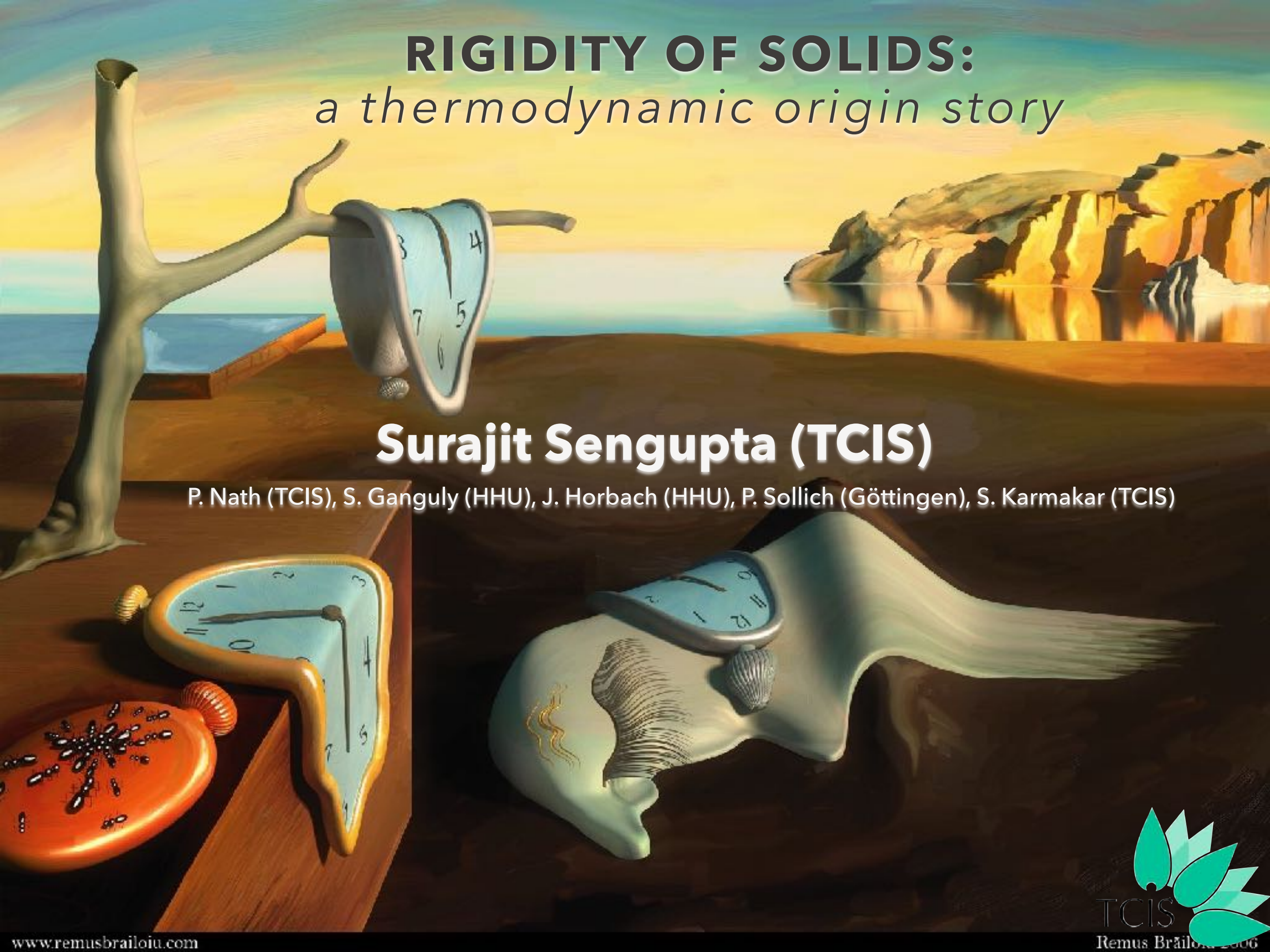


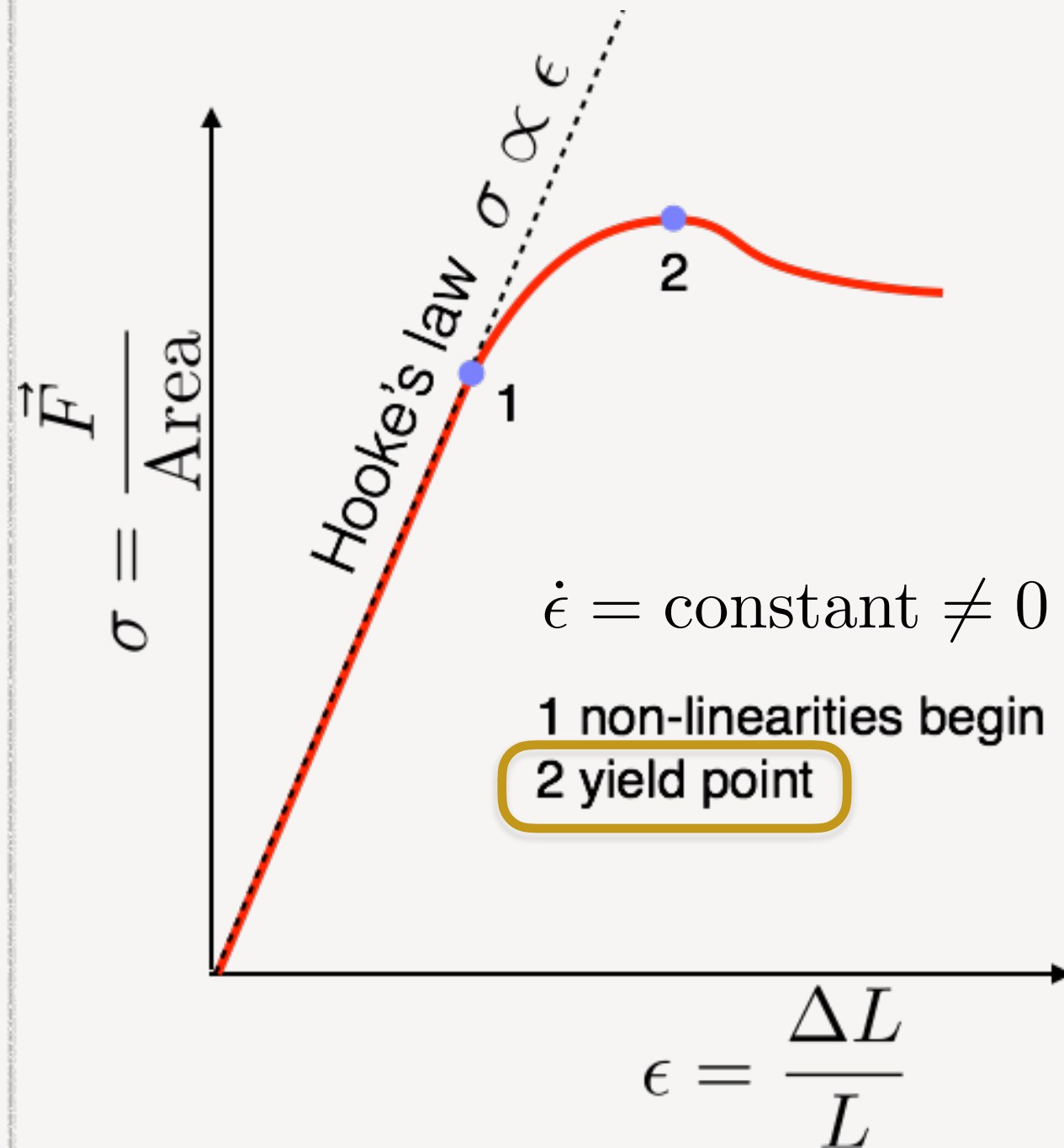
RIGIDITY OF SOLIDS: *a thermodynamic origin story*

Surajit Sengupta (TCIS)

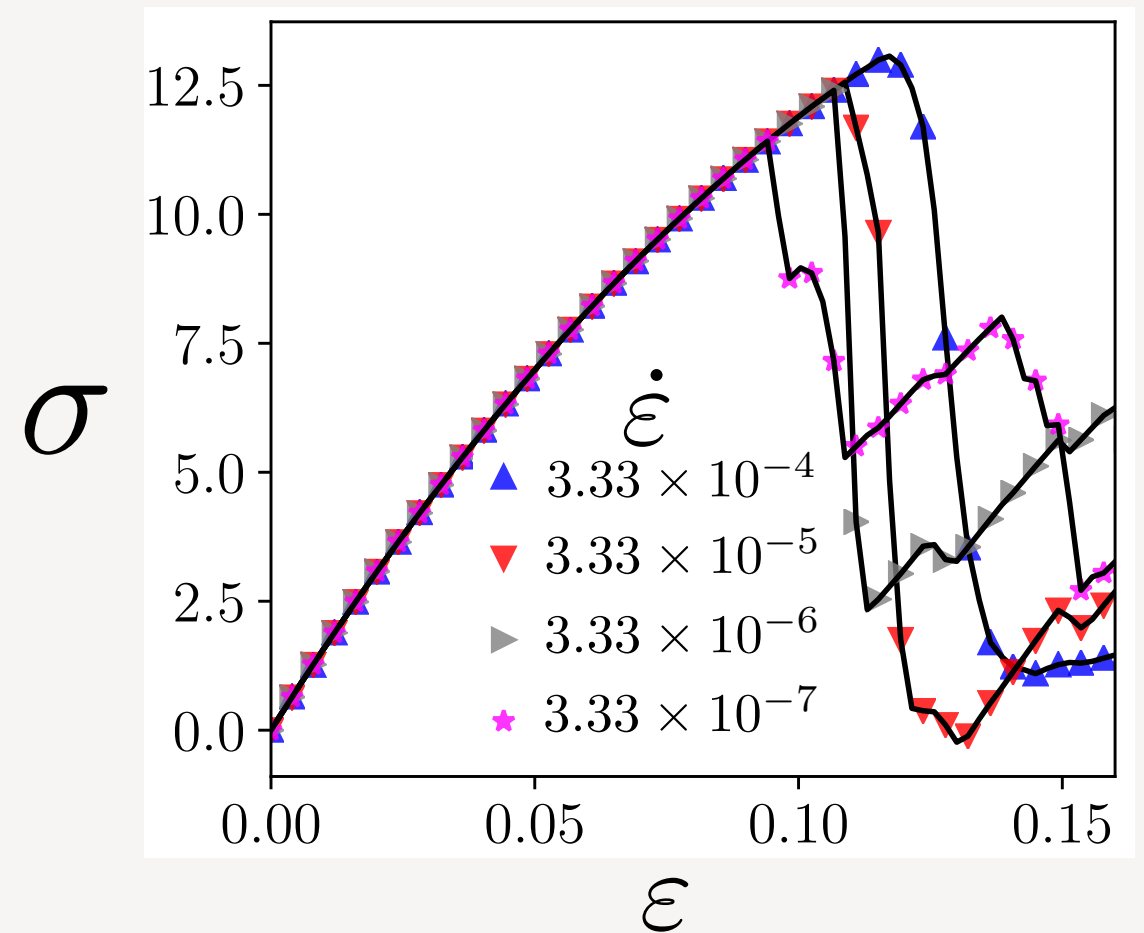
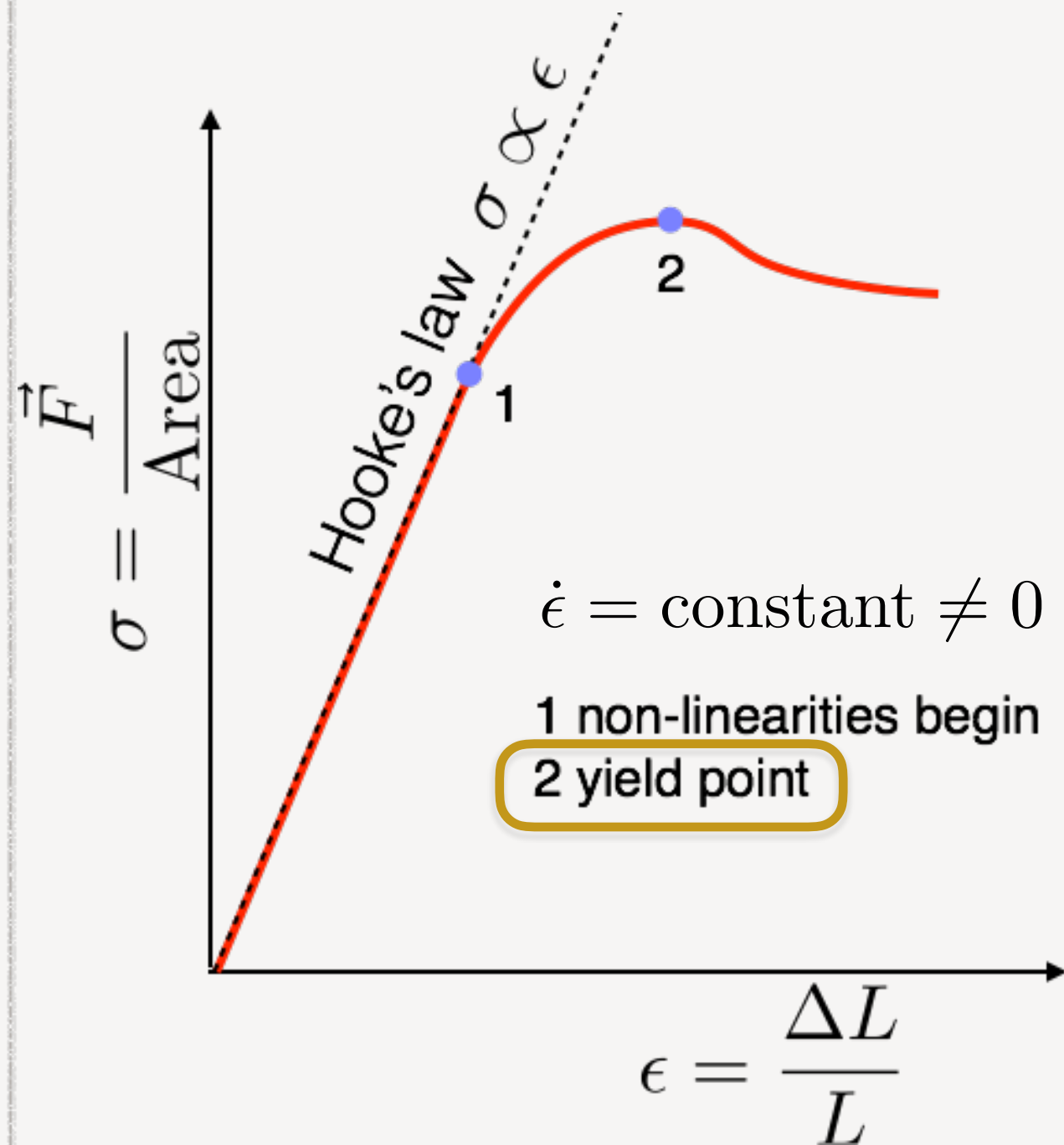
P. Nath (TCIS), S. Ganguly (HHU), J. Horbach (HHU), P. Sollich (Göttingen), S. Karmakar (TCIS)



STATING THE PROBLEM:

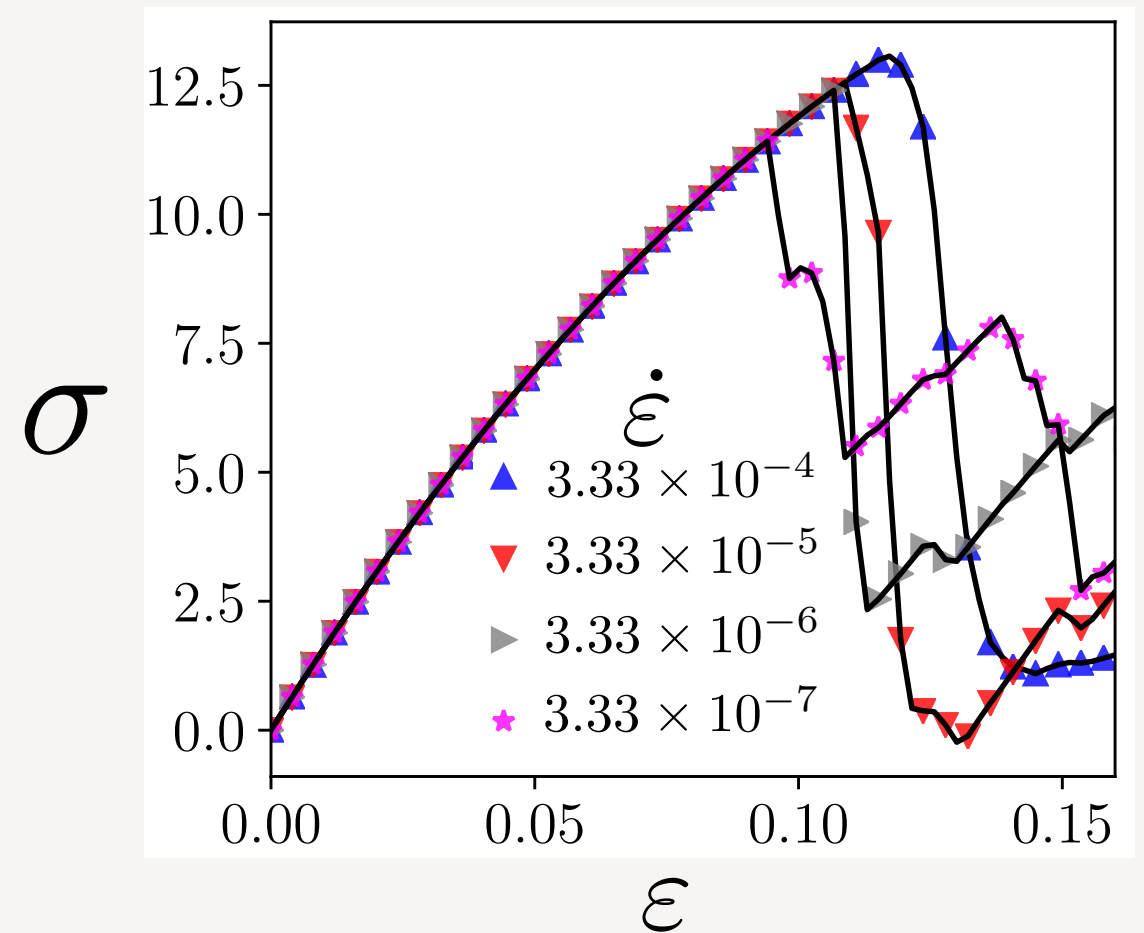
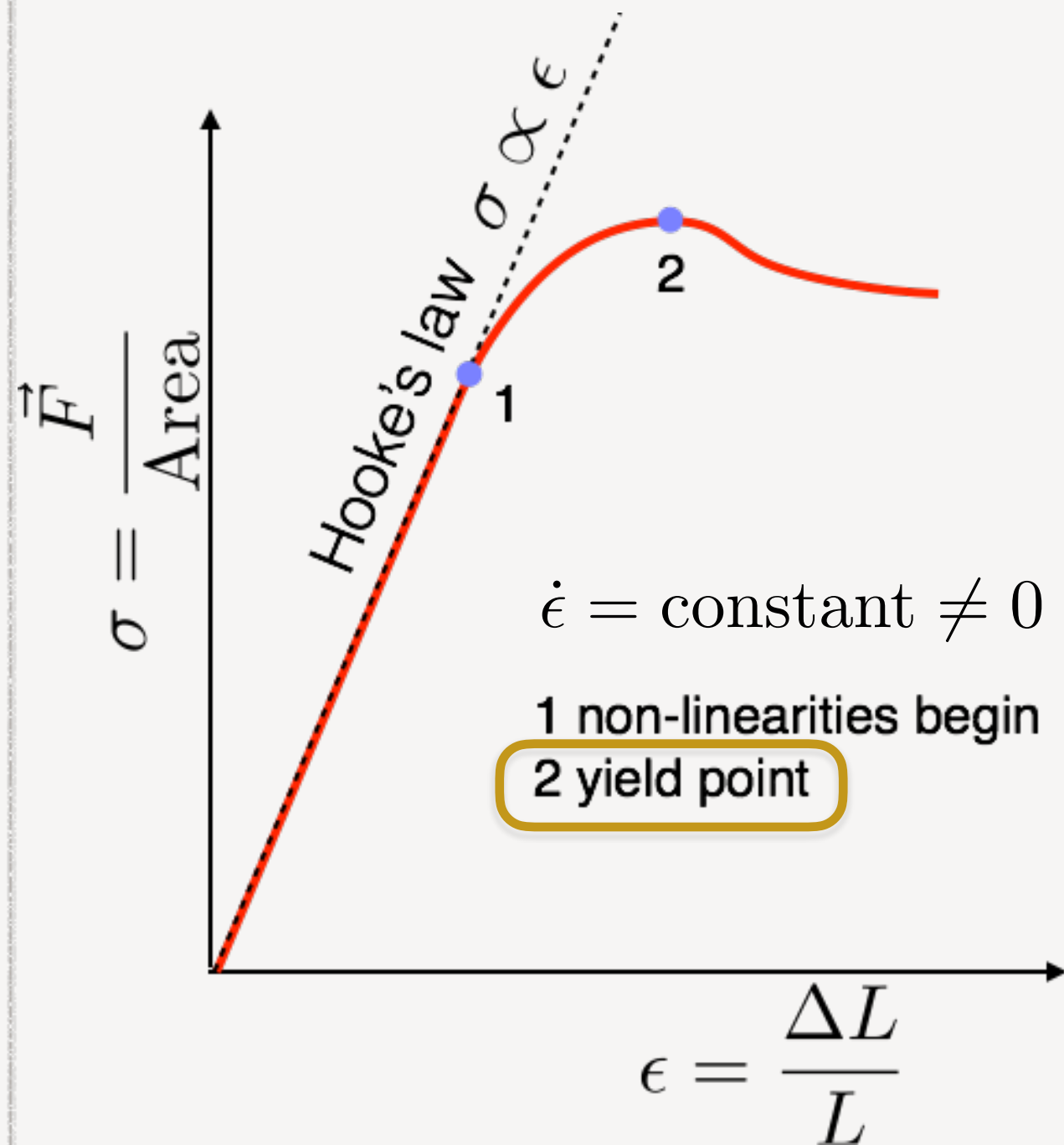


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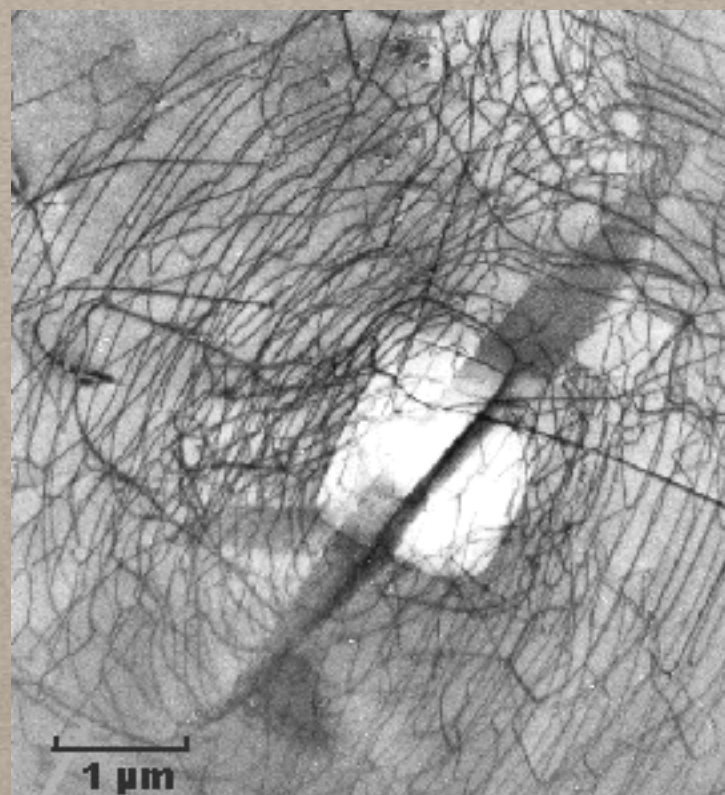
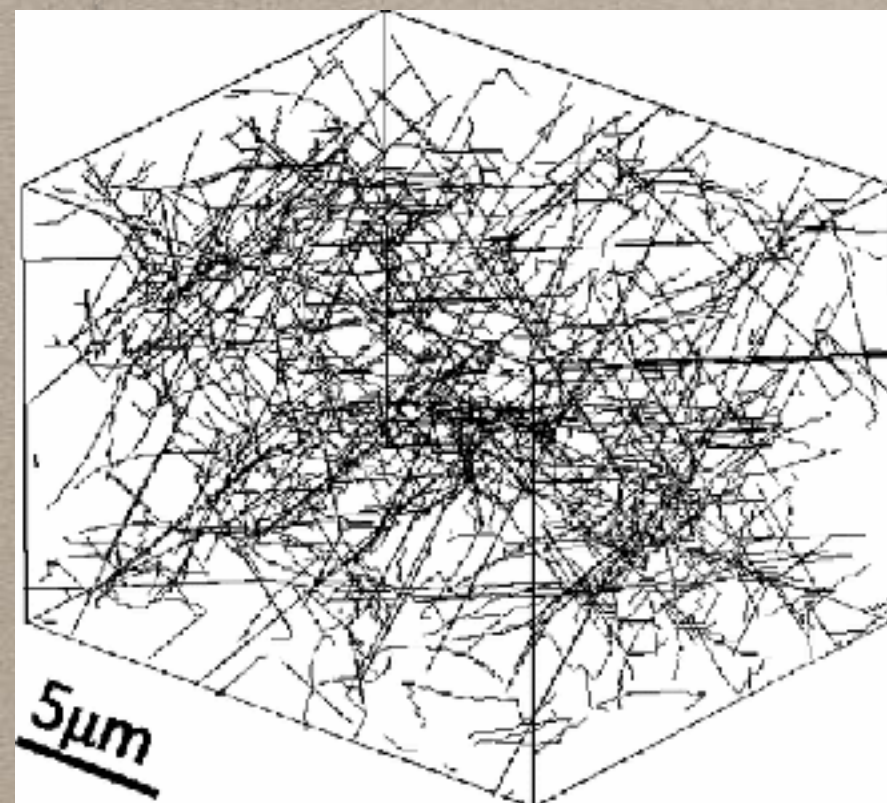
MD simulations of a 2d LJ (triangular) solid, which is *initially* defect free, under pure shear.

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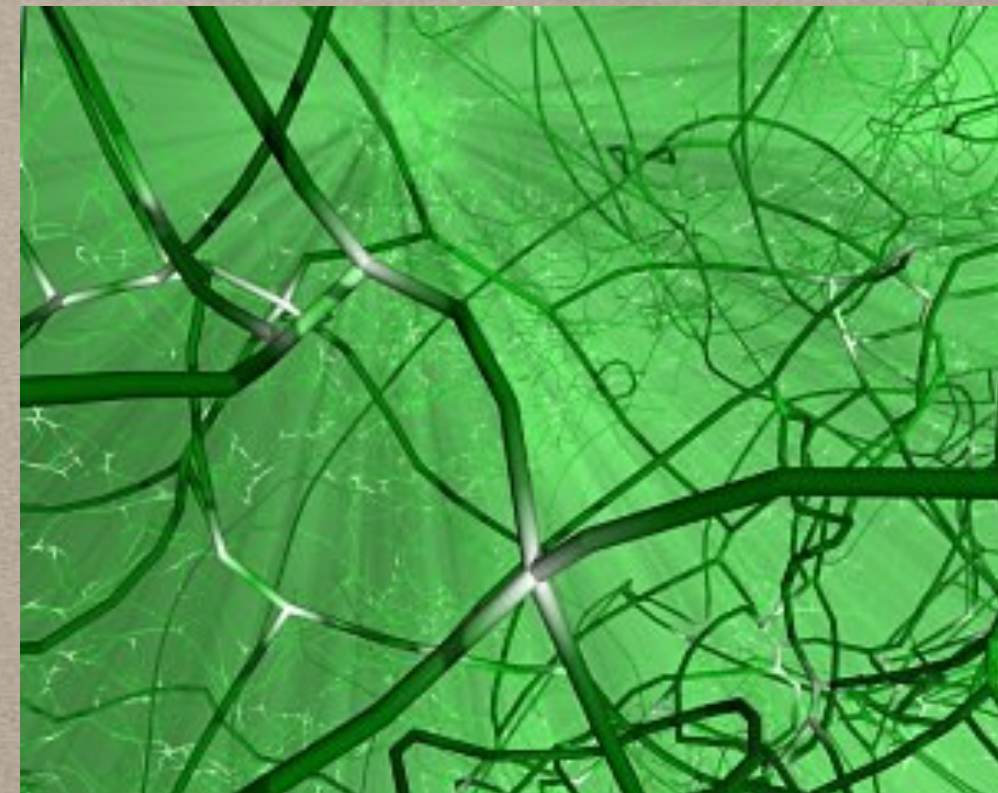
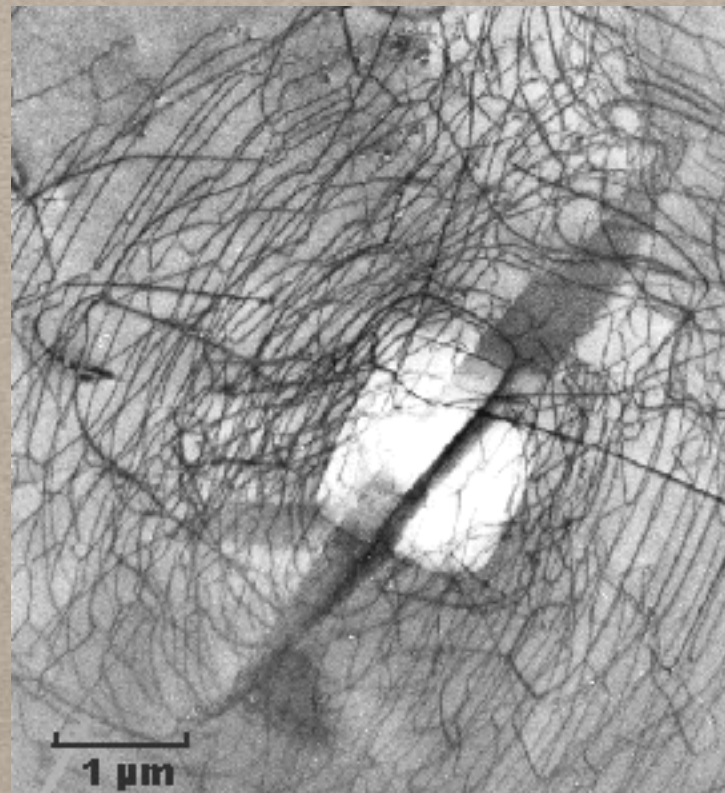
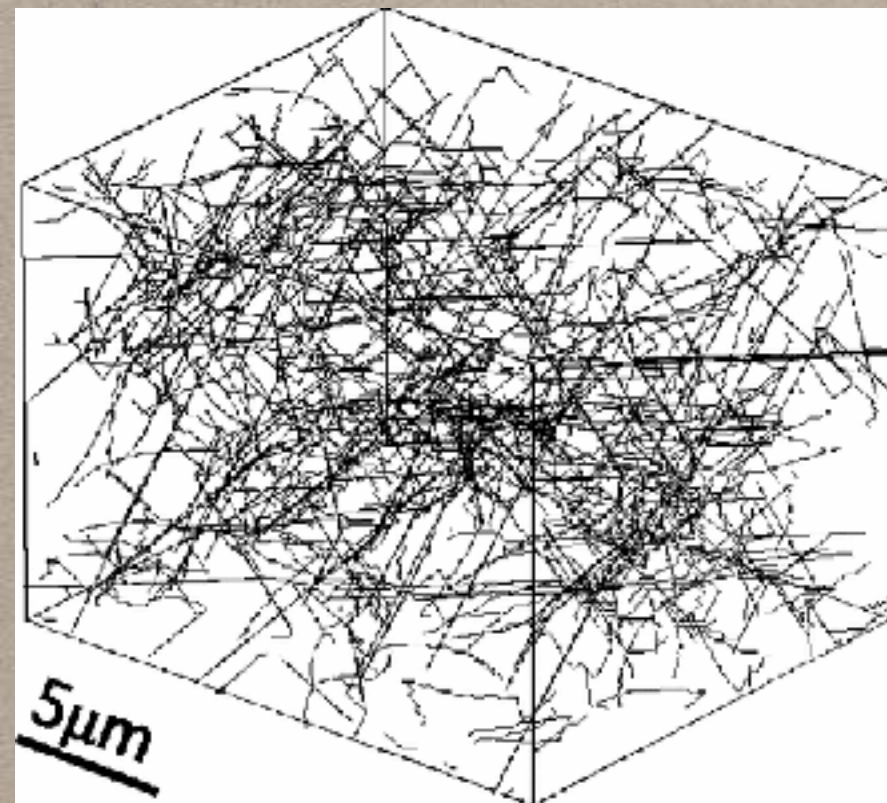


MD simulations of a 2d LJ (triangular) solid, which is *initially* defect free, under pure shear.

What leads to loss of rigidity and onset of plasticity in a crystalline solid?



Crystalline solids are rigid but lose this property at some fixed (large) stress value - the so called yield stress - due to nucleation and dynamic de-pinning/un-jamming of dislocations.



