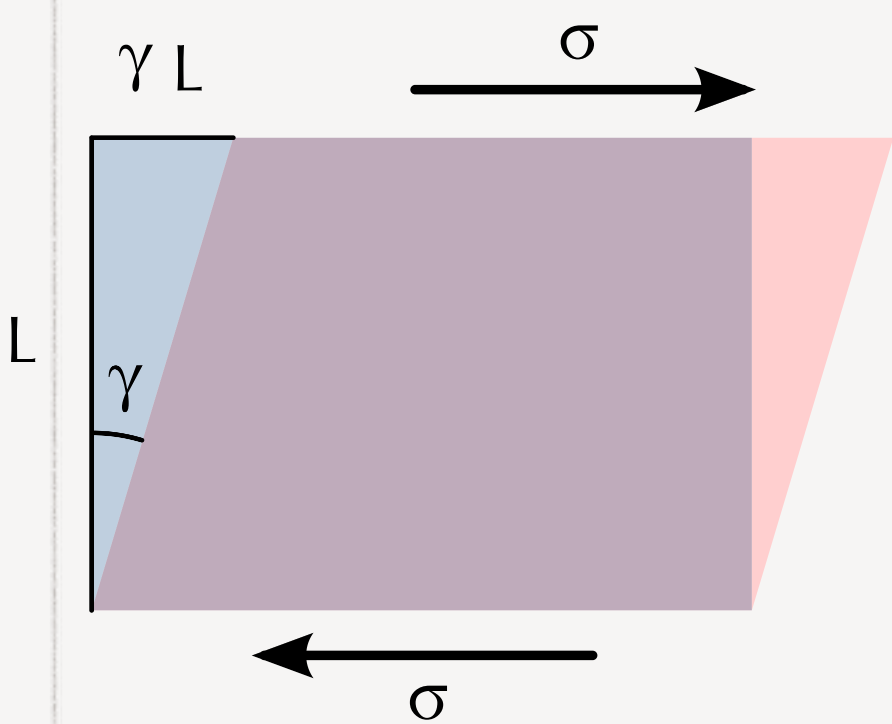
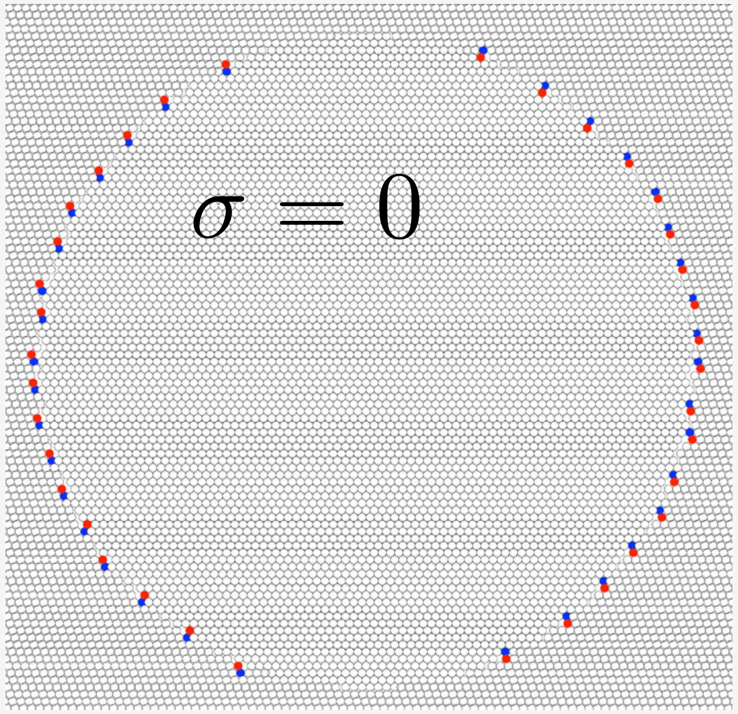
A DROPLET CALCULATION



rearrange atoms, relieve stress, introduce defects at surface to fit the patch →



Sausset, Biroli, Kurchan, J. Stat Phys 140, 718 (2010)

$$\Delta\mathcal{F}(R) = R^{d-1}\Omega(\sigma) - R^d\frac{\sigma^2}{2G_P} \qquad \tau^* = \tau_0 \exp\left(c\left(\frac{\sigma_y}{\sigma}\right)^{2d-2}\right)$$

- No yield point !
- essential singularity at $\sigma = 0$
- no singularity for $\sigma > 0$.

similar calculation in 2d by Bruinsma, Halperin, Zeppelius (1982) gives a power law with, in general, non-universal exponents.

PUZZLE:

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- Expectation: crystalline solid is *stable* upto yield point but fails for larger stresses. (e.g. Huber-von Mises criterion). Is there such a definite *critical strain* - the yield point?

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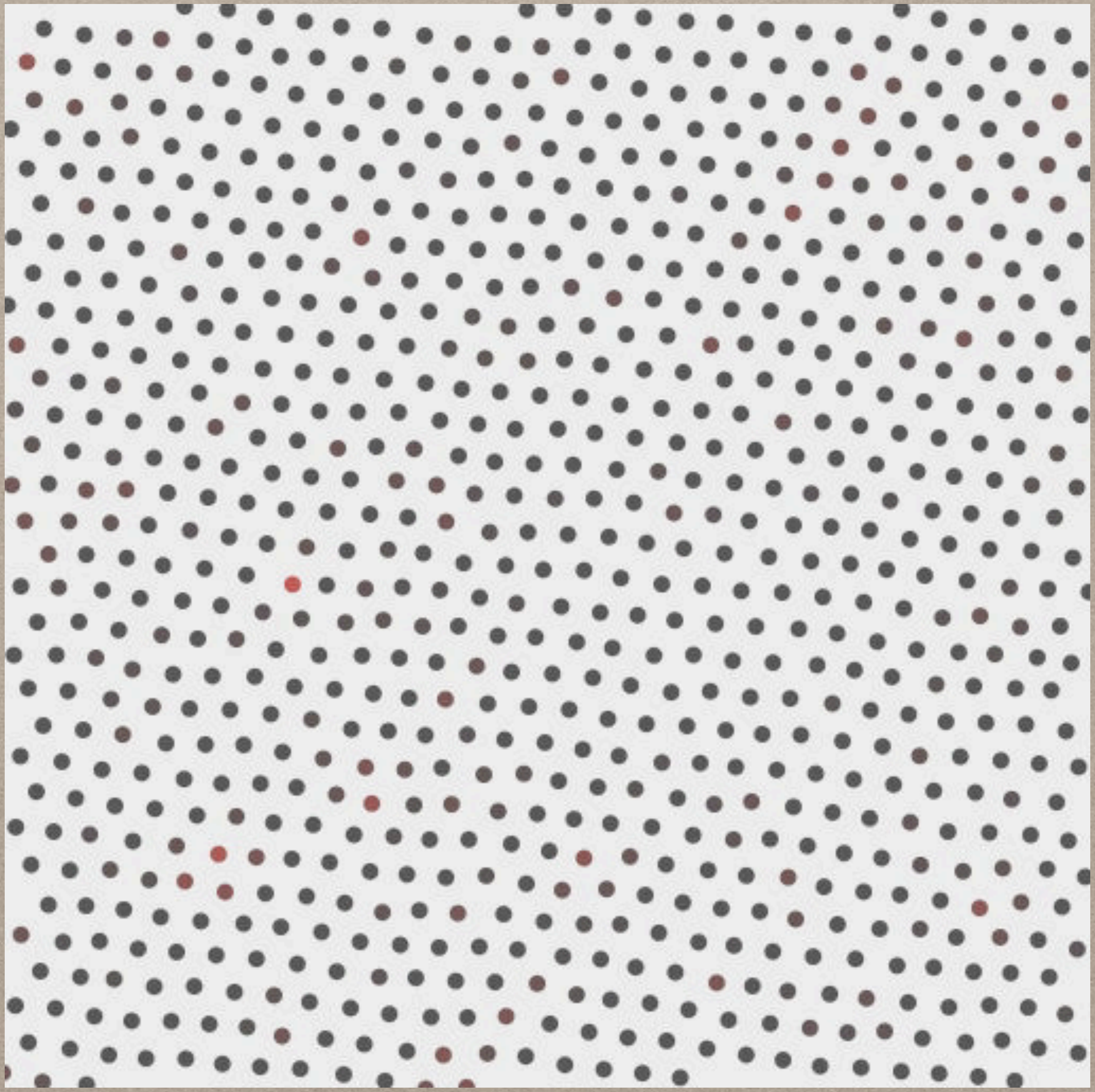
2D TRIANGULAR LATTICE OF CLASSICAL, *distinguishable*, COLLOIDAL PARTICLES



Courtesy: K. Franzrahe, data from the group of G. Maret, U. Konstanz

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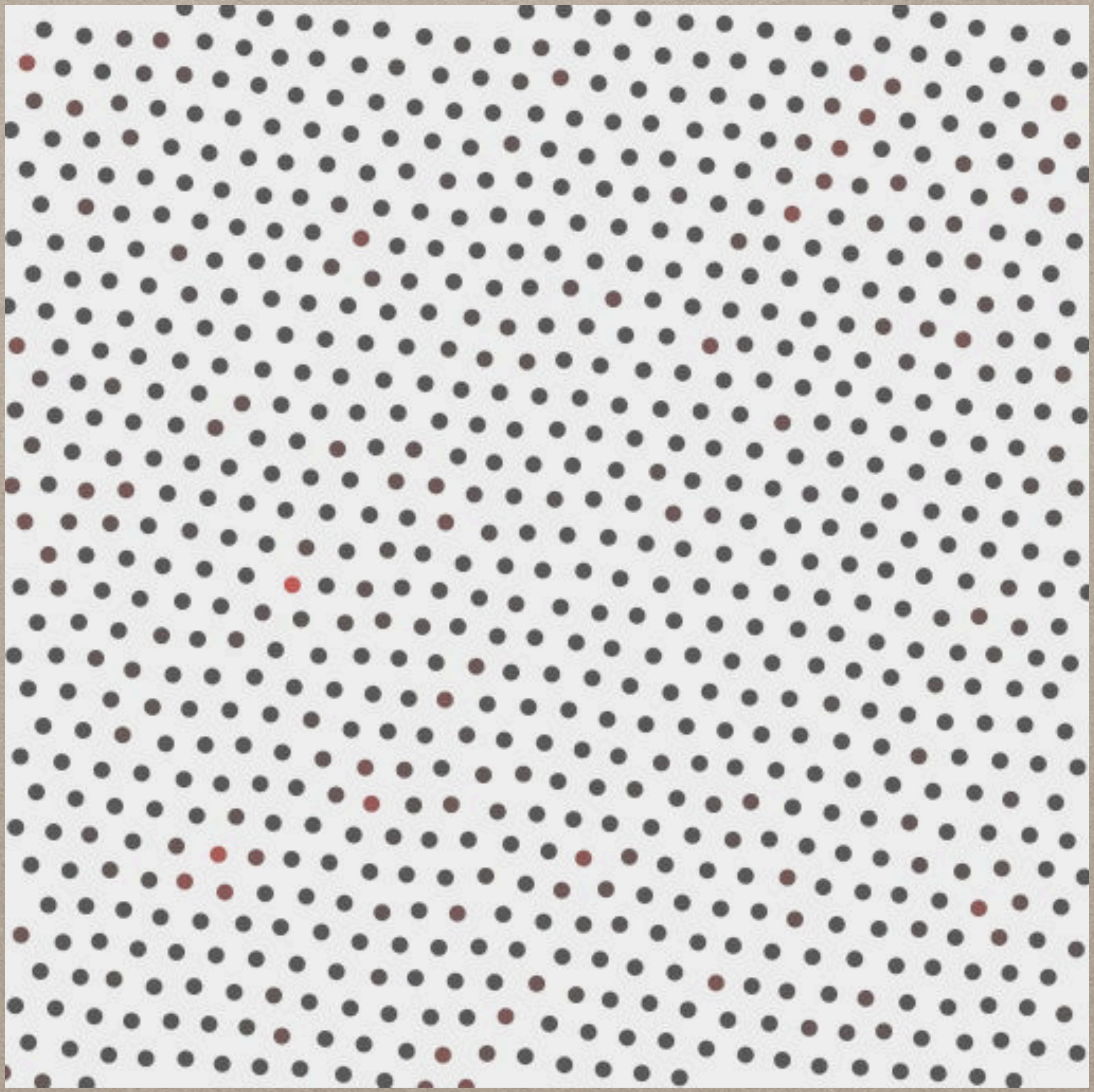

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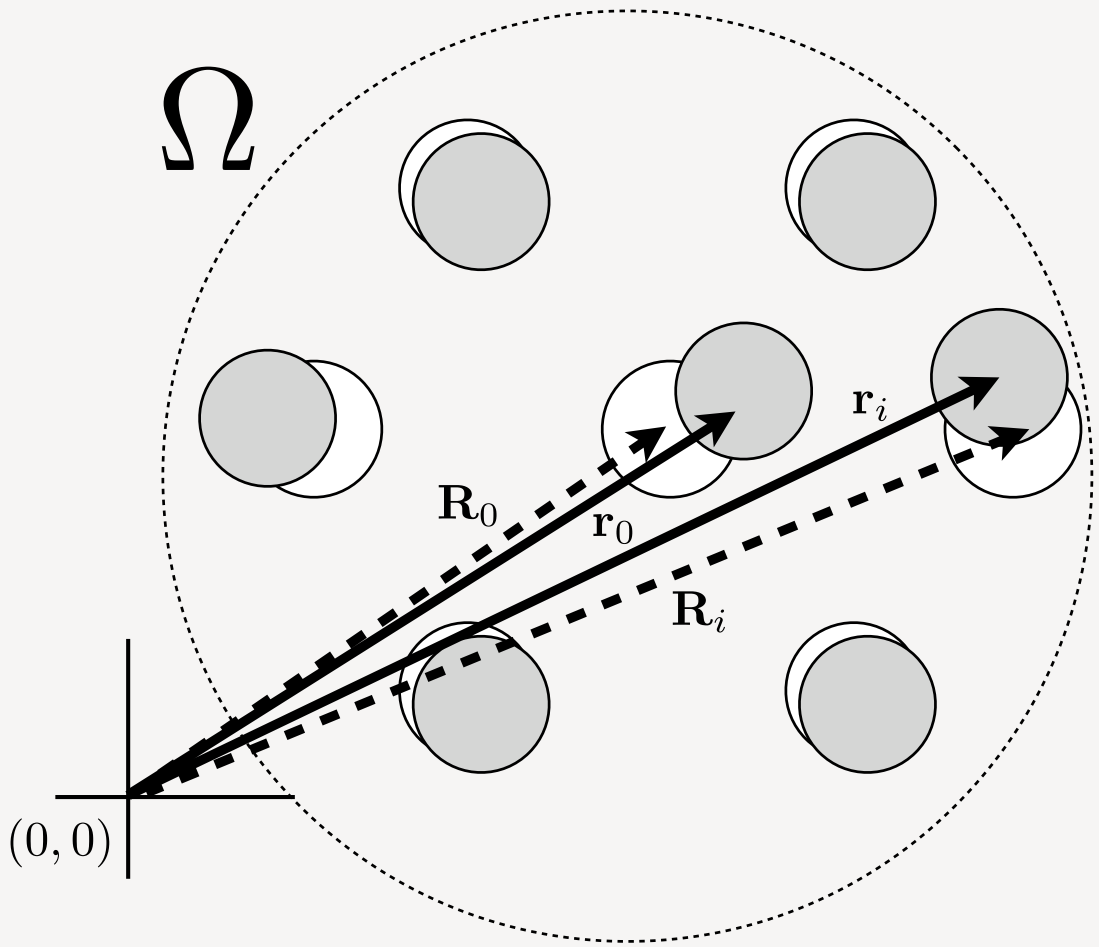
LOCAL NON-AFFINITY



Particle positions $\mathbf{r}_i$

Reference positions $\mathbf{R}_i$

Displacements $\mathbf{u}_i = \mathbf{r}_i - \mathbf{R}_i$

$$\Delta_i = \mathbf{u}_i - \mathbf{u}_0$$

$$\chi_0 = \min_D \sum_i [\boldsymbol{\Delta}_i - \mathsf{D}(\mathbf{R}_i - \mathbf{R}_0)]^2$$

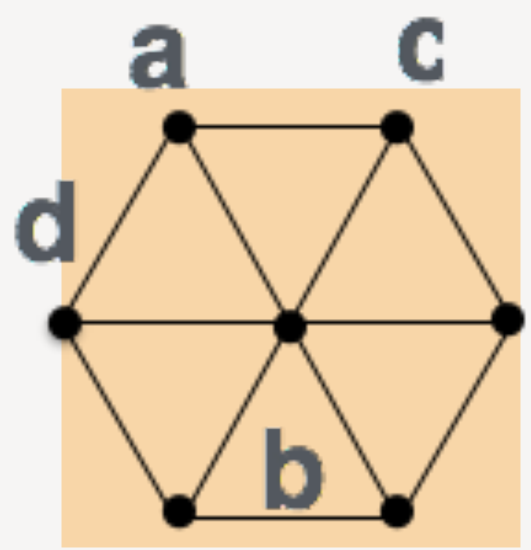
D = closest locally affine deformation

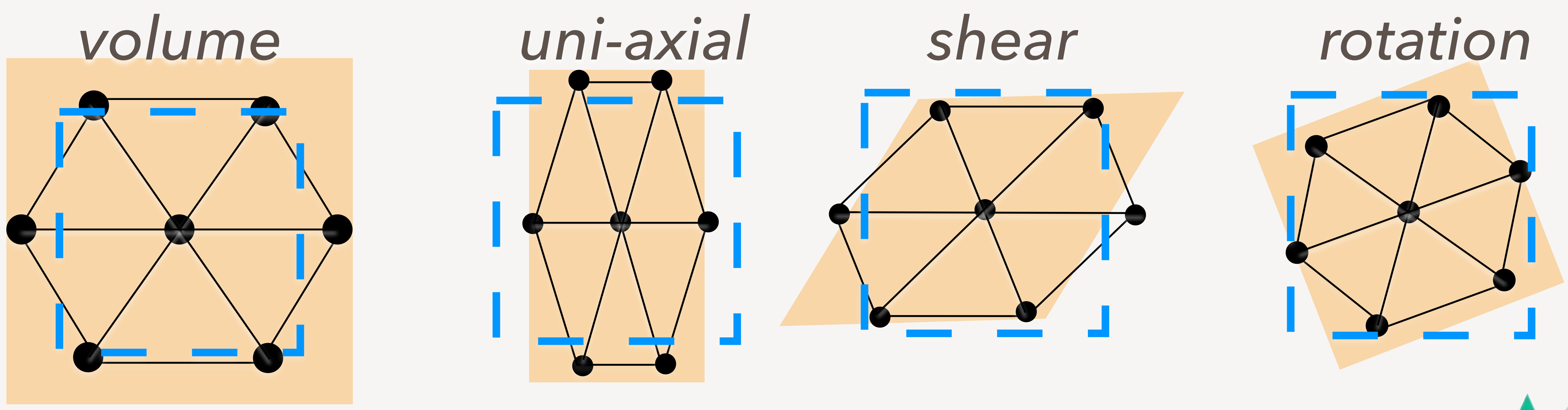
Rearrange $\{\boldsymbol{\Delta}_i\} \to$ vector Δ, similarly $\mathsf{D} \to$ vector $\mathbf{e}$:

$$\boxed{\mathbf{e} = \mathsf{Q}\Delta}, \boxed{\chi = (\mathsf{P}\Delta)^2 = \Delta^{\mathrm{T}}\mathsf{P}^{\mathrm{T}}\mathsf{P}\Delta = \Delta^{\mathrm{T}}\mathsf{P}\Delta}$$

Non-affine projector P, affine projector Q, both calculated from the $\{\mathbf{R}_i\}$