THEORIES OF YIELDING

PRL 102, 175501 (2009)

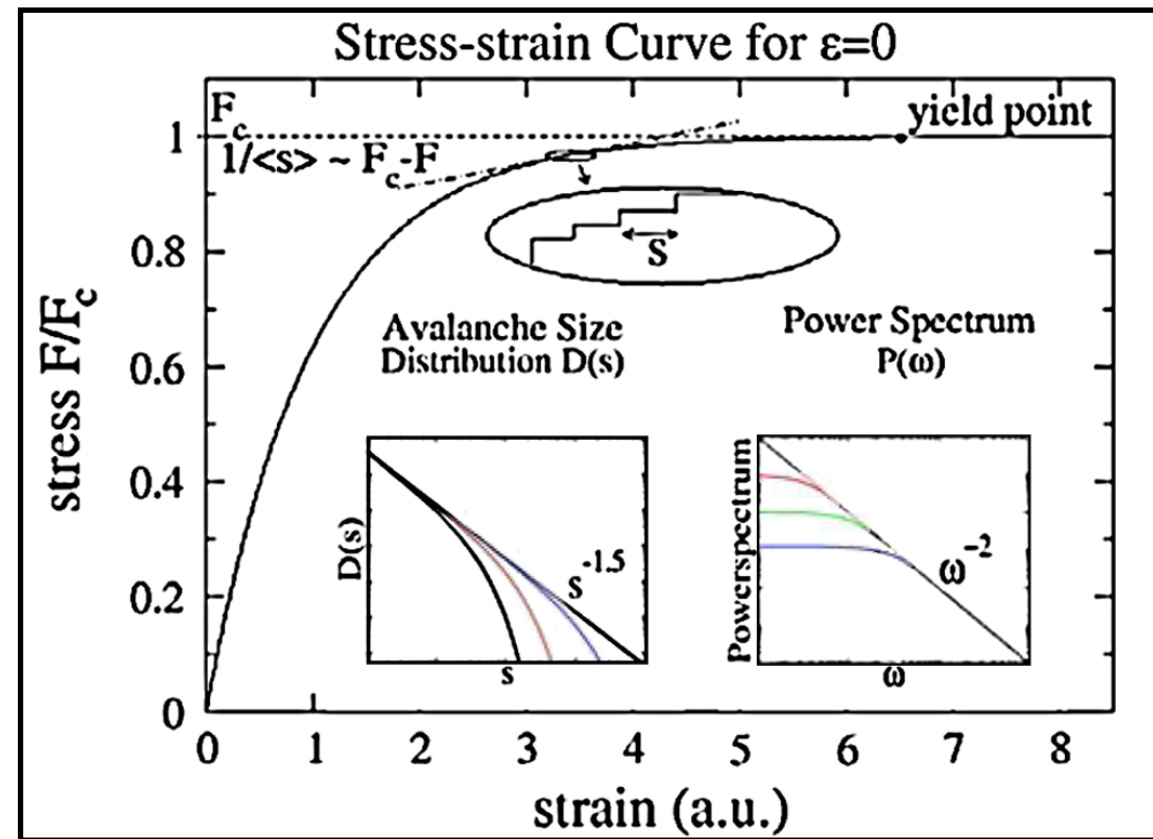
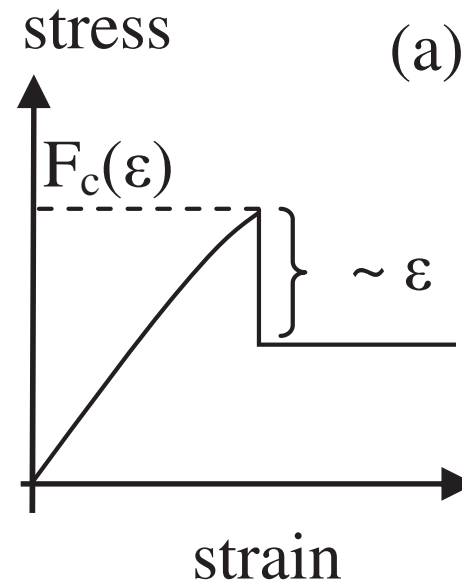
PHYSICAL REVIEW LETTERS

week ending
1 MAY 2009

Micromechanical Model for Deformation in Solids with Universal Predictions for Stress-Strain Curves and Slip Avalanches

Karin A. Dahmen, Yehuda Ben-Zion, and Jonathan T. Uhl

*Department of Physics, University of Illinois at Urbana Champaign, Urbana, Illinois 61801, USA,
and Department of Earth Sciences, University of Southern California, Los Angeles, California 90089-0740, USA*
(Received 23 May 2008; published 27 April 2009)



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

Determination of the universality class of crystal plasticity

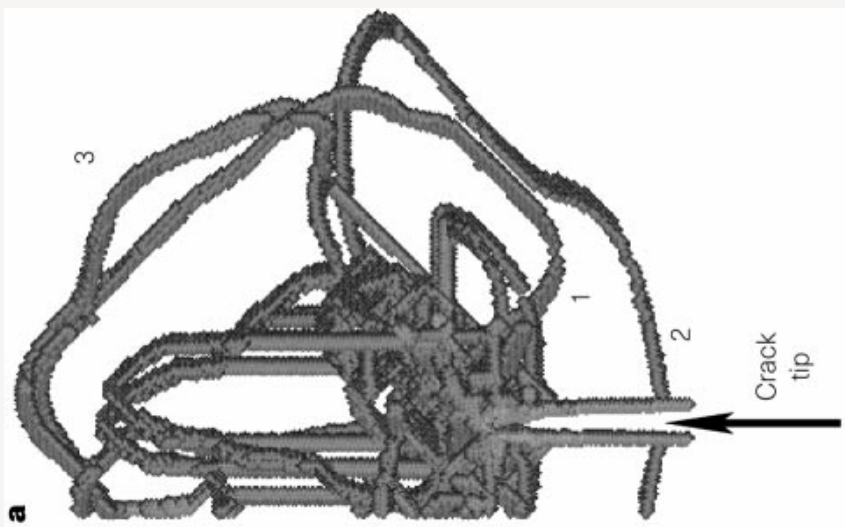
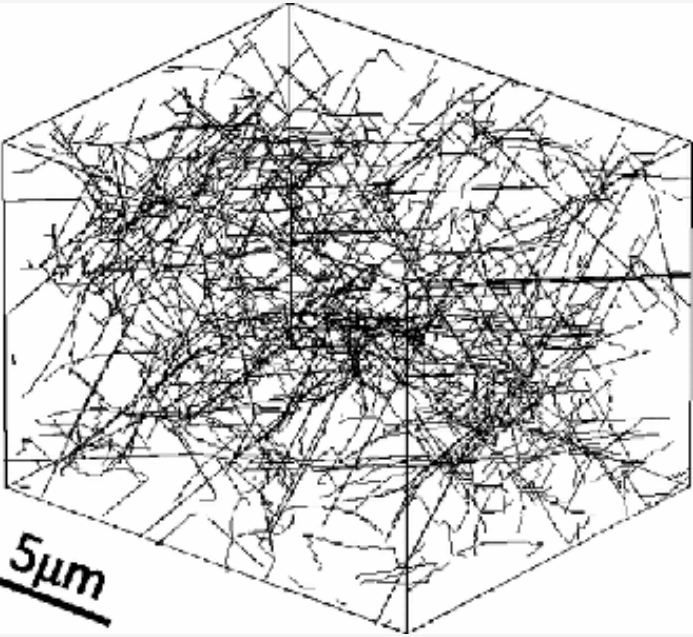
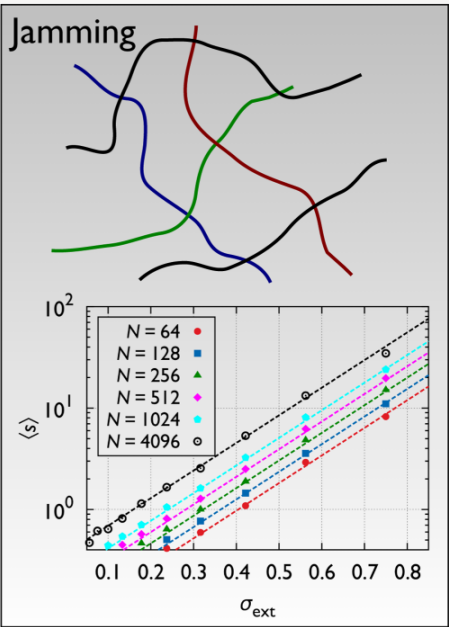
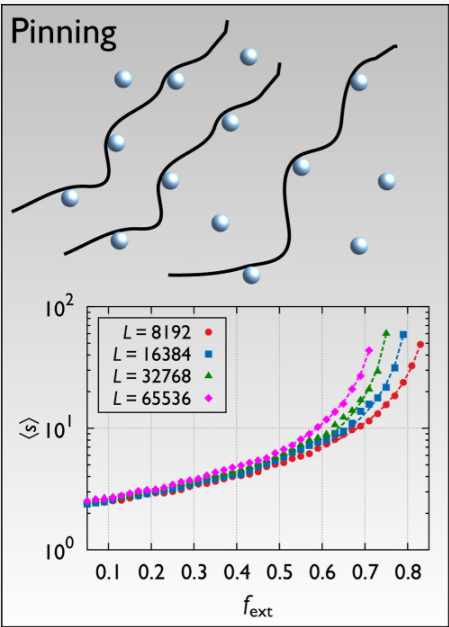
G. TSEKENIS, J. T. UHL, N. GOLDENFELD and K. A. DAHMEN

*Department of Physics, University of Illinois at Urbana-Champaign, Loomis Laboratory of Physics
1110 West Green Street, Urbana, IL, 61801-3080, USA*

- N elastically connected elements
- Starting from zero stress external stress is increased till system undergoes a de-pinning transition
- When local stress exceeds a threshold stress is reset to zero locally
- Stress is redistributed, which may cause avalanches
- Avalanches show power law distribution with “interface de-pinning” exponents
- Can explain some experimental phenomenology
- Not a microscopic theory ! Yielding (output) is incorporated in the stress thresholds (input)

Avalanches in 2D Dislocation Systems: Plastic Yielding Is Not Depinning

Péter Dusán Ispánovity,^{1,*} Lasse Laurson,² Michael Zaiser,³ István Groma,¹ Stefano Zapperi,⁴ and Mikko J. Alava²



letters to nature

VOLUME 89, NUMBER 25

PHYSICAL REVIEW LETTERS

16 DECEMBER 2002

Connecting atomistic and
mesoscale simulations
of crystal plasticity

Vasily Bulatov^{*}, Farid F. Abraham[†], Ladislav Kubin[‡],
Benoit Devincre[‡] & Sidney Yip^{*}

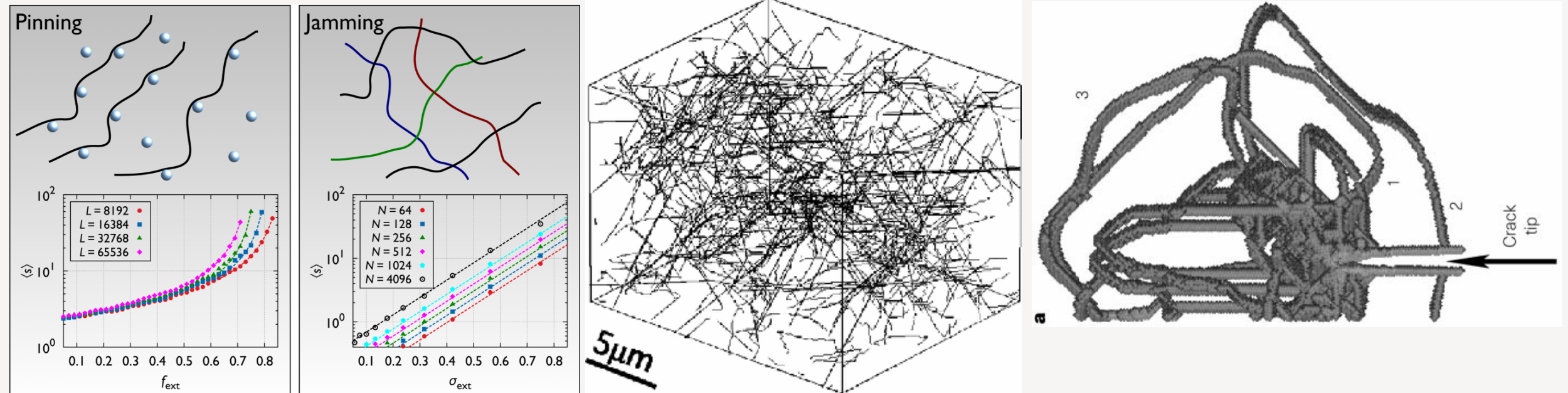
From Dislocation Junctions to Forest Hardening

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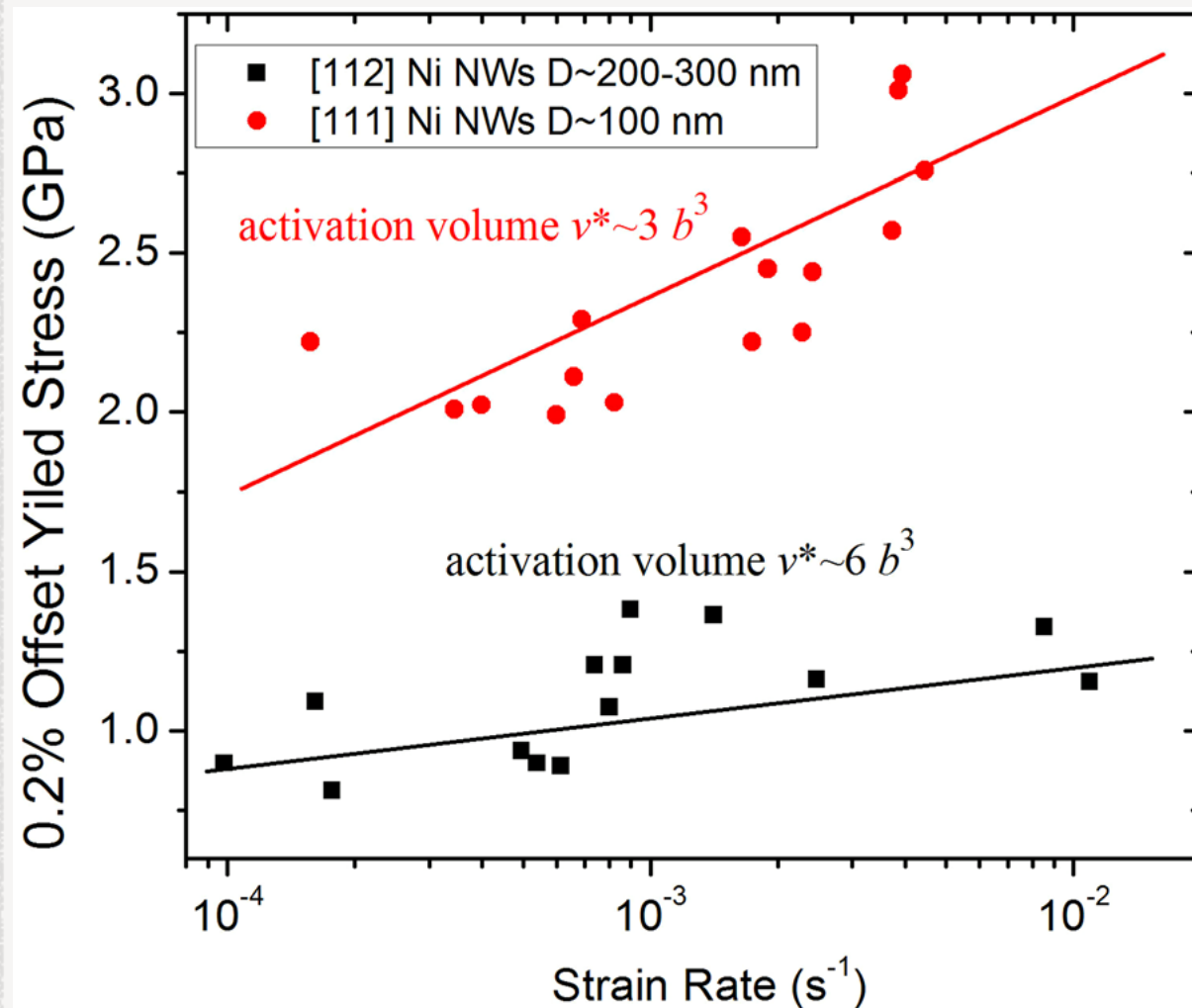
R. Madec, B. Devincre, and L. P. Kubin

A quantitative description of plastic deformation in crystalline solids requires a knowledge of how an assembly of dislocations—the defects responsible for crystal plasticity—evolves under stress¹. In this context, molecular-dynamics simulations ...

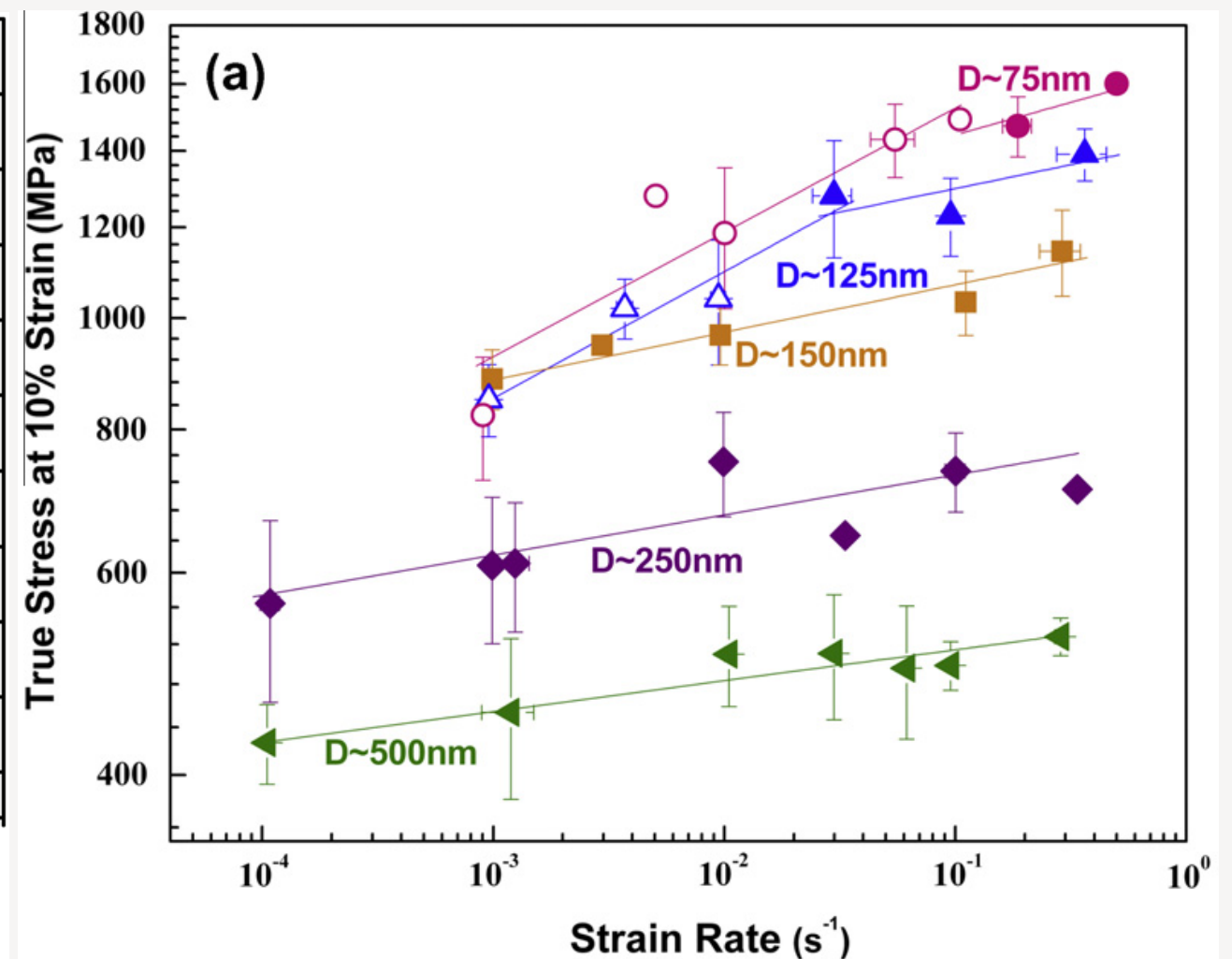
STRAIN RATE SENSITIVITY AND CREEP?

STRAIN RATE SENSITIVITY

Ni nano-wires



Cu nano-pillars



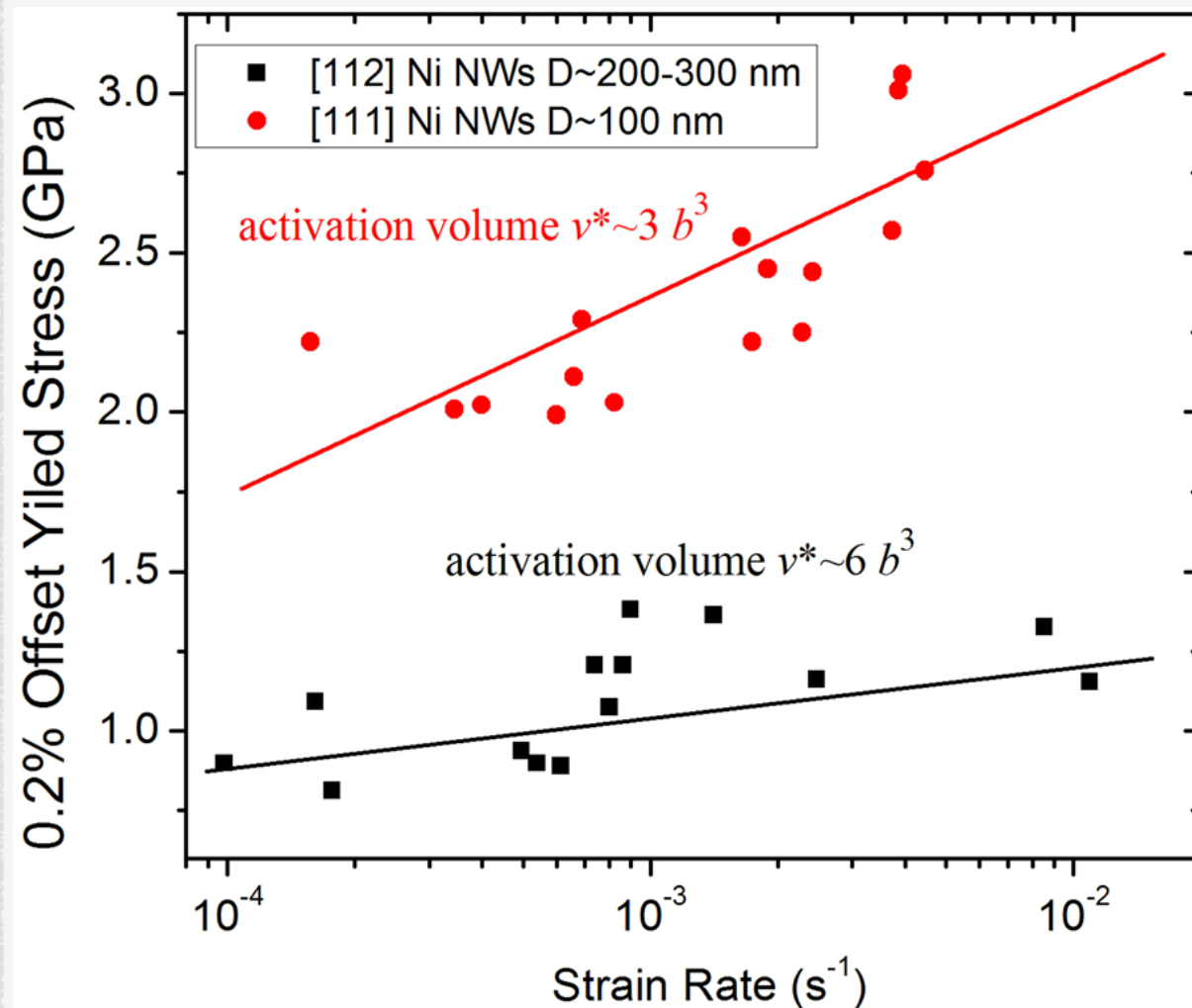
Peng et al. *Appl. Phys. Lett.* **102**, 083102 (2013)

Jennings et al. *Acta Mat.* **59**, 5627 (2011)

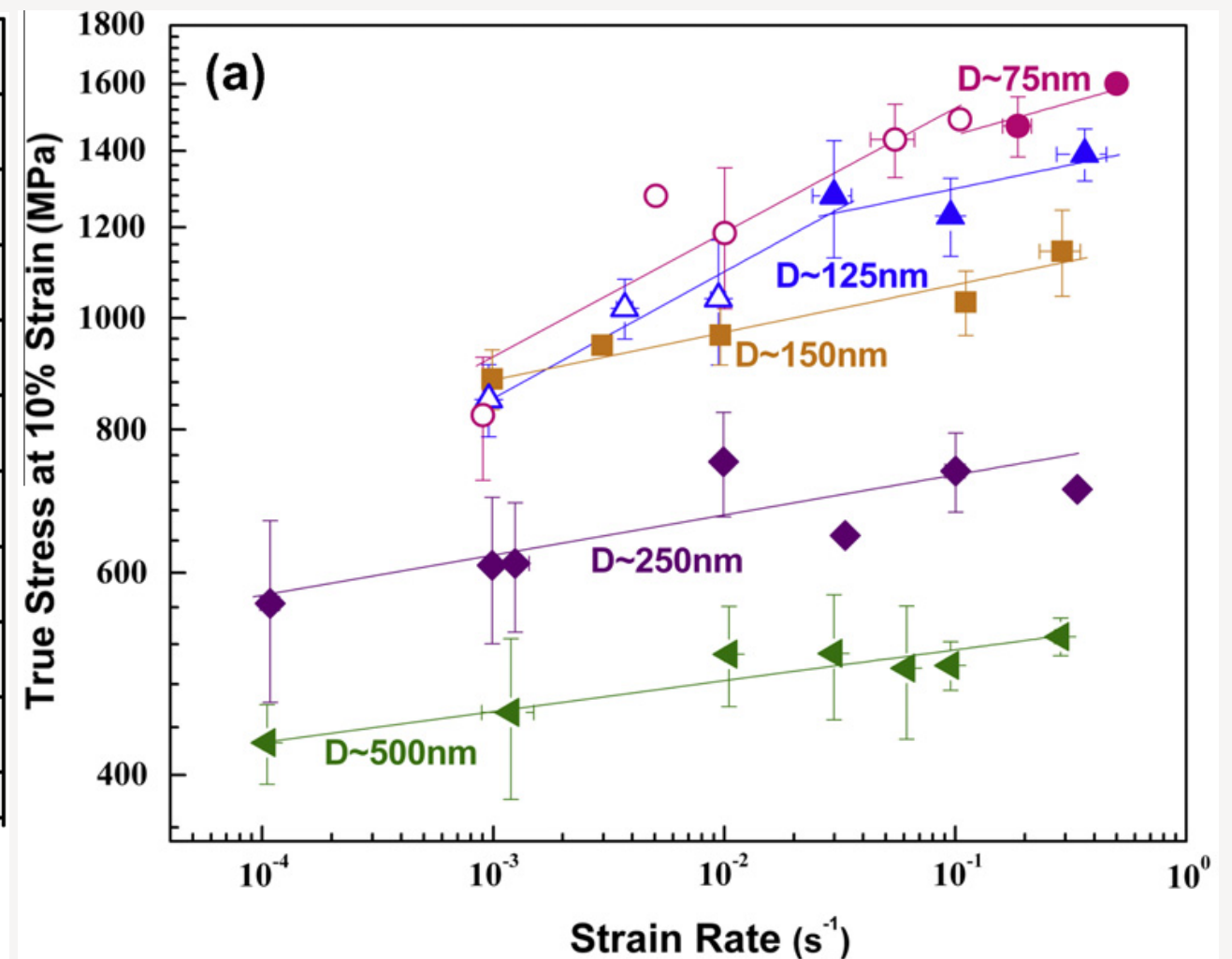
$$\sigma = \sigma_0 \dot{\epsilon}^m \quad 0.03 \lesssim m \lesssim 0.06$$

STRAIN RATE SENSITIVITY

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Cu nano-pillars



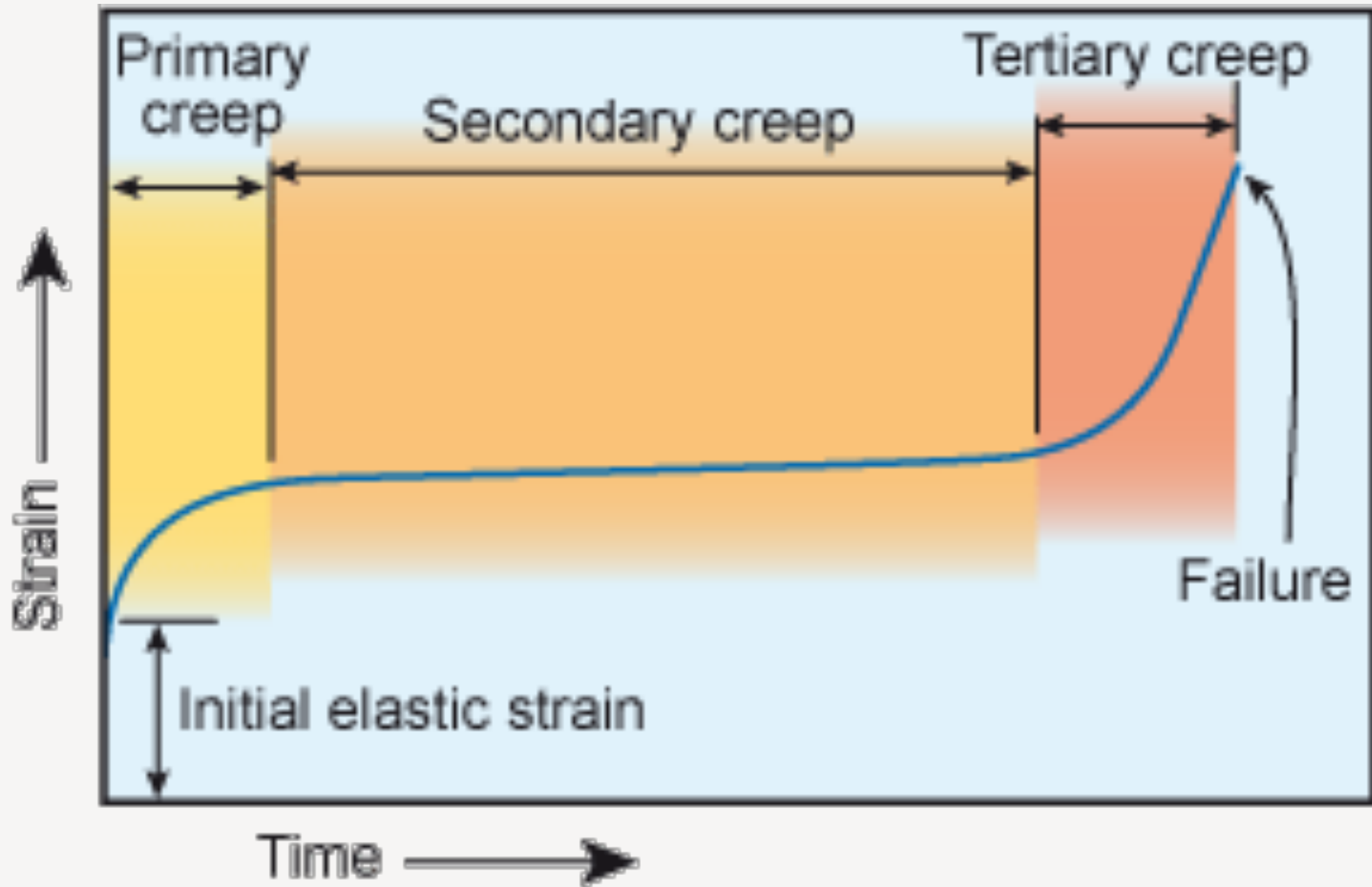
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CREEP



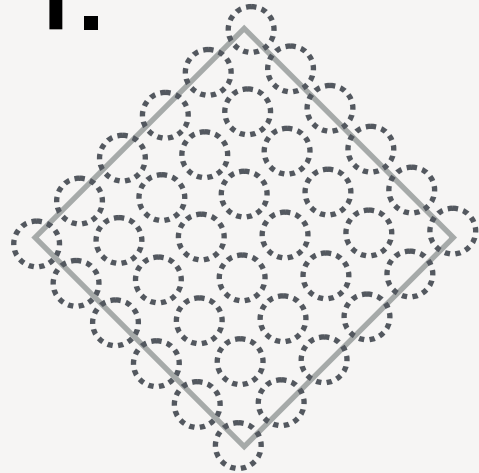
Equilibrium, *bulk*, free energy is independent of the shape of the boundary

D. Ruelle, *Statistical Mechanics: Rigorous Results* (Benjamin, New York, 1969).

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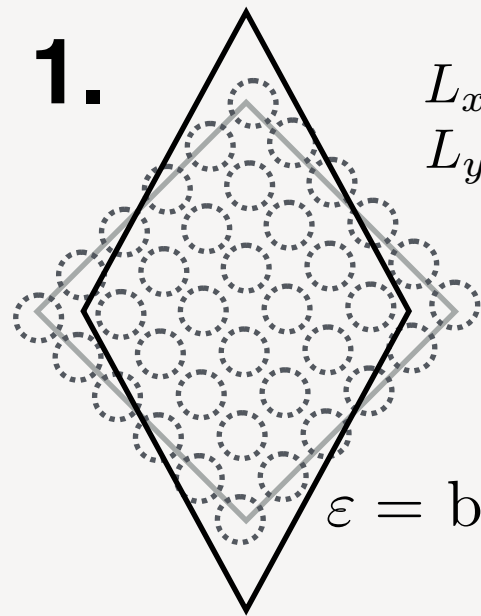
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$$L_x \rightarrow L_x(1 - \varepsilon)$$

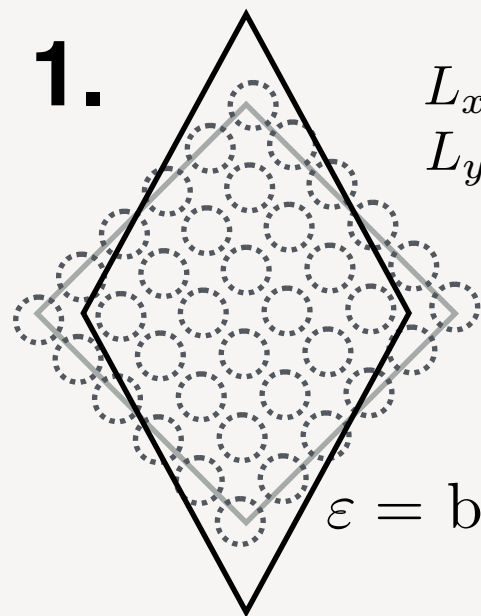
$$L_y \rightarrow L_y(1 + \varepsilon)$$

ε = boundary shape

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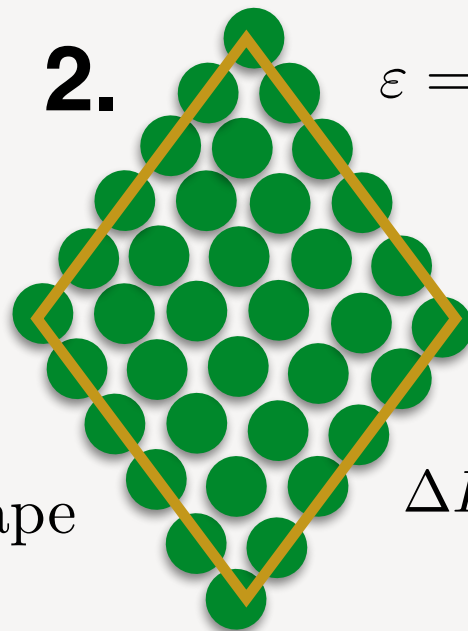
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$$\begin{aligned} L_x &\rightarrow L_x(1 - \varepsilon) \\ L_y &\rightarrow L_y(1 + \varepsilon) \end{aligned}$$

$\varepsilon = \text{boundary shape}$

2.

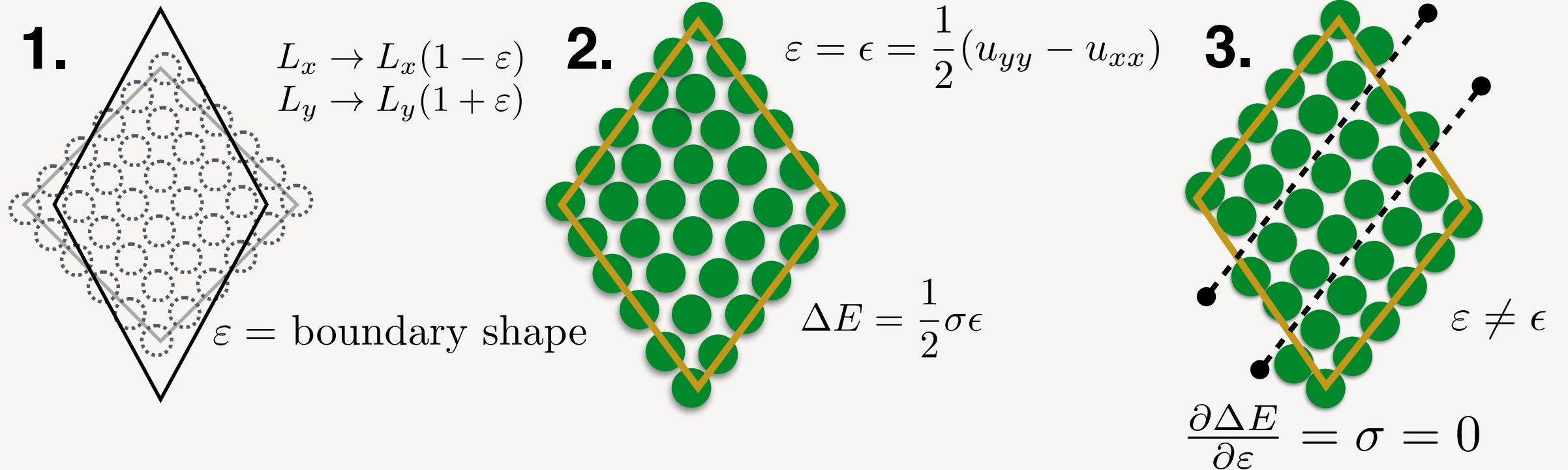


$$\varepsilon = \epsilon = \frac{1}{2}(u_{yy} - u_{xx})$$

$$\Delta E = \frac{1}{2}\sigma\epsilon$$

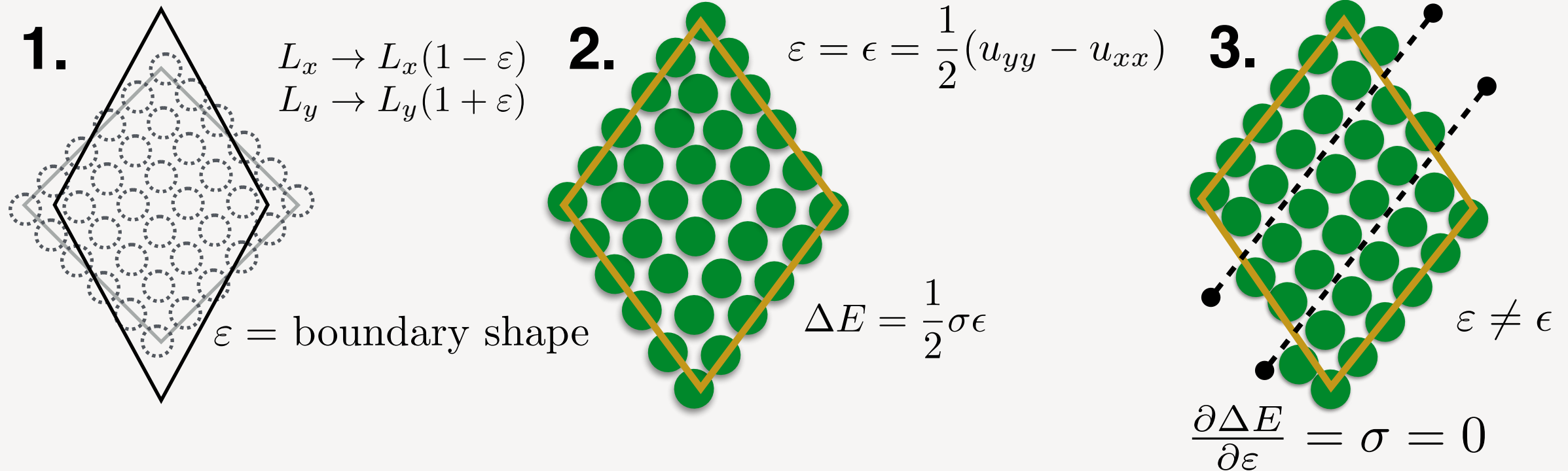
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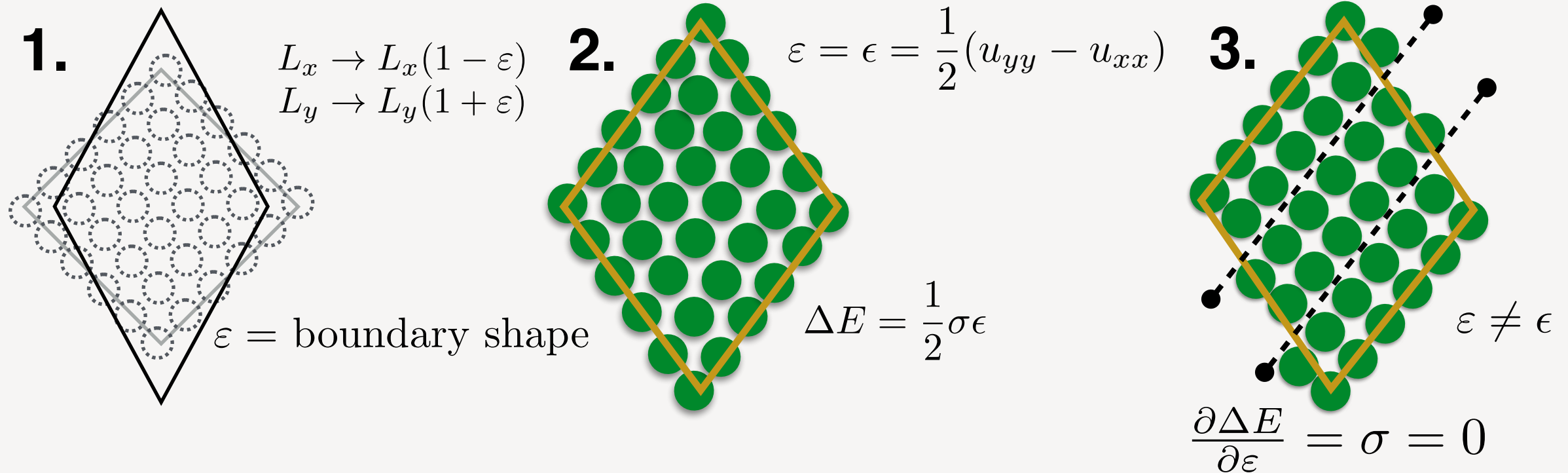
Non-zero stress only from constrained minimisation

O. Penrose, Markov Processes Relat. Fields **8**, 351 (2002).

S. Shaw and P. Harrowell, Phys. Rev. Lett. **116**, 137801 (2016)

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Or a finite time average:

F. Sausset, G. Biroli, and J. Kurchan, J. Stat. Phys. **140**, 718 (2010).

R. Bruinsma, B. I. Halperin and A. Zippelius Phys. Rev. B **25**, 579 (1982)

OUTLINE

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- First-order phase transitions

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- Affine and *non affine* atomic displacements: a new collective variable for plastic deformation.
- Rigidity: consequence of an “*invisible*” first order phase transition involving non-affine displacements
- Yielding as the *visible, dynamic* consequence of this transition
- Can understand *initiation* of plasticity in an *initially ideal crystal* without invoking properties of dislocations! (Remember: no dislocations in glasses)

FIRST ORDER TRANSITION

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- Sharp *discontinuous* changes; latent heat

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- Sharp **discontinuous** changes; latent heat
- Phase **coexistence** for choice of external parameters

FIRST ORDER TRANSITION

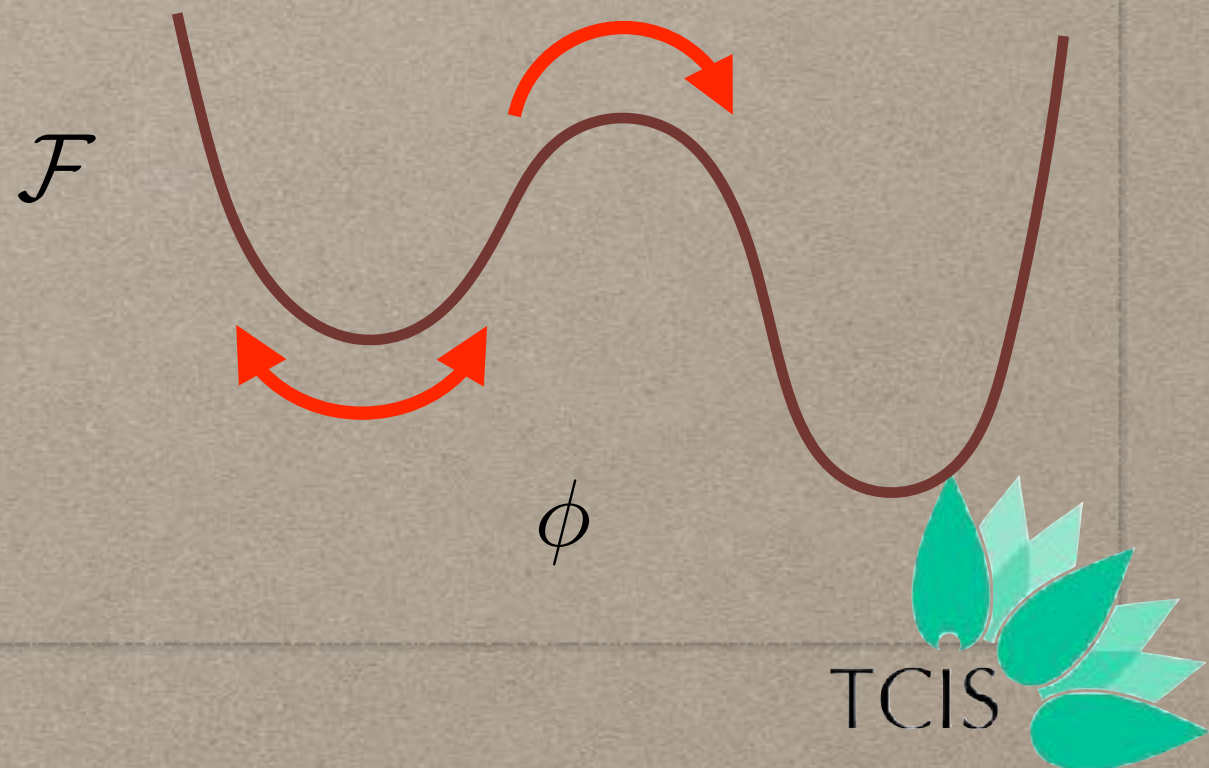
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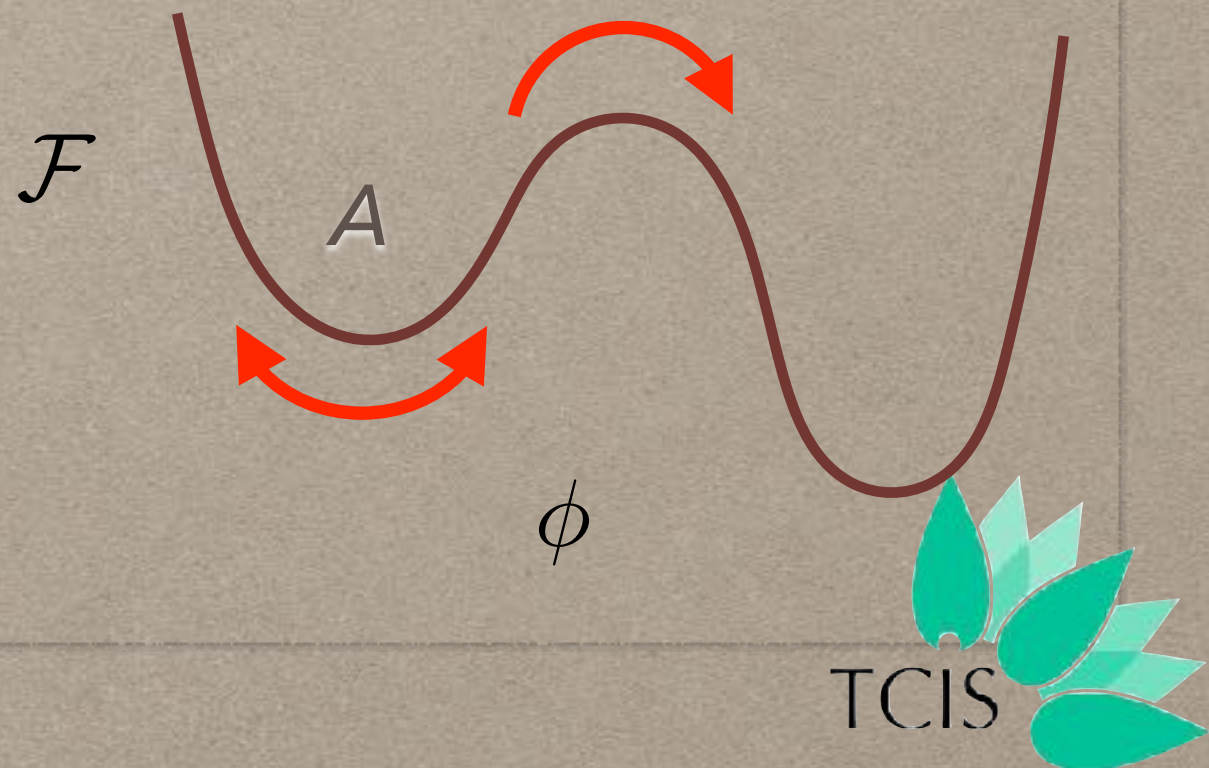
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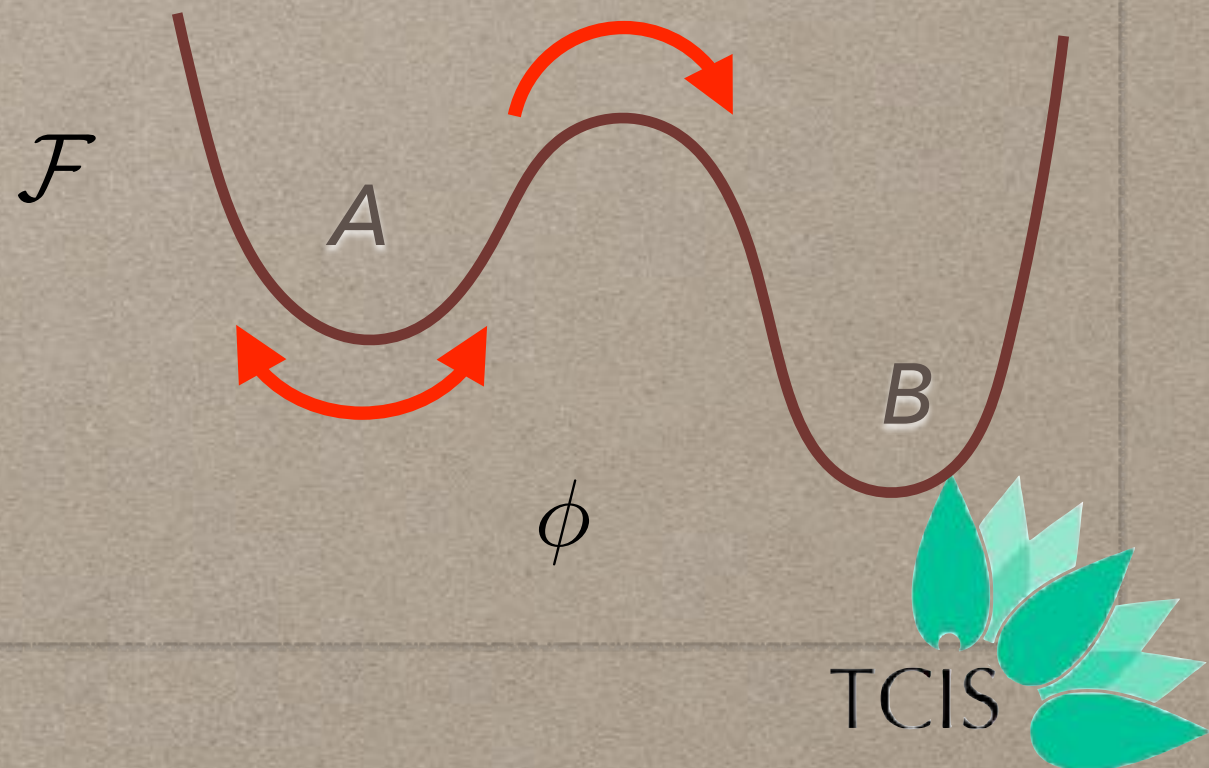
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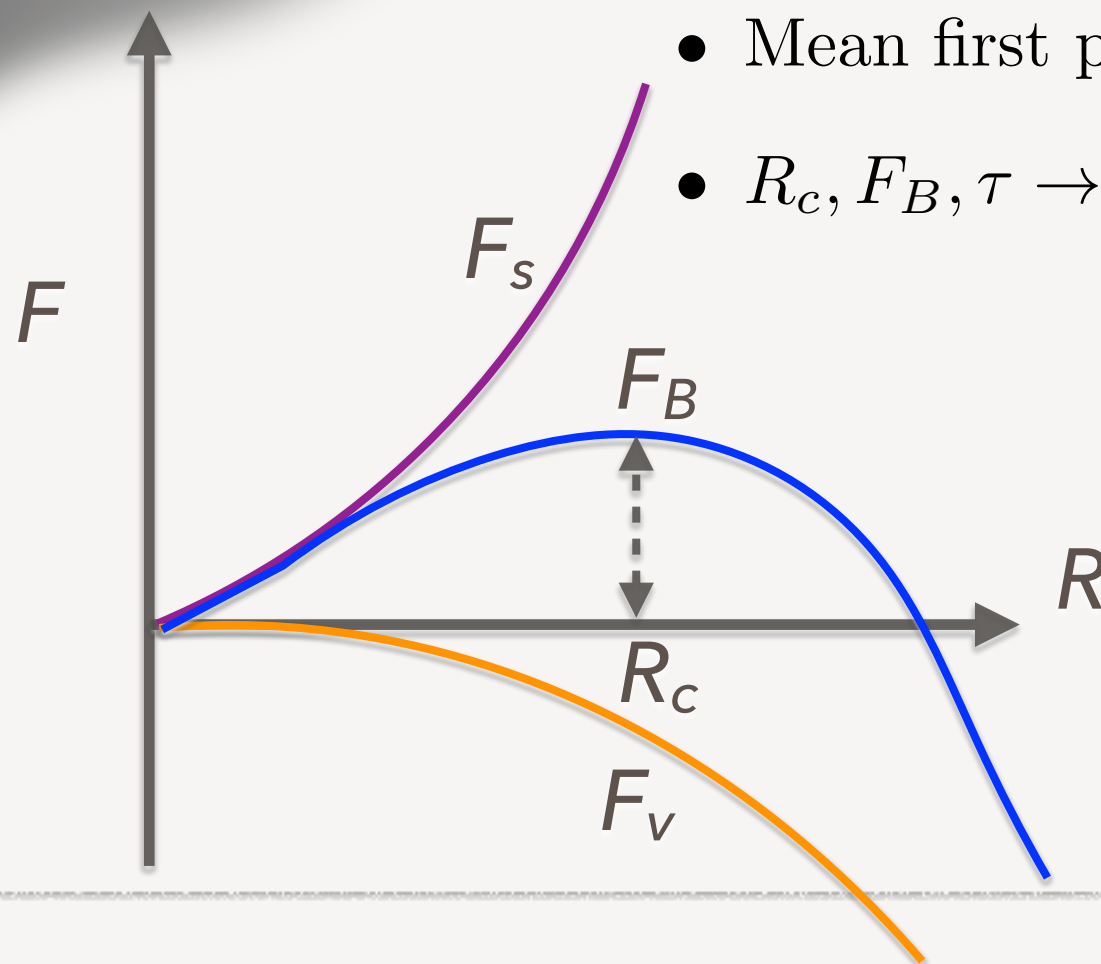
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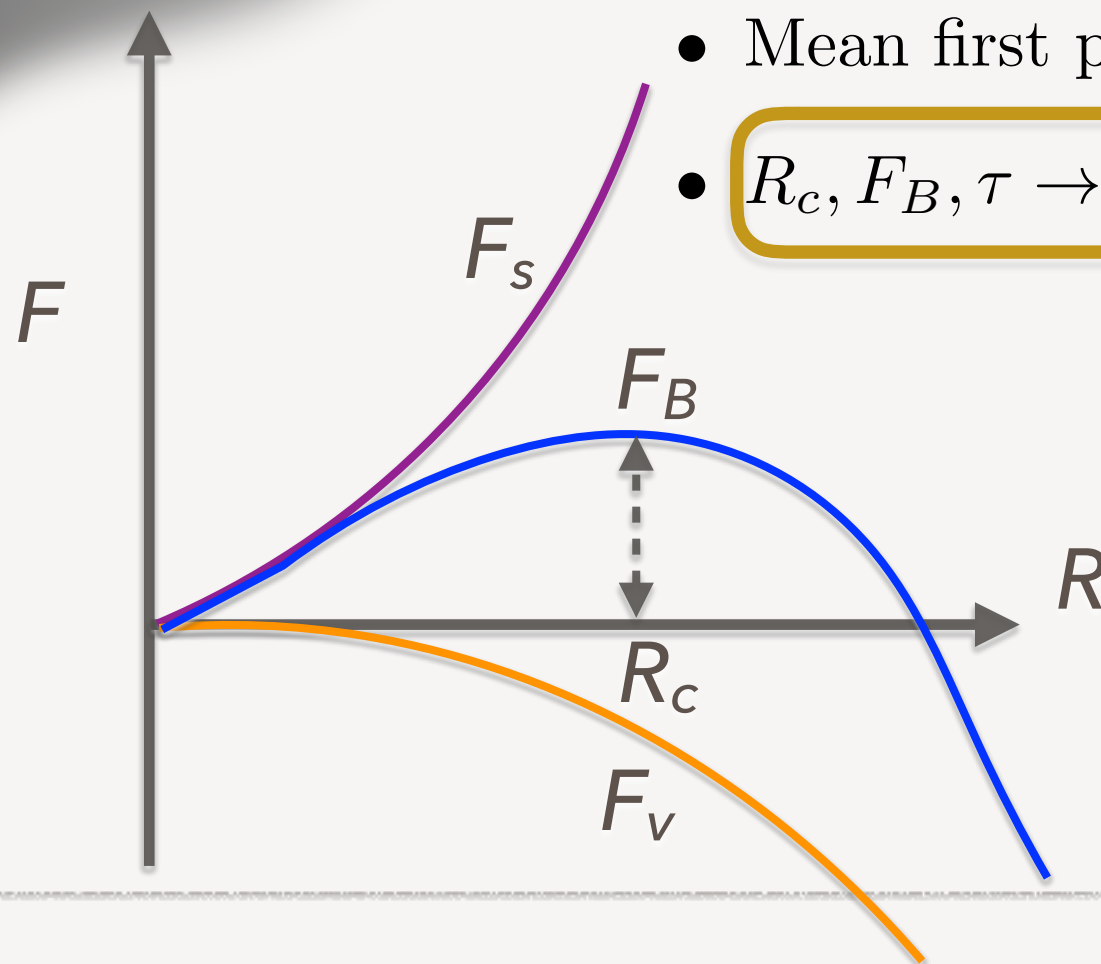
CLASSICAL NUCLEATION THEORY

- Free energy gain $F_V = \Delta F \frac{4}{3}\pi R^3$
- Free energy cost $F_S = \gamma 4\pi R^2$
- Total free energy $F = F_V + F_S$
- Critical radius R_c and free energy barrier F_B
- $R_c \propto \gamma/\Delta F$, $F_B \propto \gamma^3/\Delta F^2$
- Mean first passage time $\tau = \tau_0 e^{\beta F_B}$
- $R_c, F_B, \tau \rightarrow \infty$ as $\Delta F \rightarrow 0$.



CLASSICAL NUCLEATION THEORY

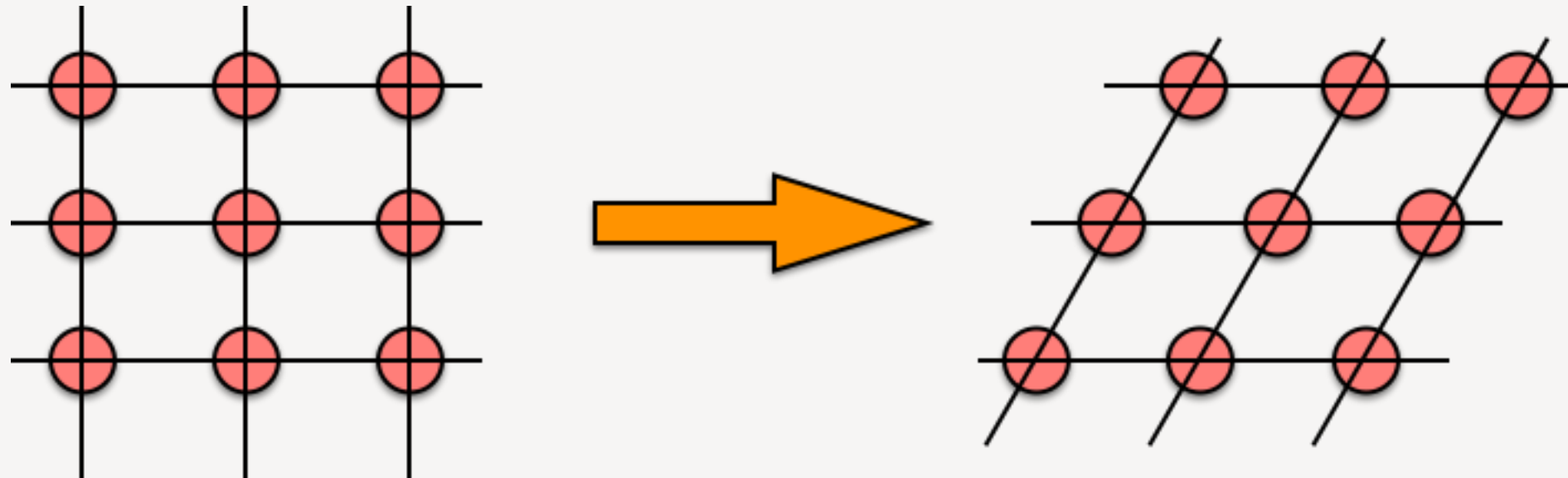
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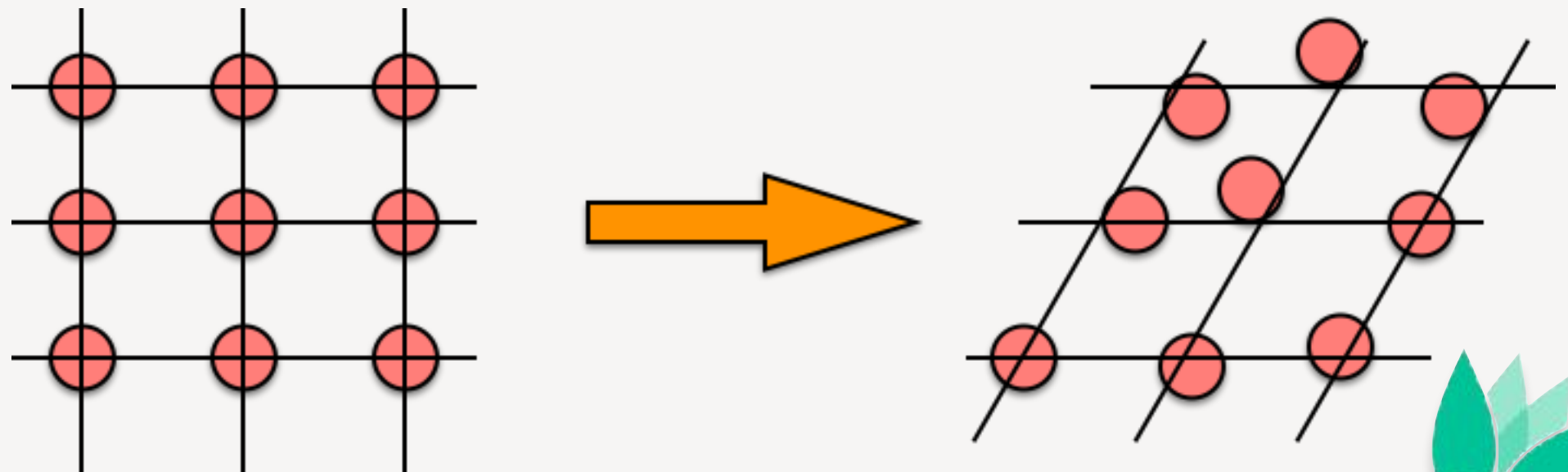
AFFINE AND NON-AFFINE

$$\{\mathbf{R}_i\} \rightarrow \{\mathbf{r}_i\} : (\mathbf{r}_i - \mathbf{r}_j) = \mathcal{D}(\mathbf{R}_i - \mathbf{R}_j)$$

Matrix $\mathcal{D}$ may be scalings, shear or rotations.



Displacements which cannot be represented using $\mathcal{D}$ are non-affine



3 SOURCES OF NON-AFFINE DISPLACEMENTS

- Thermal fluctuations (Ganguly et al. , PRE 2013)
- Elastic heterogeneities (Di Donna and Lubensky, PRE 2005 and many others)
- Rearrangements (Nath et al. PNAS 2018)

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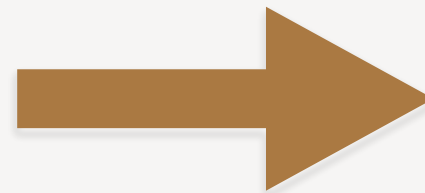
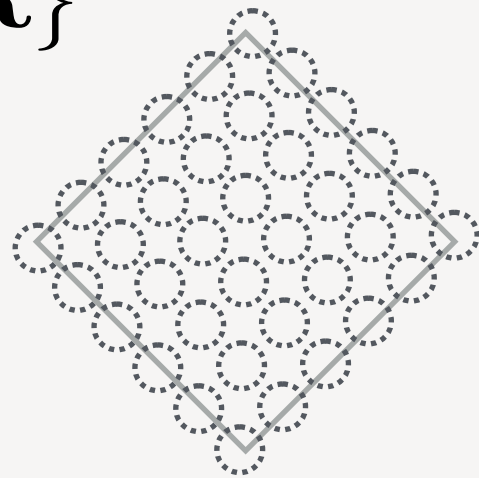
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SPECIFICALLY

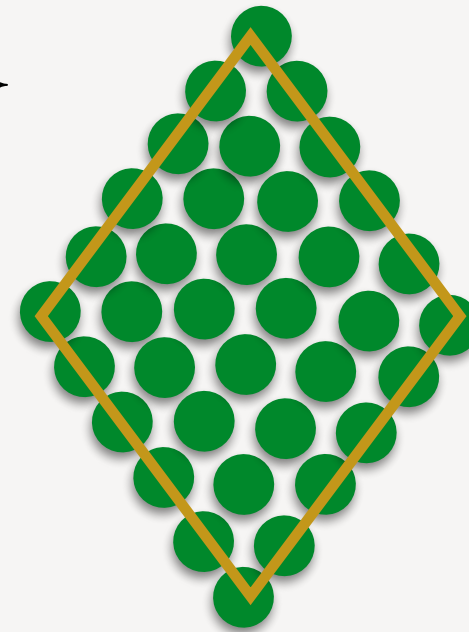
$$\exists \chi_{\Omega}(\{\mathbf{R}, \mathbf{r}\}) \quad \forall \{\mathbf{R}\}, \{\mathbf{r}\}$$

$\{\mathbf{R}\}$



Affine

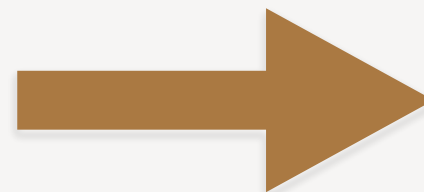
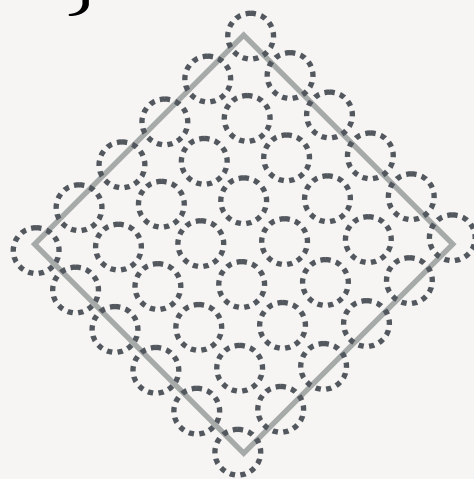
$\{\mathbf{r}\}$



$$\chi \approx 0$$

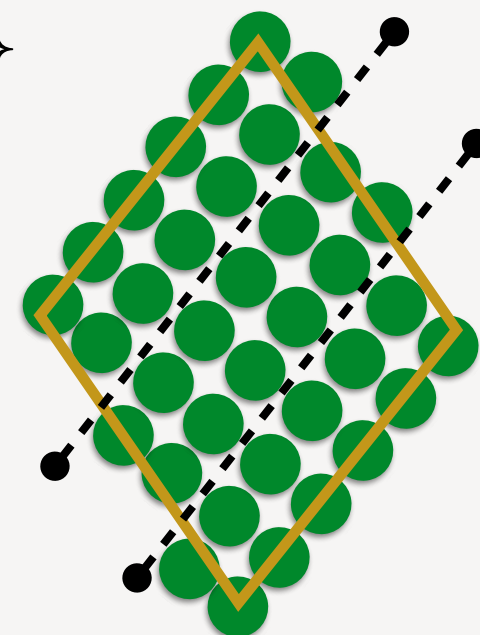
rearrangements cause non-affine-ness, measured by χ

$\{\mathbf{R}\}$



Non-affine

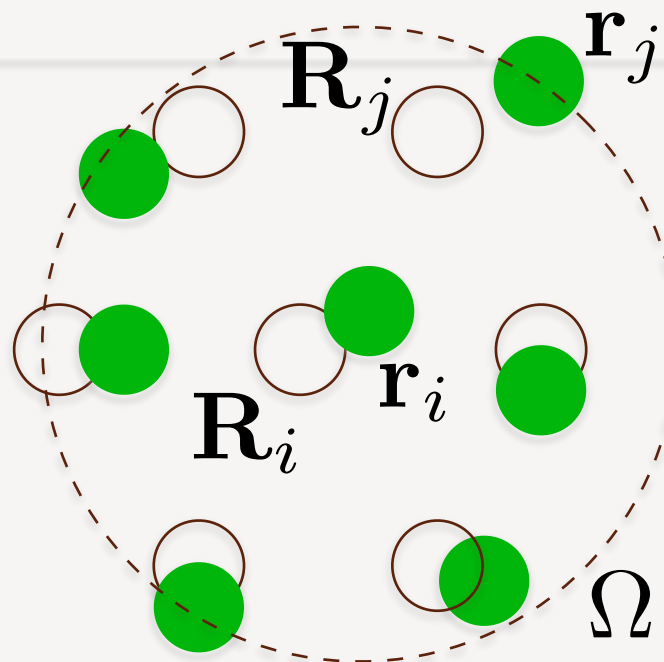
$\{\mathbf{r}\}$



$$\chi > 0$$

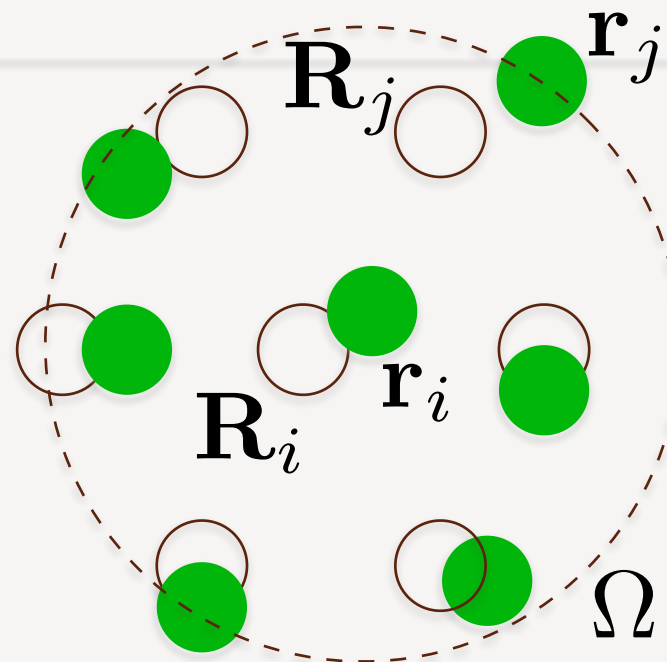
NON AFFINE DISPLACEMENTS

- Choose coarse graining volume Ω around a particle i .