AFFINE FLUCTUATION MODES





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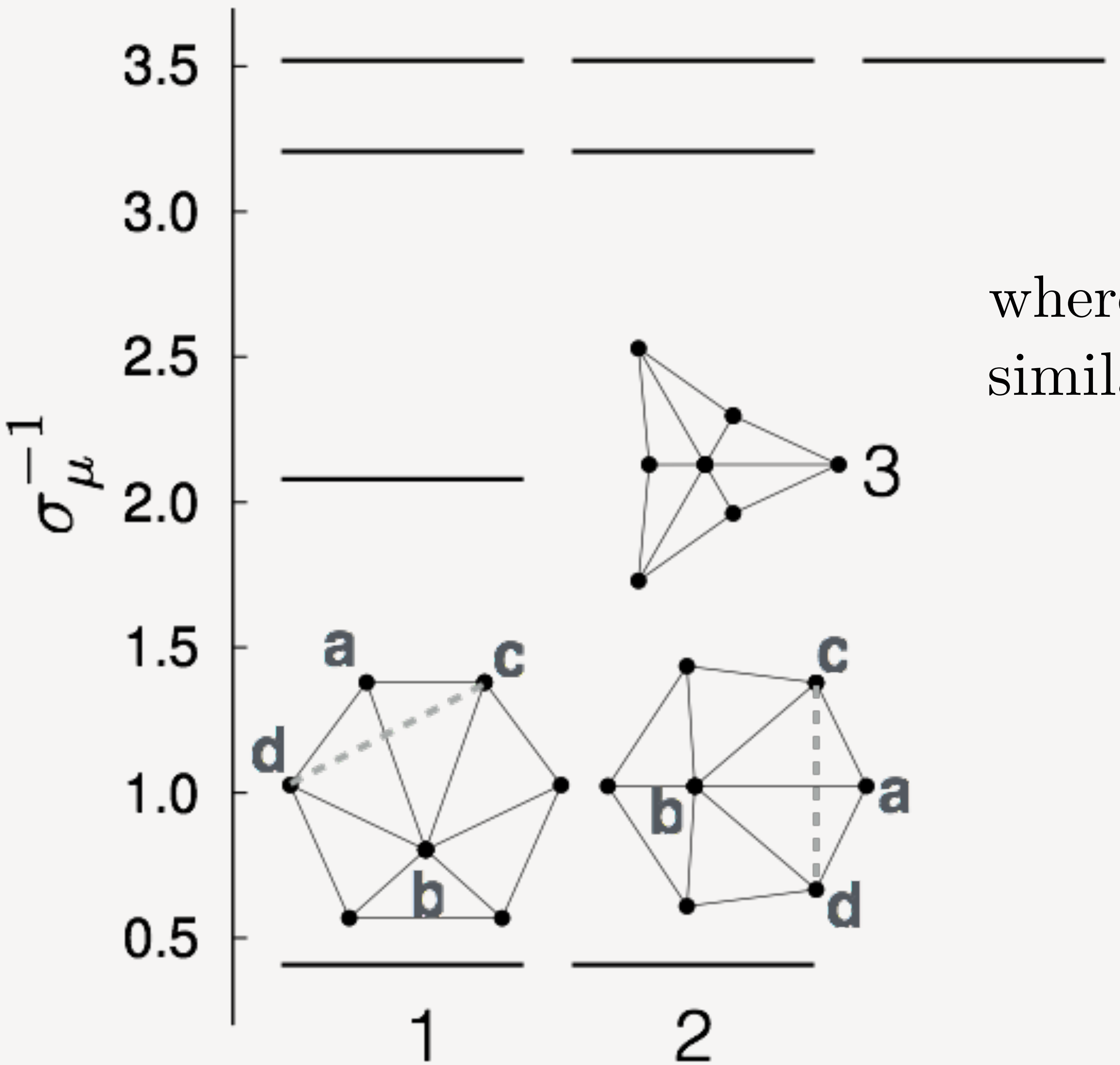
NON AFFINE FLUCTUATION MODES?

- $\chi = \Delta^{\mathrm{T}} \mathsf{P} \Delta = \mathrm{Tr} \mathsf{P} \Delta \Delta^{\mathrm{T}} \mathsf{P}$ so, $\langle \chi \rangle = \mathrm{Tr} \mathsf{PCP}$
- $\mathsf{C} = \langle \Delta \Delta^{\mathrm{T}} \rangle$ correlation matrix of displacement fluctuations
- Non-affine modes: eigenvectors of PCP

Ganguly,SS,Sollich,Rao PRE (2013) TCIS

NON-AFFINE SPECTRUM AND MODES



$$\langle \chi \rangle = \sum_{\mu=1}^{8} \sigma_\mu$$

where σ_μ are the eigenvalues of PCP. similarly $\mathbf{e}_\mu$ are the eigenvectors.

Ganguly, Sengupta, Sollich Soft Matter (2015)

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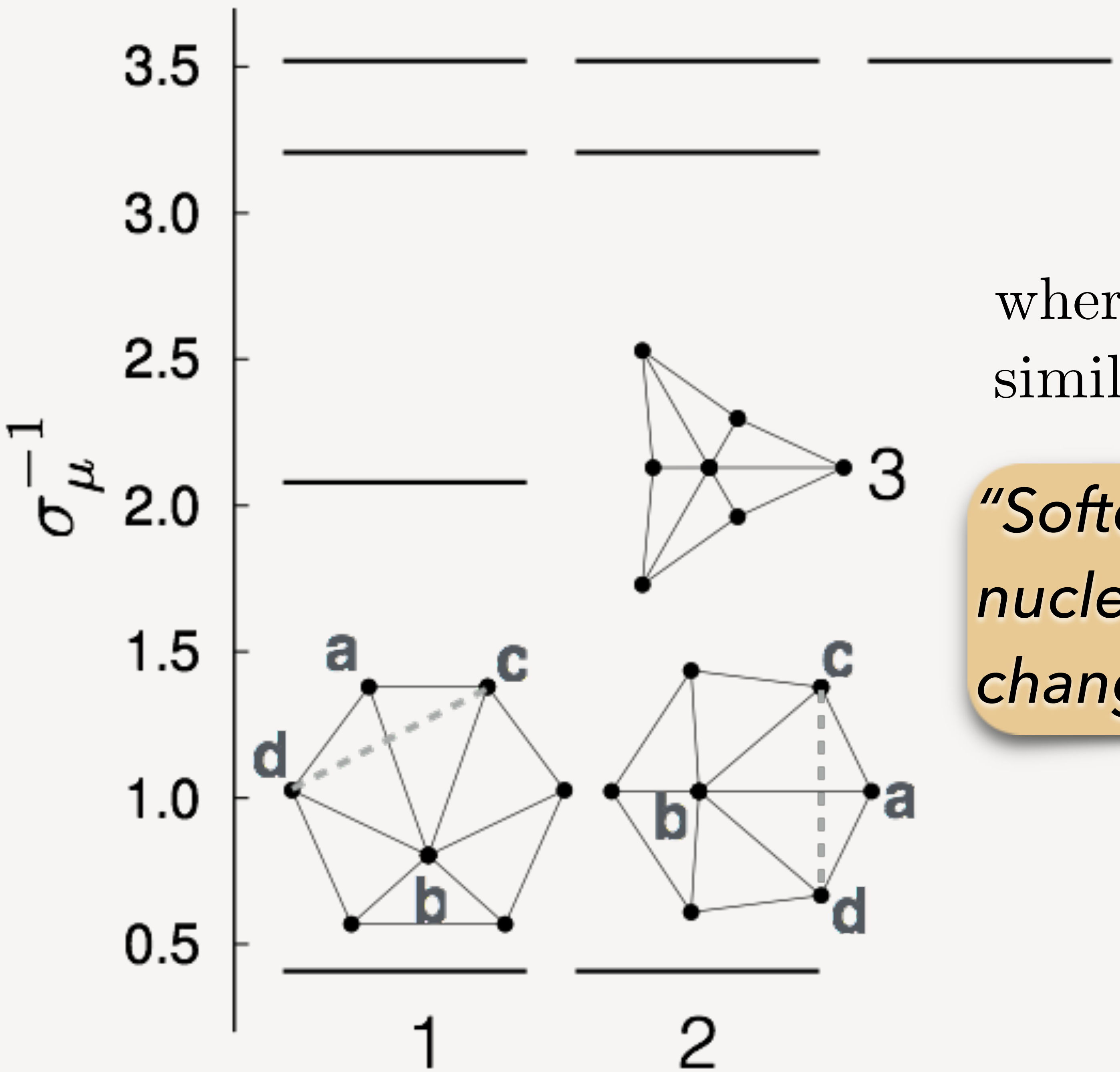

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"Softest" non-affine modes tend to nucleate defect dipoles leading to changes in neighbourhood.

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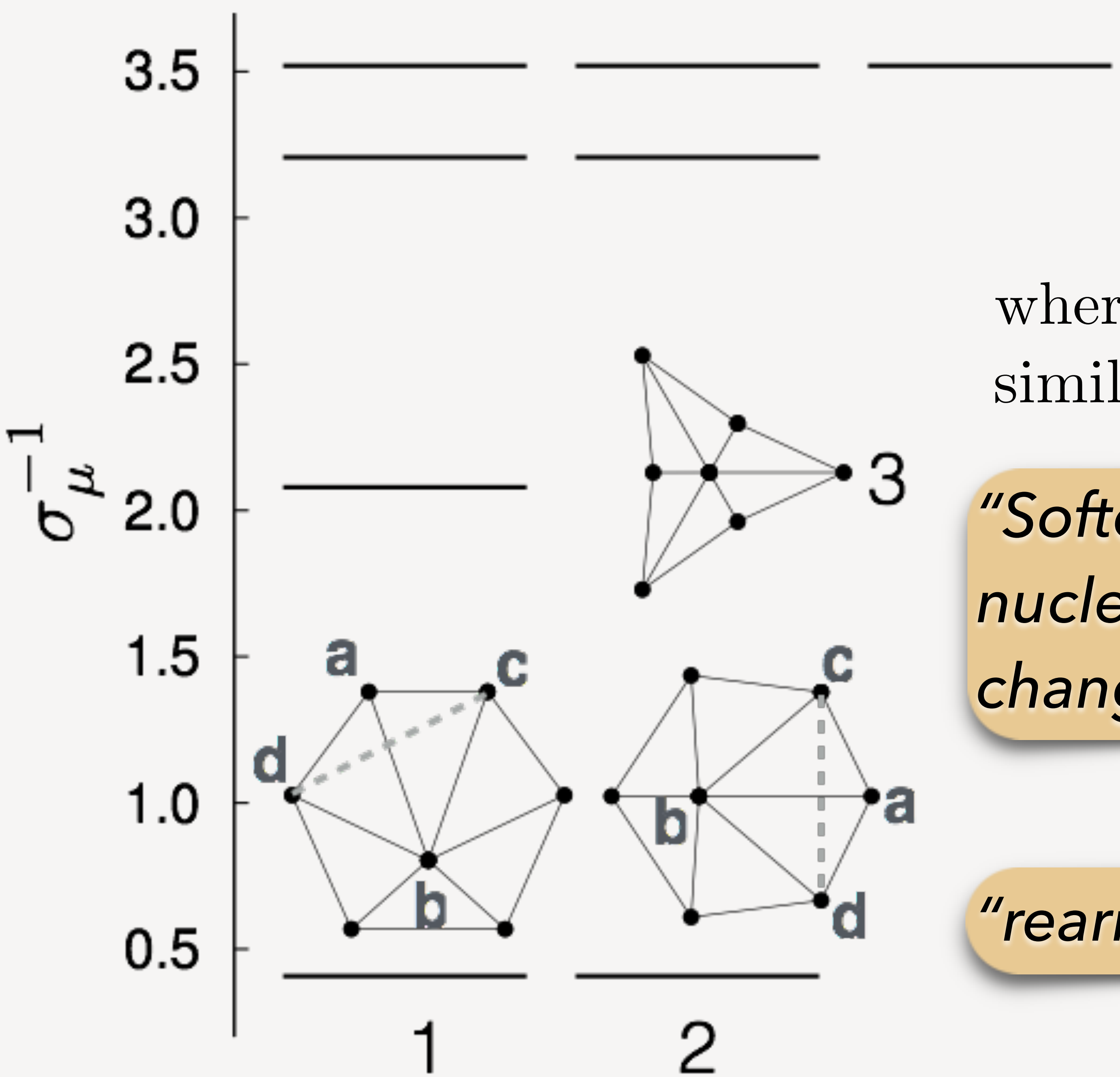
NON-AFFINE SPECTRUM AND MODES



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"rearrangements" create χ.

Ganguly, Sengupta, Sollich Soft Matter (2015)

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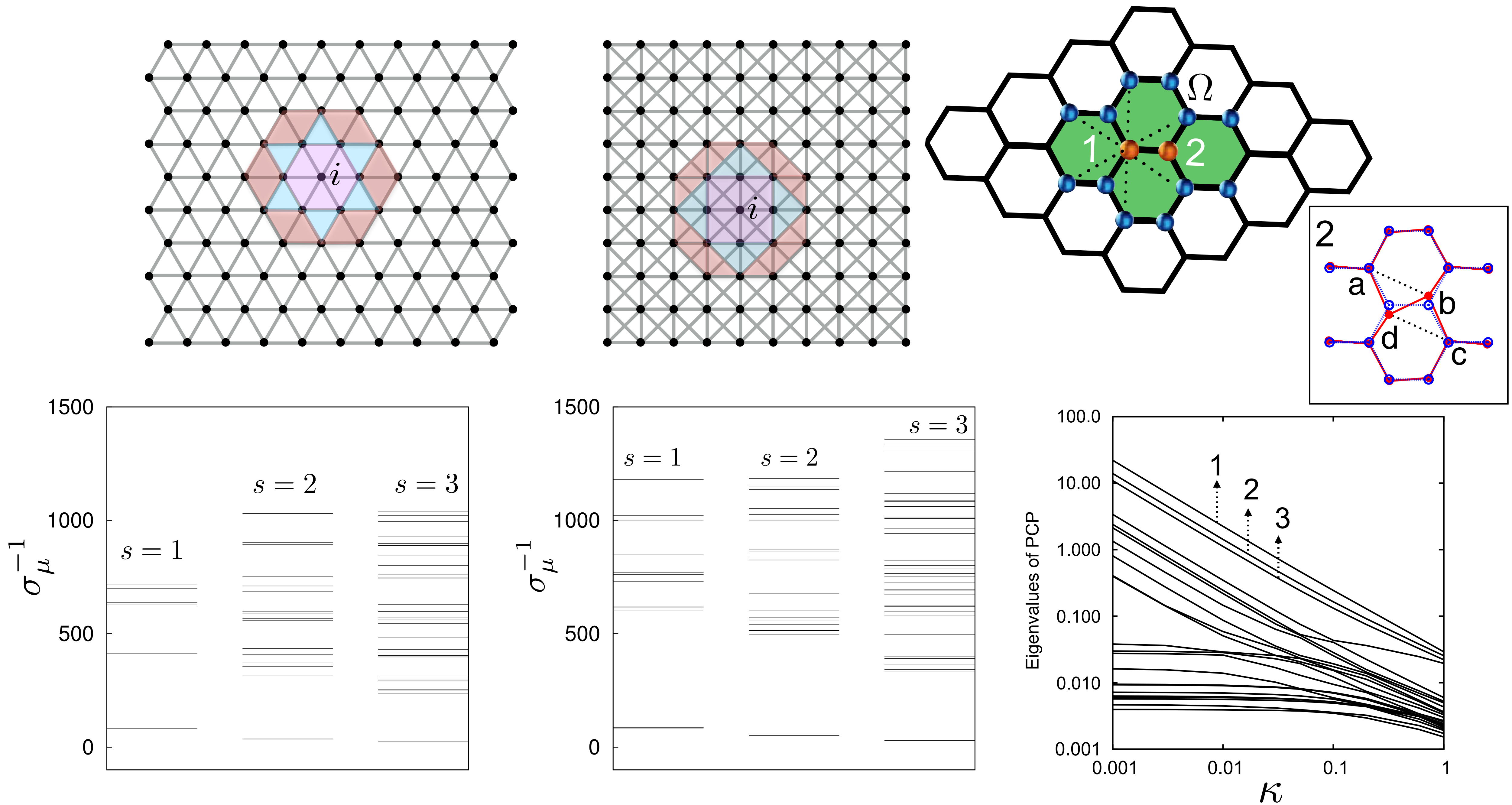

- Soft non-affine modes remain associated with defect precursors
  (Stone-Wales defect in planar honeycomb)
- Separated by a gap from other modes

*S. Ganguly et al. Soft Matter, **11**, 4517 (2015); A. Mitra, et al. J. Stat. Mech. P06025, (2015)*

BIASING NON-AFFINITY

THE "FICTITIOUS" FIELD

- Define global non-affinity $X = N^{-1}\sum_i \chi_i$
- $P(X)$ is a Gaussian entered at $\langle\chi\rangle$ with width $\sim 1/\sqrt{N}$
- Add bias term $-Nh_X X$ to the Hamiltonian, h_X non-affine field

$$Nh_X X = h_X \sum_i \sum_{j,k\in\Omega} (\mathbf{u}_j - \mathbf{u}_i)^{\mathrm{T}} \mathsf{P}_{j-i,k-i}(\mathbf{u}_k - \mathbf{u}_i)$$

- Two-body interactions between next nearest neighbours
- No coupling to affine deformations - those couple to stress
- Interaction $\mathsf{P}_{\cdot,\cdot}$ in bias term involves particle reference position $\{\mathbf{R}_i\}$
- Note: translational symmetry, $\mathbf{u}_i \to \mathbf{u}_i + \text{constant}$, is preserved.

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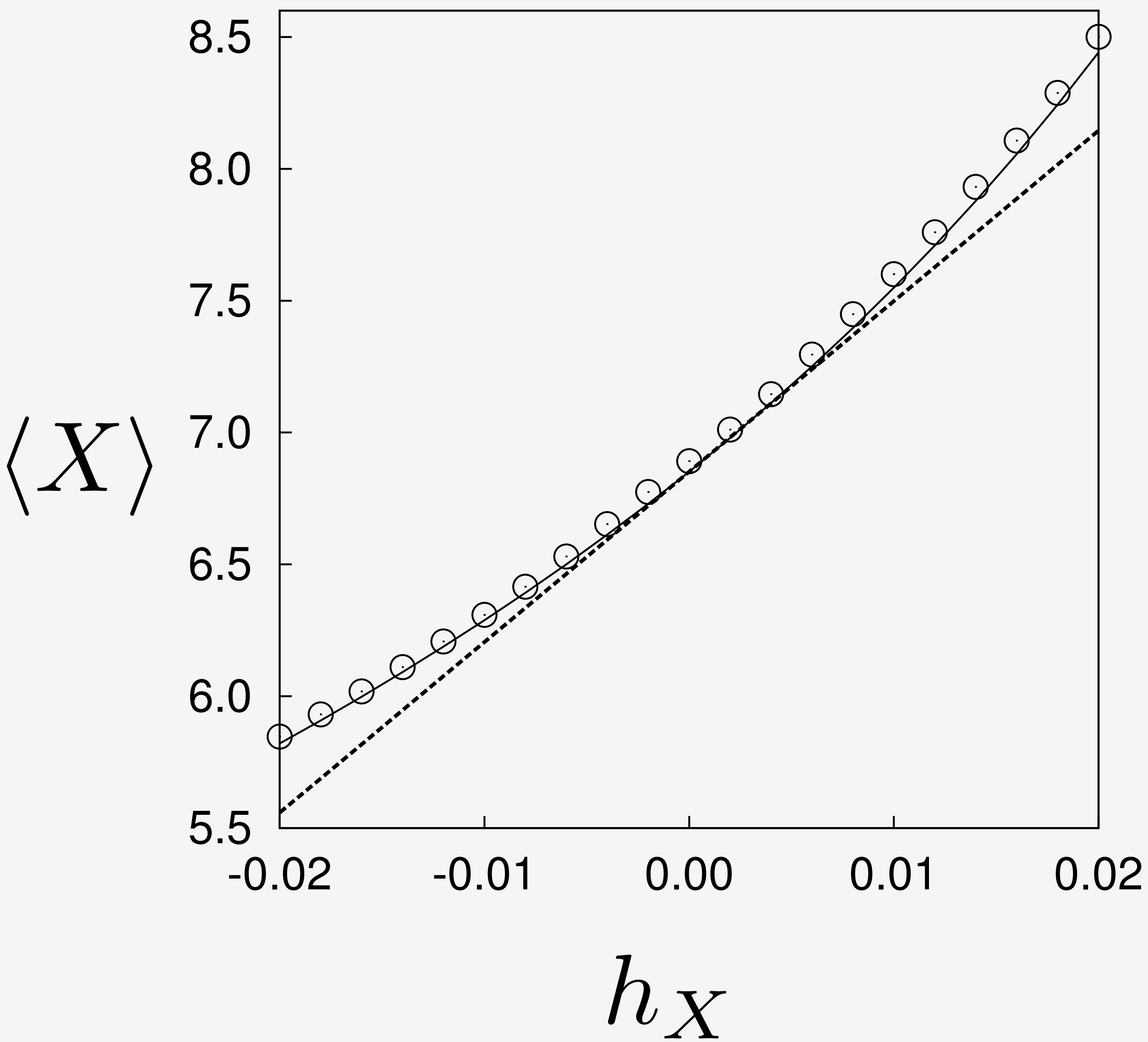
SMALL FIELDS: FLUCTUATION RESPONSE



$X(h_X) = X(0) + \langle \Delta\chi^2 \rangle \sum_{\mathbf{R}} C_\chi(\mathbf{R}, 0)$ where $C_\chi(\mathbf{R}, 0)$ is the equal time, spatial correlation of χ.