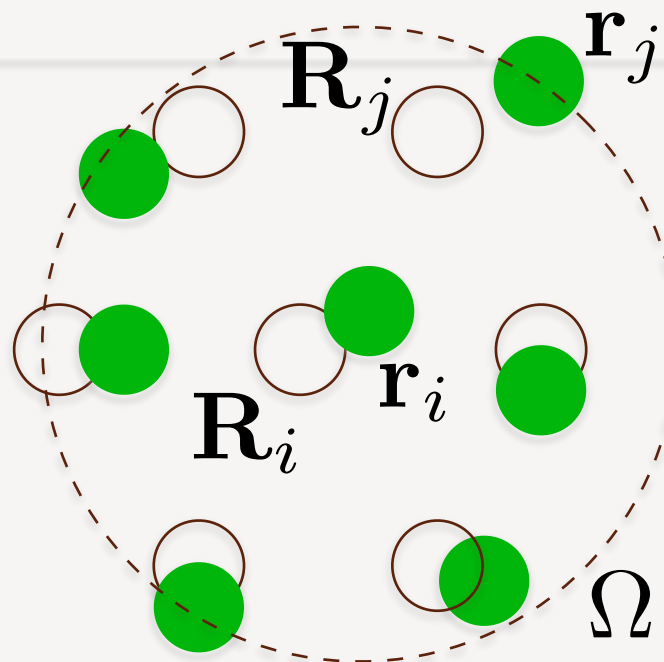
NON AFFINE DISPLACEMENTS

- Choose coarse graining volume Ω around a particle i .
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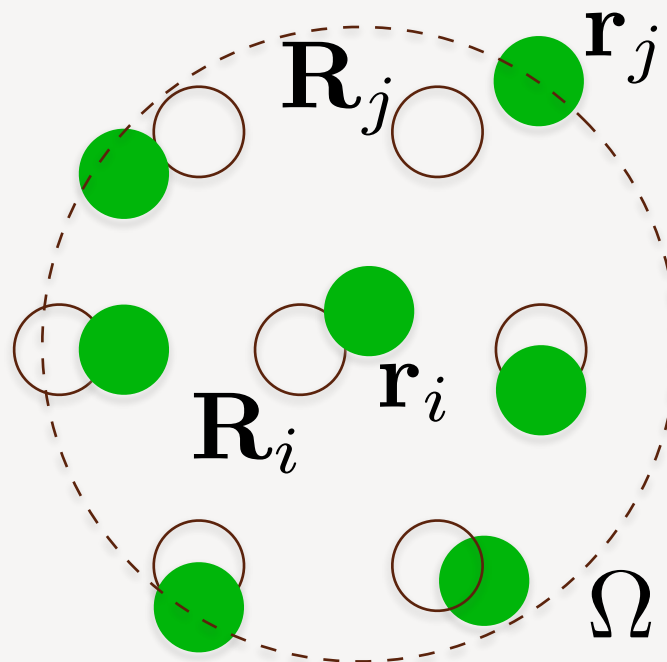
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- Minimisation = projection; $\chi_i = (\Delta\mathbf{u})^T \mathbf{P}(\{\mathbf{R}\})(\Delta\mathbf{u})$; and ensemble average $\langle \chi \rangle = \text{Tr} \mathbf{P} \mathbf{C} \mathbf{P}$; $\mathbf{C} = \langle \Delta\mathbf{u}^T \Delta\mathbf{u} \rangle$ the displacement correlator.



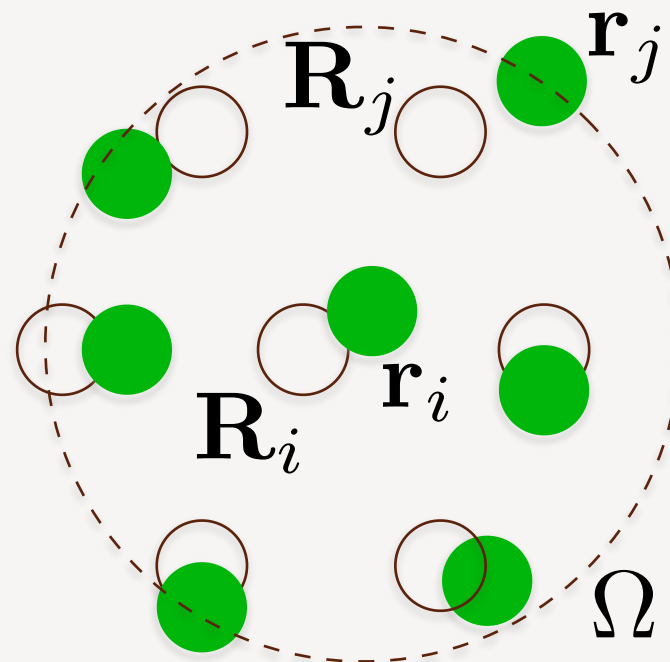
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- Eigenvectors of $\mathbf{P} \mathbf{C} \mathbf{P}$ give “non-affine displacement modes” which are *orthogonal* to the affine displacements viz. volume, rectangular distortion (ε), shear and rotation.



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2d triangular lattice has
12 normal modes with
4 affine and 8 non-affine

BIASING NON-AFFINITY

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- Define **global non-affinity** $X = N^{-1} \sum_i \chi_i$

BIASING NON-AFFINITY

- Define **global non-affinity** $X = N^{-1} \sum_i \chi_i$
- $P(X)$ is a Gaussian centered at $\langle \chi \rangle$ with width $\sim 1/\sqrt{N}$

BIASING NON-AFFINITY

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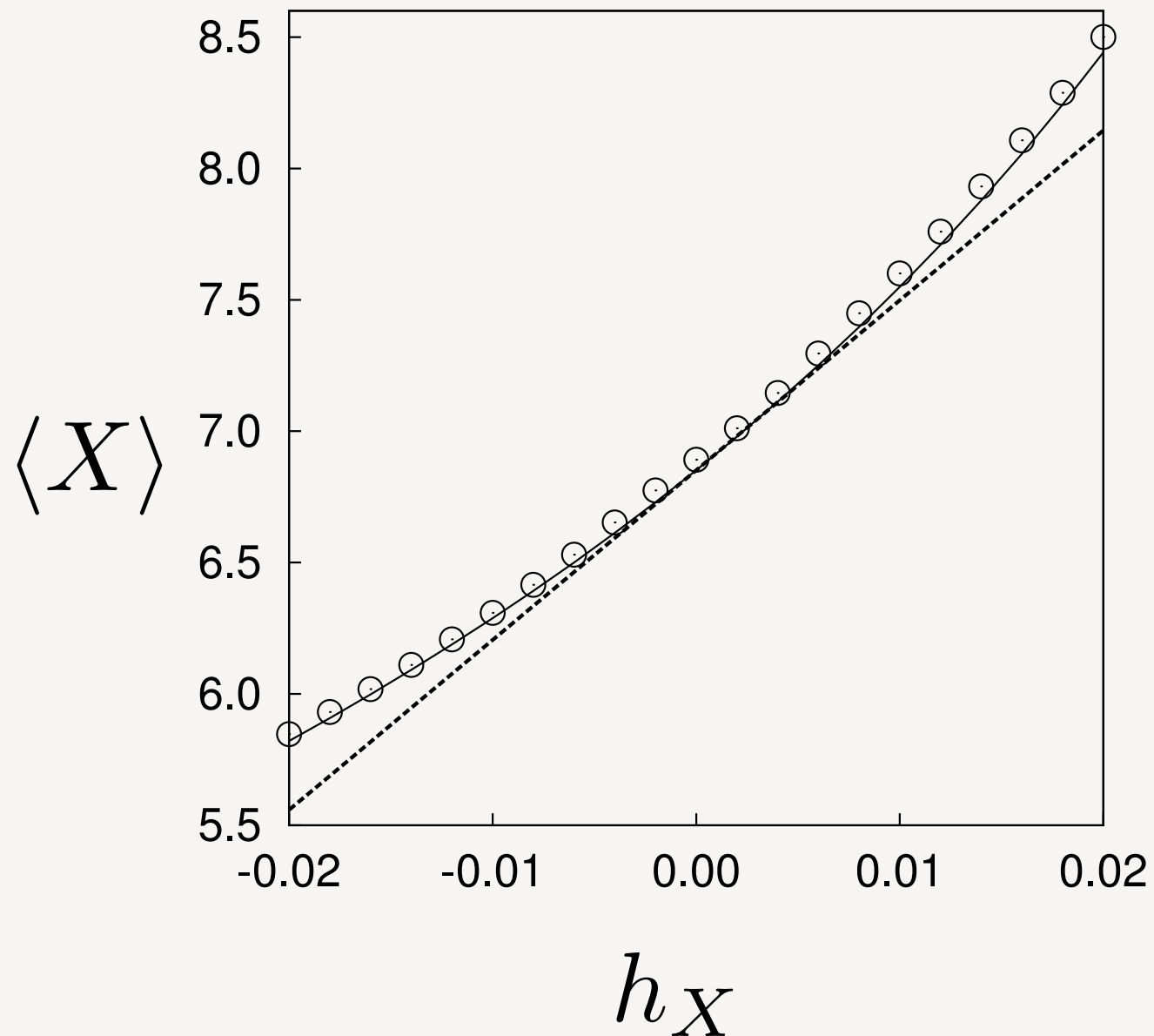
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- Note: **translational symmetry**, $\mathbf{u}_i \rightarrow \mathbf{u}_i + \text{constant}$, is preserved.

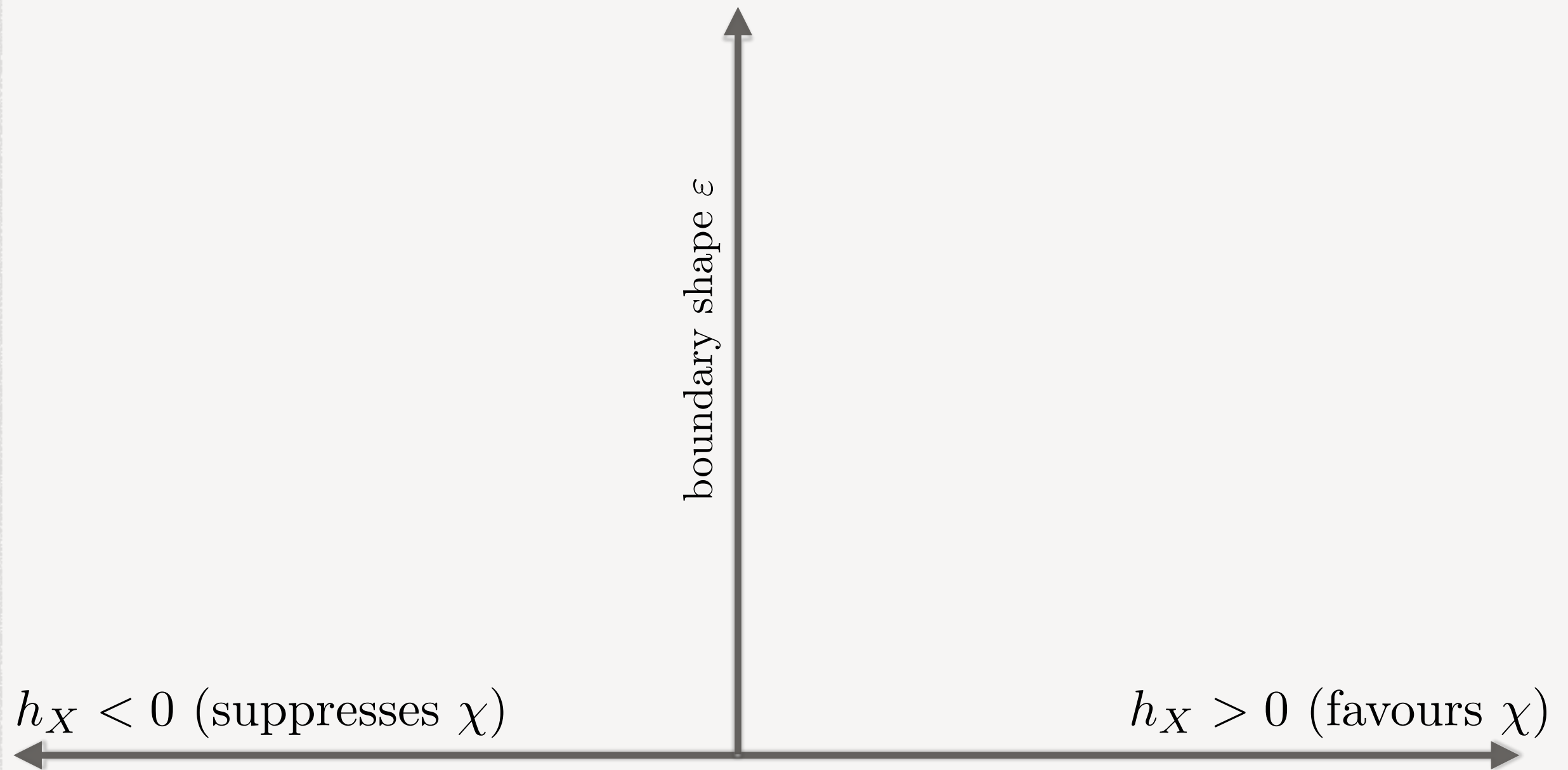
SMALL FIELDS: FLUCTUATION RESPONSE



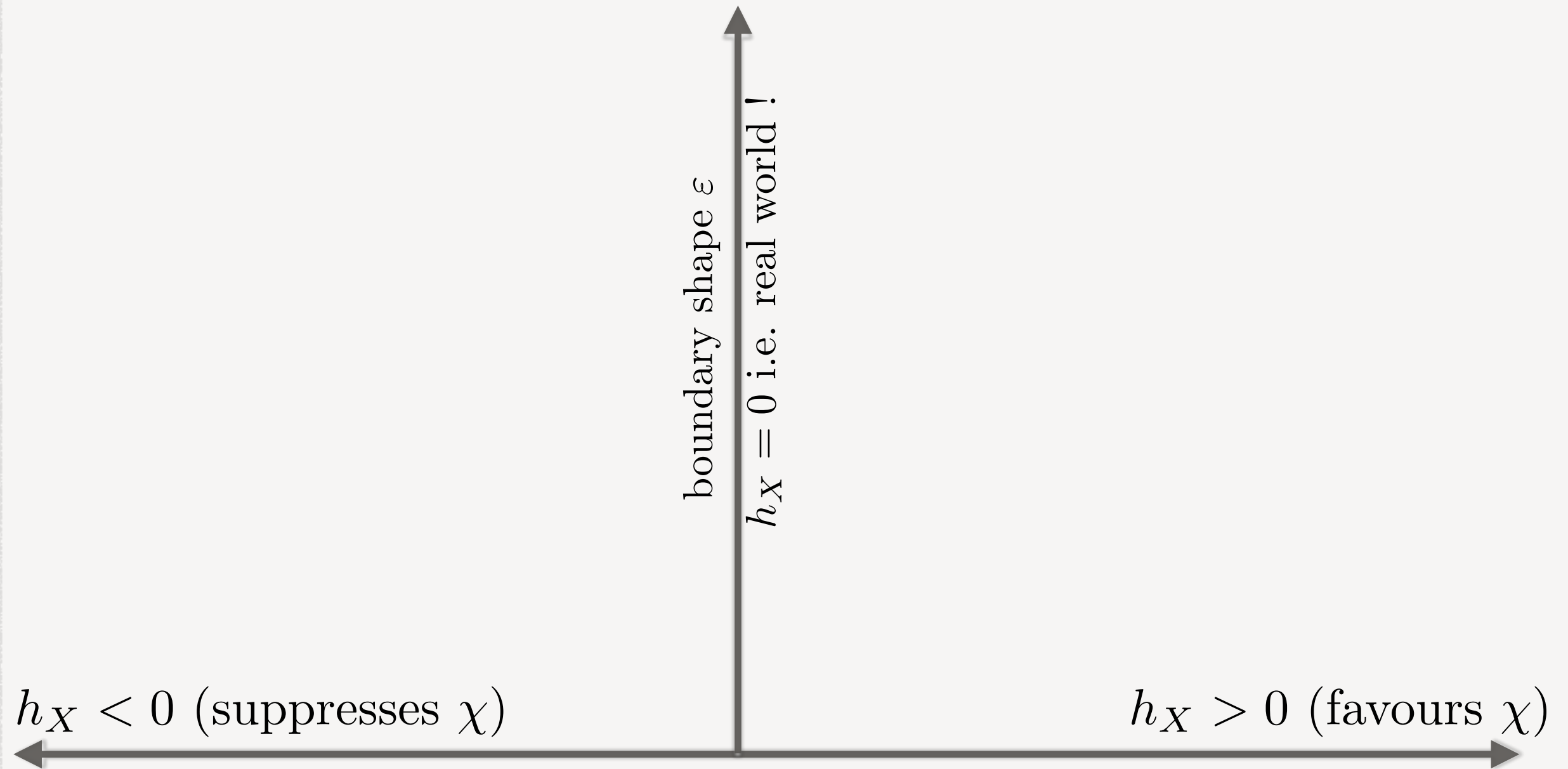
$X(h_X) = X(0) + \langle \Delta \chi^2 \rangle \sum_{\mathbf{R}} C_{\chi}(\mathbf{R}, 0)$ where $C_{\chi}(\mathbf{R}, 0)$ is the equal time, spatial correlation of χ .



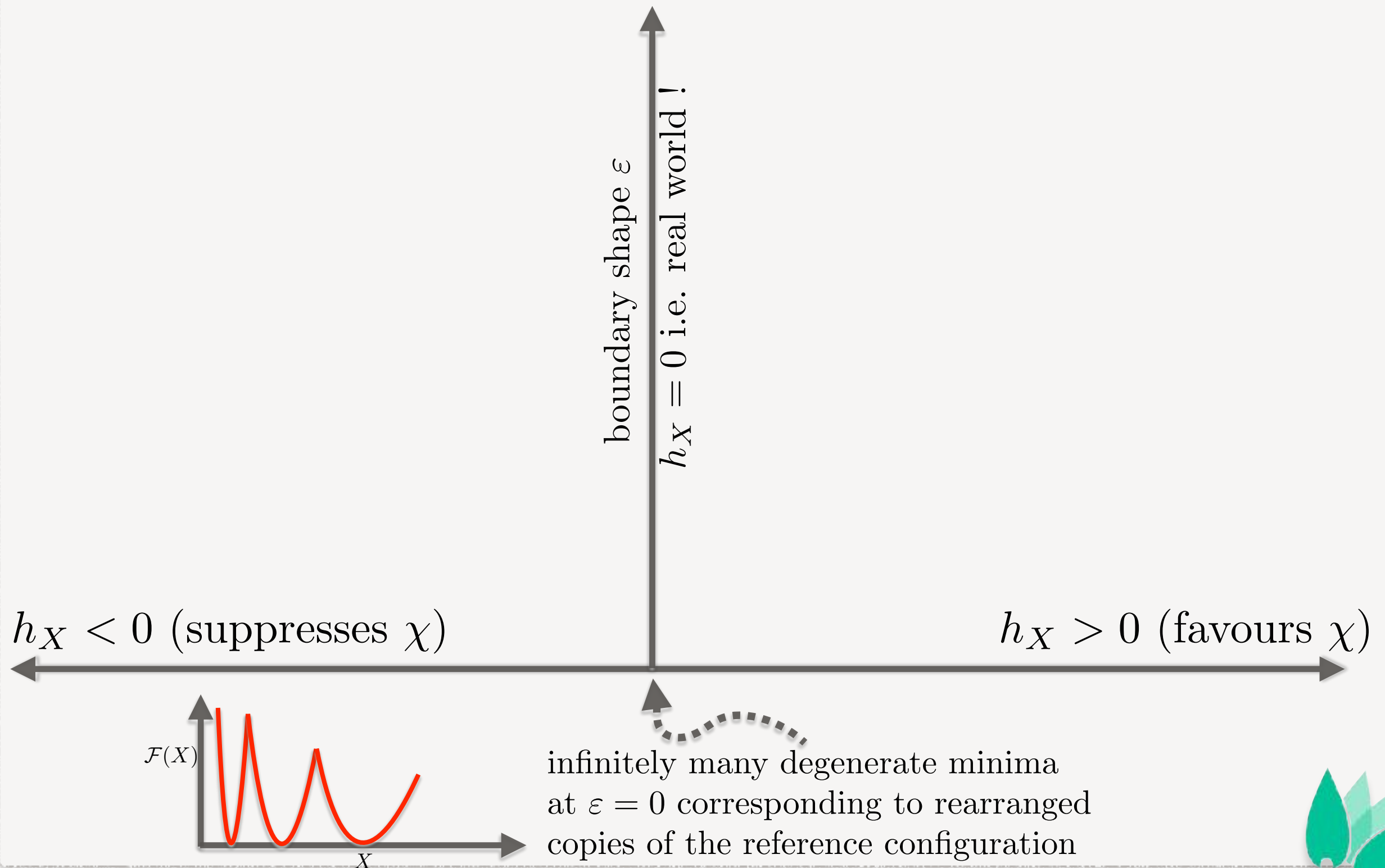
LARGE FIELDS: GLOBAL THERMO-DYNAMICS



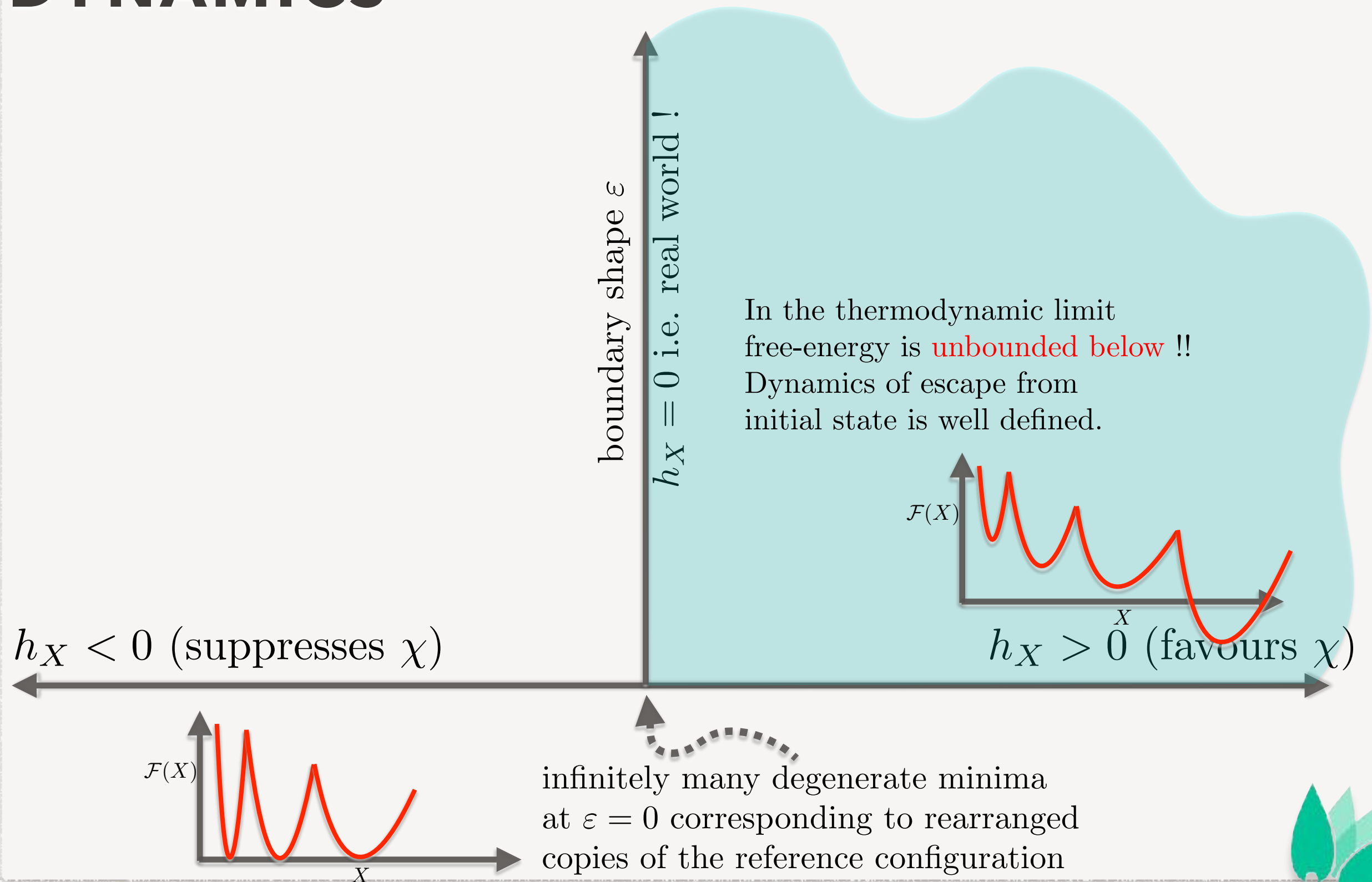
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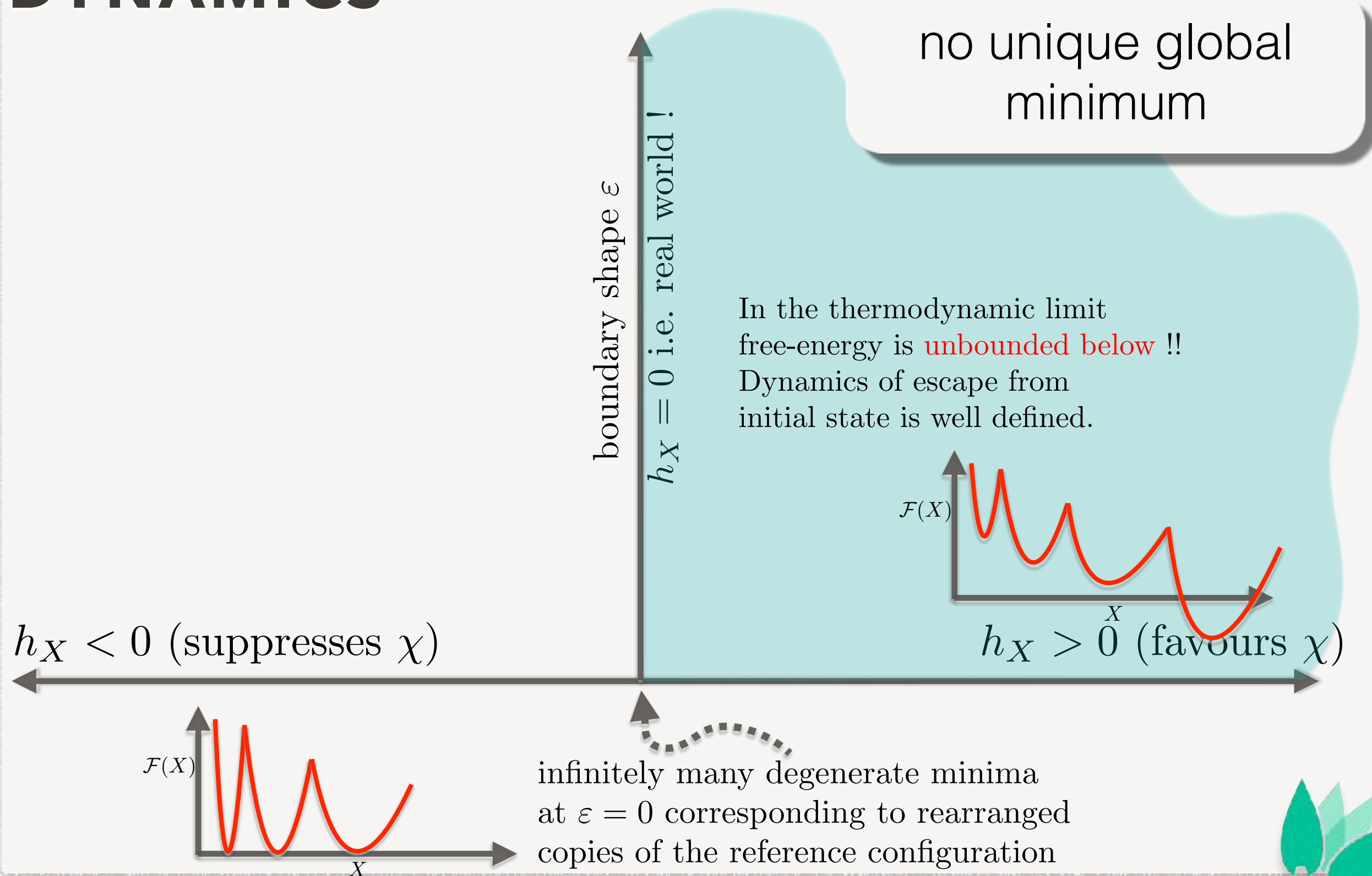
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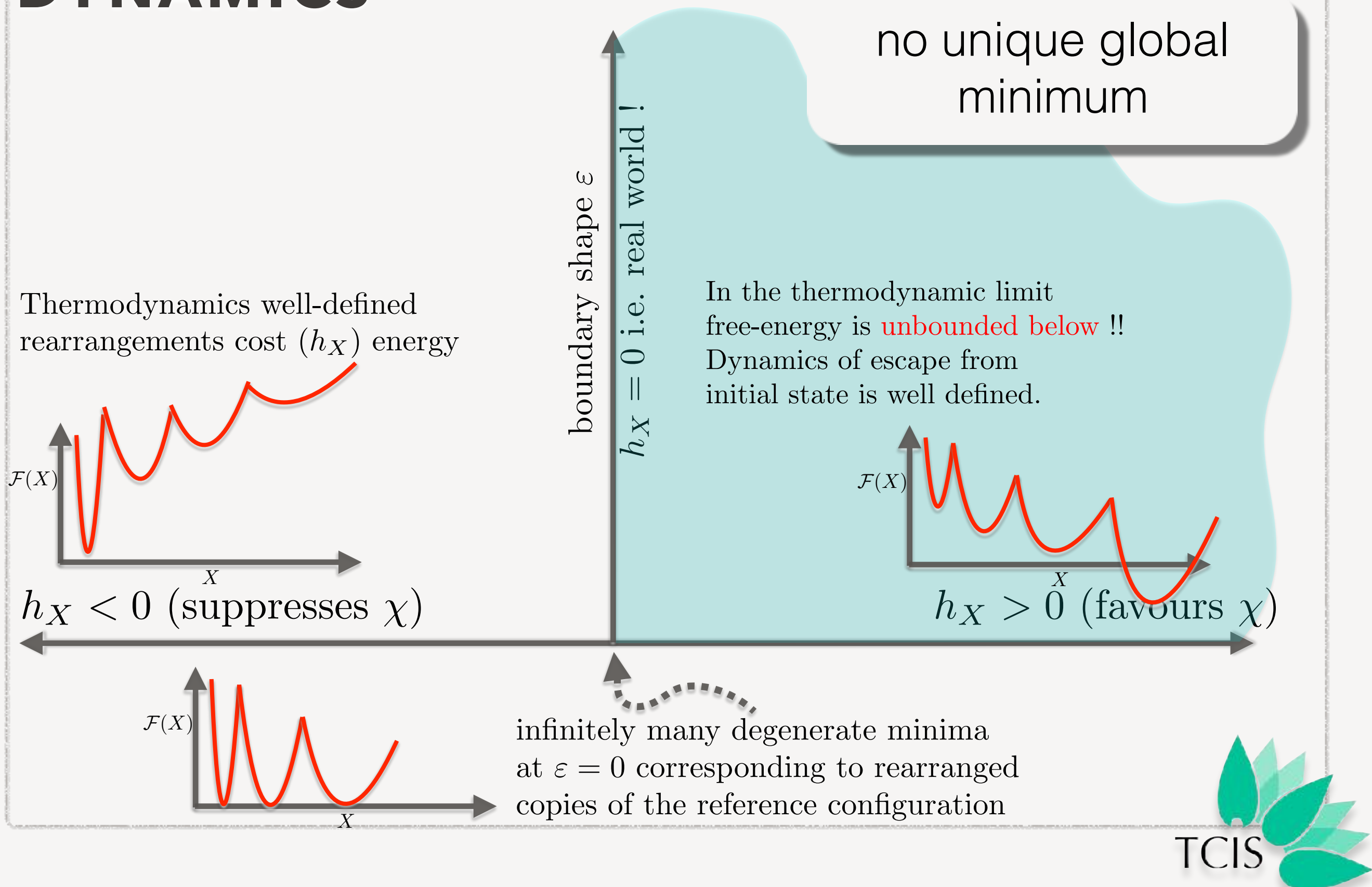
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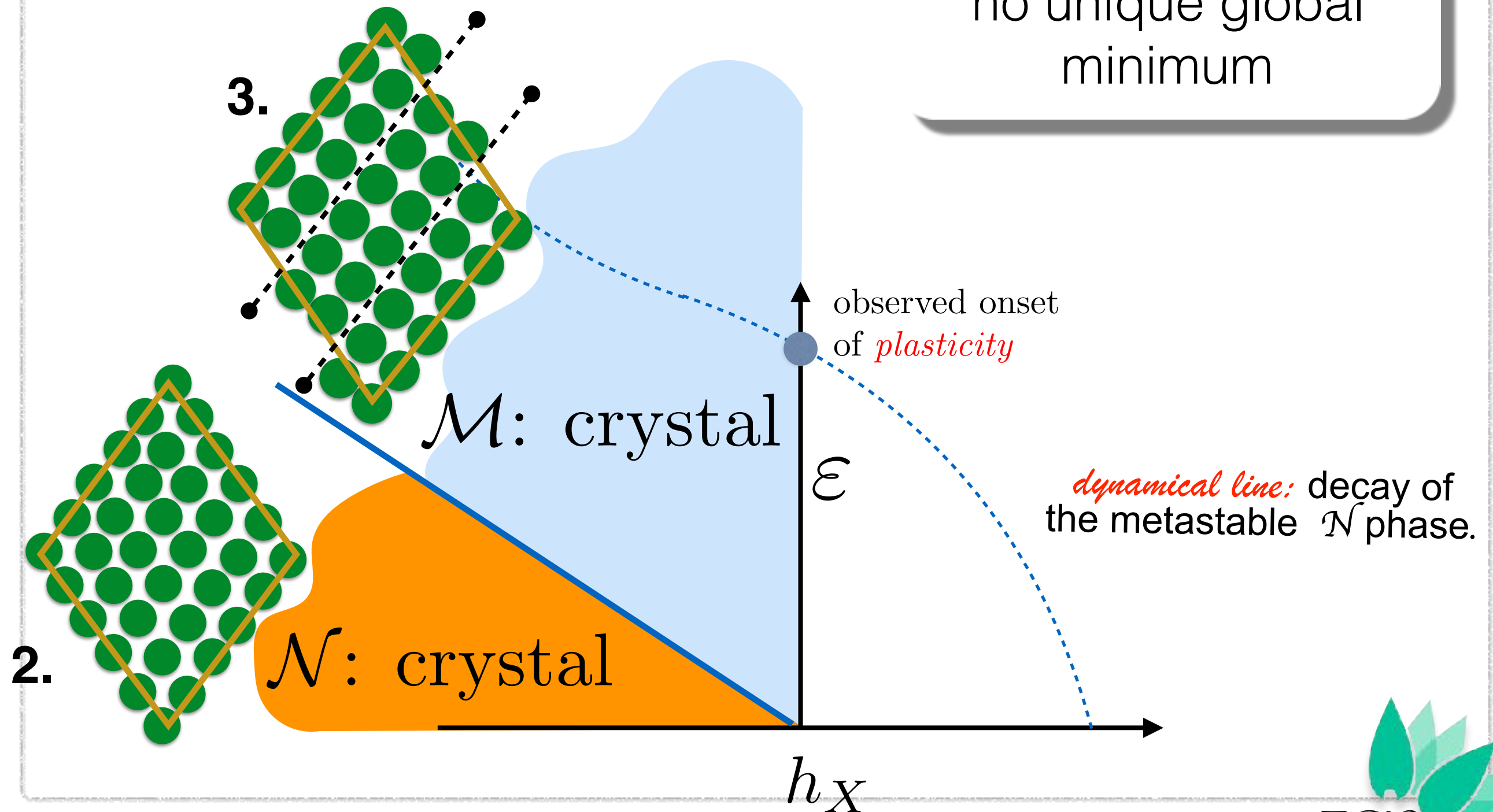
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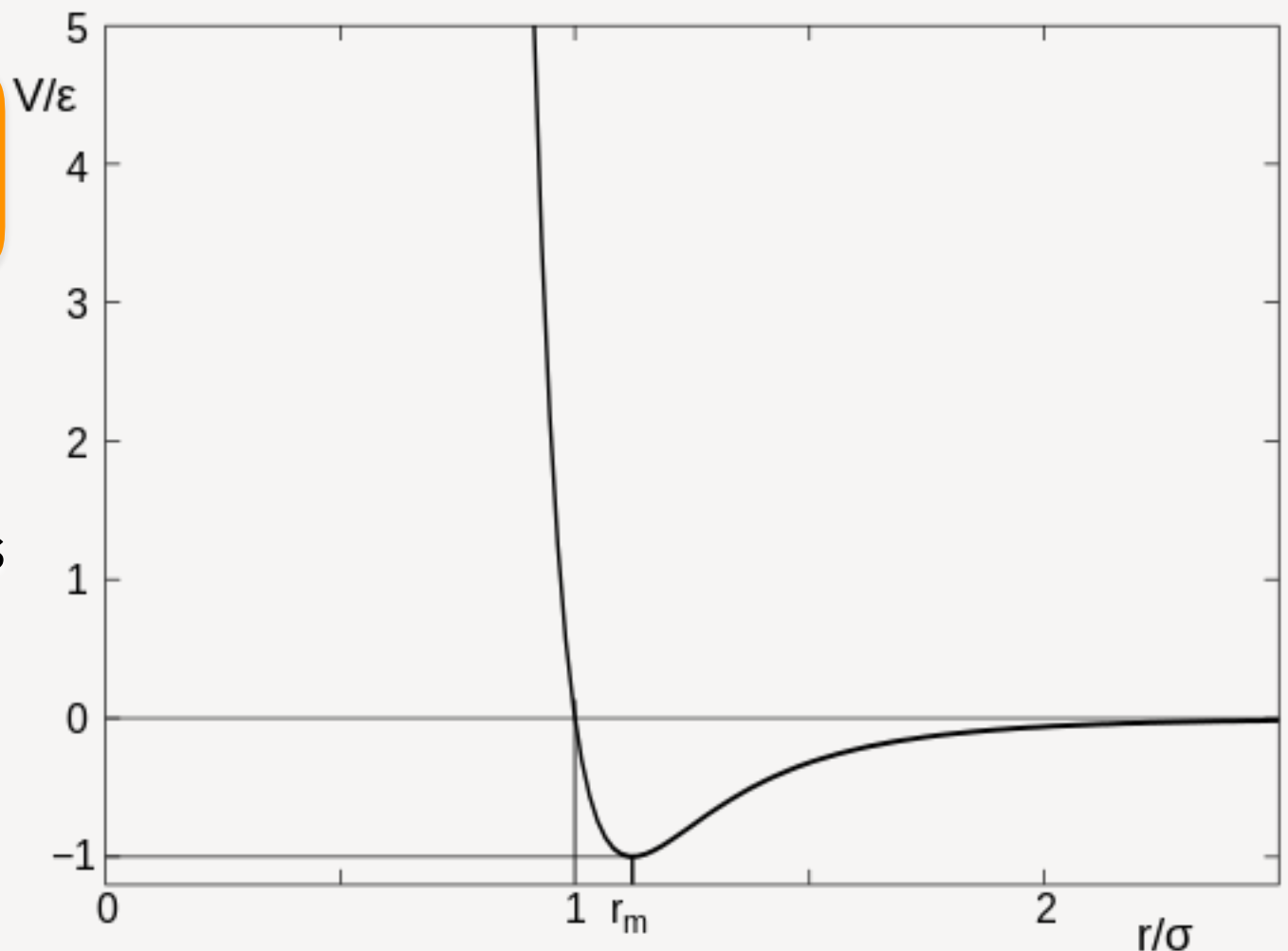
no unique global minimum



TWO DIMENSIONAL IDEAL LENNARD-JONES CRYSTAL

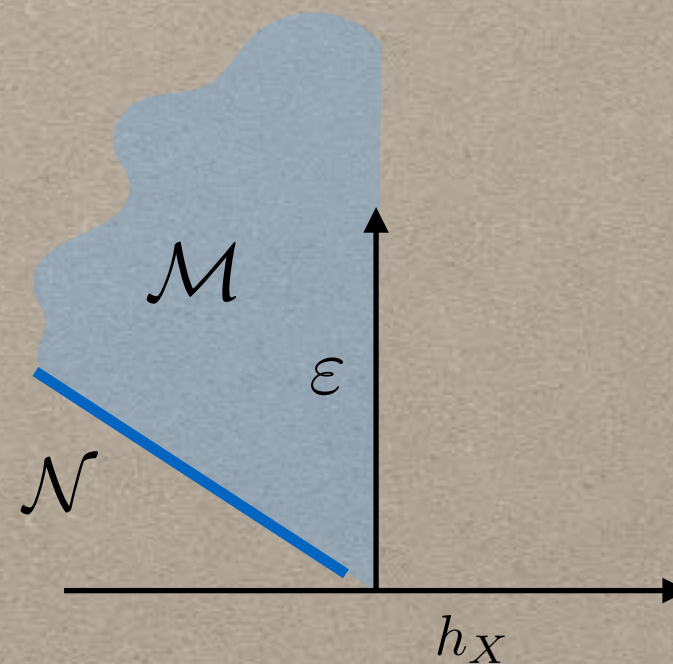
$$V(r_{ij}) = 4\epsilon \left[r_{ij}^{-12} - r_{ij}^{-6} \right]$$

- no pre-existing defects
- periodic boundary conditions
- constant NVT
- uniform (pure shear) by deforming the box.

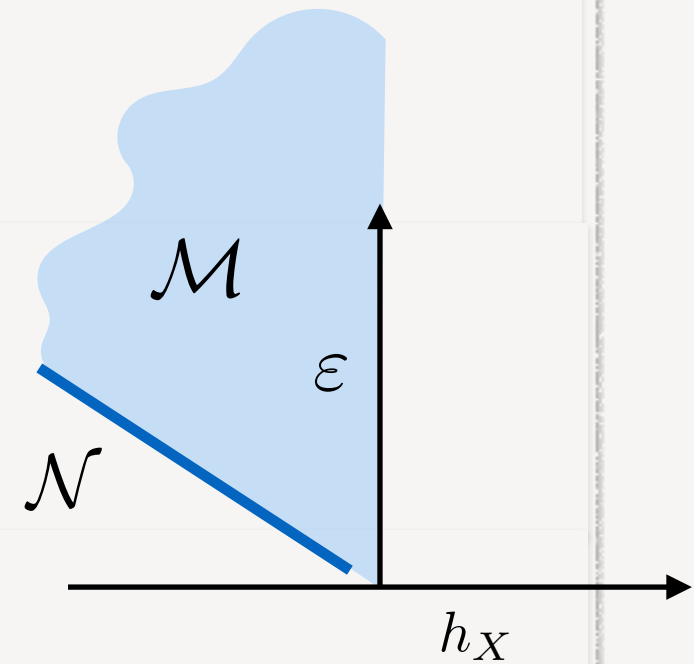


Equilibrium → sequential umbrella sampling Monte Carlo
Dynamics → molecular dynamics simulations

THE **EQUILIBRIUM** TRANSITION: "X" as the order parameter

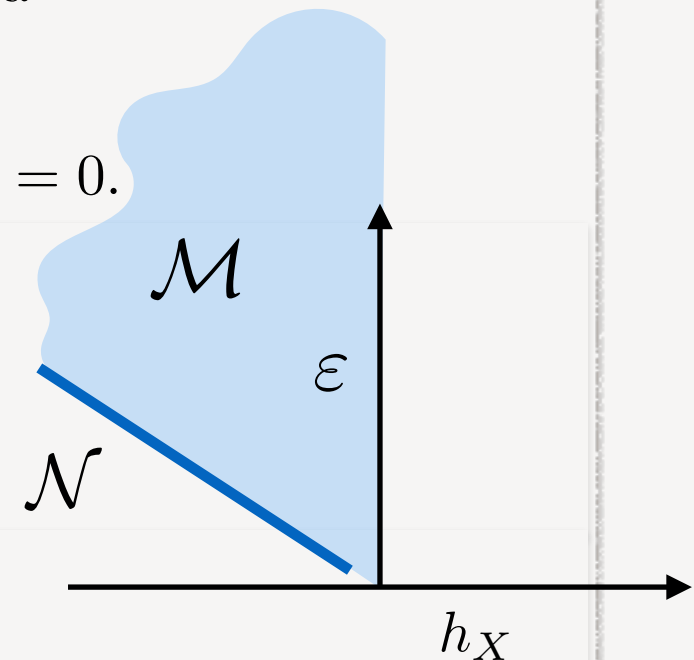


ENERGY BALANCE AND $T=0$ PHASE BOUNDARY



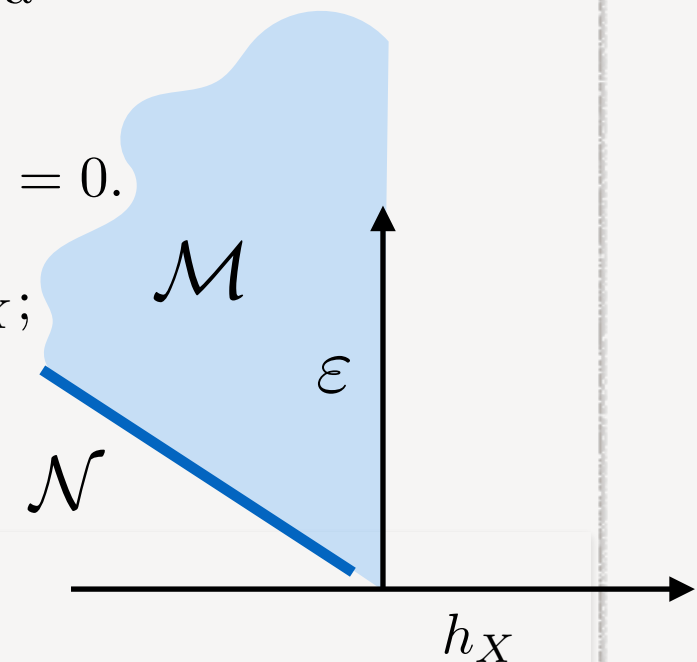
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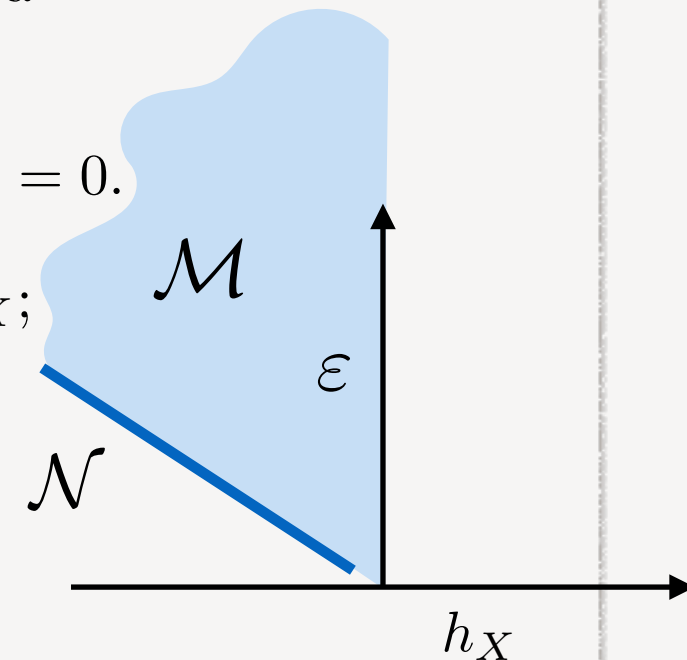
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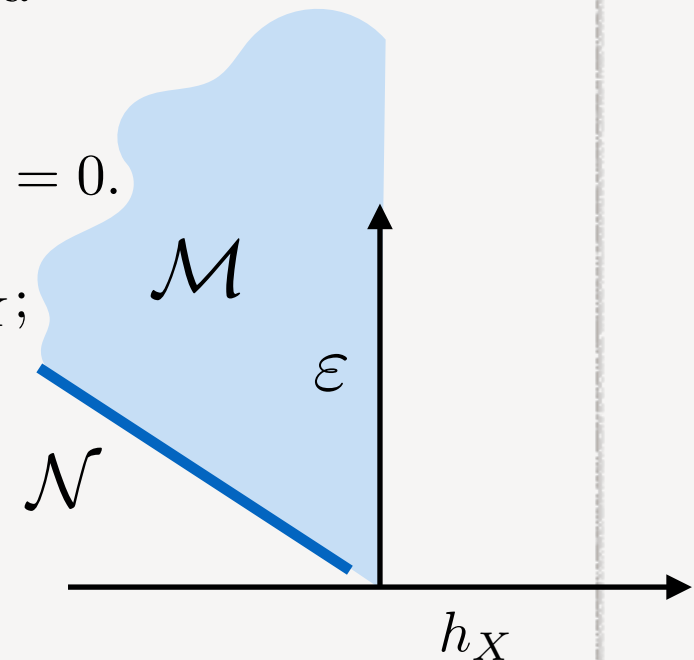
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- Note: Total energy may be written as $\Delta E = \frac{1}{2}\varsigma\varepsilon$, where $\varsigma = \sigma + 2 (\partial X/\partial \varepsilon)_{h_X} (\partial X/\partial h_X)_{\varepsilon}^{-1} X(\varepsilon)$.
- $\varsigma \times (\text{area})$ is the **true thermodynamic conjugate** to ε .
- $\varsigma = \sigma$ in the $\mathcal{N}$ crystal while it is $\propto X$ in the $\mathcal{M}$ crystal.

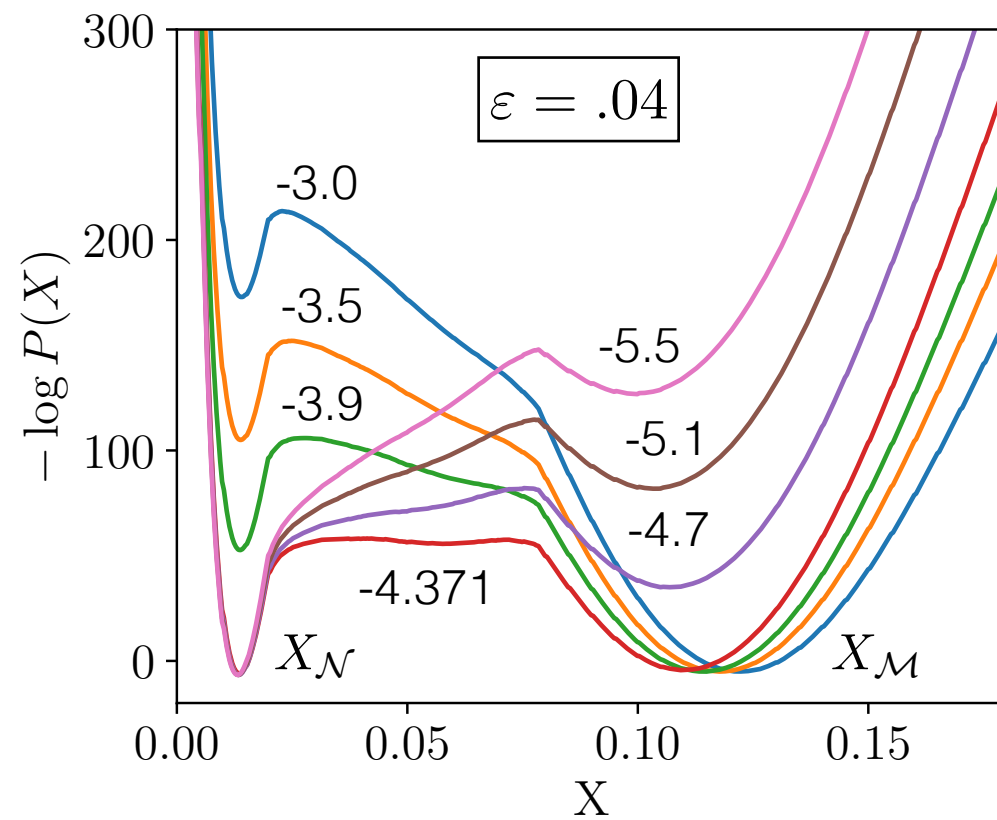


PHASE DIAGRAM AT $T > 0$

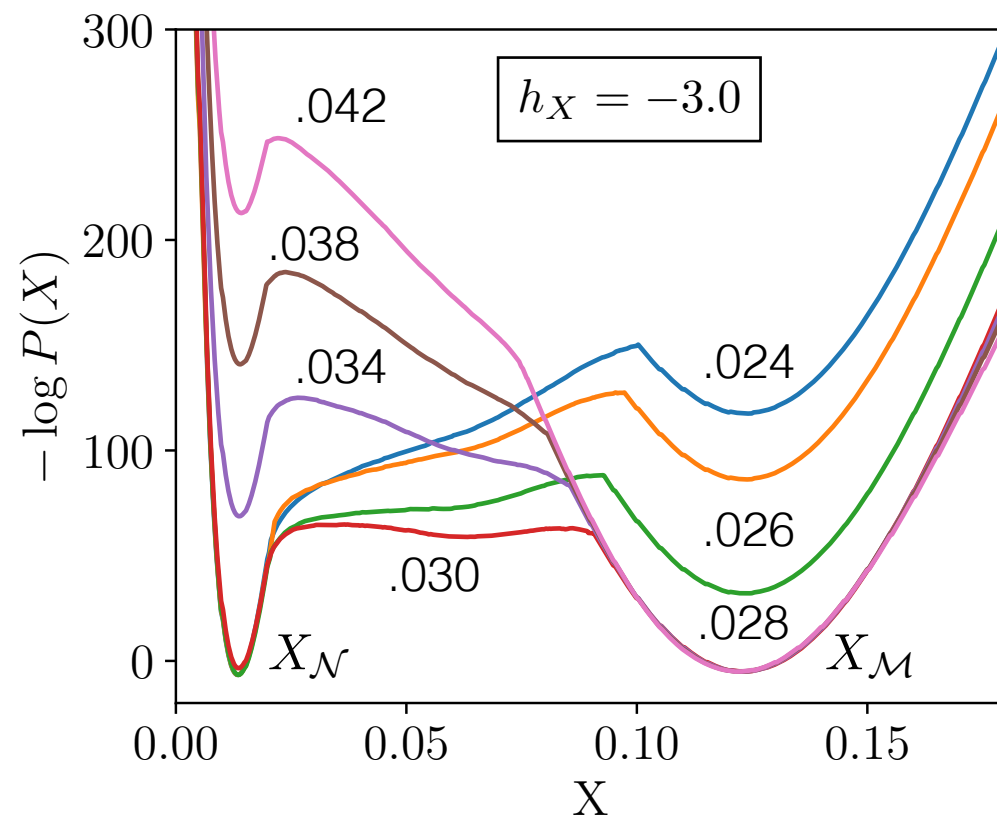
- N particles with Lennard Jones interactions in 2d **plus** non-affine field.
- constant $N, V(\text{shape}), T$, ensemble.
- cut-off at 2.5 times particle diameter, truncated and shifted, $T^* = 0.8, \rho = 2/\sqrt{3}$.
- Large energy barriers between $\mathcal{N}$ and $\mathcal{M}$ crystals.
- **Sequential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

First order transition

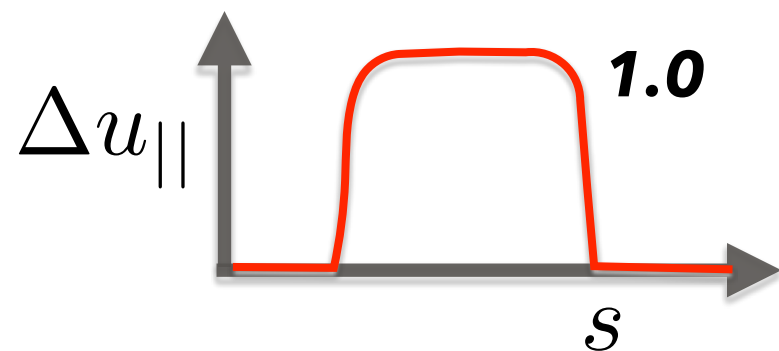
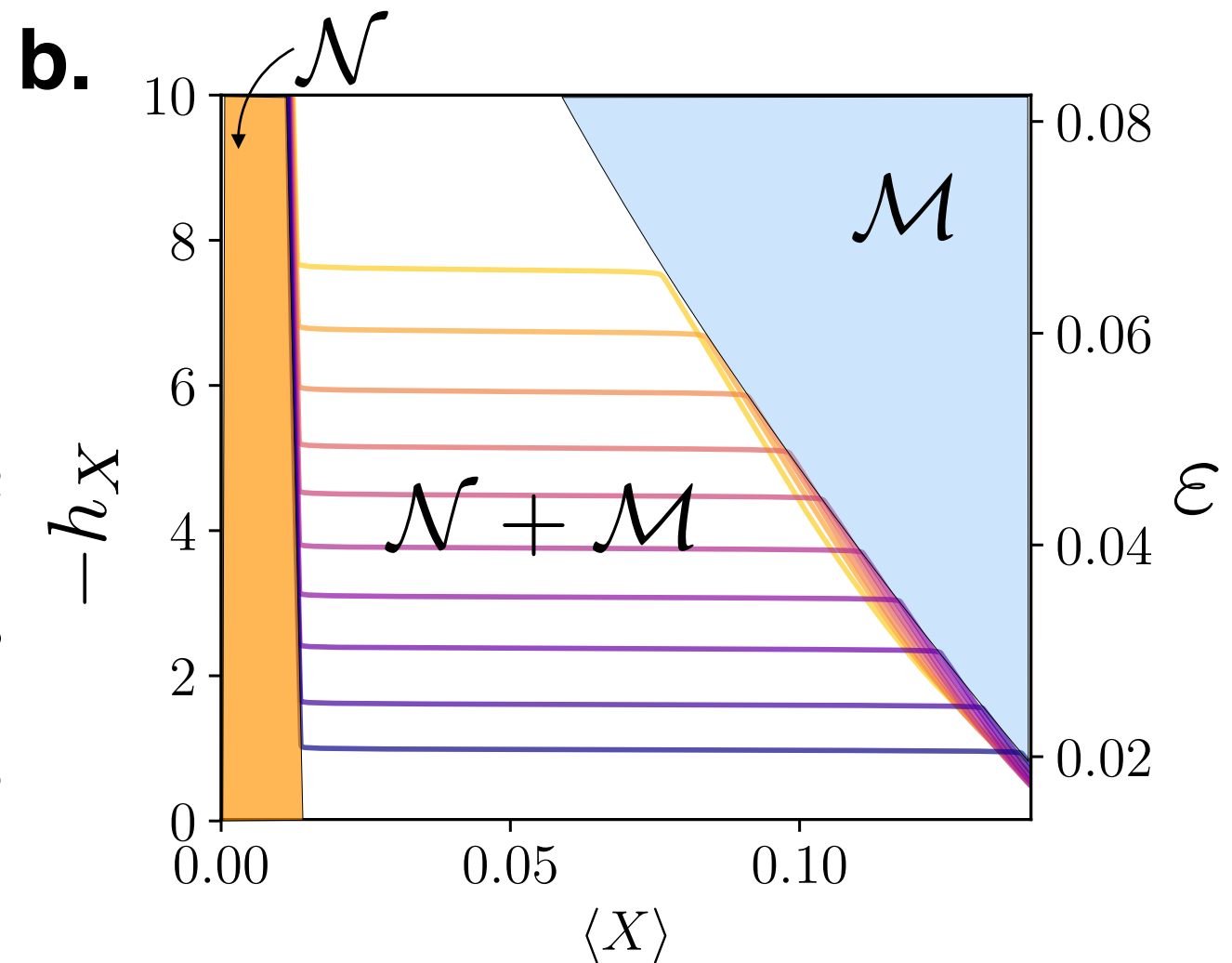
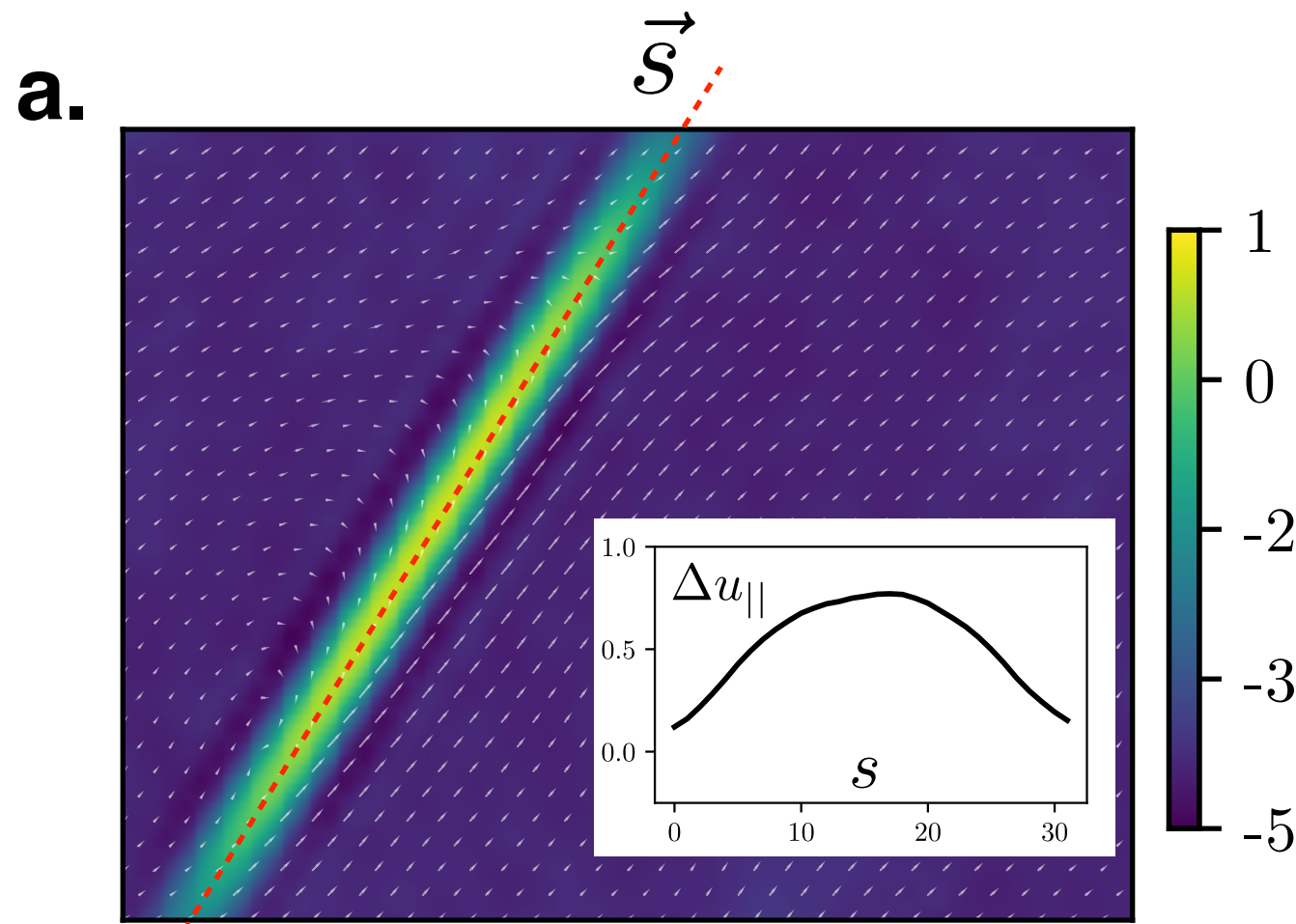
a.



b.