S. Ganguly et al. Soft Matter, ***11****, 4517 (2015)* TCIS

LARGE FIELDS: GLOBAL THERMO-DYNAMICS

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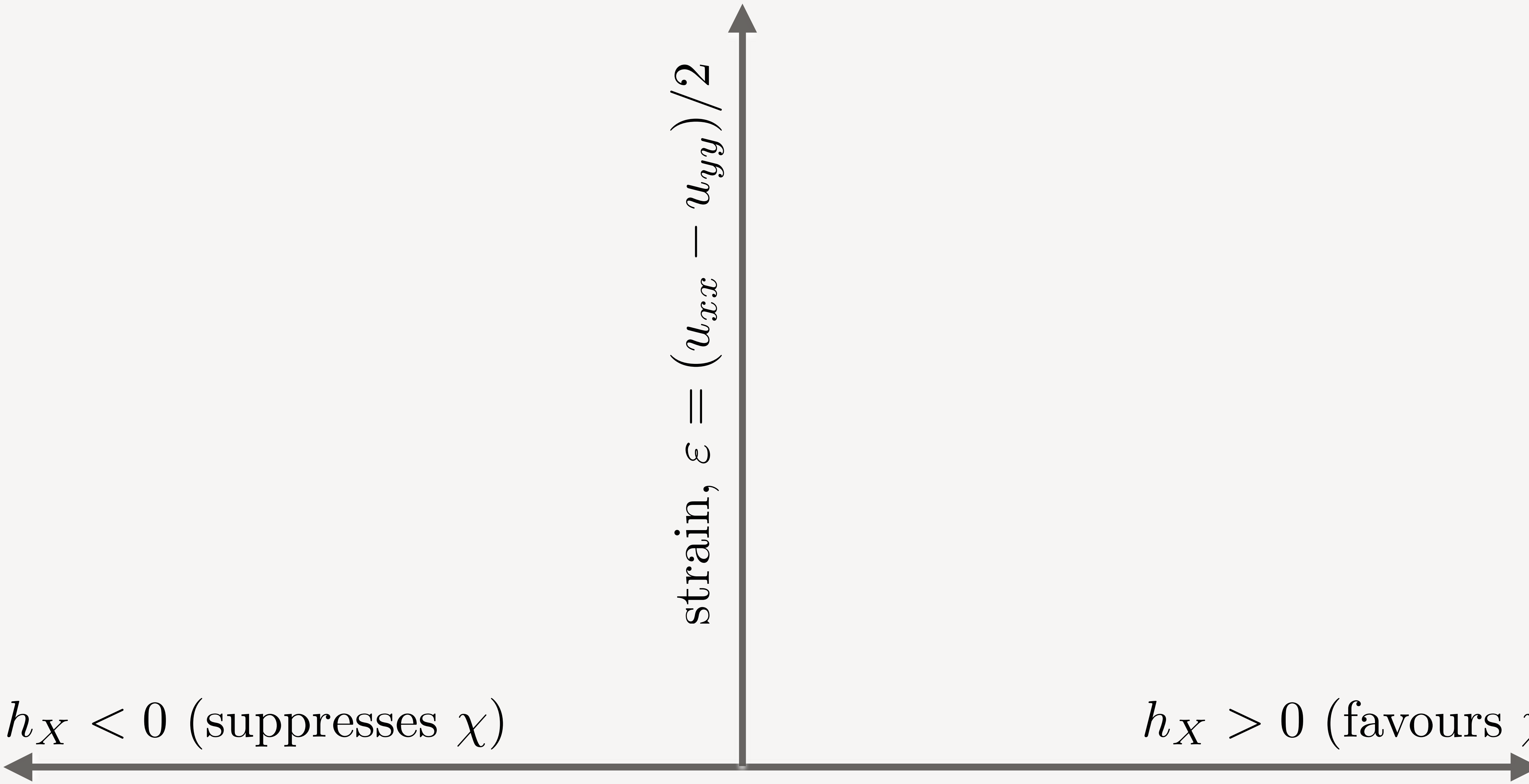
LARGE FIELDS: GLOBAL THERMODYNAMICS



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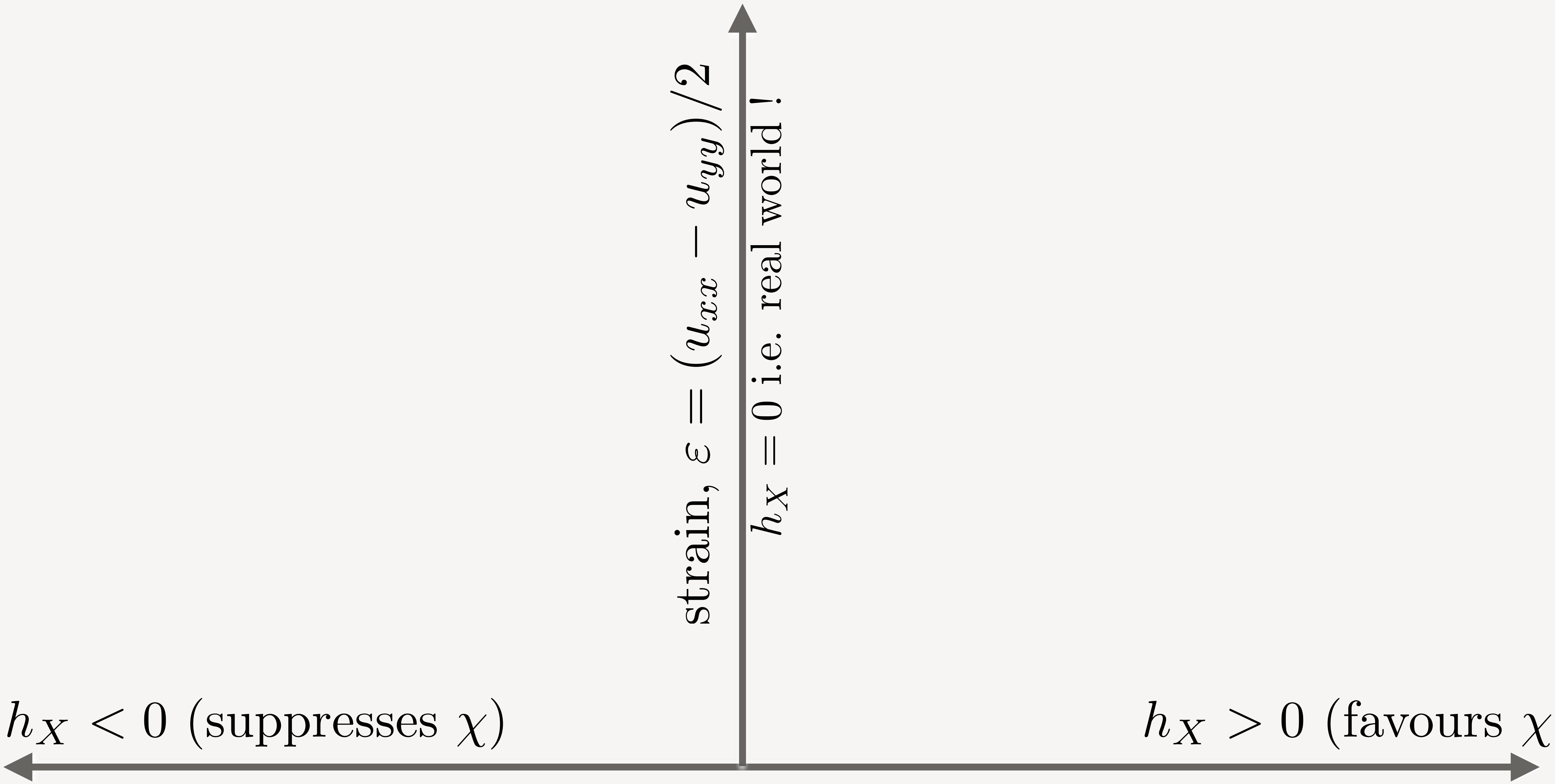

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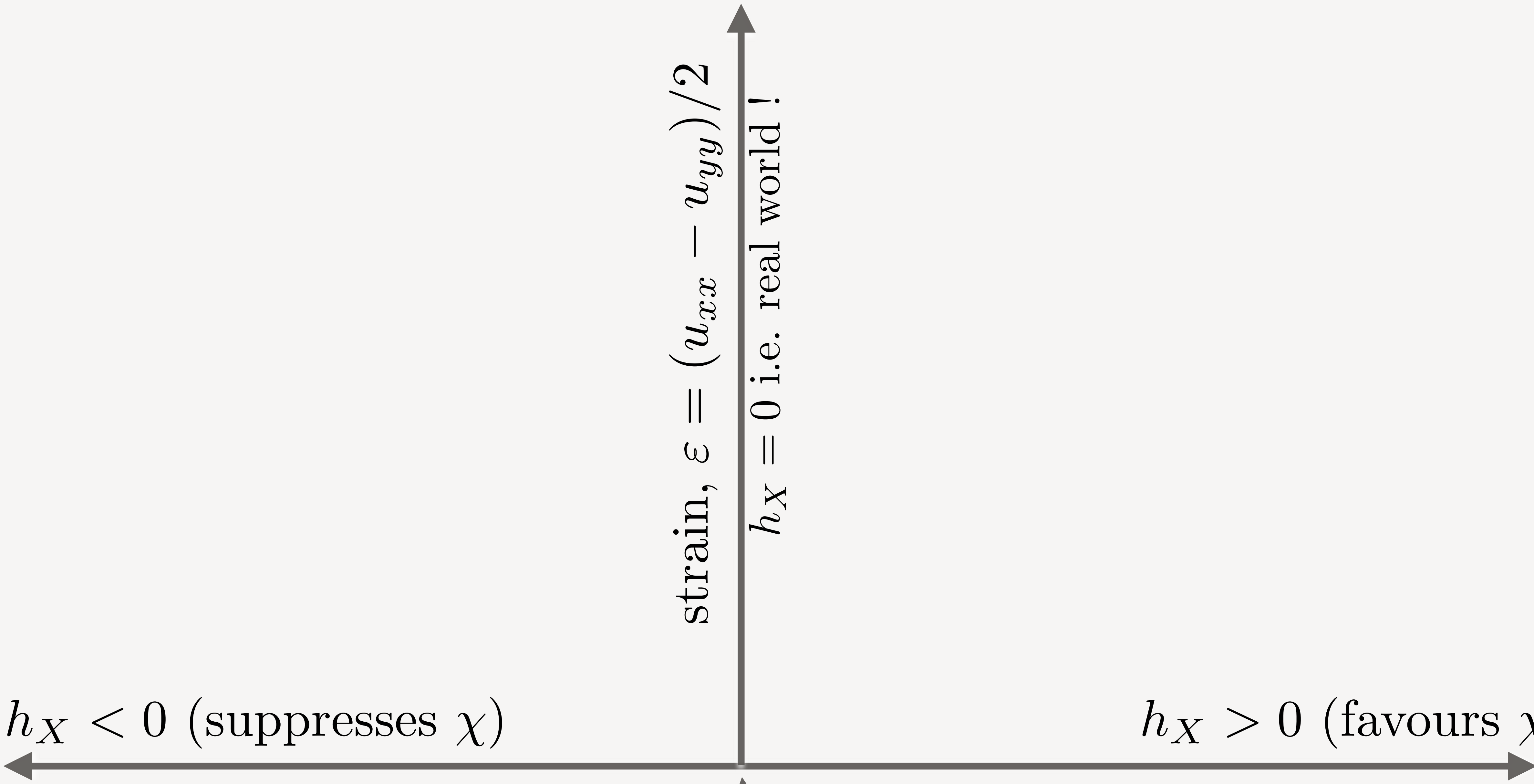

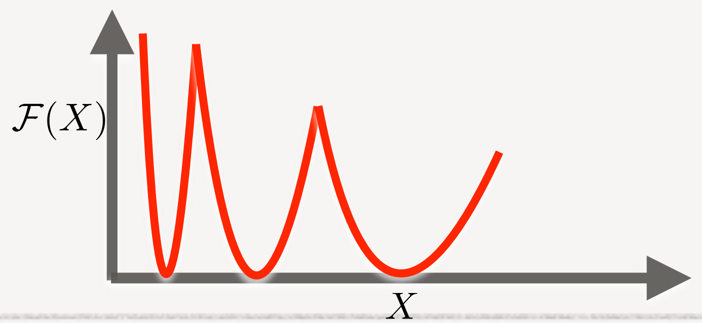

infinitely many degenerate minima
at $\varepsilon = 0$ corresponding to rearranged
copies of the reference configuration

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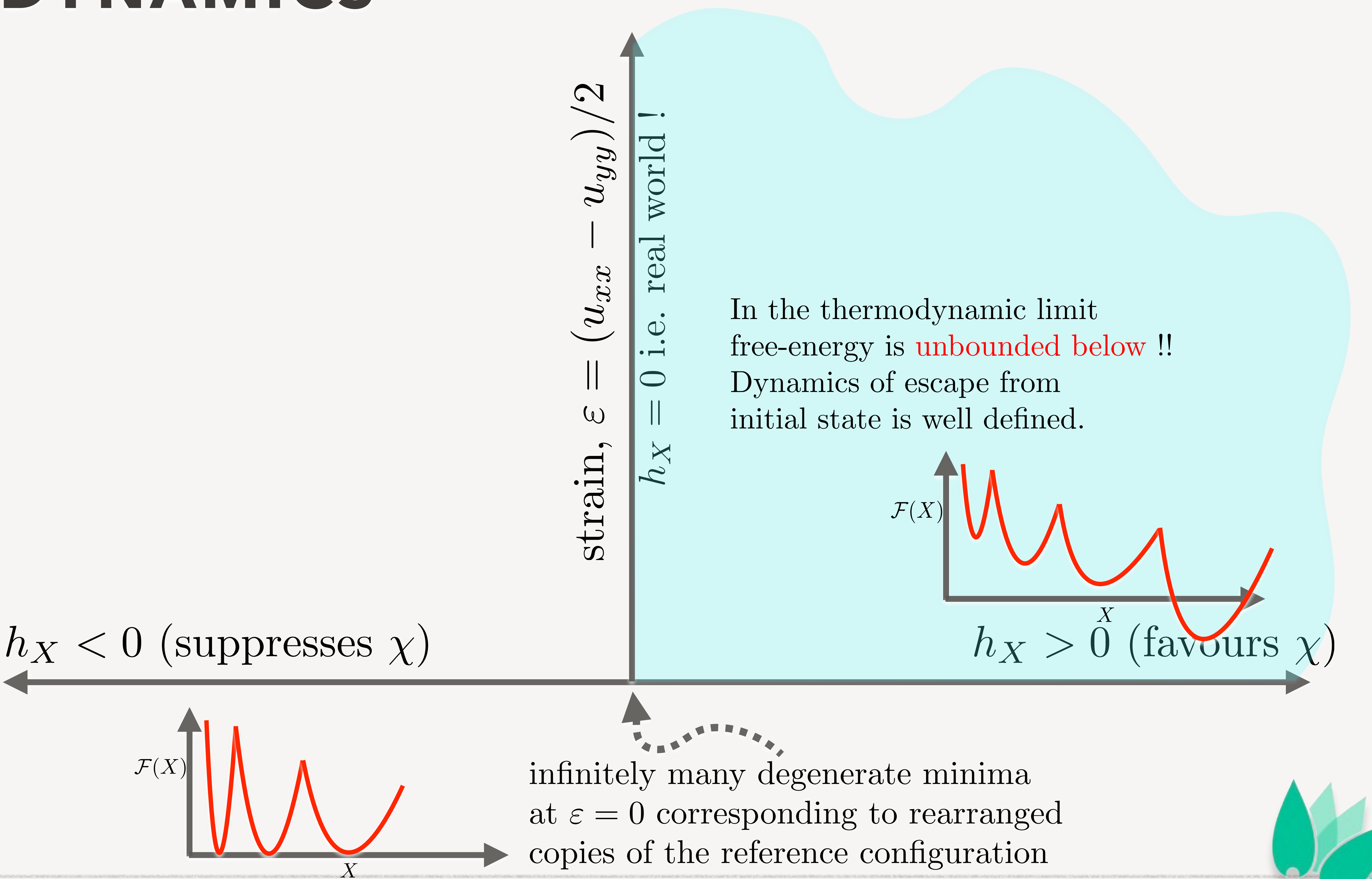
LARGE FIELDS: GLOBAL THERMO-DYNAMICS



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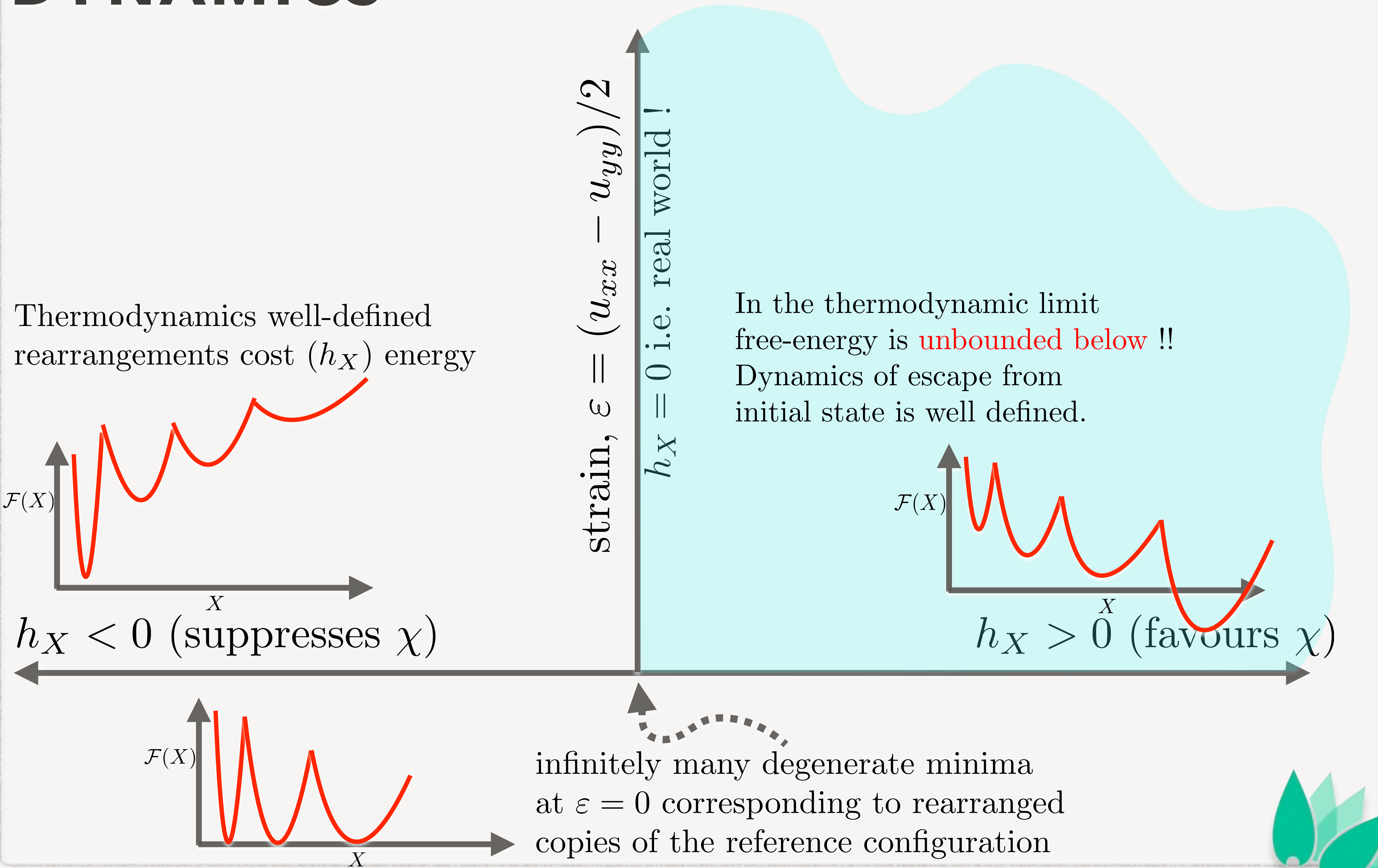