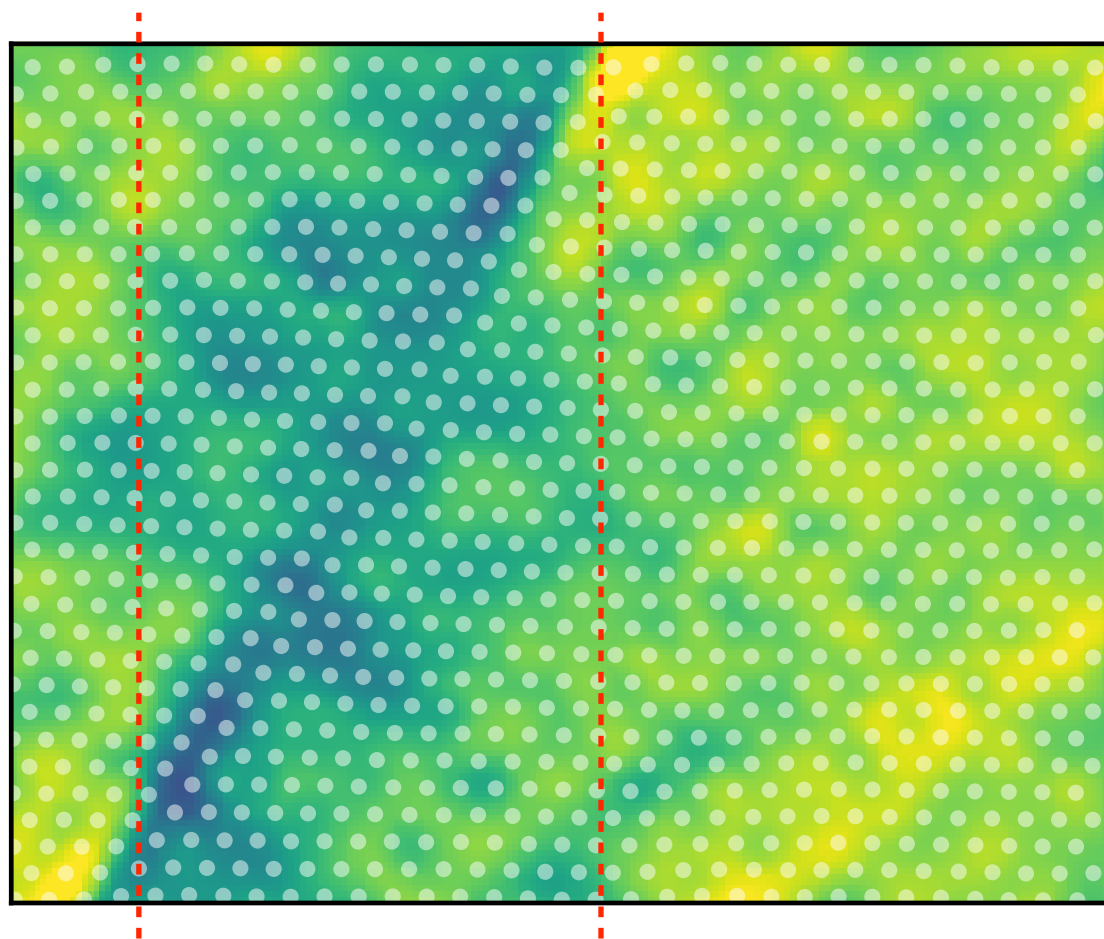


Slip bands, equation of state and phase diagram

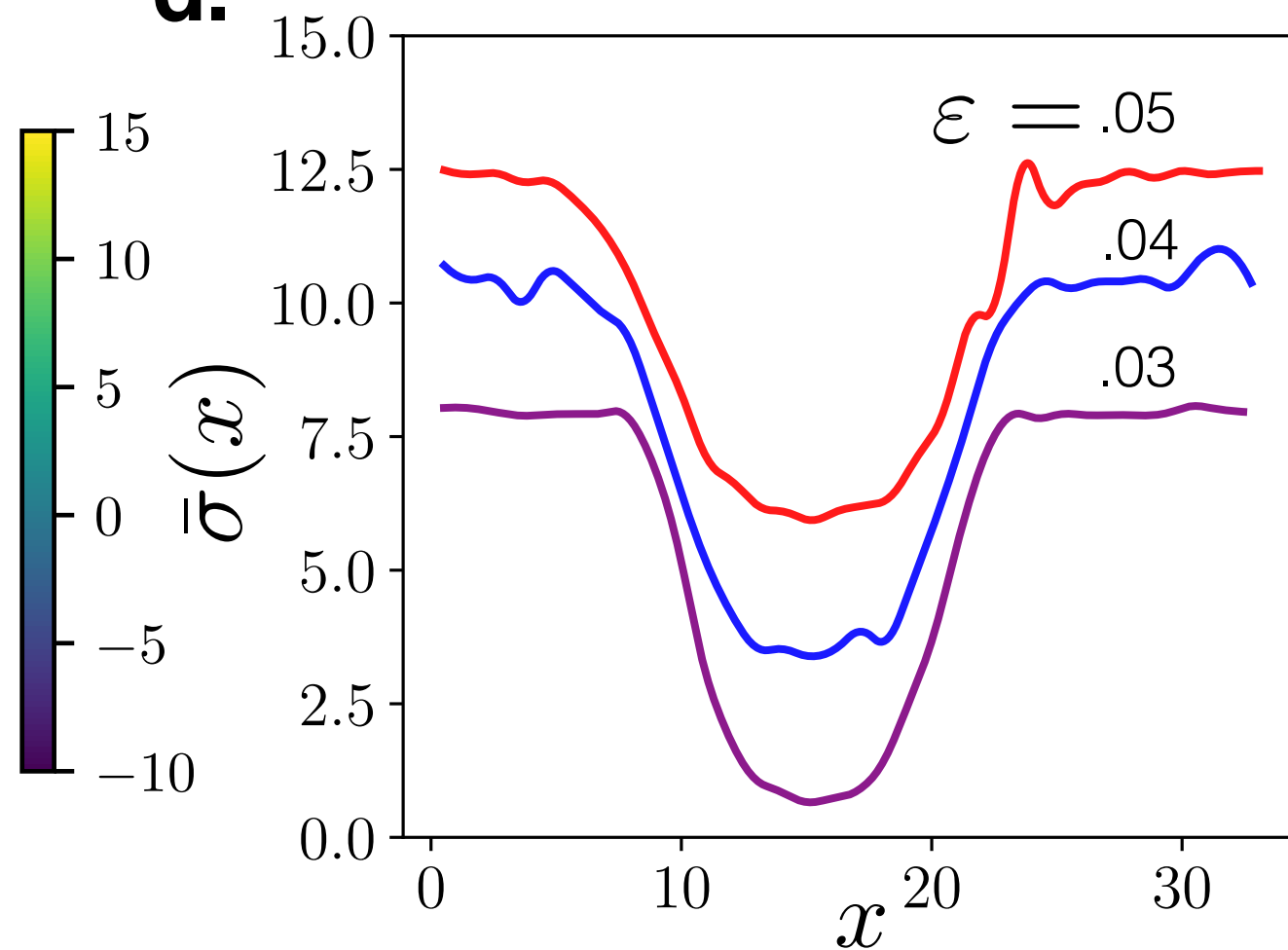


Stress interface

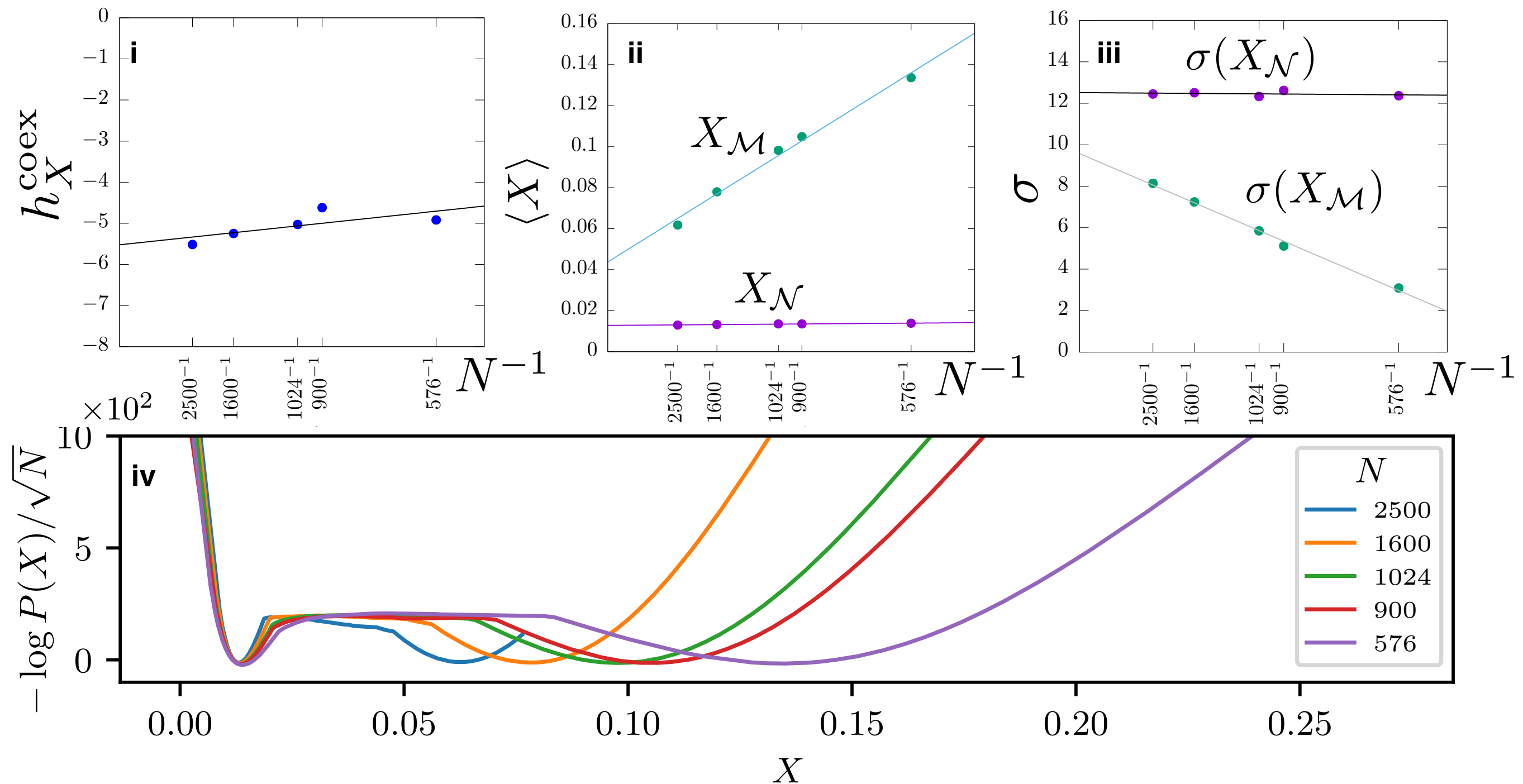
c.



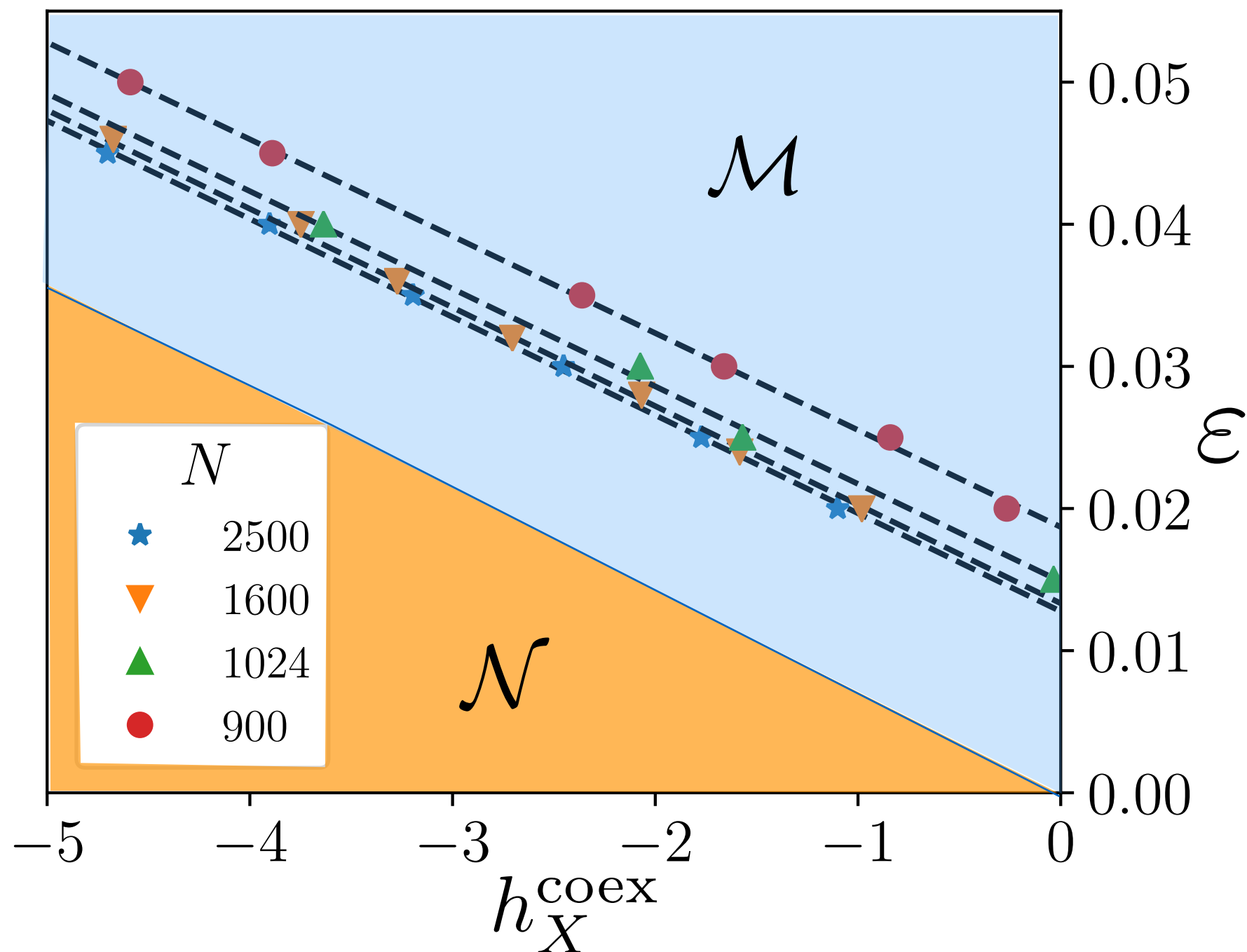
d.



Finite size scaling



The phase diagram



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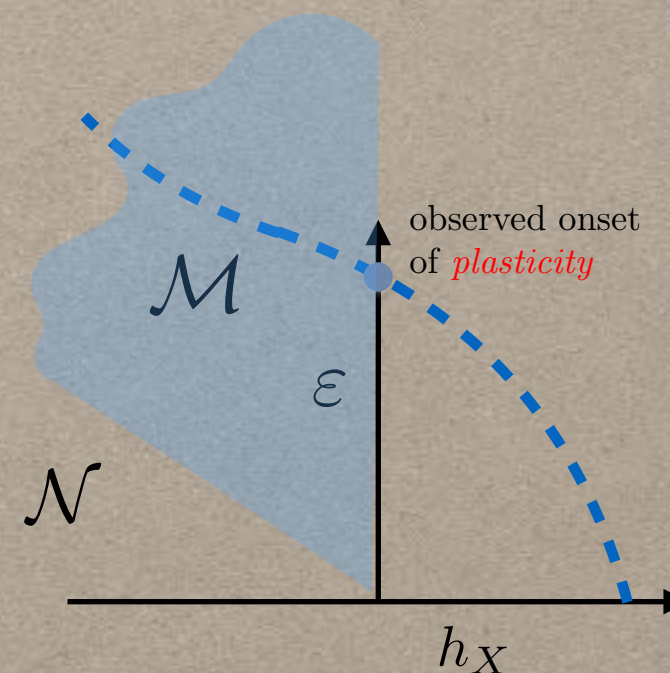
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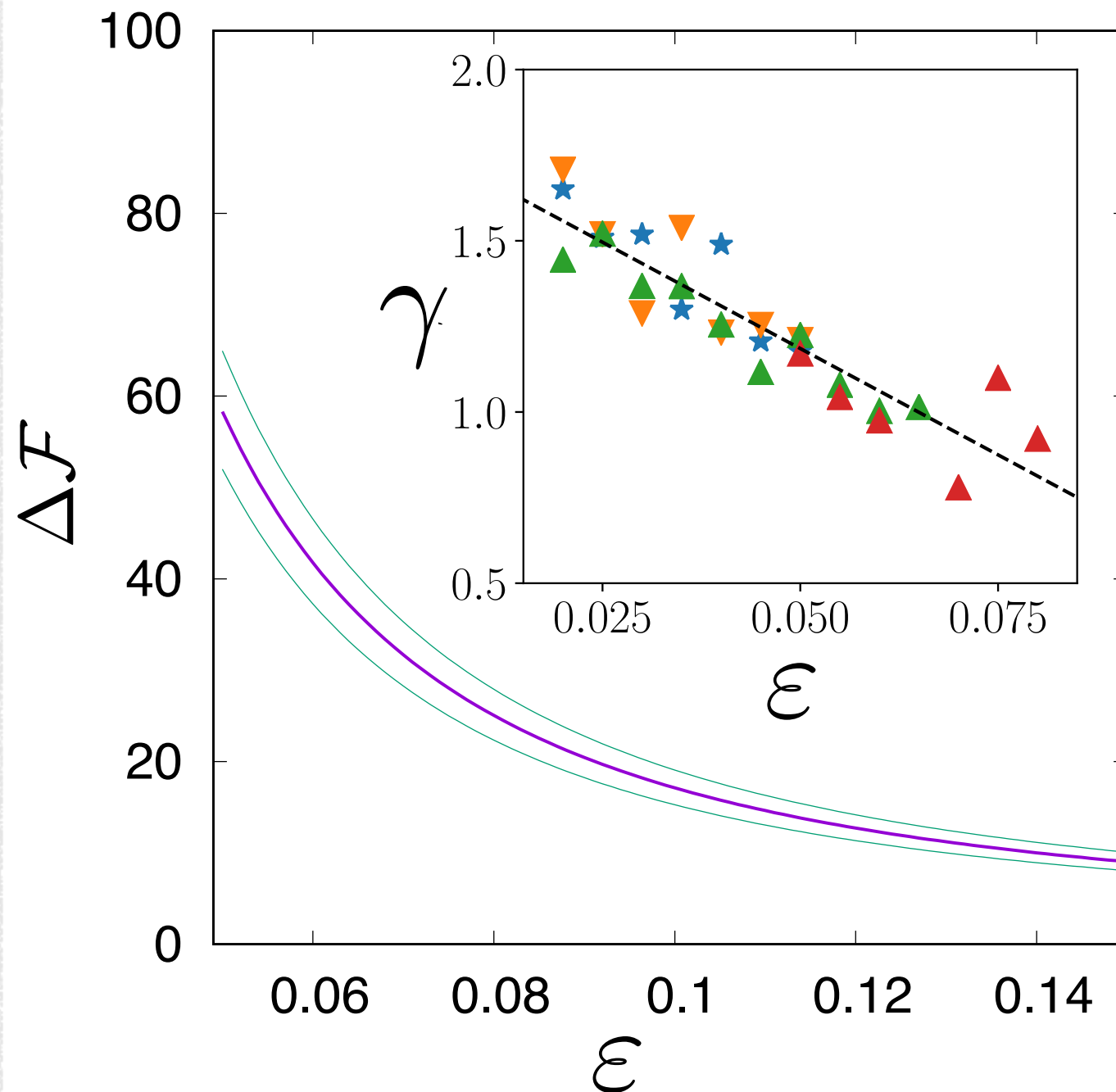
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- The rigid crystal is metastable for all values of stress for $h_X = 0$.

THE **DYNAMICS** AT FINITE STRAIN RATE: "X" as a reaction coordinate



NUCLEATION BARRIERS AT $h_x=0$



$$\mathcal{F} = -\pi R^2 \Delta_b + 2\pi R\gamma$$

$$\Delta_b = \frac{1}{2}\sigma\varepsilon$$

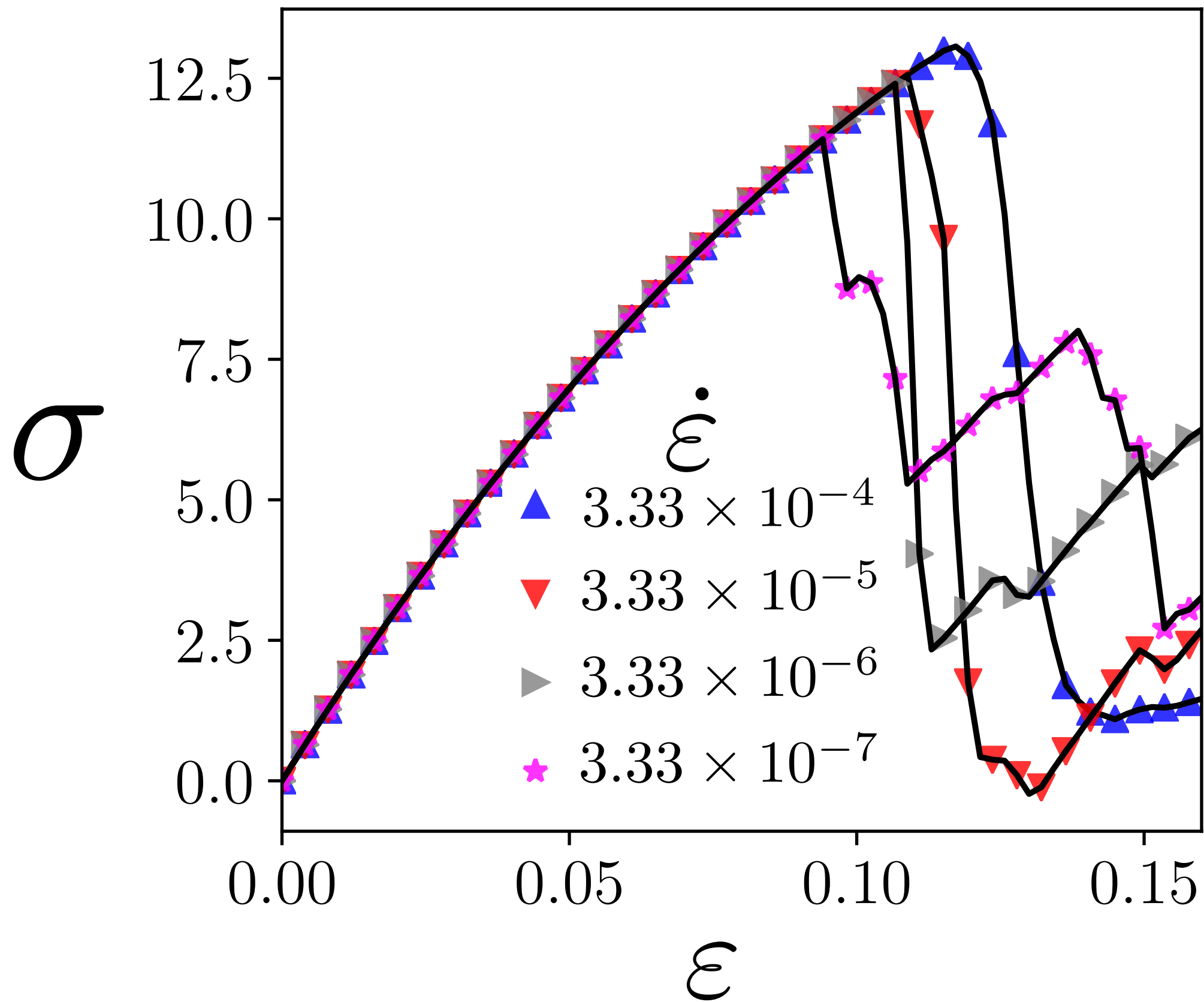
γ from finite size scaling of SUS

$$\Delta\mathcal{F} = \frac{\pi\gamma^2}{\Delta_b}$$

Critical barrier height

MD SIMULATIONS OF LJ SOLID

- $N = 128 \times 128 = 16384$ particles
- $a = 1.0, 0.2 < T < 1.2$
- MD time step $\delta t = 0.001, = .0001$ near yielding.
- Berendsen thermostat
- equilibration for $t = 1500$
- strain rate $\dot{\epsilon} = 3.33 \times 10^{-5}$ till yielding
- results averaged over 4 independent runs.
- fast GPU based in-house parallel code - checked against LAMMPS whenever possible.



SELF CONSISTENT CNT

Strain ramped up in time $\rightarrow$ barrier $\Delta\mathcal{F}(t)$ is *time-dependent*.

$\therefore$ demand self consistency $\tau_{FP} = \tau_0 \exp [\Delta\mathcal{F}(\tau_{FP})]$

multiply by $\dot{\epsilon}$ and use, $\dot{\epsilon} \tau_{FP} = \epsilon^*$

take logarithm $\Delta\mathcal{F}(\epsilon^*) = \log(\epsilon^*) - \log(\dot{\epsilon}\tau_0)$

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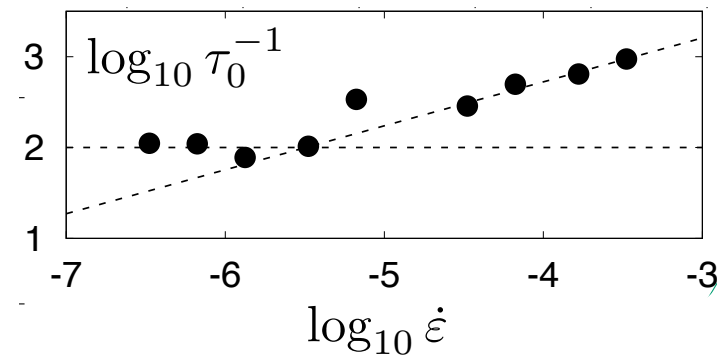
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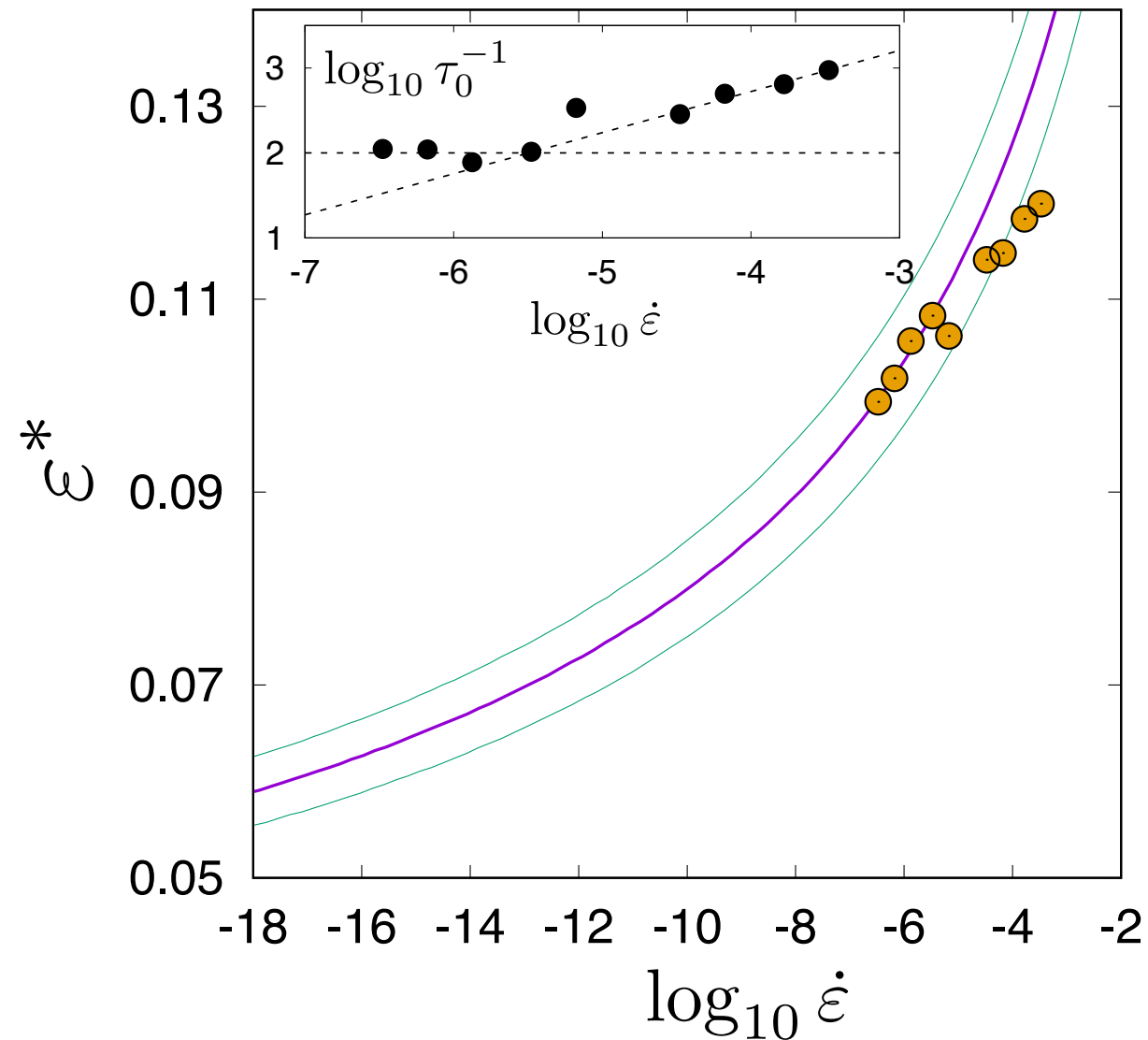
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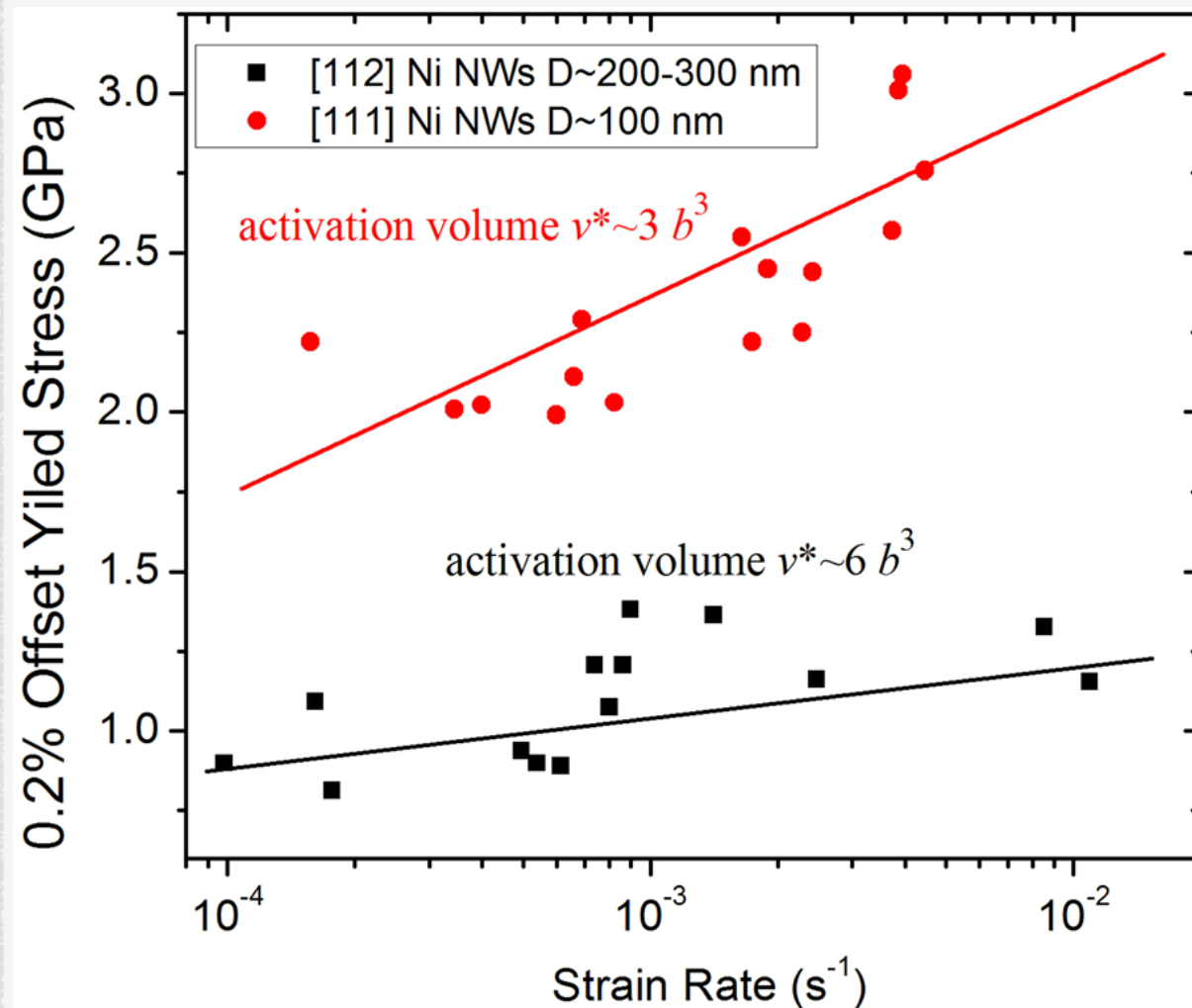
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STRAIN RATE SENSITIVITY