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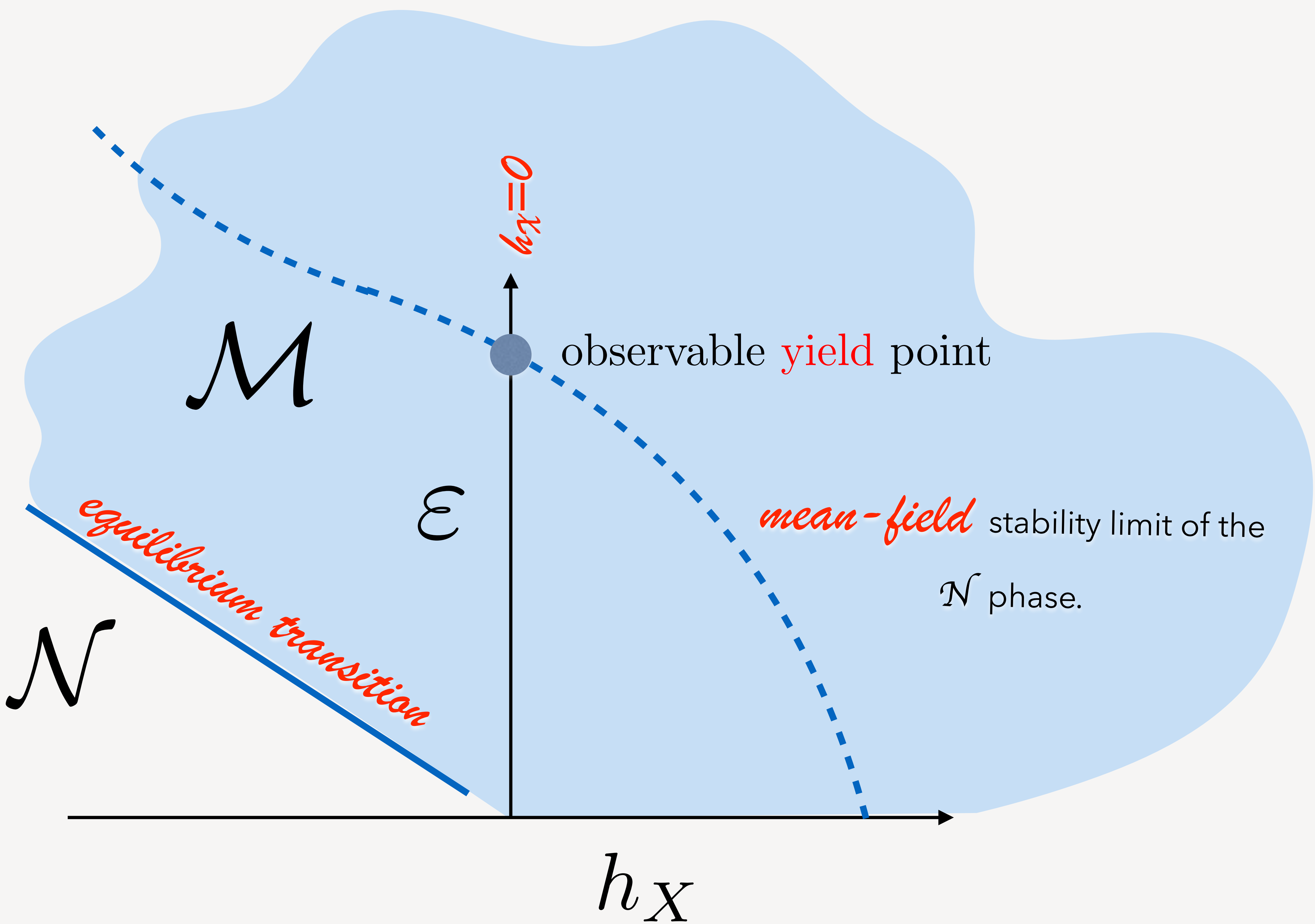
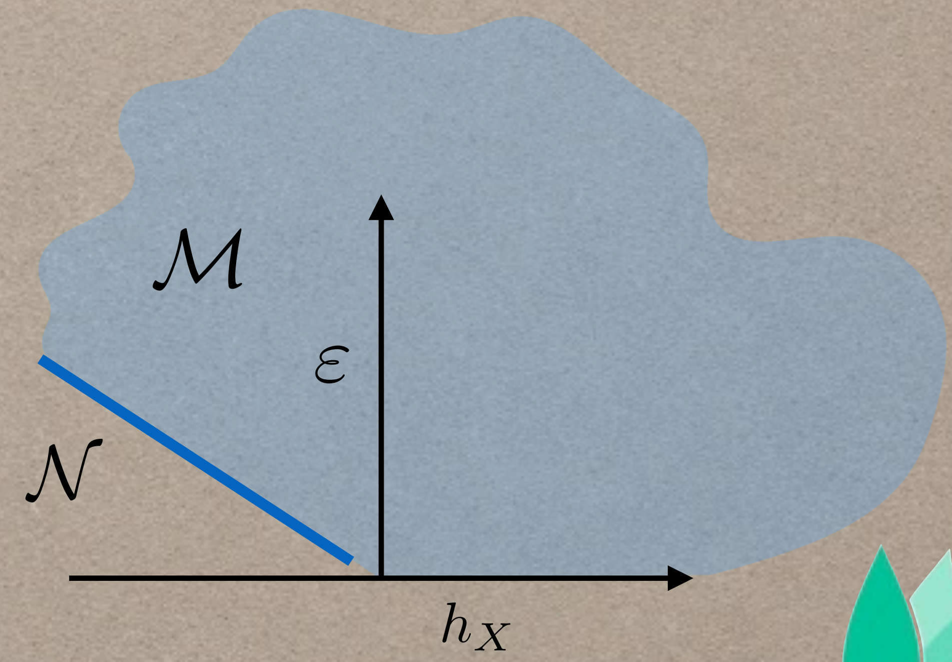
THE STORY

At the yield point the $\mathcal{N}$ phase becomes unstable w.r.t. *non-affine* displacement fluctuations



THE EQUILIBRIUM TRANSITION



T=0 PHASE DIAGRAM

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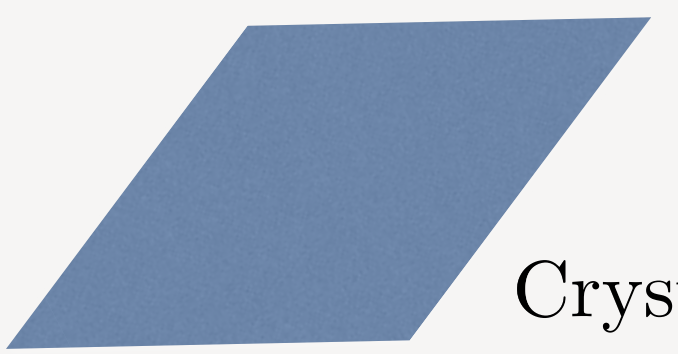
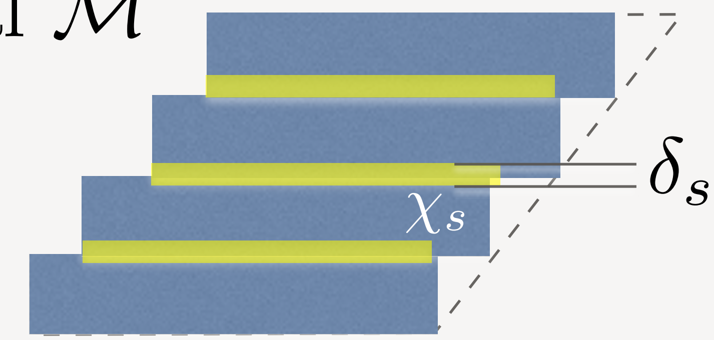
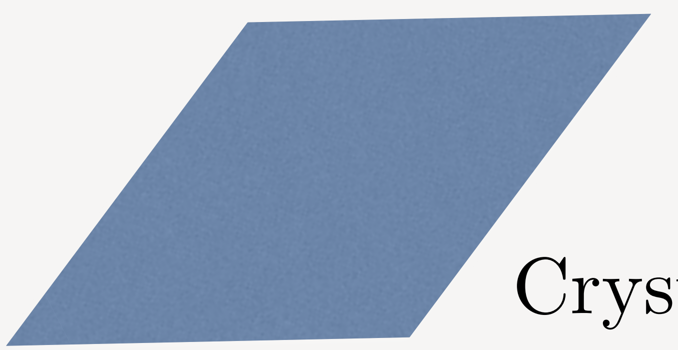


Crystal $\mathcal{N}$

T=0 PHASE DIAGRAM

Crystal $\mathcal{M}$





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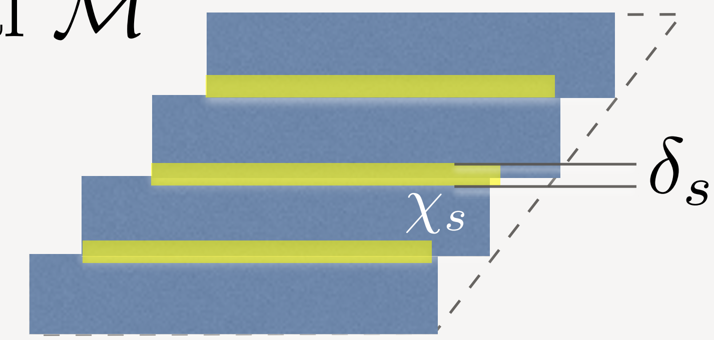

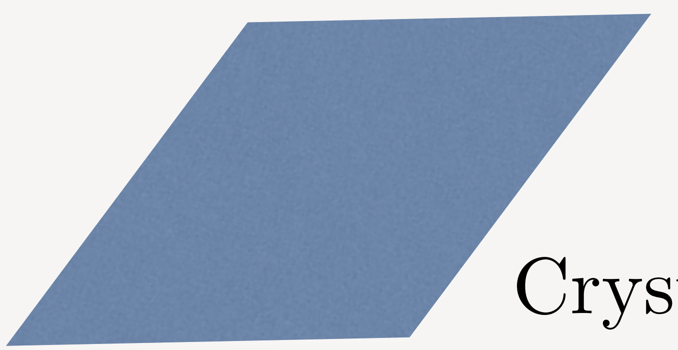

Crystal $\mathcal{N}$

- For any strain $\varepsilon > 0$ crystal $\mathcal{N}$ has stress $\sigma = G\varepsilon$.
- Stress in crystal $\mathcal{M}$ is always 0.
- Crystal $\mathcal{N}$ is metastable for all $h_X > 0$.
- For $h_X < 0$: possibility of a phase transition.
- Stress relaxation by N_s slip planes $GN_s a/L$.
- compare $\sim \frac{1}{2}G\varepsilon^2$ to $\sim h_X|\varepsilon|\chi_s$.
- phase boundary $\boxed{h_X = -G|\varepsilon|/2\chi_s}$

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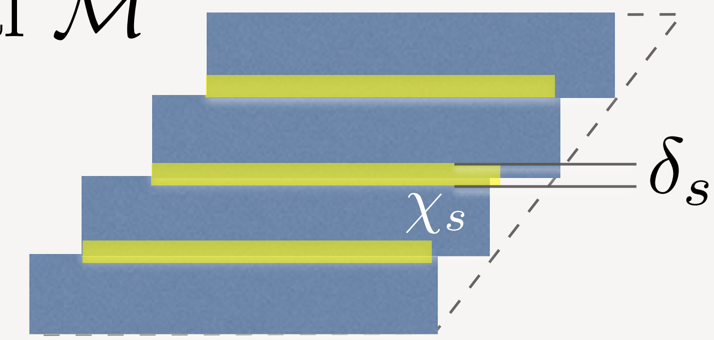
T=0 PHASE DIAGRAM

Crystal $\mathcal{M}$



strain, $\varepsilon = (u_{xx} - u_{yy})/2$

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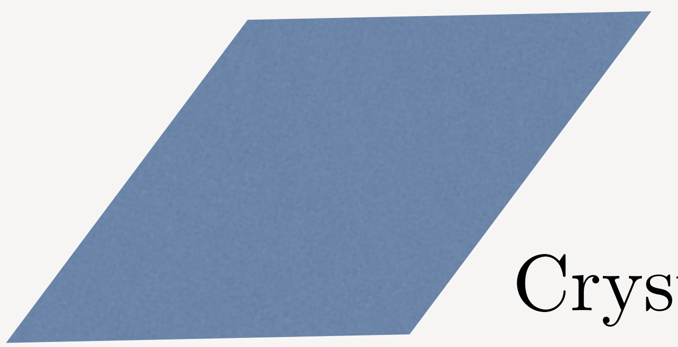

Crystal $\mathcal{N}$

$h_X < 0$ (suppresses χ) $h_X > 0$ (favours χ)

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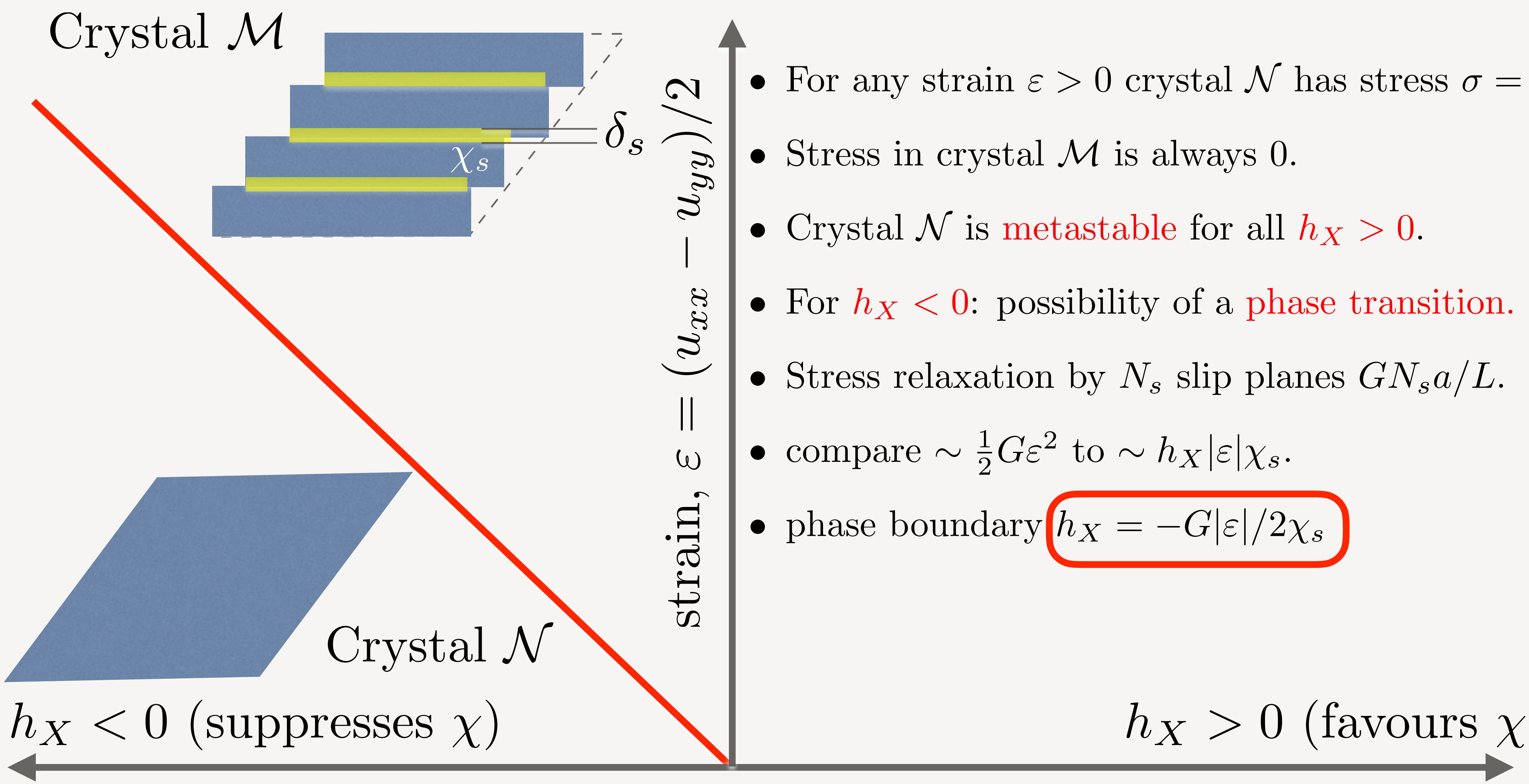
T=0 PHASE DIAGRAM



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T>0

- N particles with Lennard Jones interactions in 2d plus non-affine field.
- constant $N, V(\text{shape}), T$, ensemble.
- cut-off at 2.5 times particle diameter, truncated and shifted, $T^* = 0.8, \rho = 2/\sqrt{3}$.
- Large energy barriers between $\mathcal{N}$ and $\mathcal{M}$ crystals.
- Sequential umbrella sampling Monte Carlo (SUS-MC) technique needed.
- accurate calculation of $P(X)$ at the transition.
- transition point obtained by histogram reweighting.