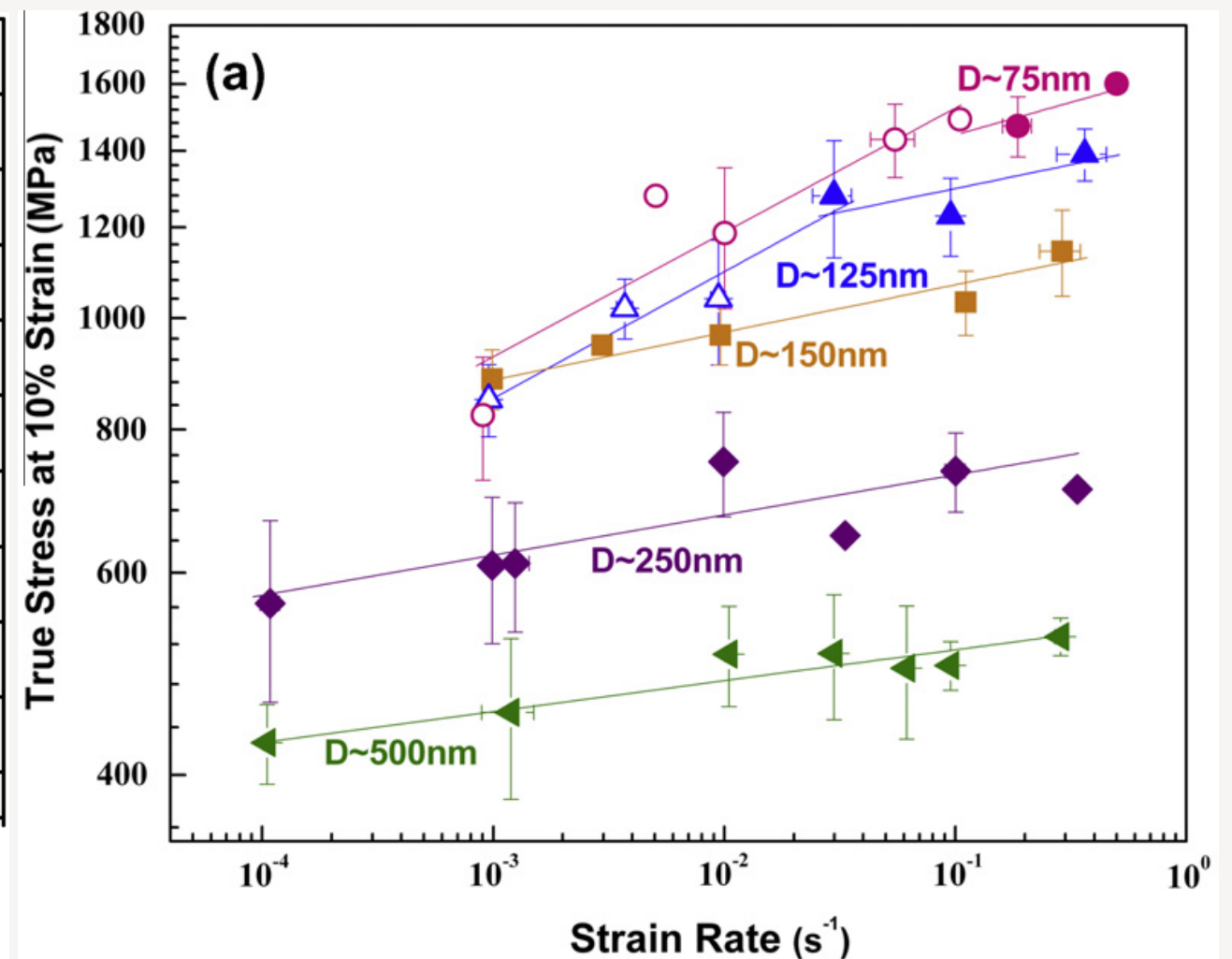
Ni nano-wires



Peng et al. *Appl. Phys. Lett.* **102**, 083102 (2013)

$$\sigma = \sigma_0 \dot{\epsilon}^m$$

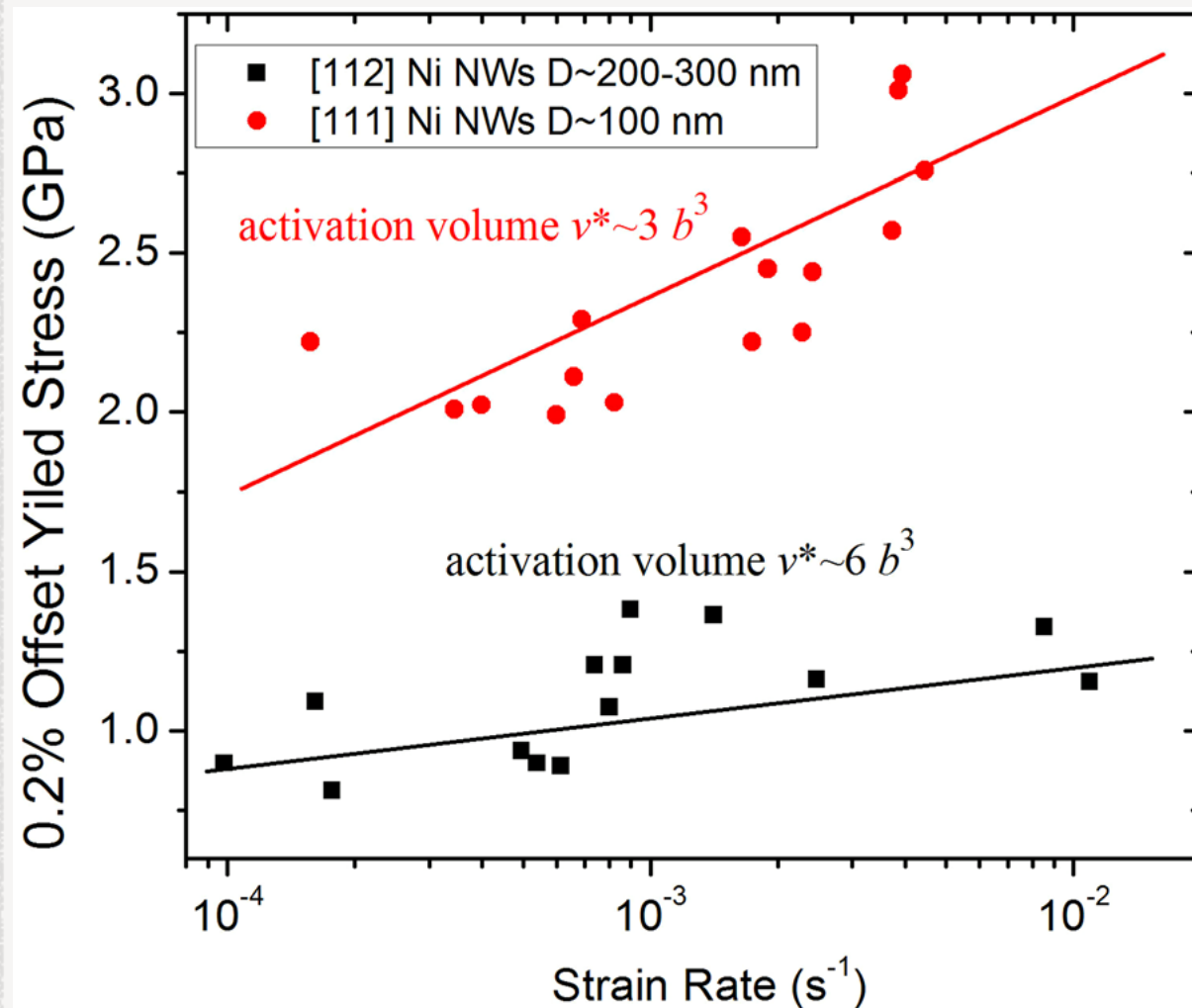
Cu nano-pillars



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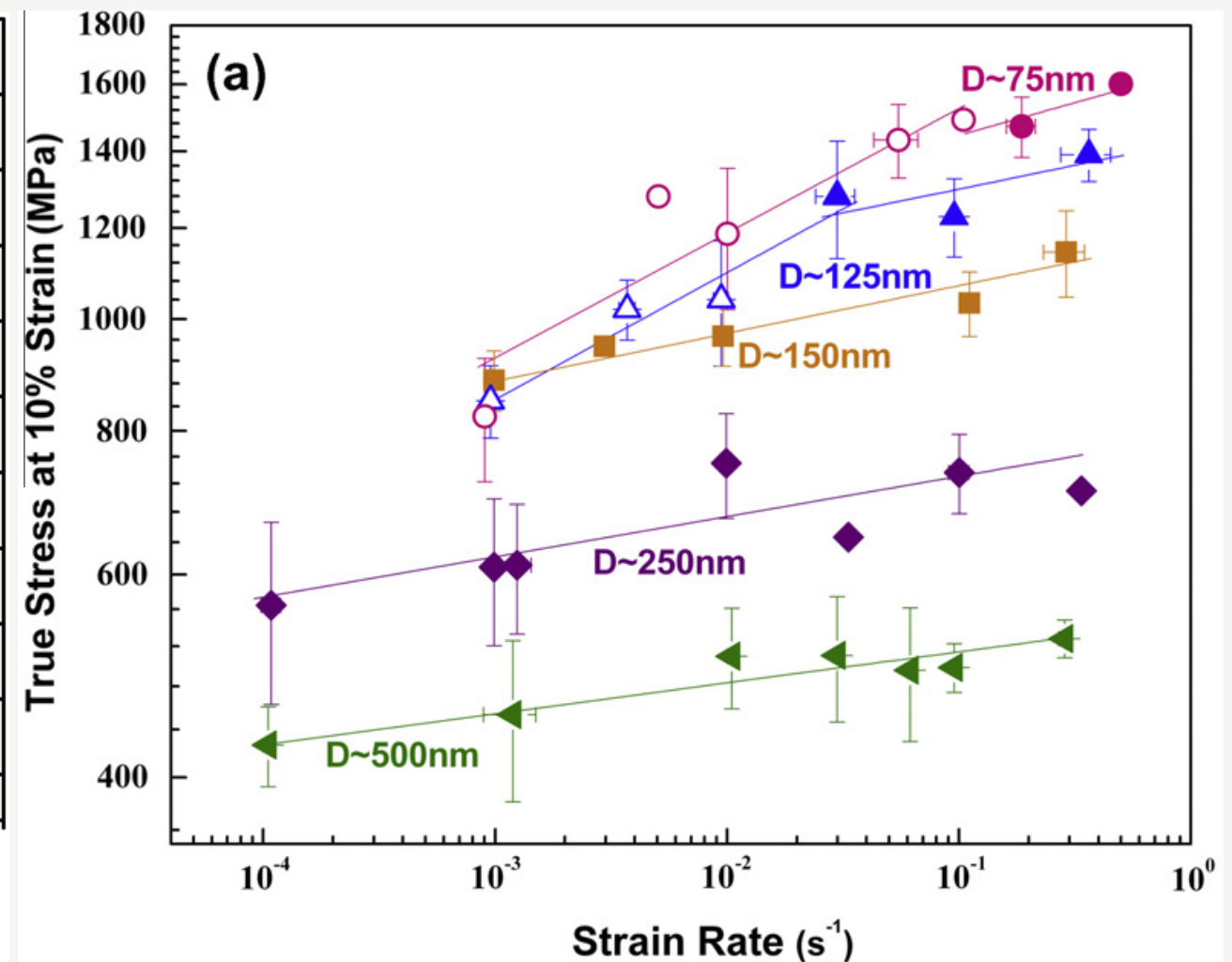
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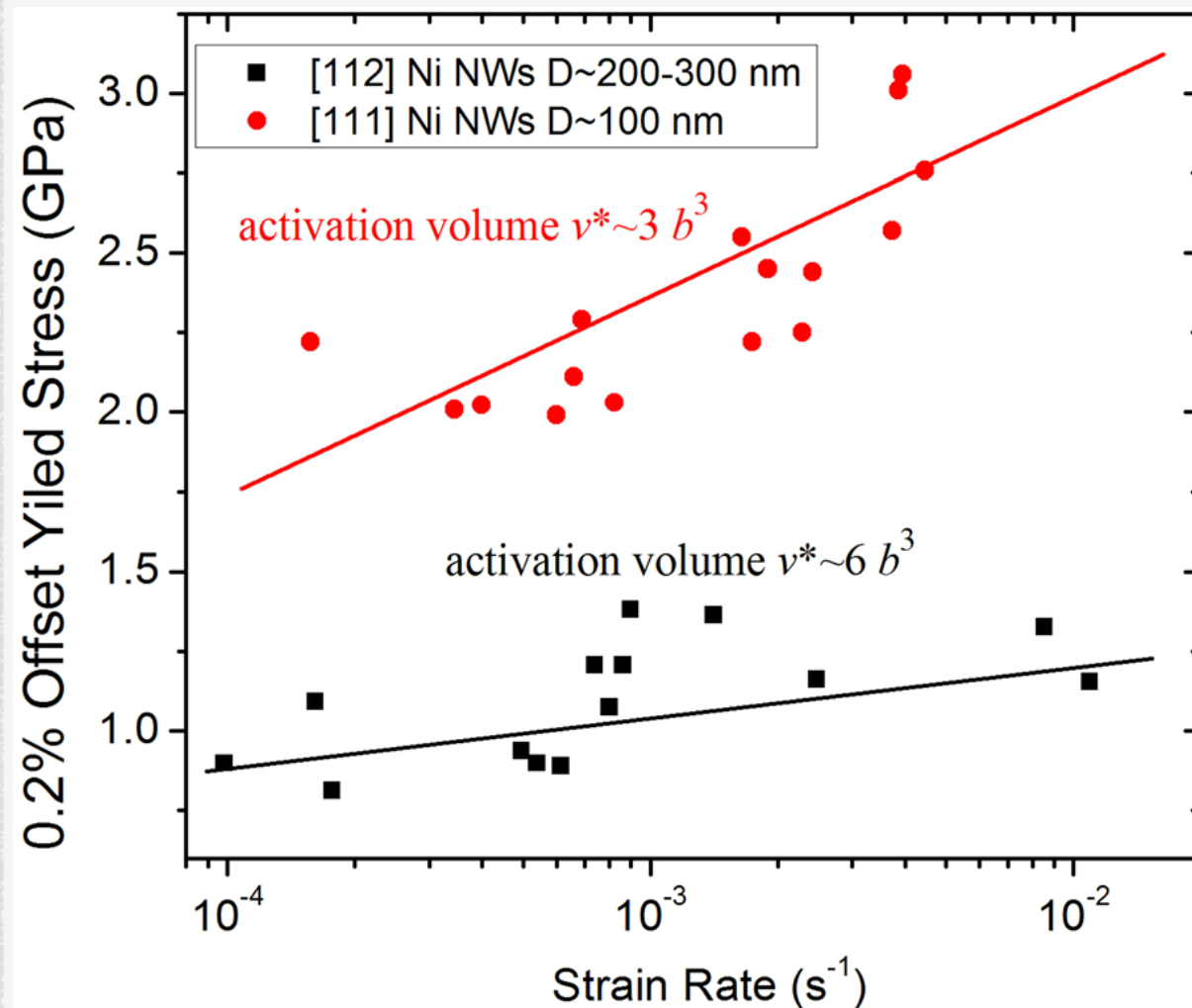
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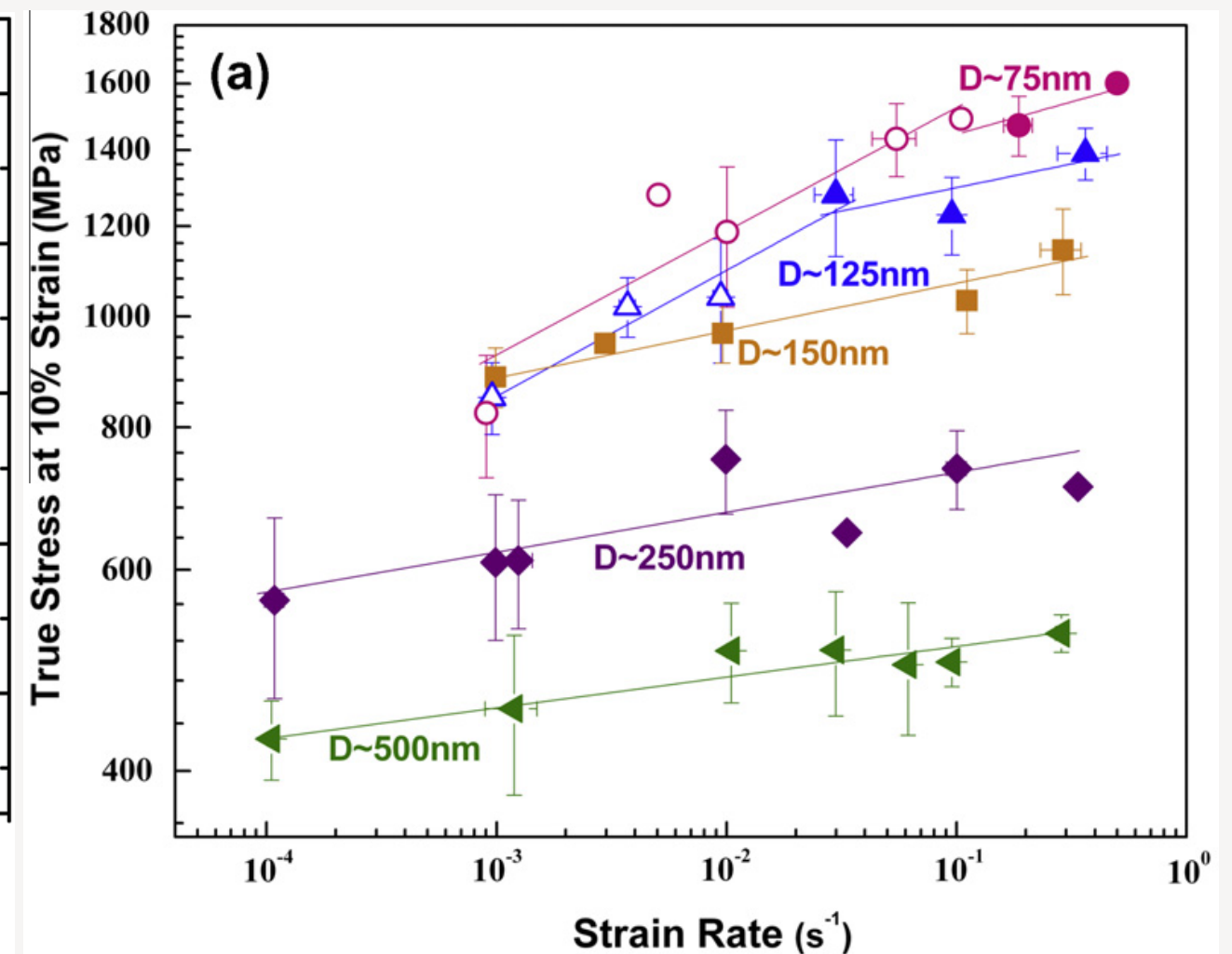
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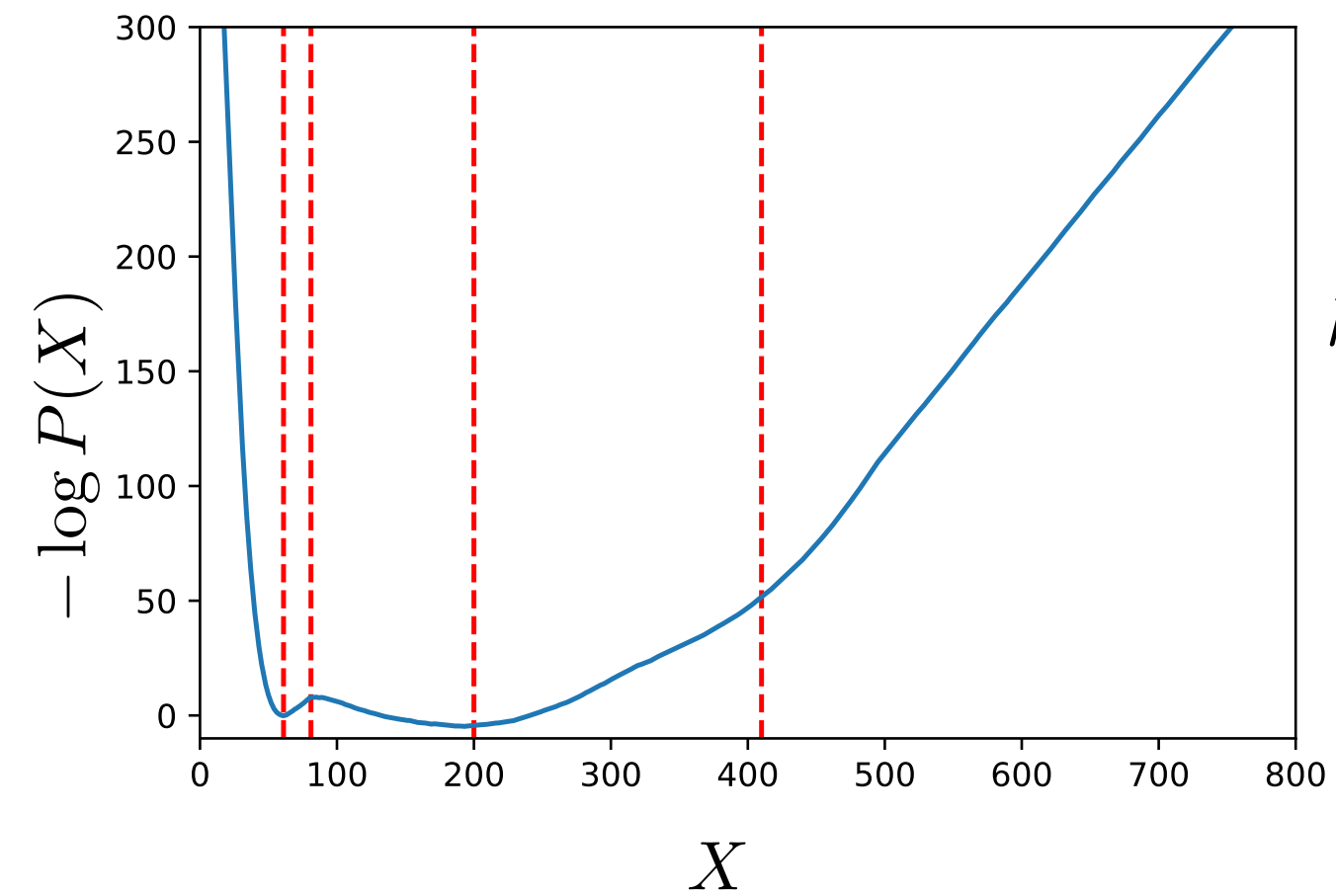
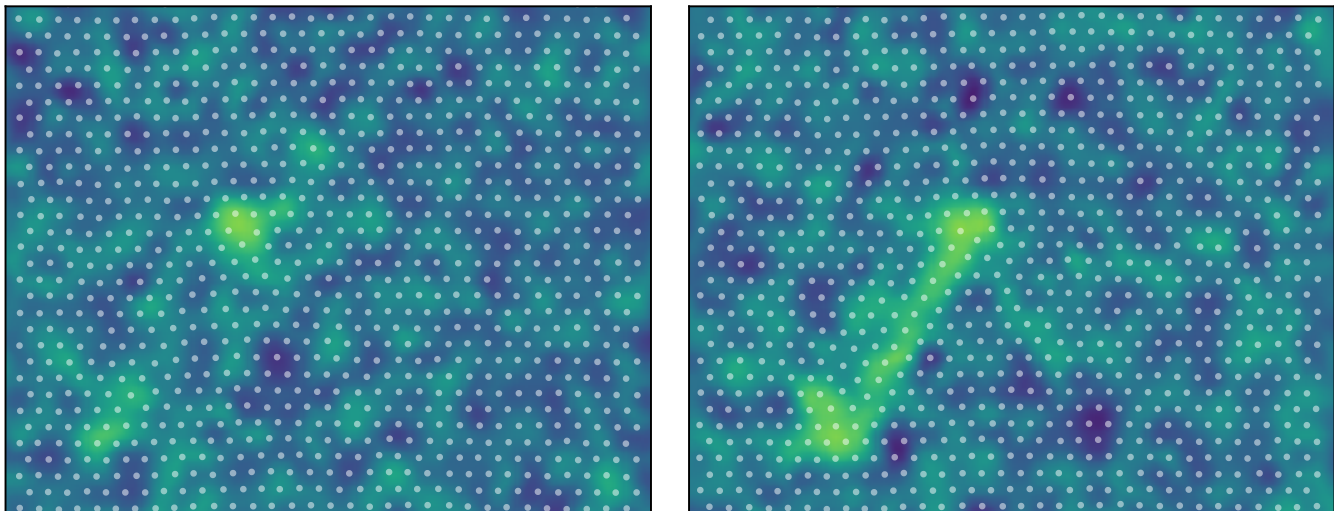
$$\sigma = f(\log \dot{\epsilon}); \lim_{x \rightarrow -\infty} f(x) = 0$$

EXPLICIT “TAKE AWAYS”

- There exists a *hidden* first order transition between a rigid and a stress free crystal. All solids flow because a rigid solid is *always* in a metastable phase, which decays over time depending on the amount of deformation.
- Both equilibrium and non equilibrium aspects of this transition may be understood using a *new collective variable* X to distinguish affine and non-affine displacements.
- *Quantitative* prediction of rate dependent initiation of plasticity for the first time. Properties of dislocations *not needed* to discuss *onset of* plasticity of ideal crystals. Dislocations appear *only at coexistence* and only at the *stress interface*.
- New “picture” for deformation. Unifying *plasticity* with *first-order phase transitions*. To understand plasticity, concentrate on the *equilibrium transition*.
- May serve as a language for *plasticity* in solids where dislocations cannot be defined (*glasses?*).

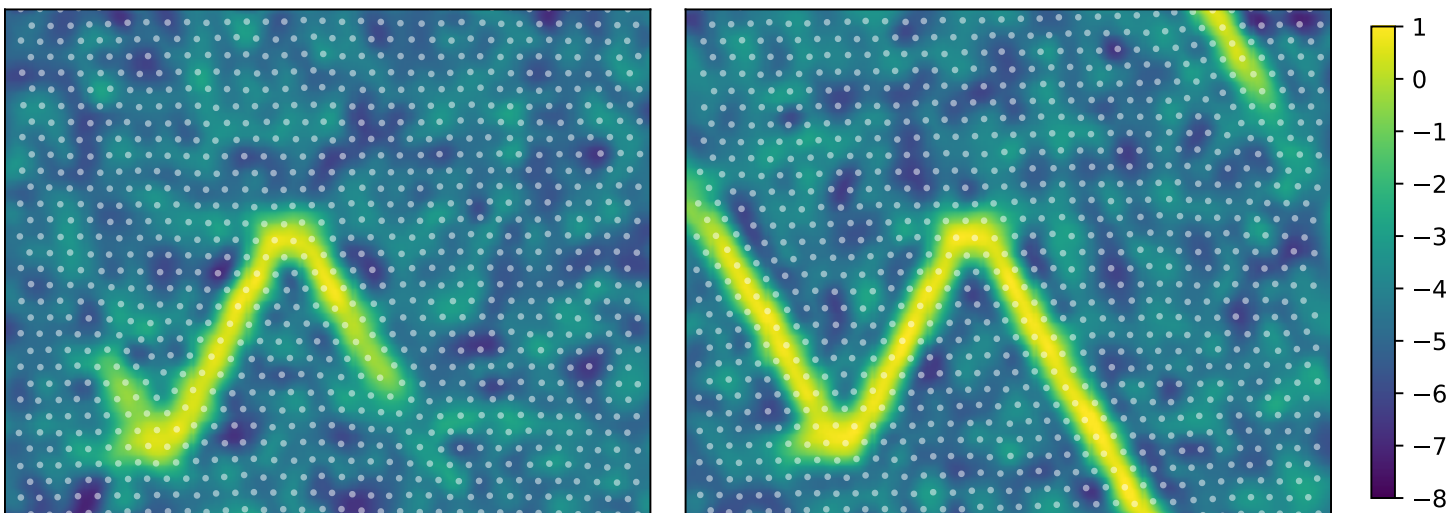
FROM CRYSTAL TO GLASS:

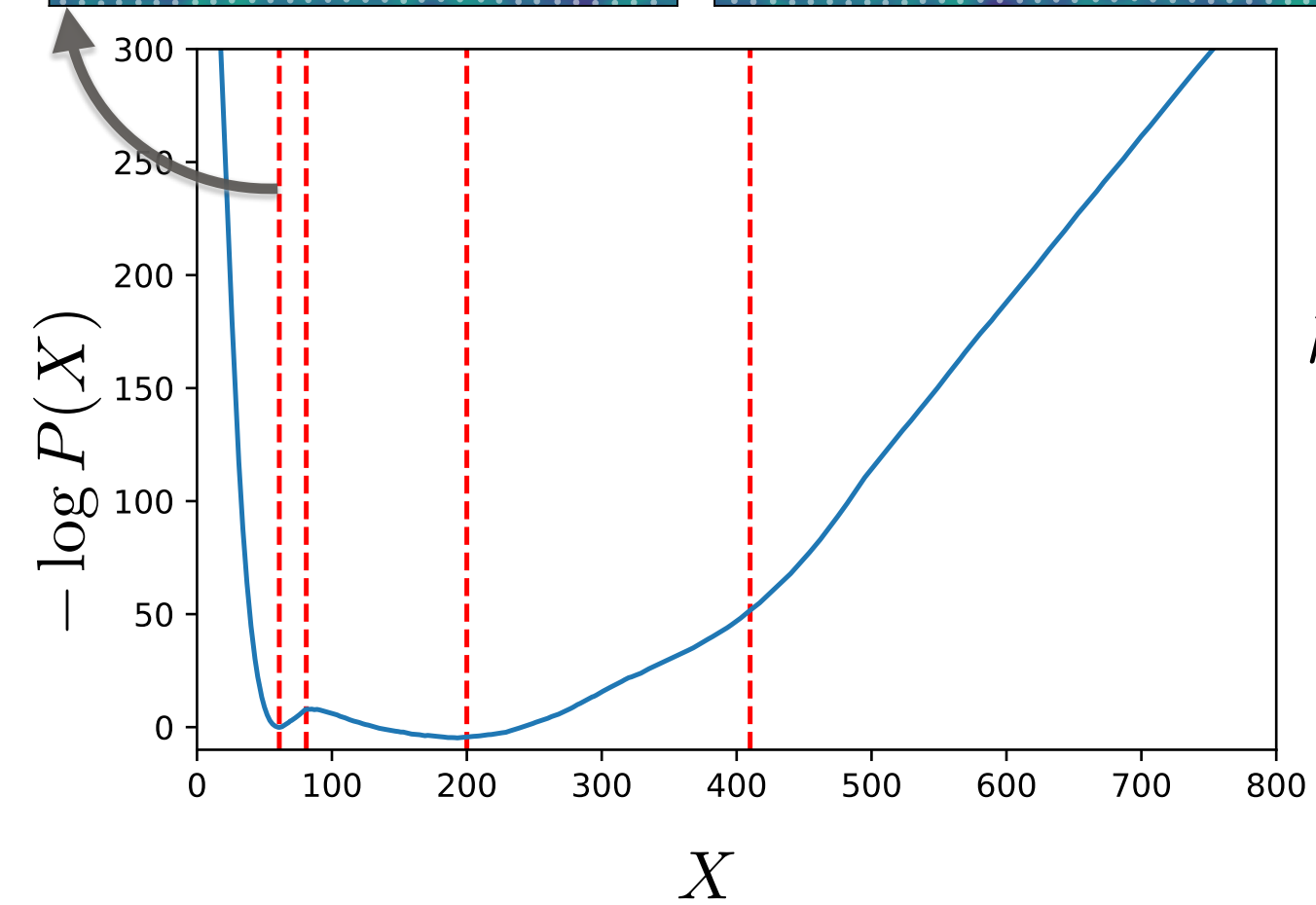
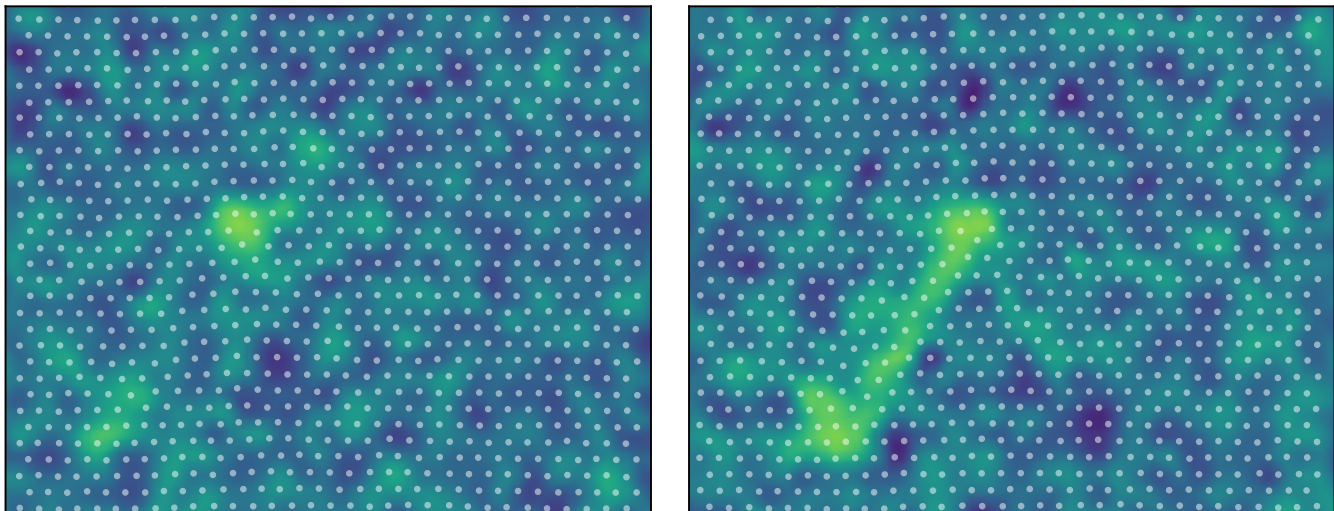
EFFECT OF A SINGLE FROZEN-IN DISLOCATION PAIR