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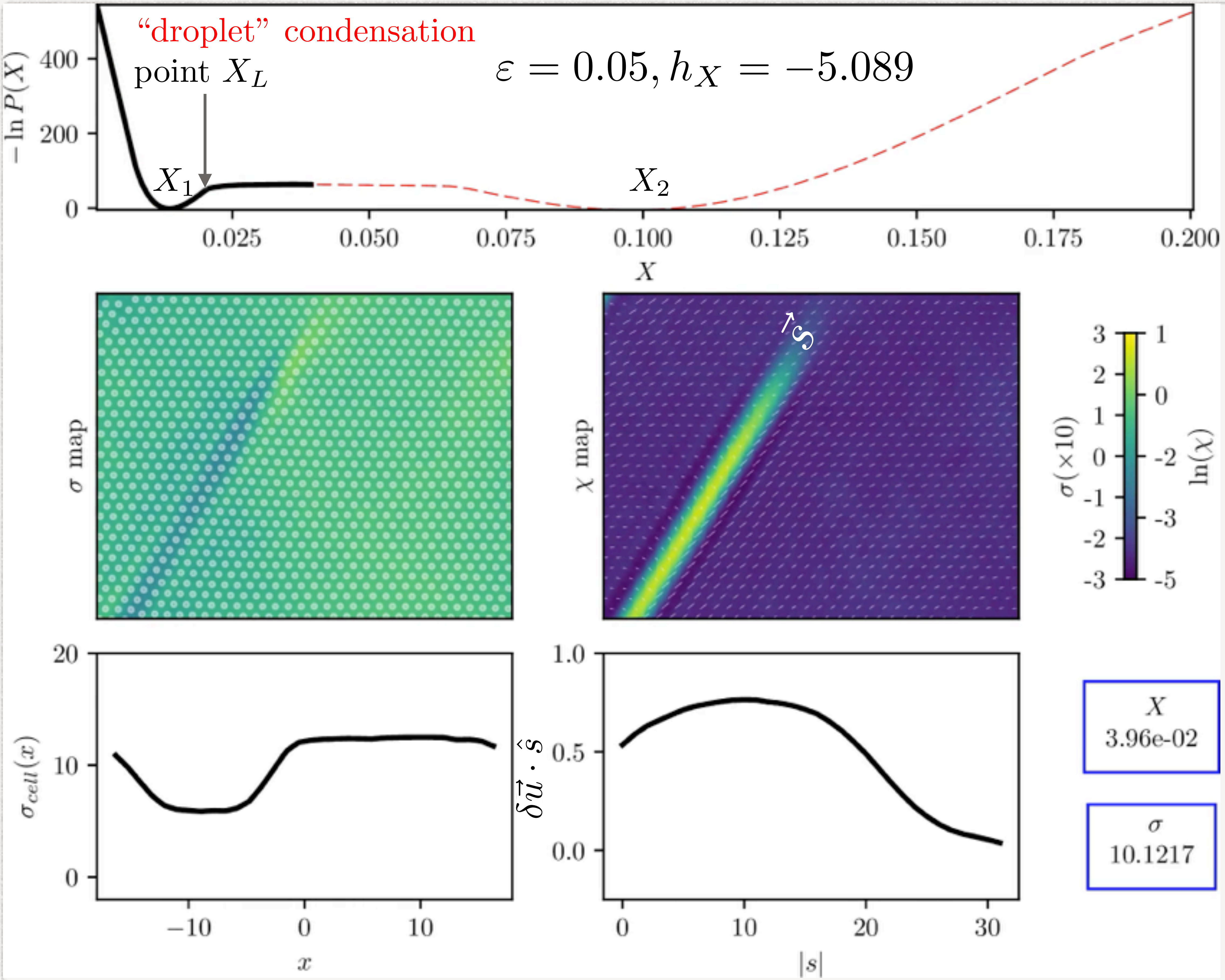

"droplet" condensation
point X_L
$\varepsilon = 0.05, h_X = -5.089$
X_1
X_2
$-\ln P(X)$
X
σ map
χ map
$\vec{s}$
$\sigma(\times 10)$
$\ln(\chi)$
$\sigma_{cell}(x)$
x
$\delta\vec{u}\cdot\hat{s}$
$|s|$
X
3.96e-02
σ
10.1217

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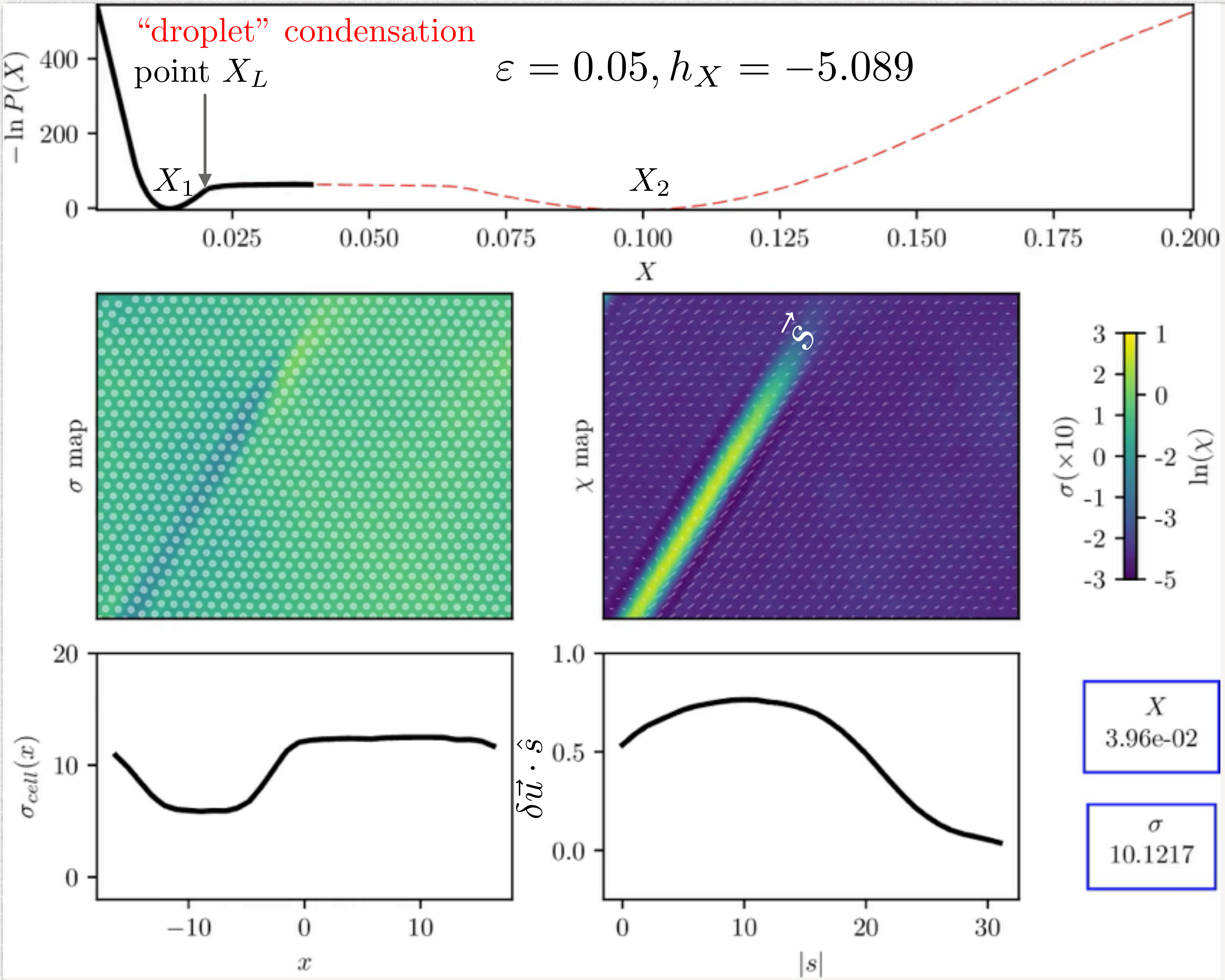

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x
$\delta\vec{u}\cdot\hat{s}$
$|s|$
X
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σ
10.1217

COMMENTS

- two minima of equal weight in the effective Hamiltonian $\mathcal{F}(\mathcal{X}) = -\ln \mathcal{P}(\mathcal{X})$
- singularity at $X = X_L \approx .02$.
- a proto- dislocation dipole / stacking fault forms at X_L
- large coexistence region between crystals $\mathcal{N}$ and $\mathcal{M}$
- novel solid-solid interface between $\mathcal{N}$ and $\mathcal{M}$ defined by local stress
- stress is *eliminated* from $\mathcal{M}$ crystal by slip

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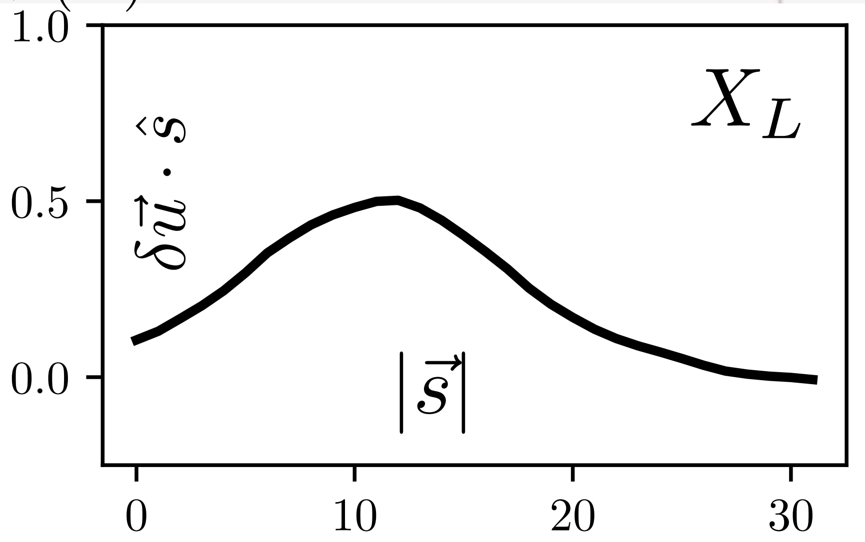

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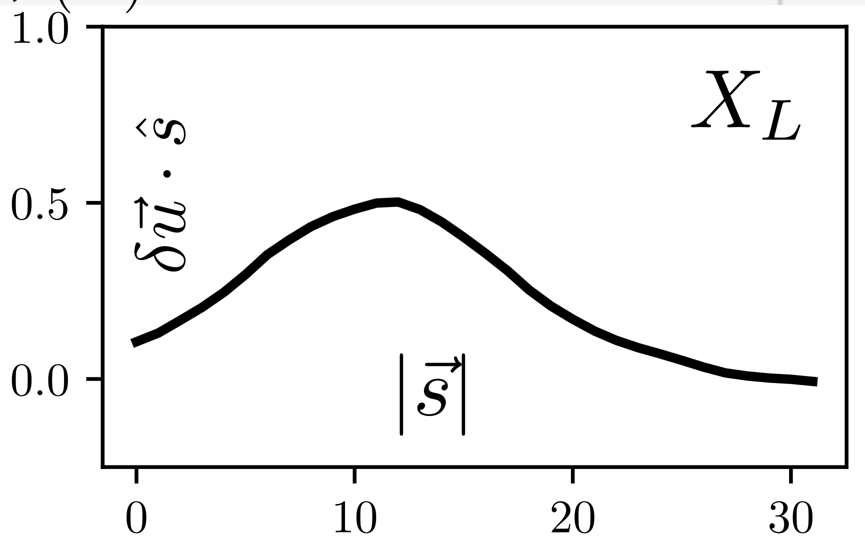
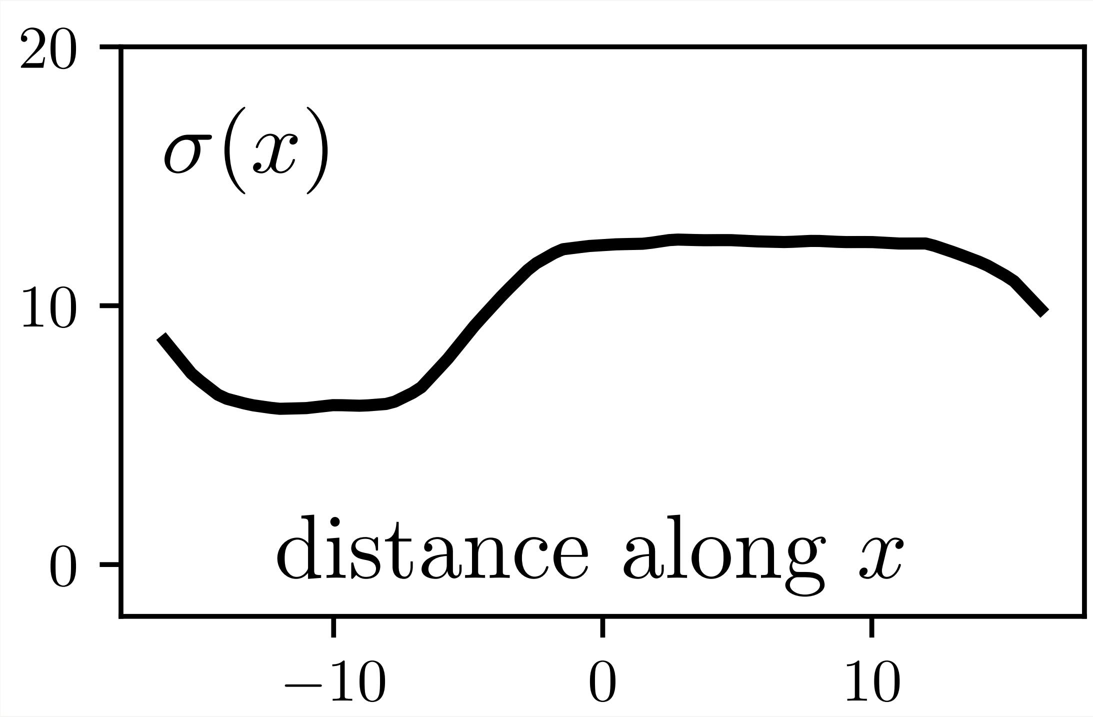
- stress is *eliminated* from $\mathcal{M}$ crystal by slip





COMMENTS

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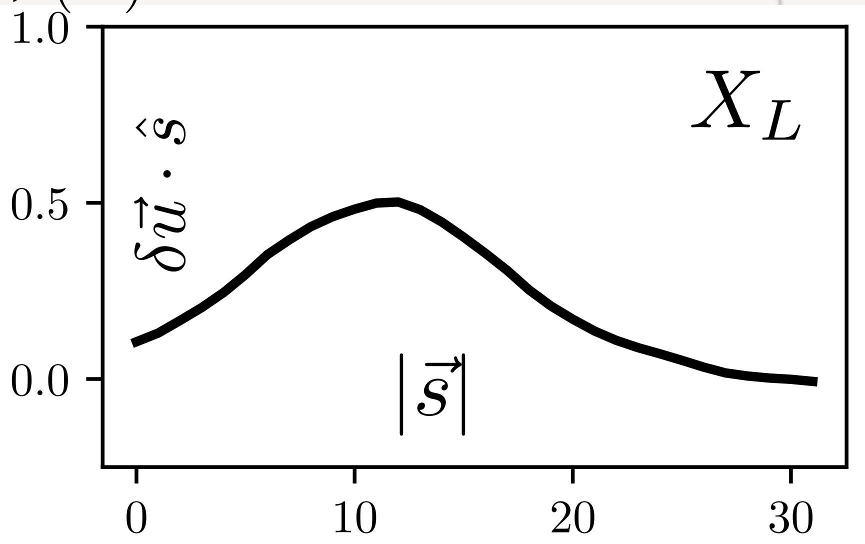

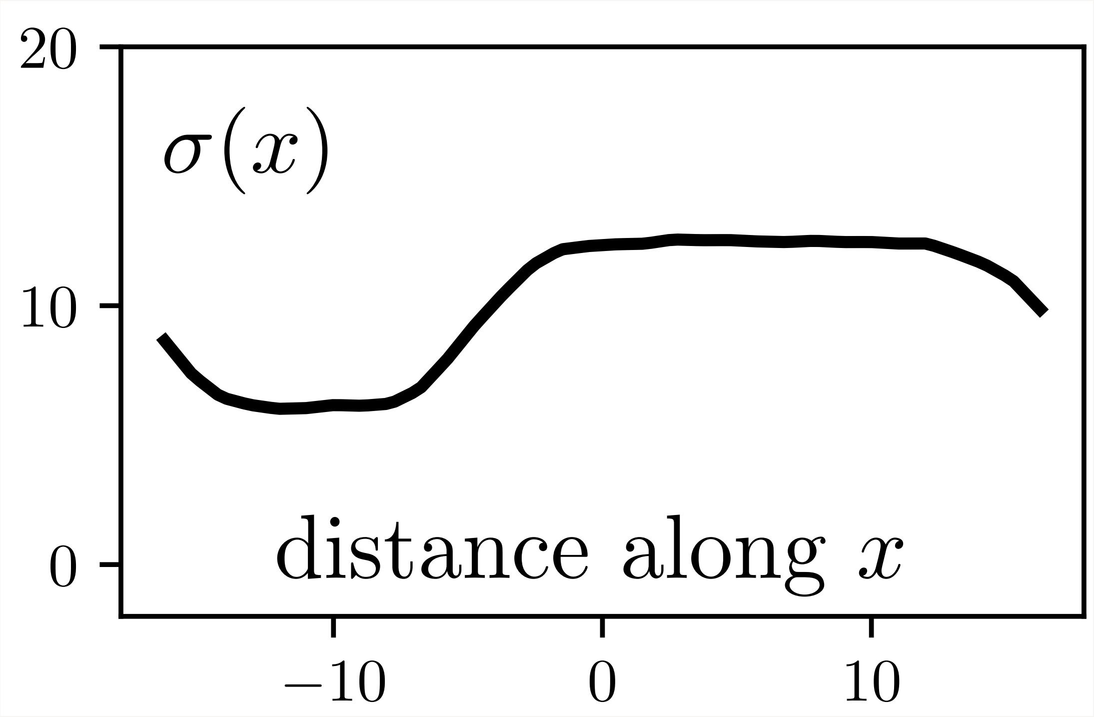

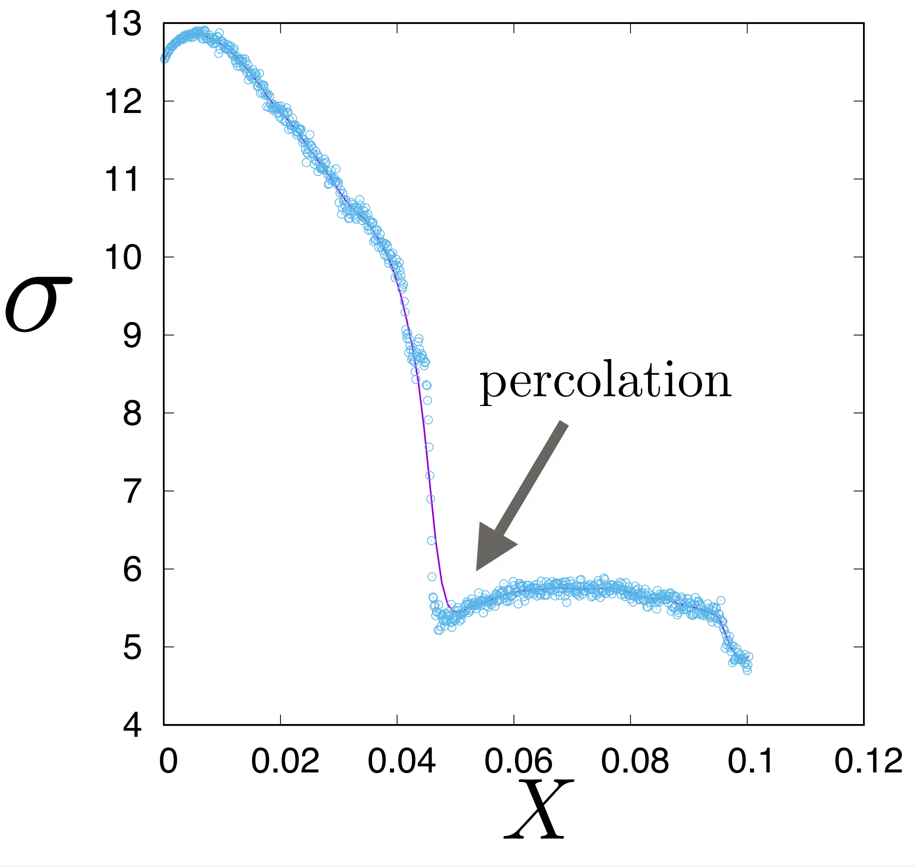

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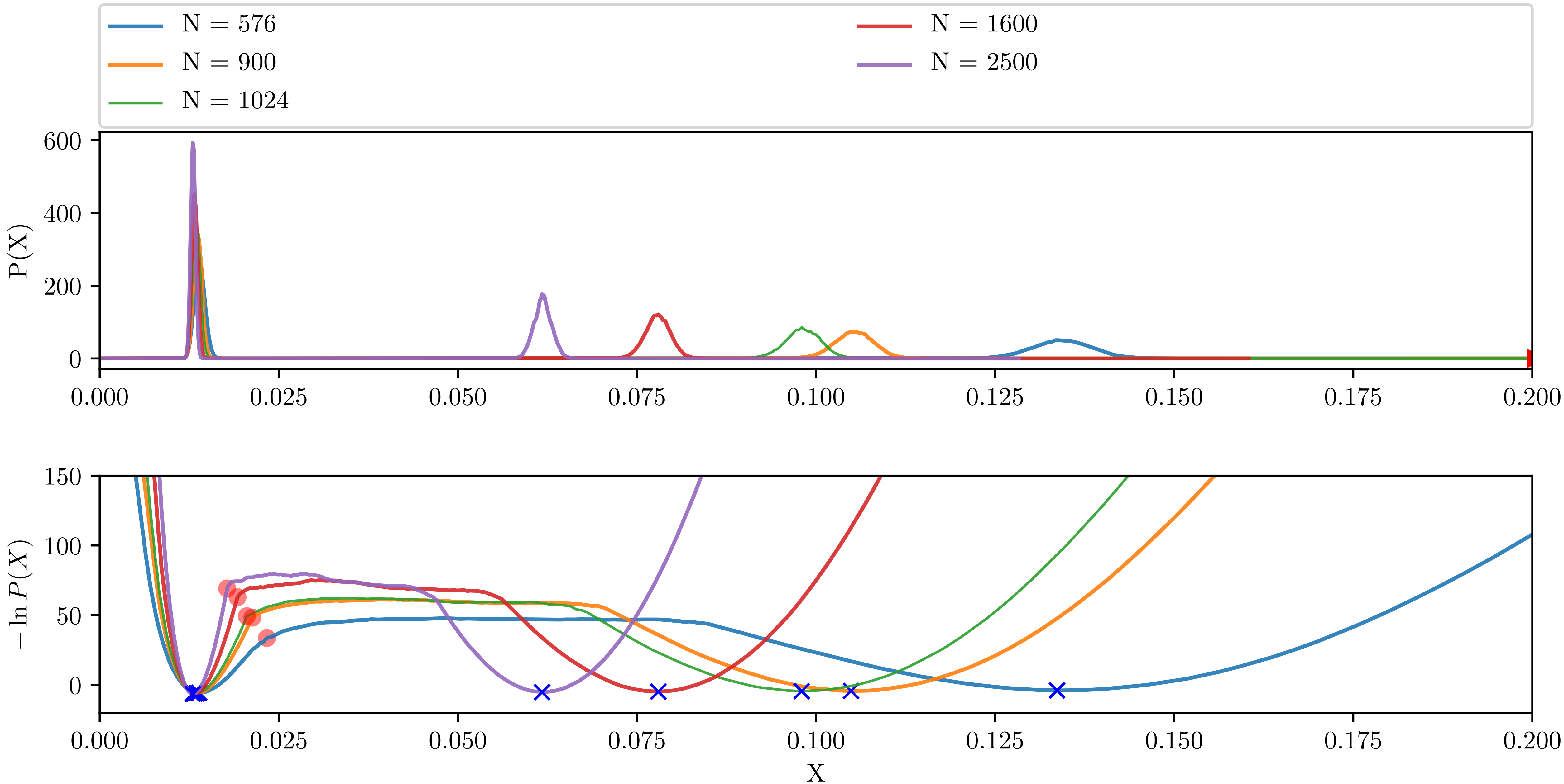
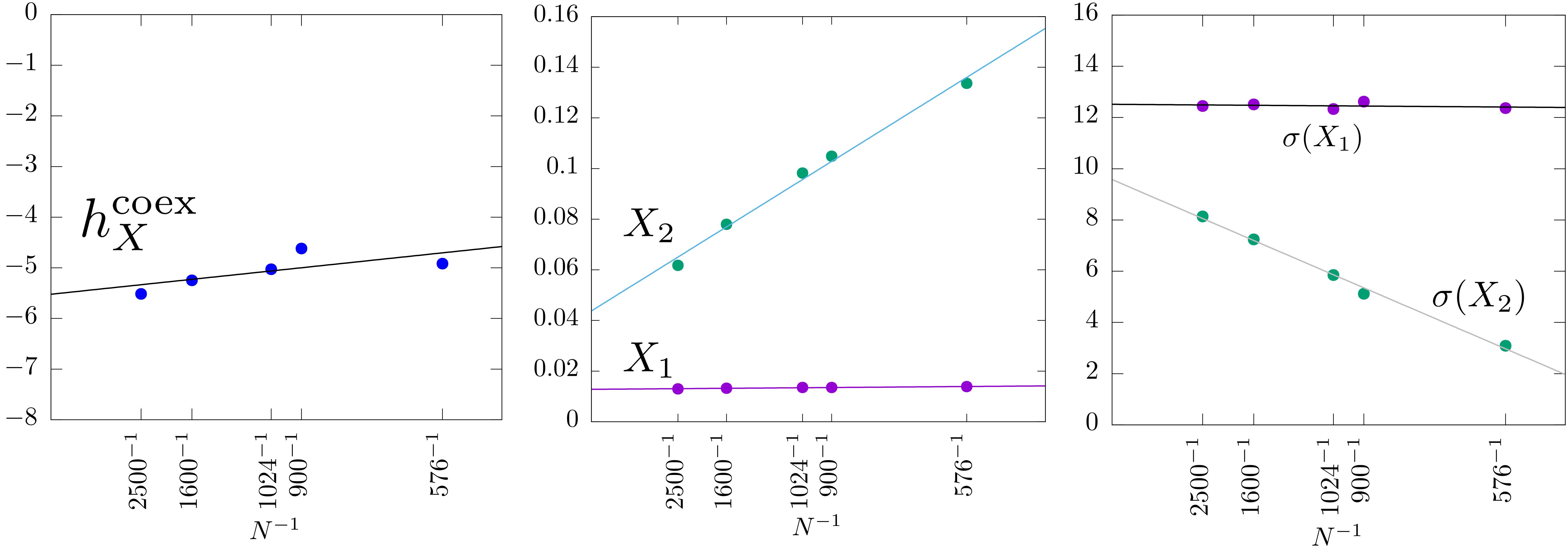
FINITE SIZE EFFECTS

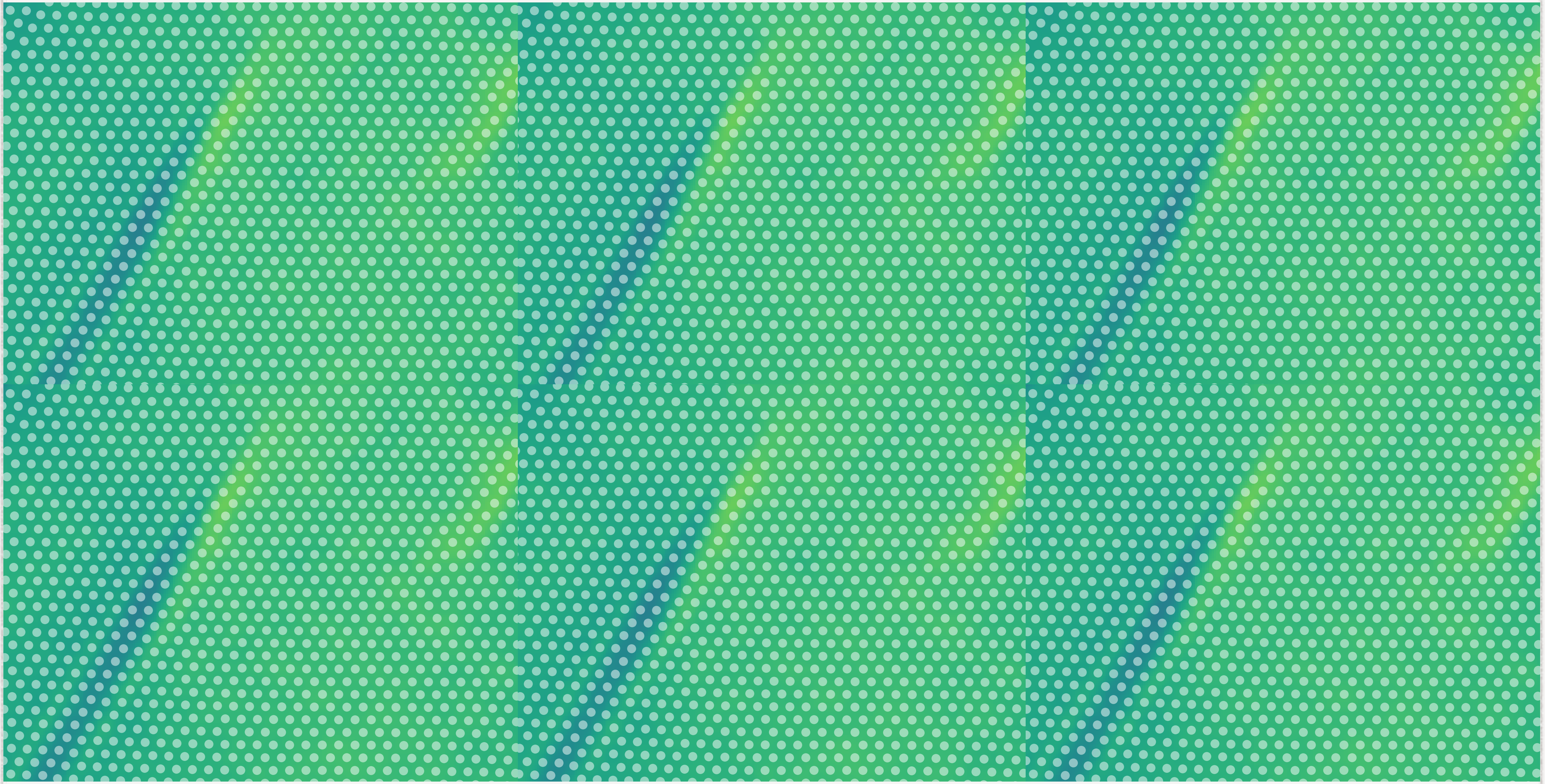


FINITE SIZE SCALING



Jump in X, σ and h_X^{coex} scales as $L^{d=2} = N$

Interfacial free energy scales as $L^{d-1} \sim \sqrt{N}$



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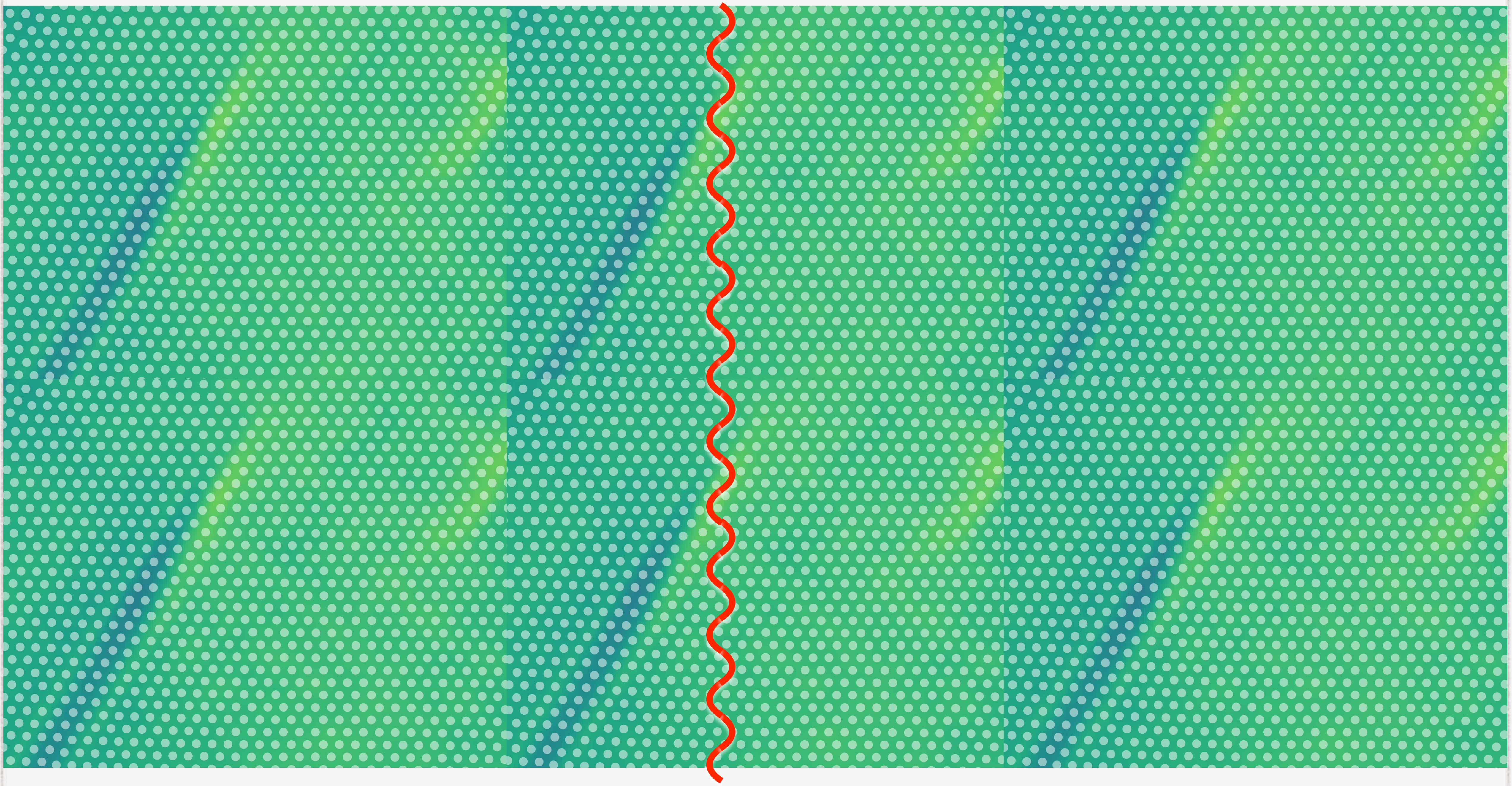

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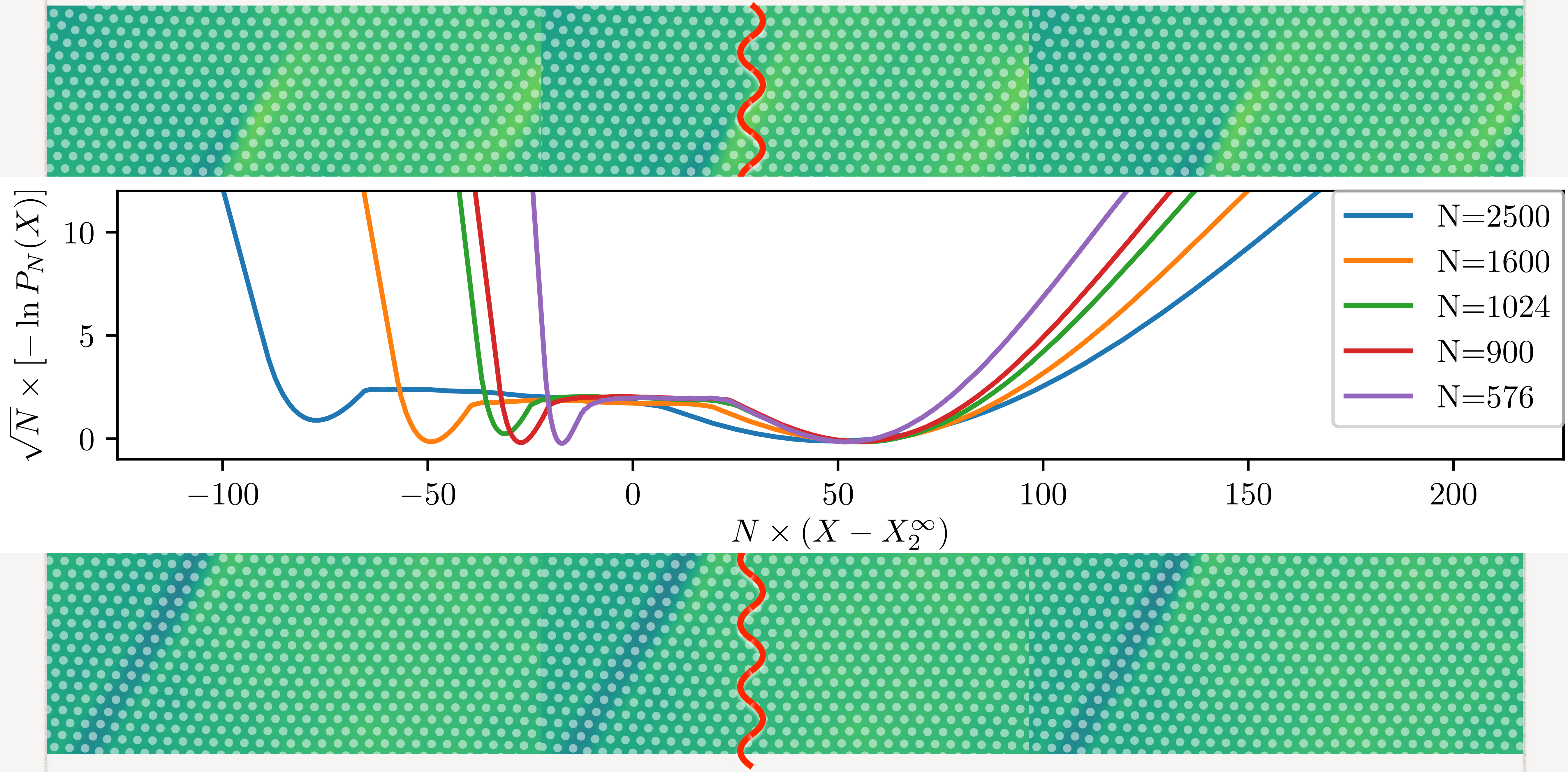

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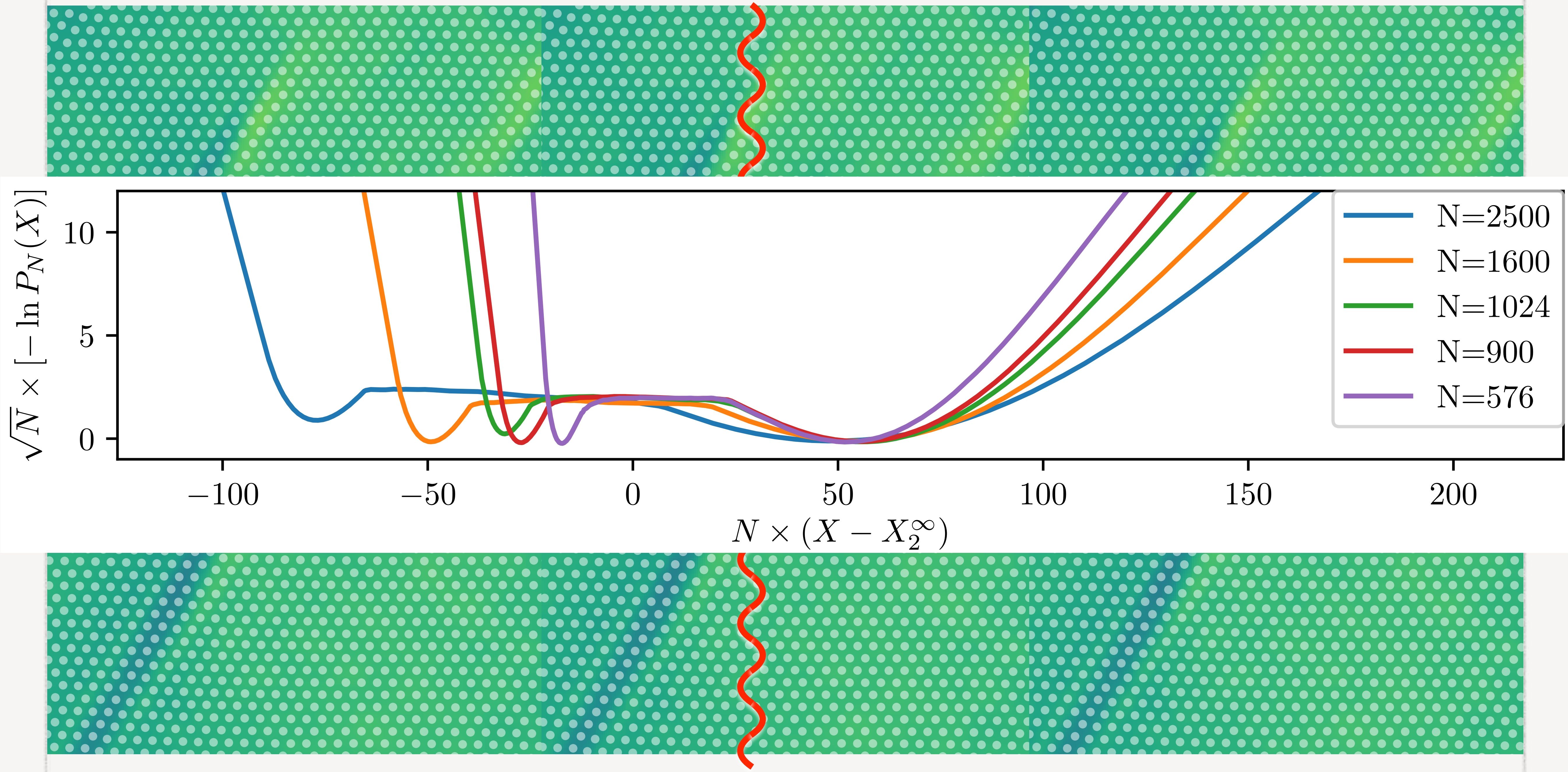

An unconventional solid-solid interface with absolutely normal finite size scaling property.

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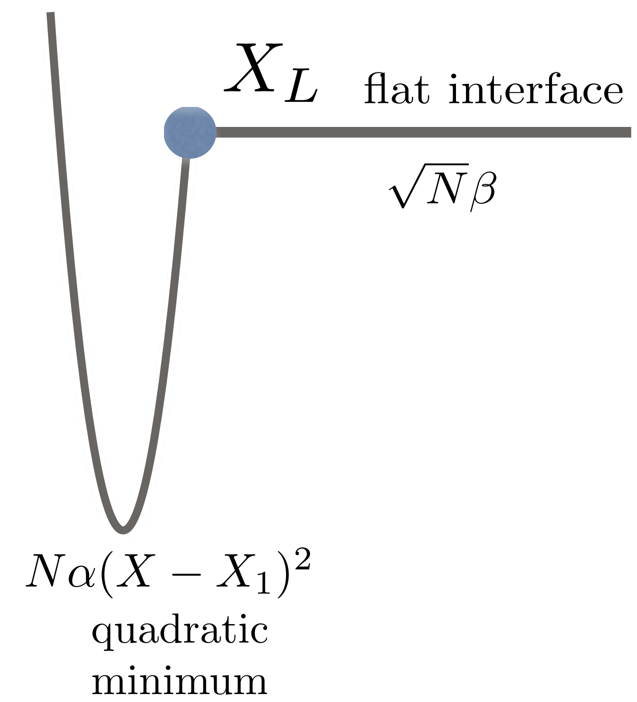
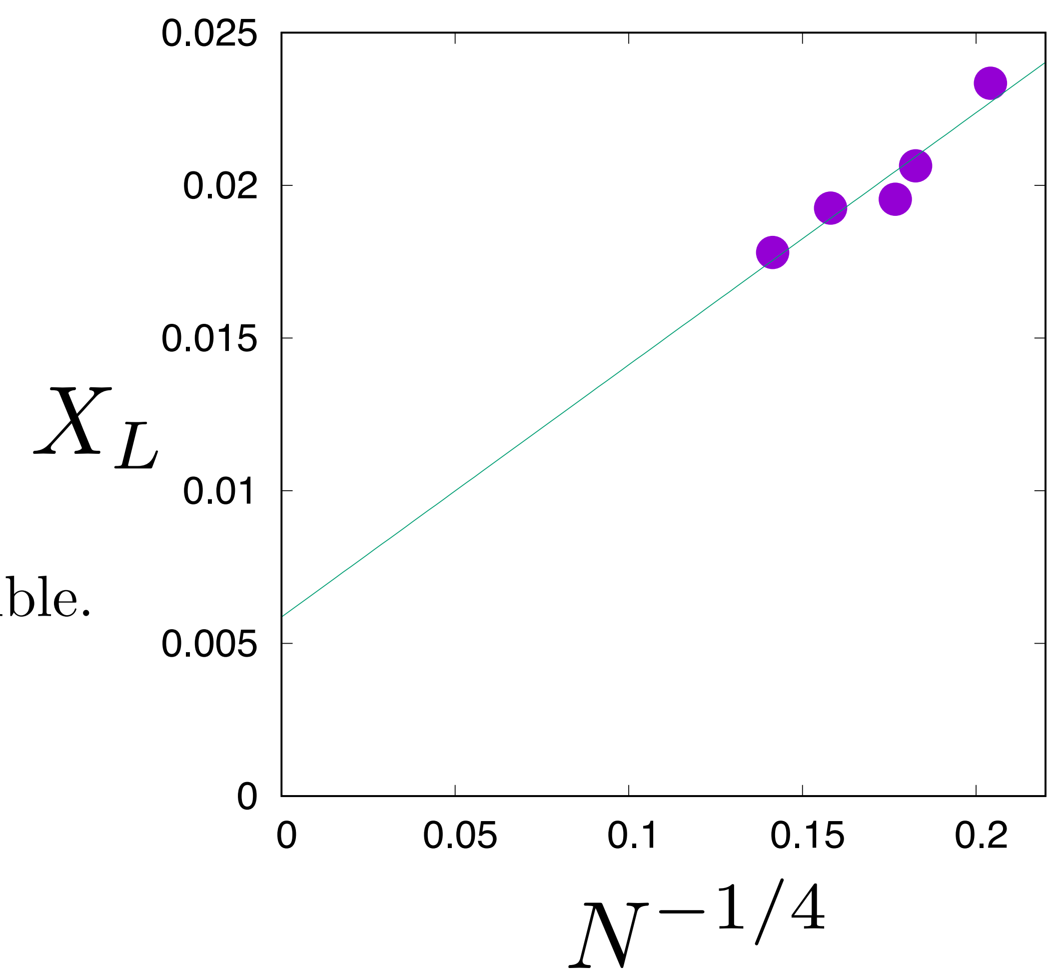
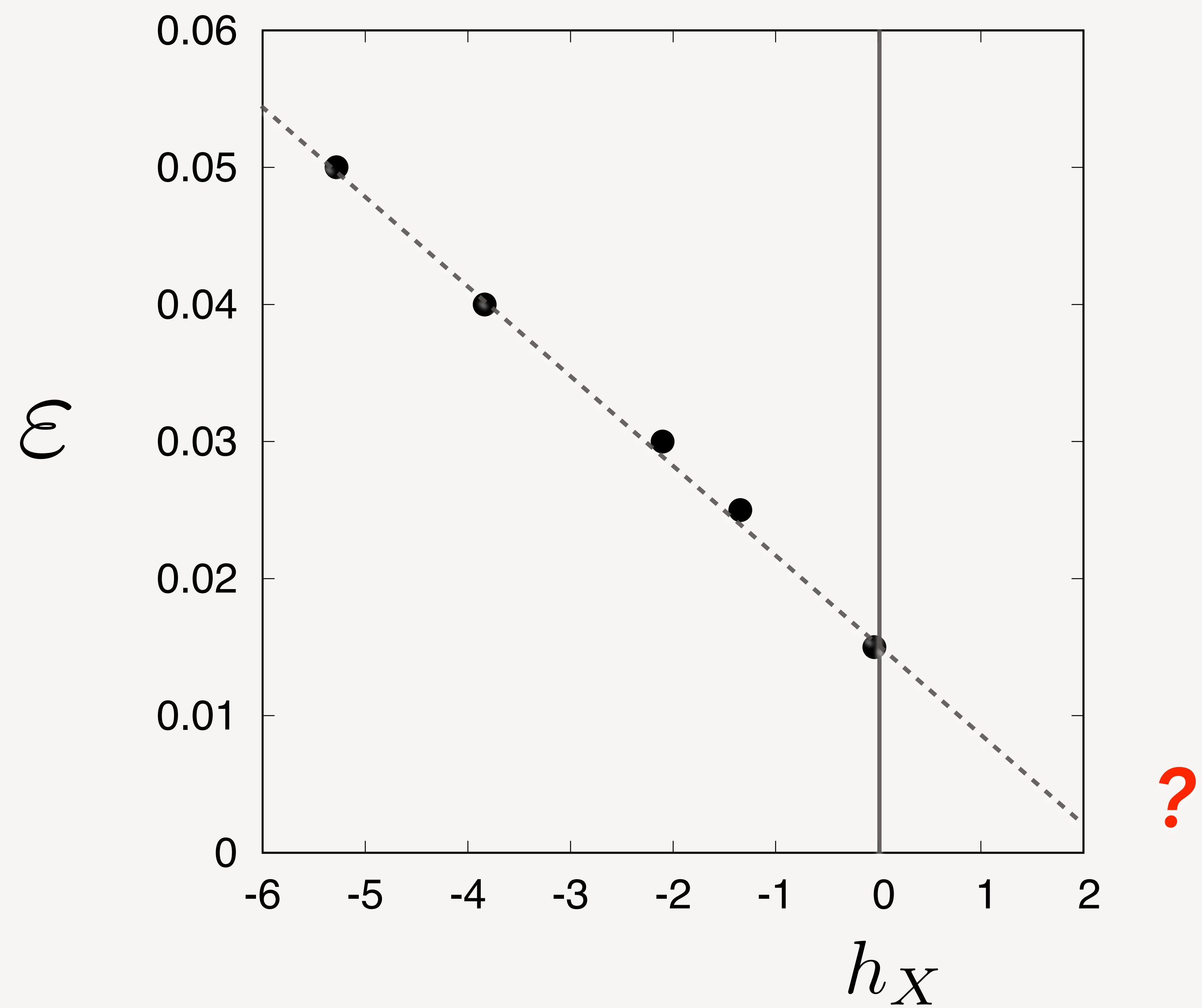
SCALING OF X_L



- X_L is the limiting value of X, an intensive quantity, upto which the crystal is stable.
- Hypothesis: X_L is given by the intersection of the quadratic minimum and the flat region in $-lnP(X)$.
- Curvature of first minimum $\sim N$ and height of interfacial contribution $\sim \sqrt{N}$.
- This gives $(X_L - X_1) = \sqrt{\frac{\beta}{\alpha}} N^{-1/4}$.
- so, $X_L \to X_1$ as $N \to \infty$.
- for large N non-flat interfaces and droplets become possible.



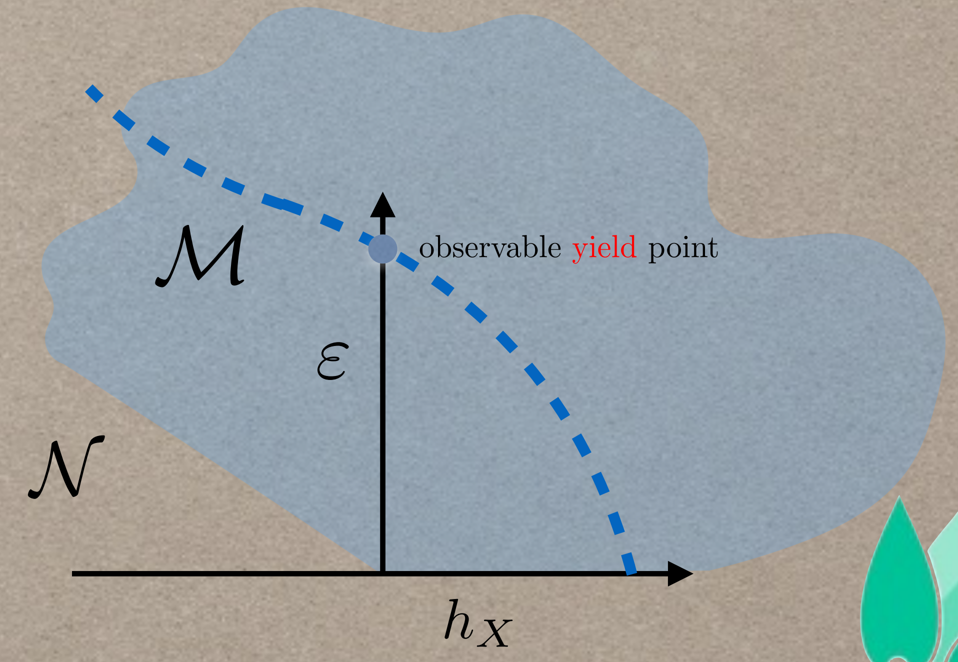
PHASE DIAGRAM FOR N=32X32



finite size effect: cannot have less than one slip band !

THE CONNECTION TO YIELDING:

a *mean field* transition at finite strain rate



IF OUR SCENARIO IS CORRECT...

- a single value of $X = X_S$ should determine yielding for any h_X and ε.
- when X reaches X_S the barrier is small enough so that thermal fluctuations are able to overcome this *within the timescale of the experiment.*
- at $T = 0$ this is the spinodal point (w.r.t non-affinity).
- since $X \propto h_X$ and $X \propto \varepsilon^2$, the stability line is a parabola for small h_X.

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MD SIMULATIONS OF LJ SOLID

- $N = 128 \times 128 = 16384$ particles
- $a = 1.0$, $T^* = 1.0$
- MD time step $\delta t = 0.001$, $= .0001$ near yielding.
- Berendsen thermostat
- equilibration for $t = 1500$
- strain rate $\dot{\varepsilon} = 3.33 \times 10^{-5}$ till yielding
- results averaged over 4 independent runs.
- fast GPU based in-house parallel code - checked against LAMMPS wherever possible.

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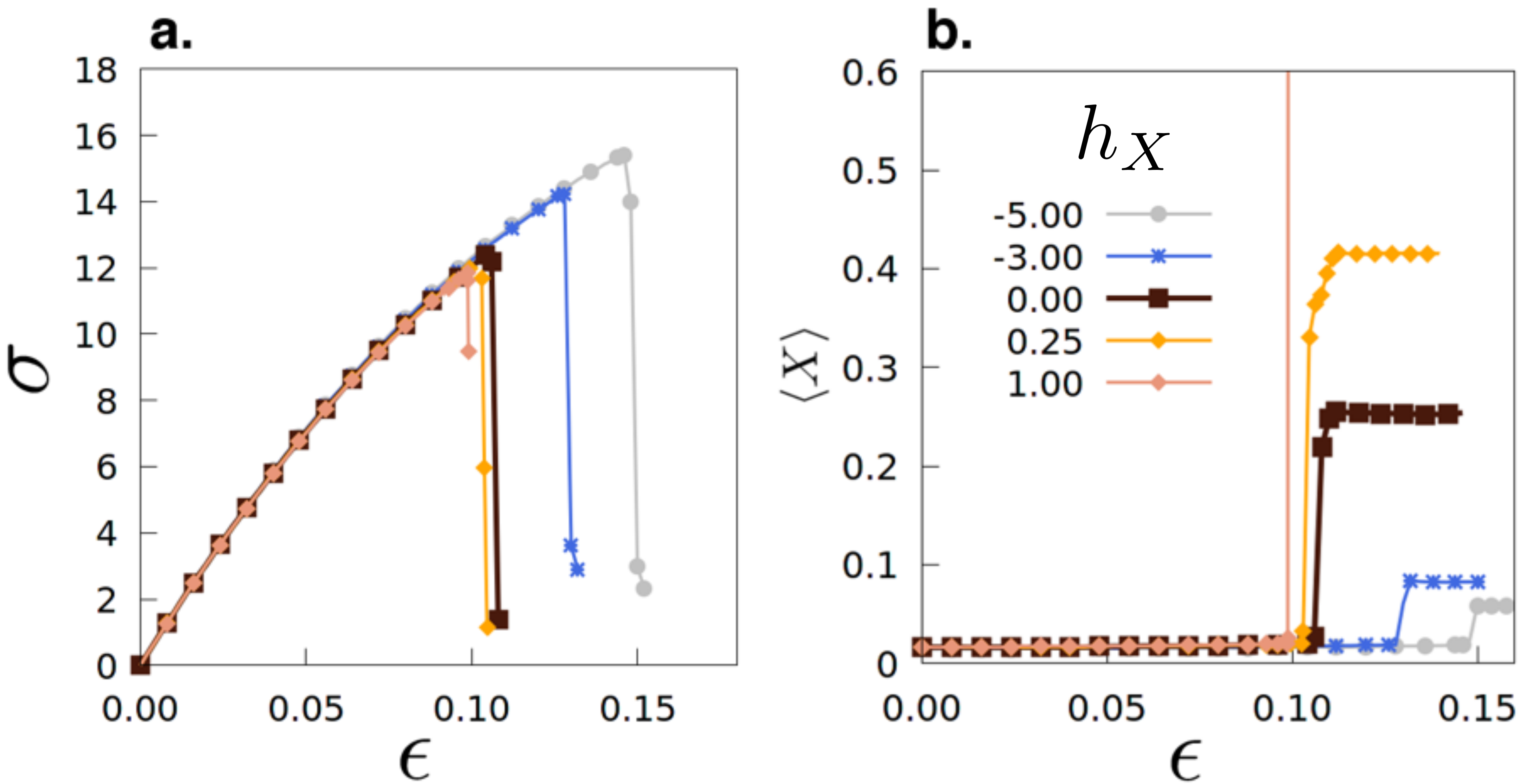
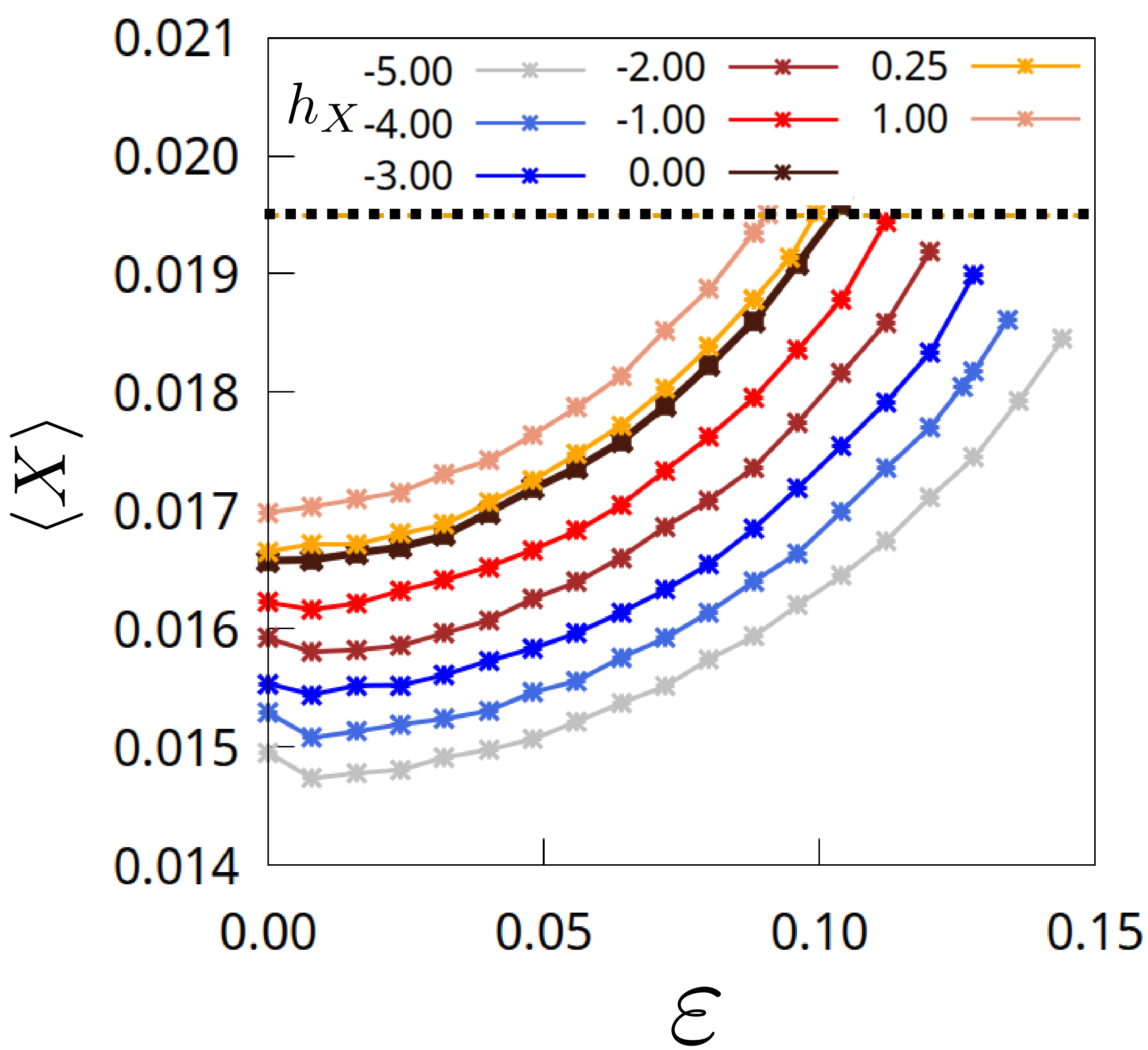
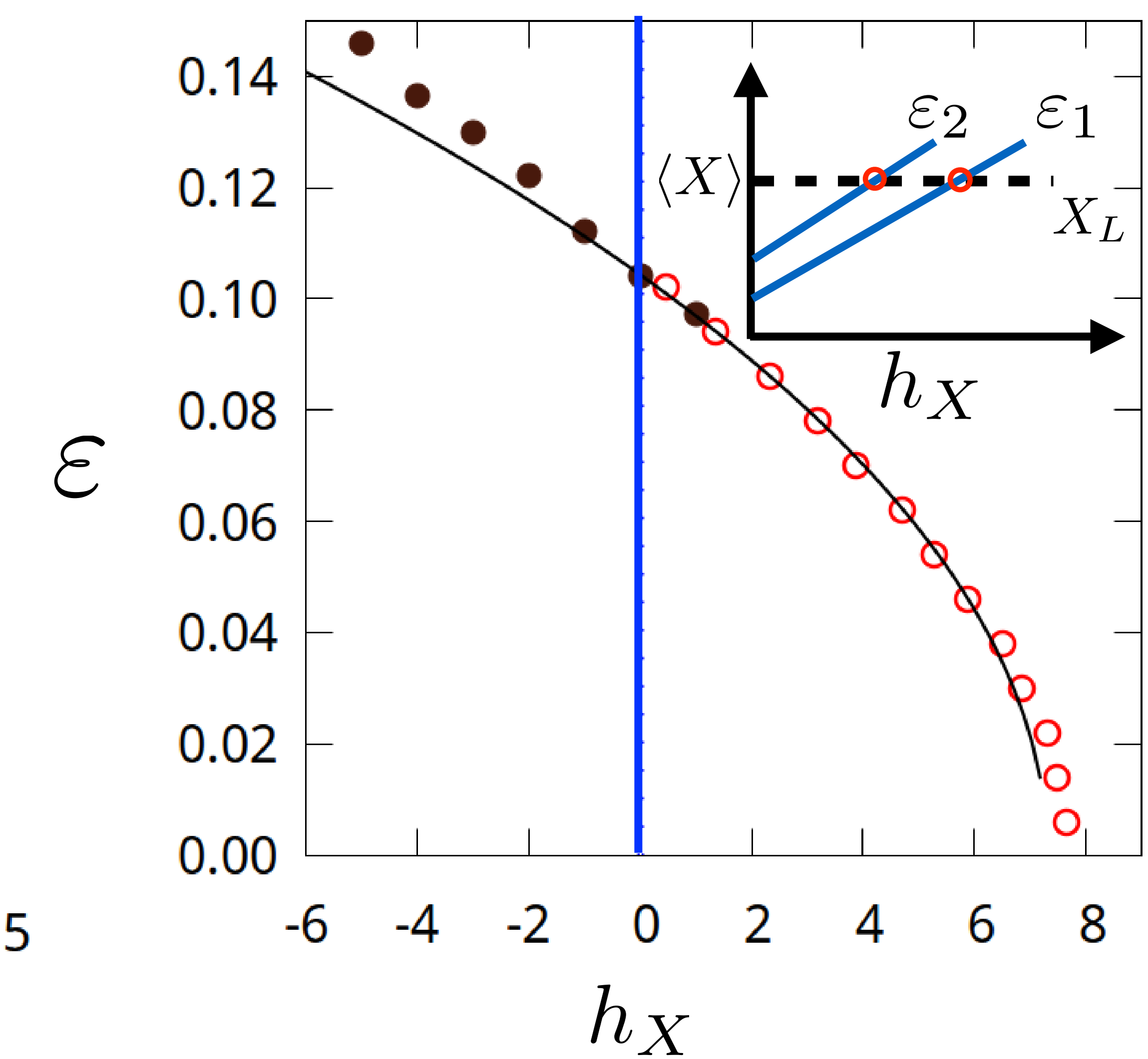
$$\rho^* = 2/\sqrt{3}, T^* = 1.0$$



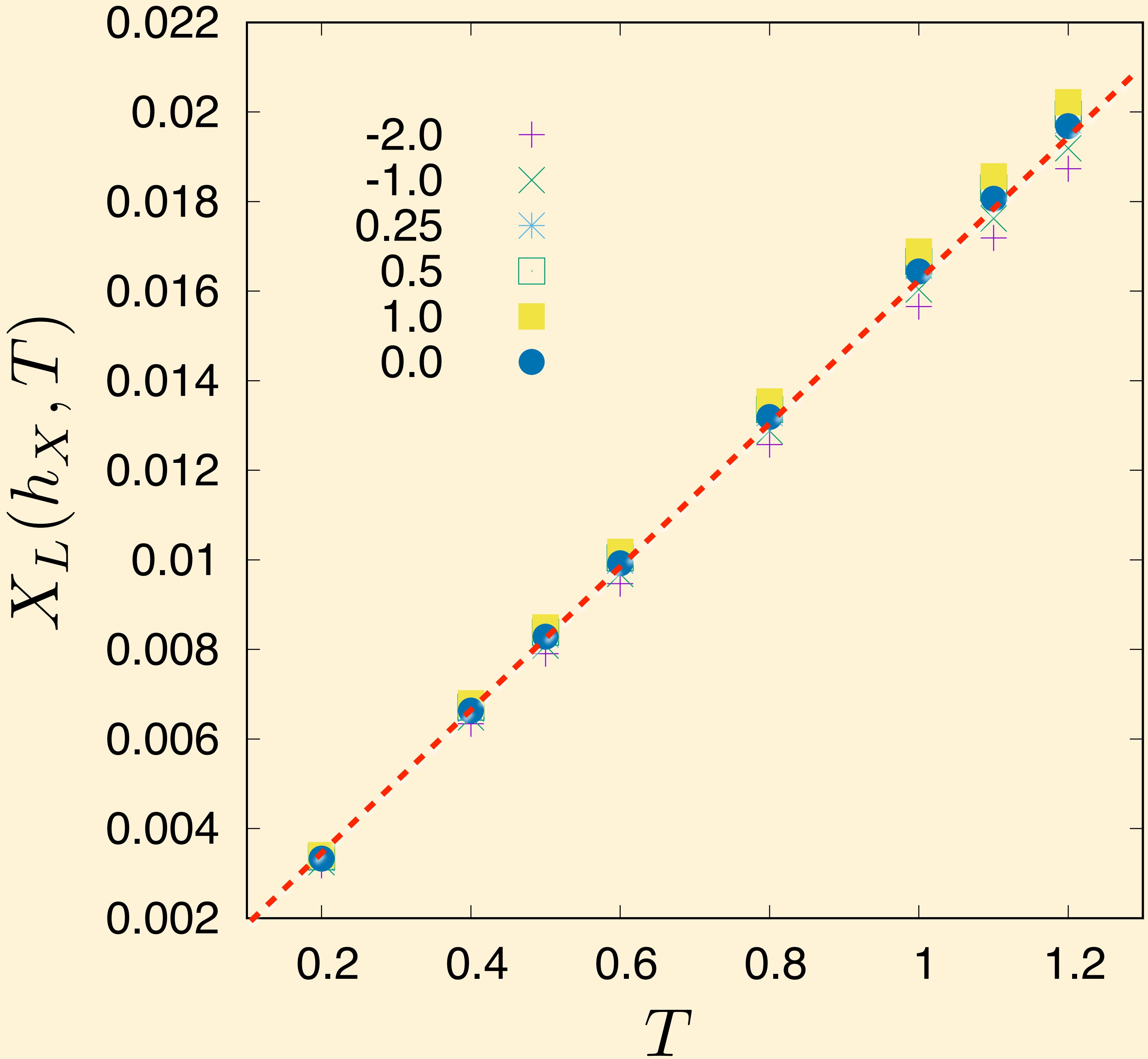
Note: Elastic properties are unchanged

- $\mathcal{N}$ phase becomes *unstable* when barrier $\rightarrow 0$ or $<< k_B T$.
- implies $\langle X \rangle \rightarrow X_S$ - a limiting value ($\neq X_L$).
- since X is positive definite instability must lie in the $h_X > 0$ quadrant at $\varepsilon = 0$.
- can calculate $\langle X(h_X, \varepsilon) \rangle$ from L.R.T. at $h_X = 0$. Only inputs are χ correlations at $h_X = 0$ and $\varepsilon > 0$.
- stability limit from LRT (open symbols) $\langle X \rangle = X_S \approx 0.019$ compared with yield points from MD (filled symbols).





OTHER TEMPERATURES ?



$\rho\beta X_L =$ constant?

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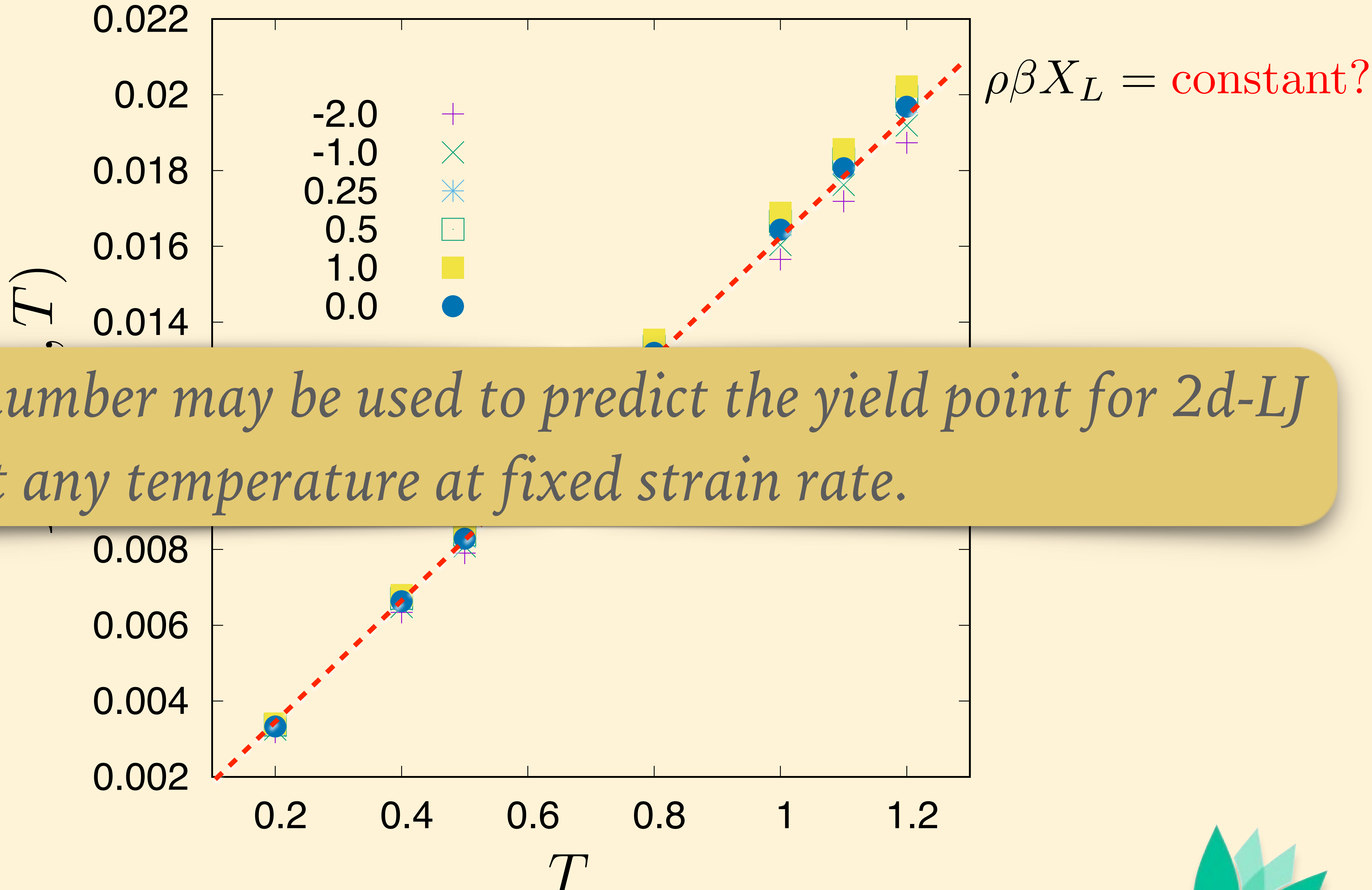
OTHER TEMPERATURES ?



Single number may be used to predict the yield point for 2d-LJ solids at any temperature at fixed strain rate.

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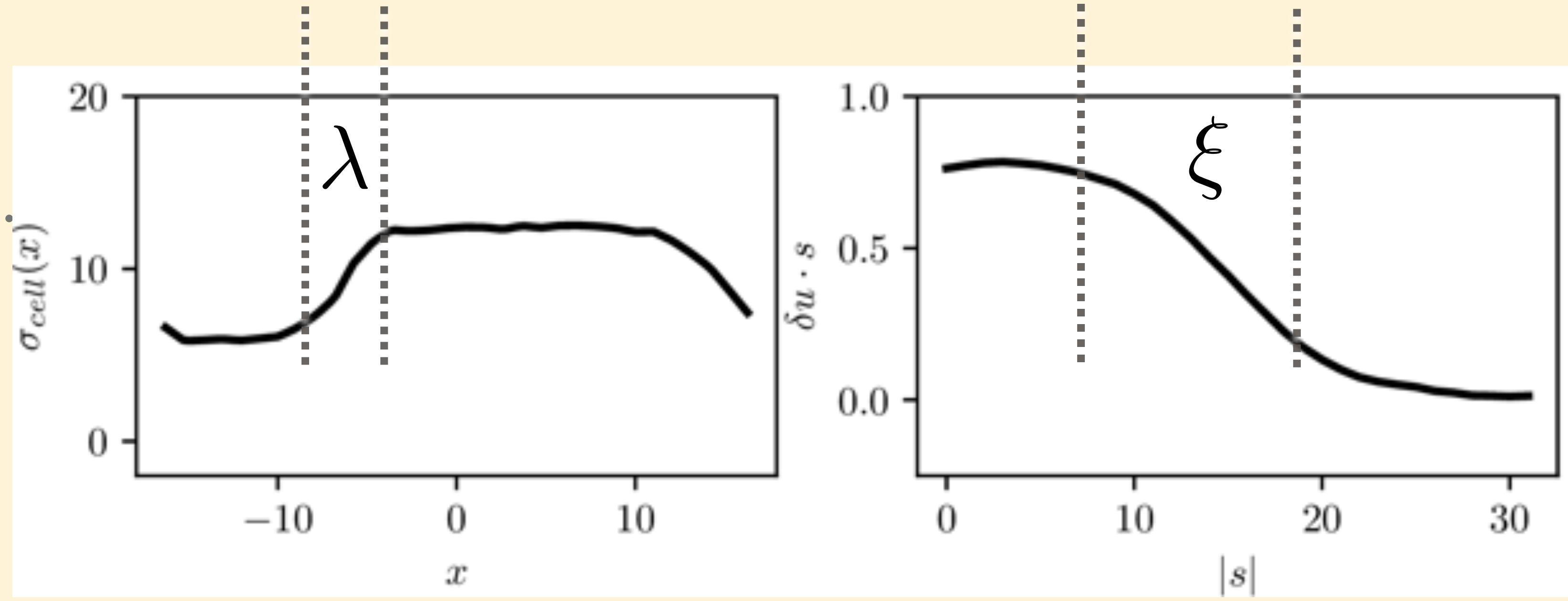
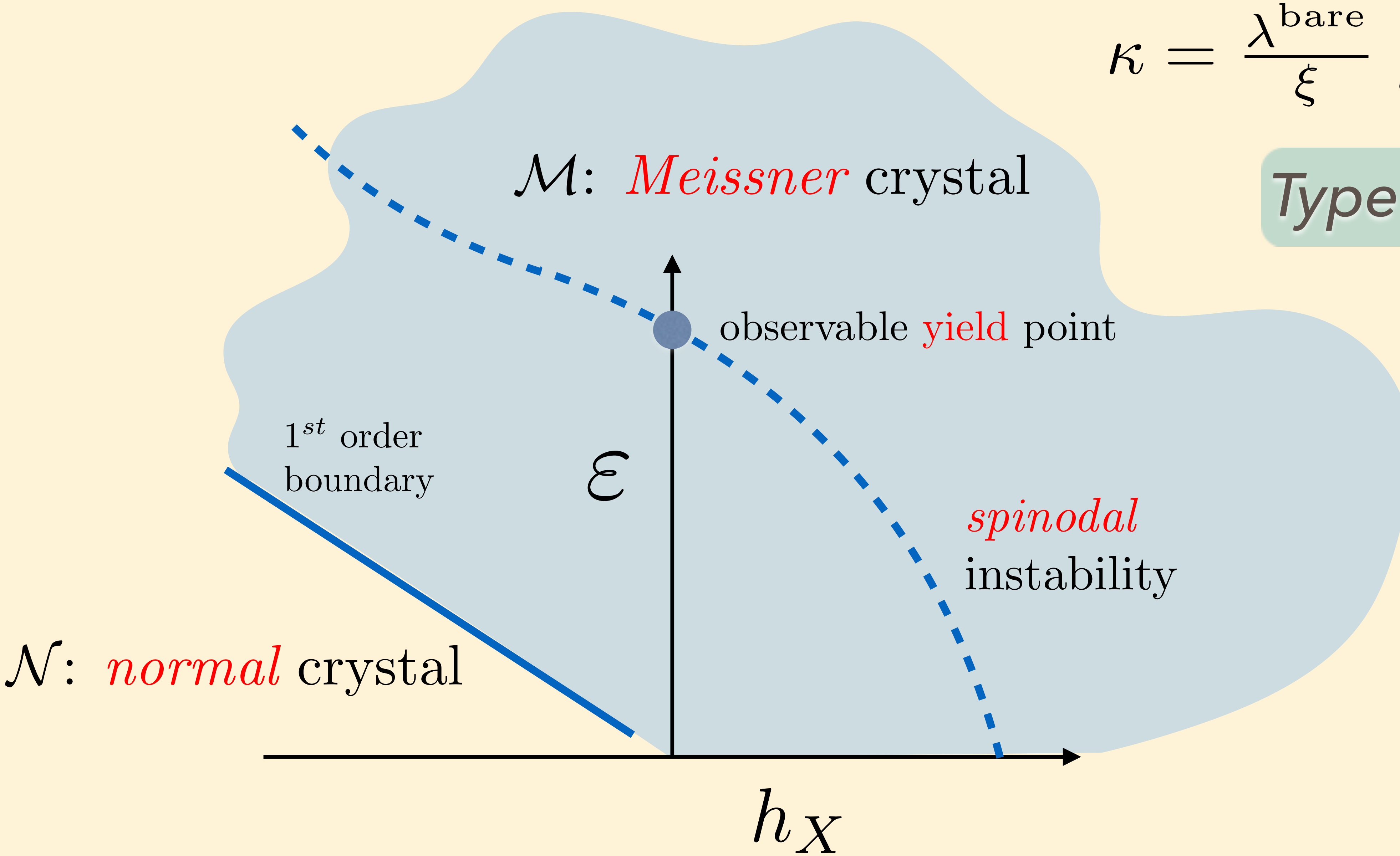
SCHEMATIC SUMMARY



$$\kappa = \frac{\lambda^{\text{bare}}}{\xi} \lesssim 0.3 < \frac{1}{\sqrt{2}}$$

Type I ??



CAN THESE BE CHECKED?

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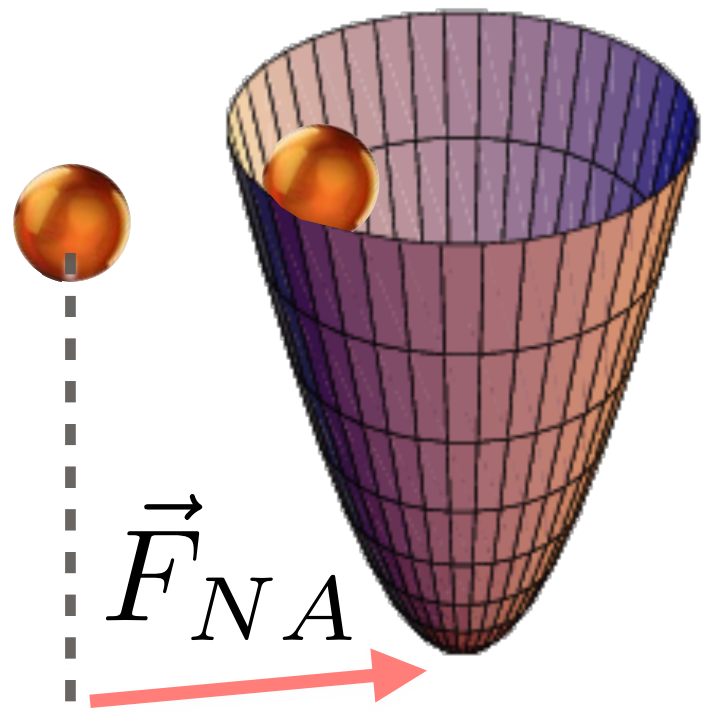
CREATE h_x USING A "FEEDBACK LOOP"

get particle coordinates using video microscopy

calculate forces using positions of neighbors



construct displaced traps to apply calculated forces

repeat at frequency larger than typical inverse colloid diffusion times

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EXPLICIT "TAKE AWAYS"

- A *free energy landscape view* for plasticity of solids.
- Recover Sausset, Biroli, Kurchan - *except* surface free energies should be obtained *at coexistence!*
- Contact with finite size, mean field, finite strain rate yielding studies - yielding as an approach to a mean field *spinodal* like instability. Quantitative *prediction* of the yield point.
- Conventional yield point can be understood *without* explicit reference to *dislocation motion*.
- Can serve as a language for yielding in solids where dislocations cannot be defined (*glasses*?).
- "Technological" *by-product* (!) - means to *control* yielding *without* changing elastic properties in colloidal crystals using dynamic laser traps.

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