$$h_X = -5, \varepsilon = .02$$

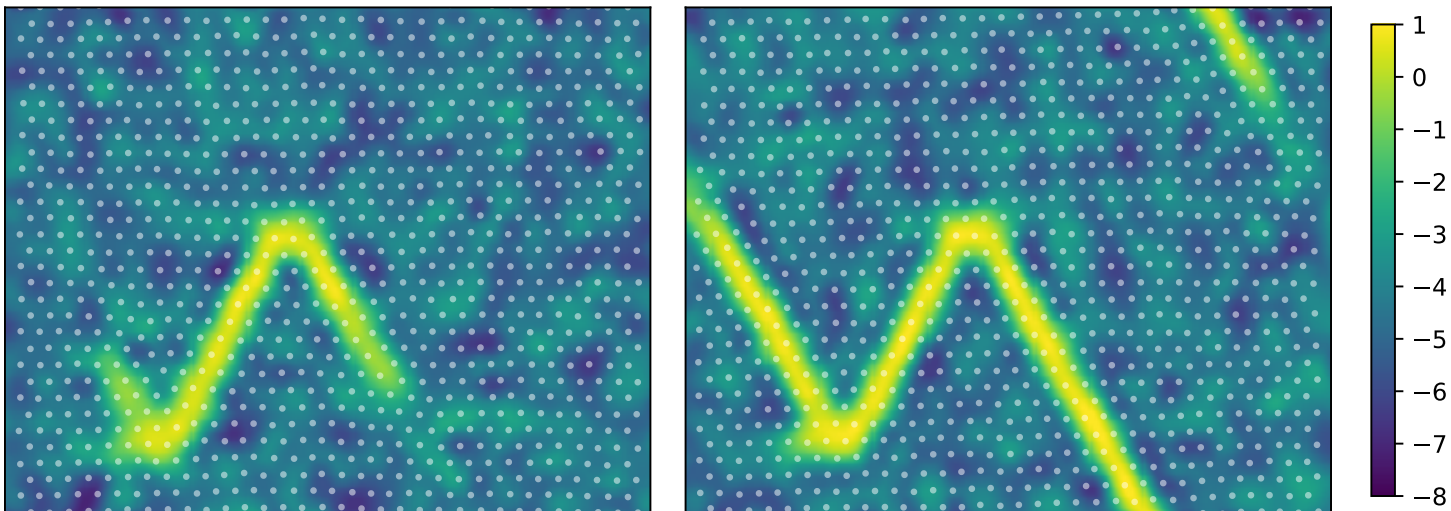
$$N = 1024$$

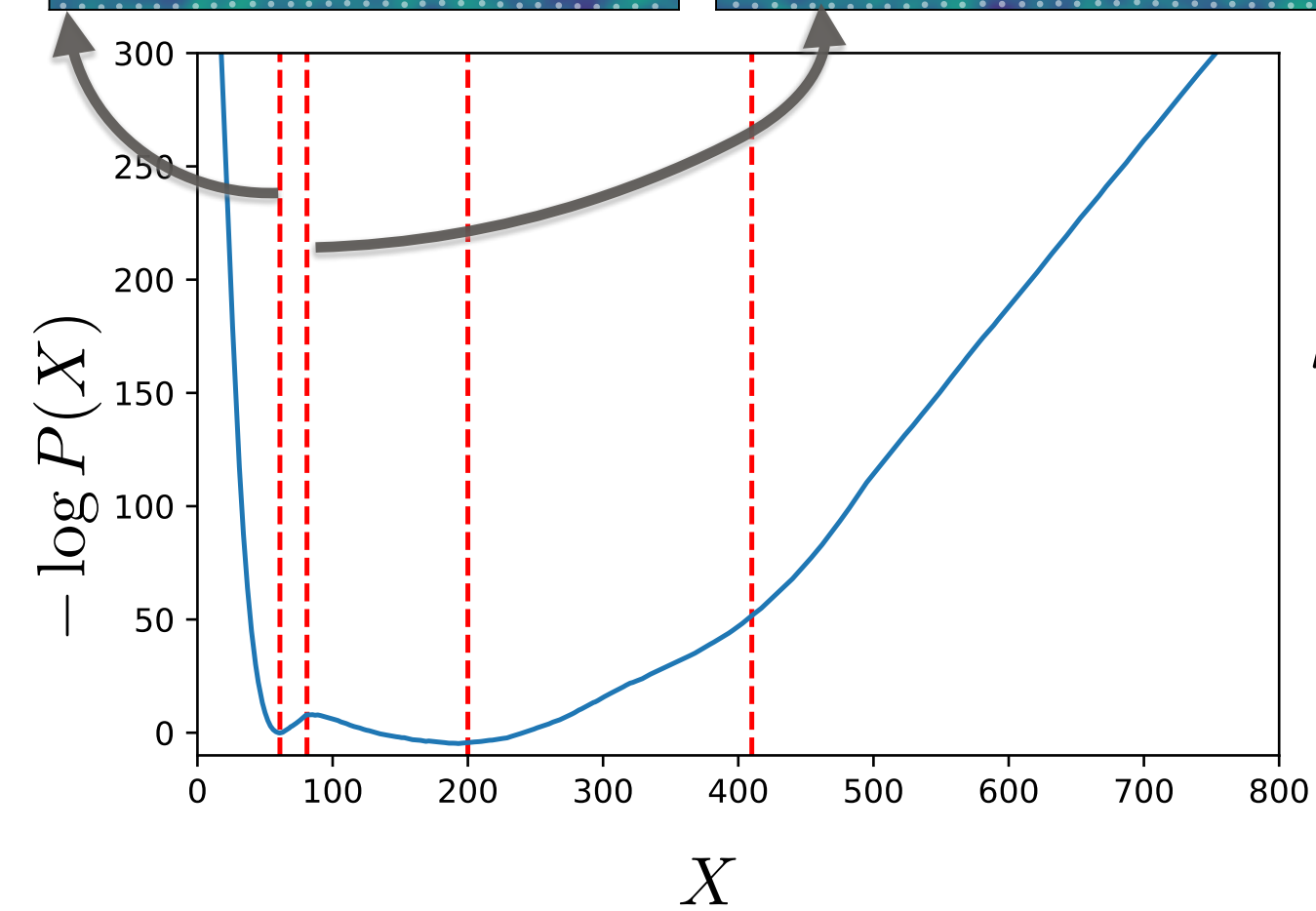
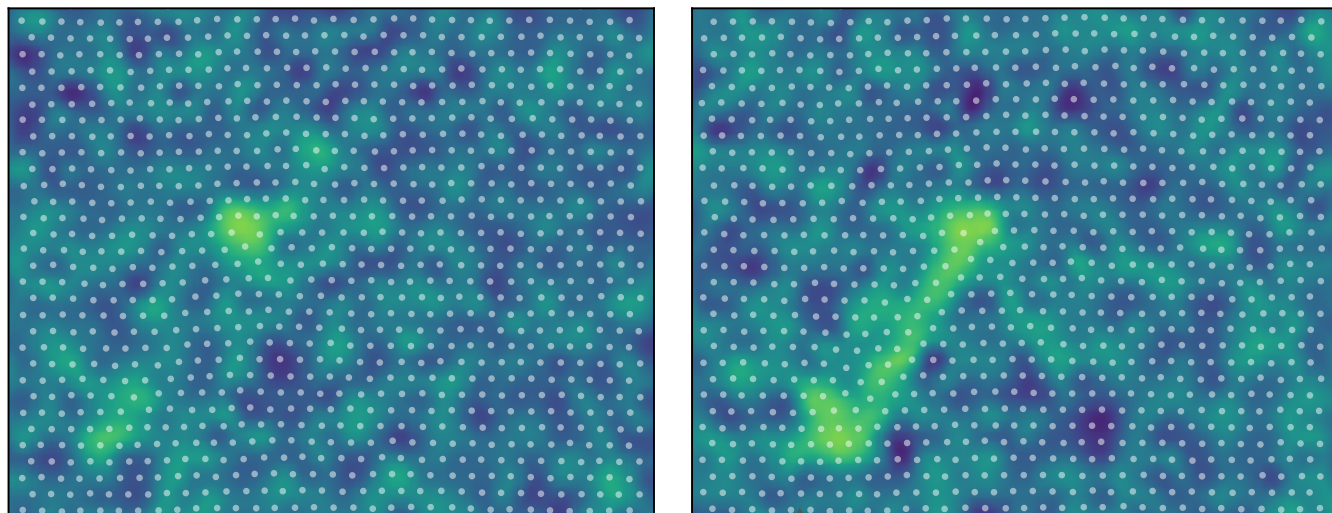




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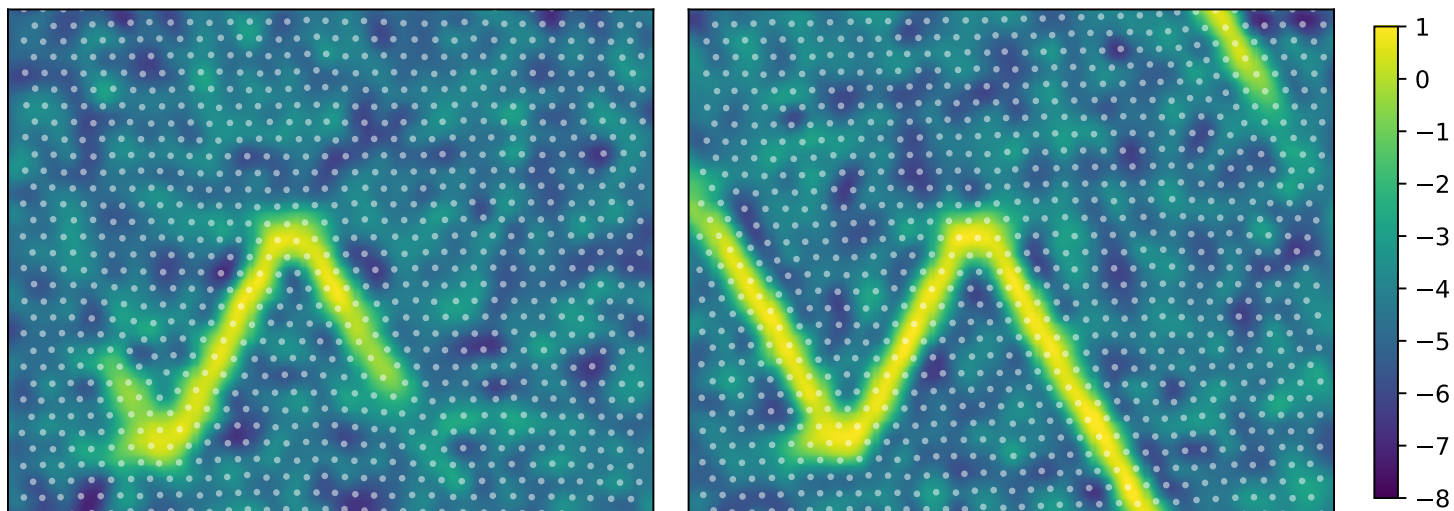
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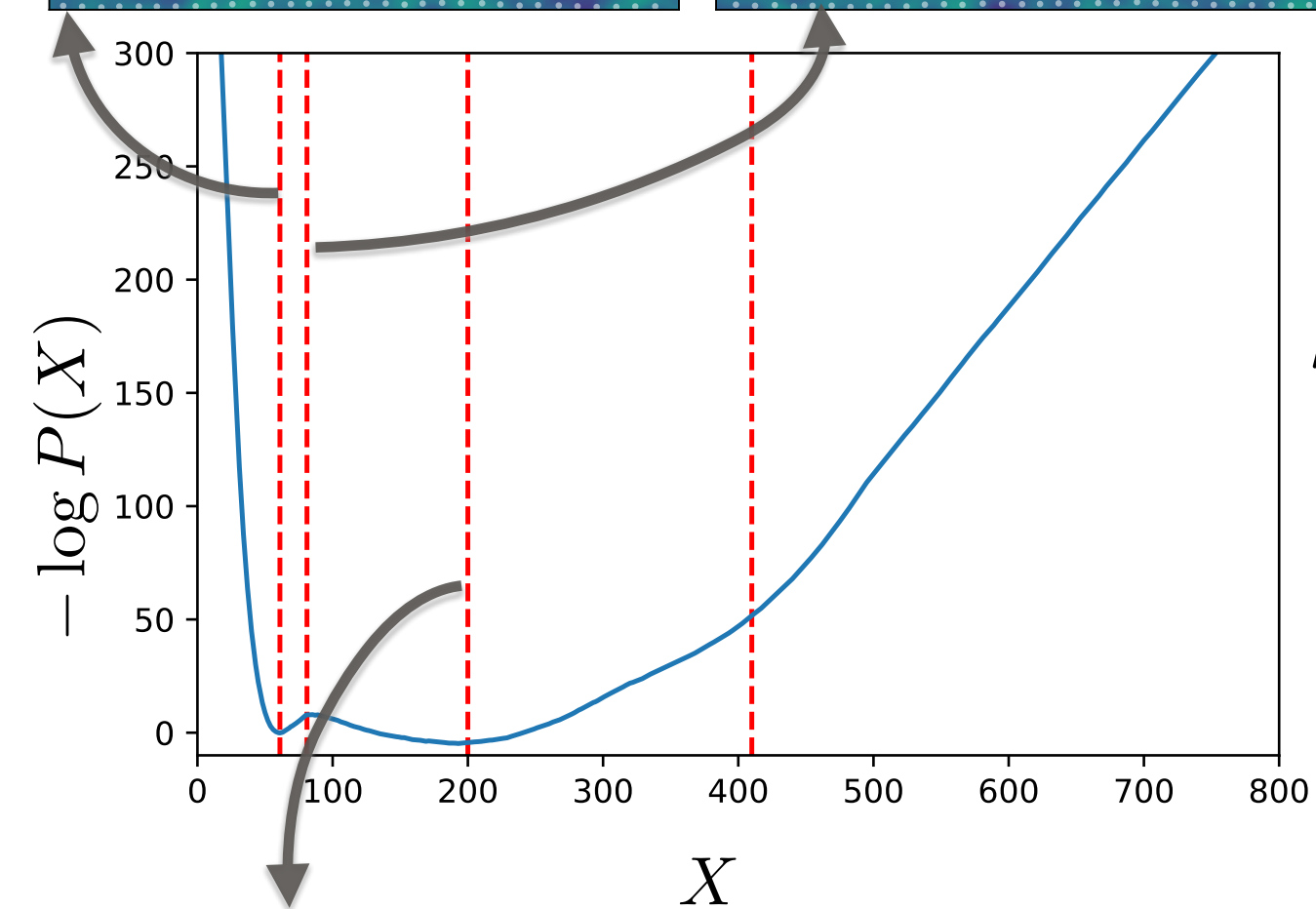
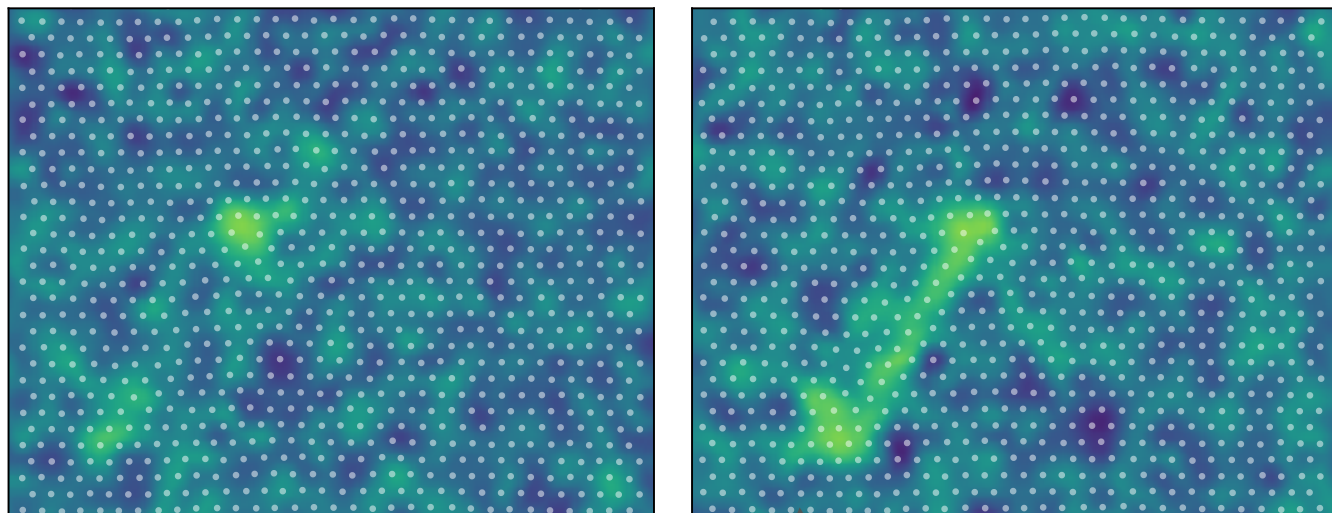




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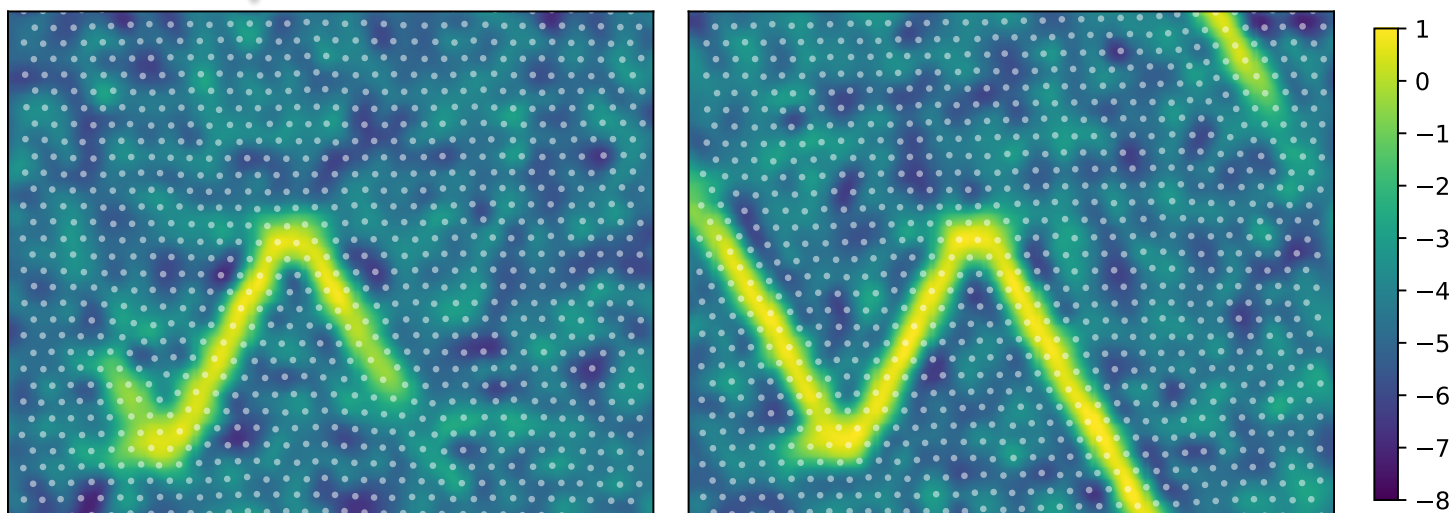
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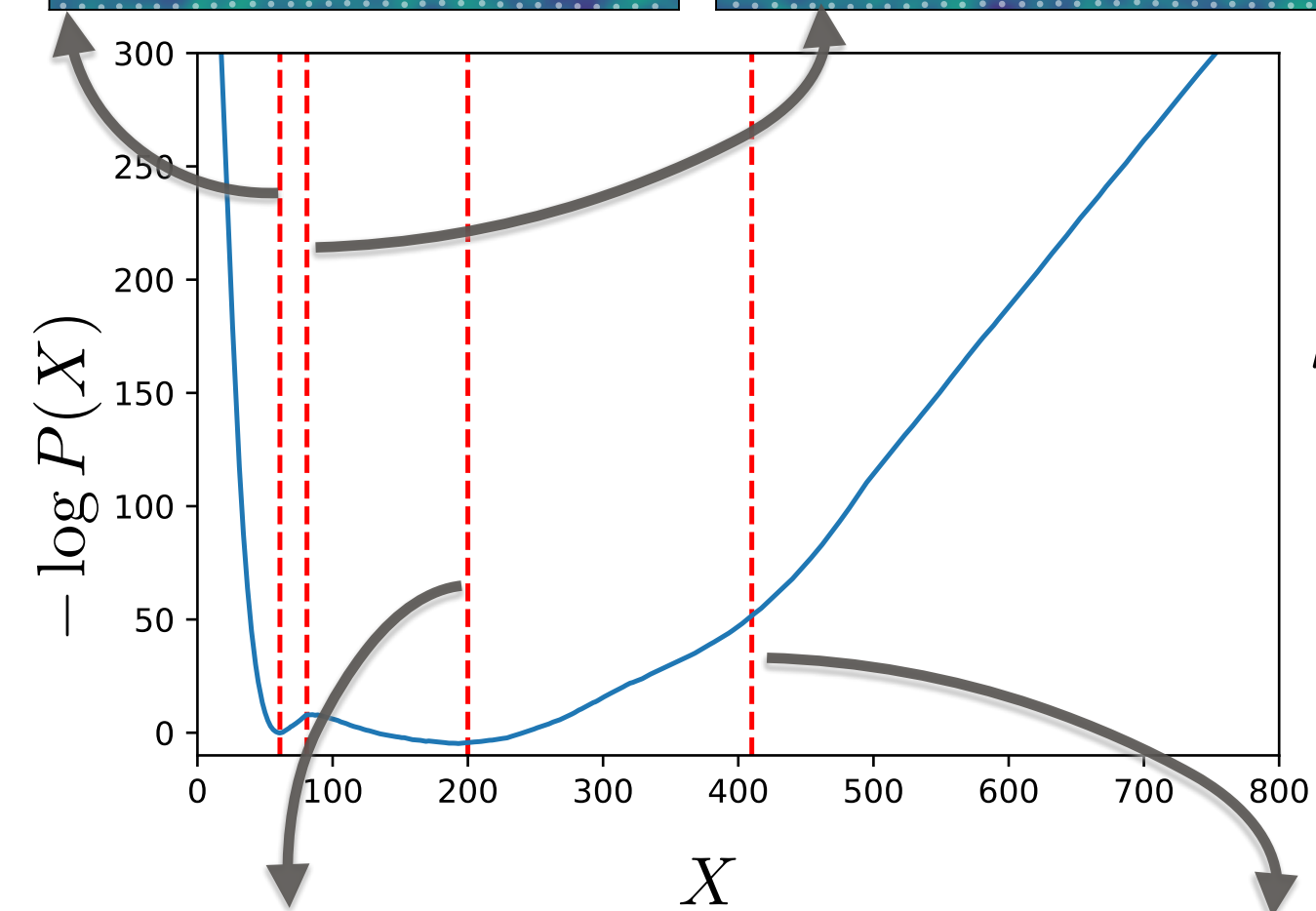
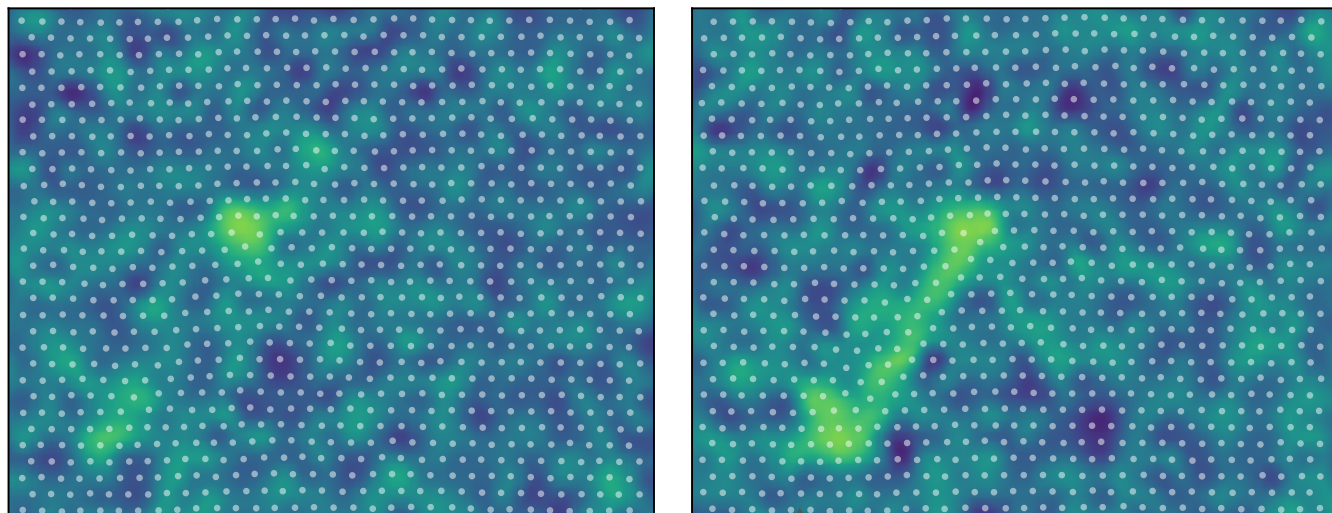




$$h_X = -5, \varepsilon = .02$$

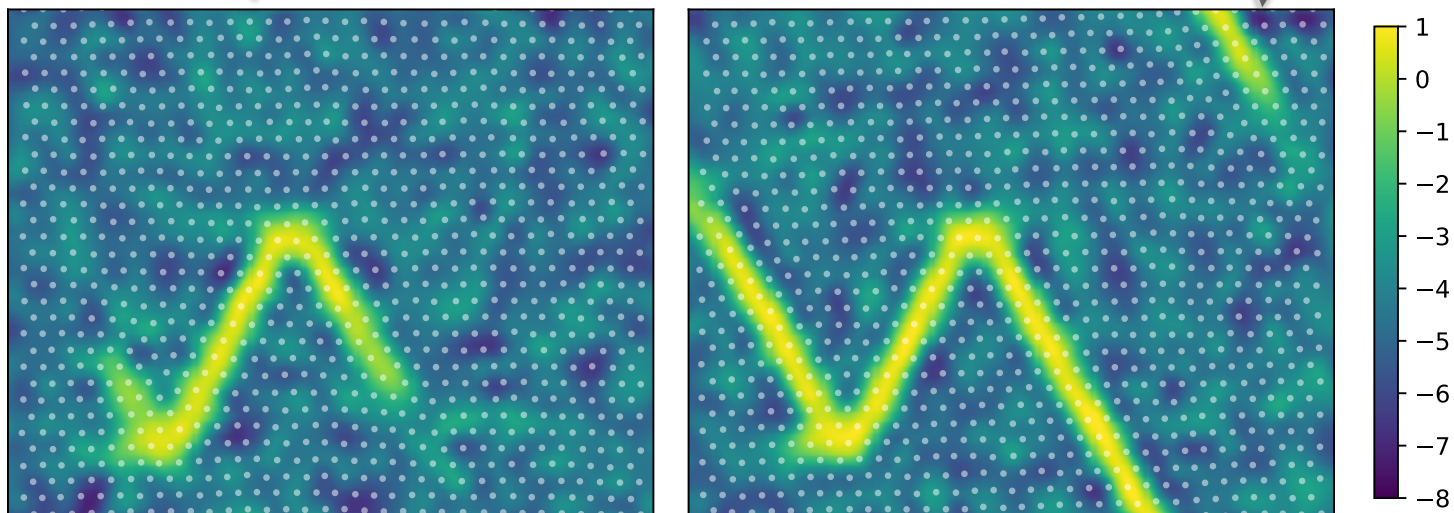
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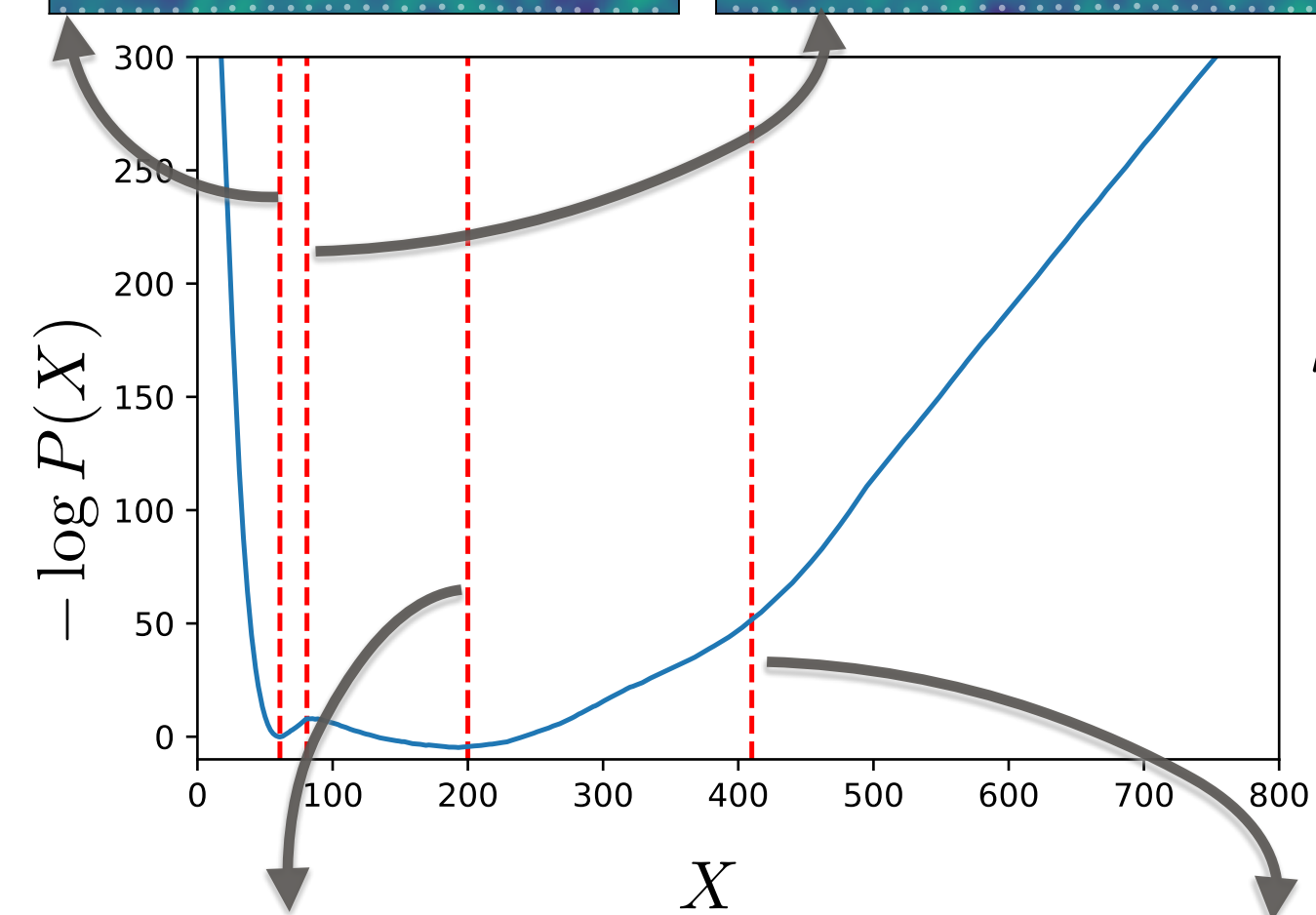
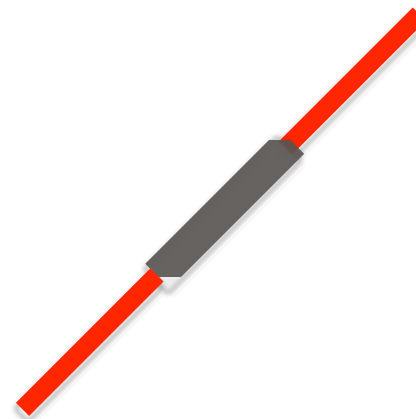
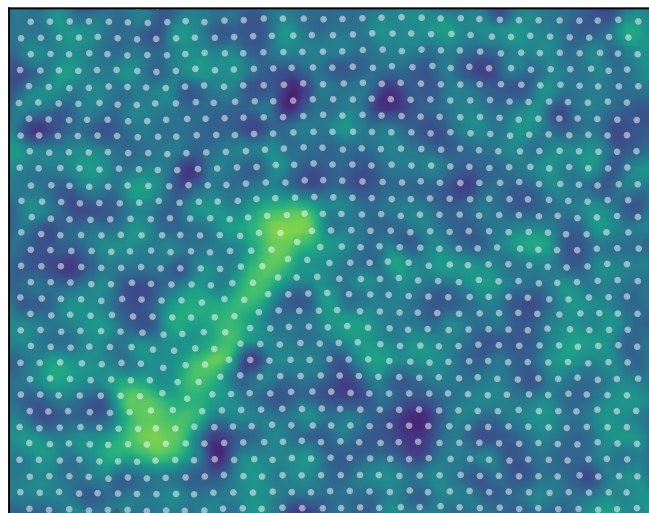
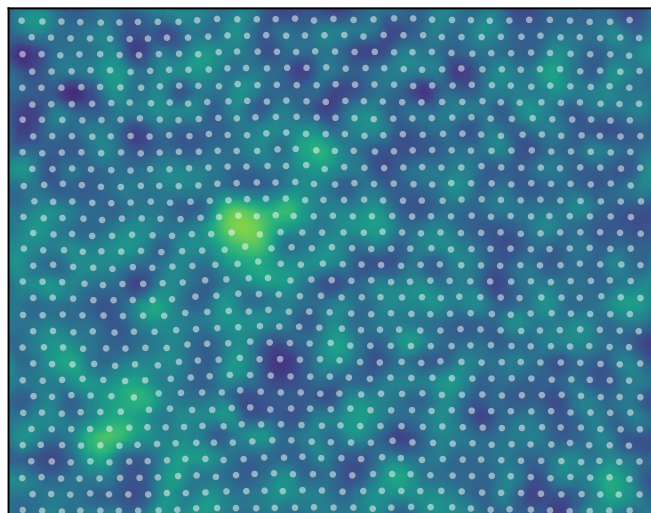




$$h_X = -5, \varepsilon = .02$$

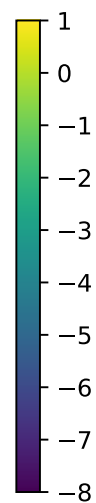
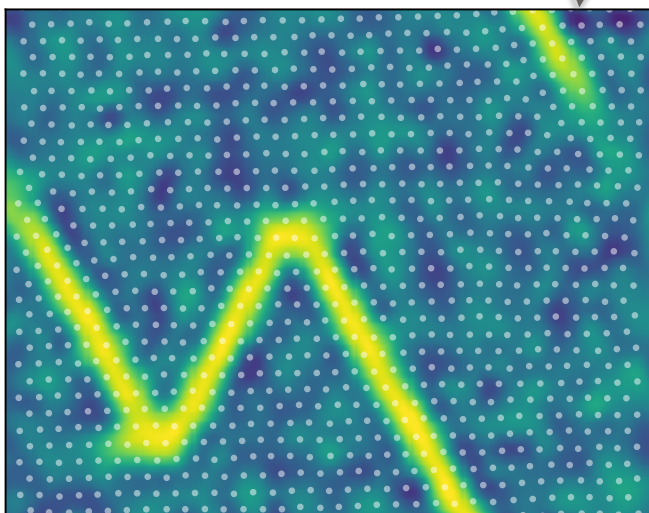
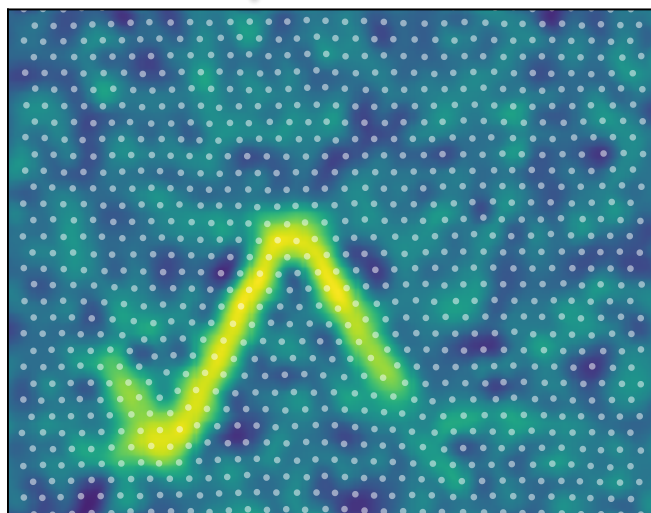
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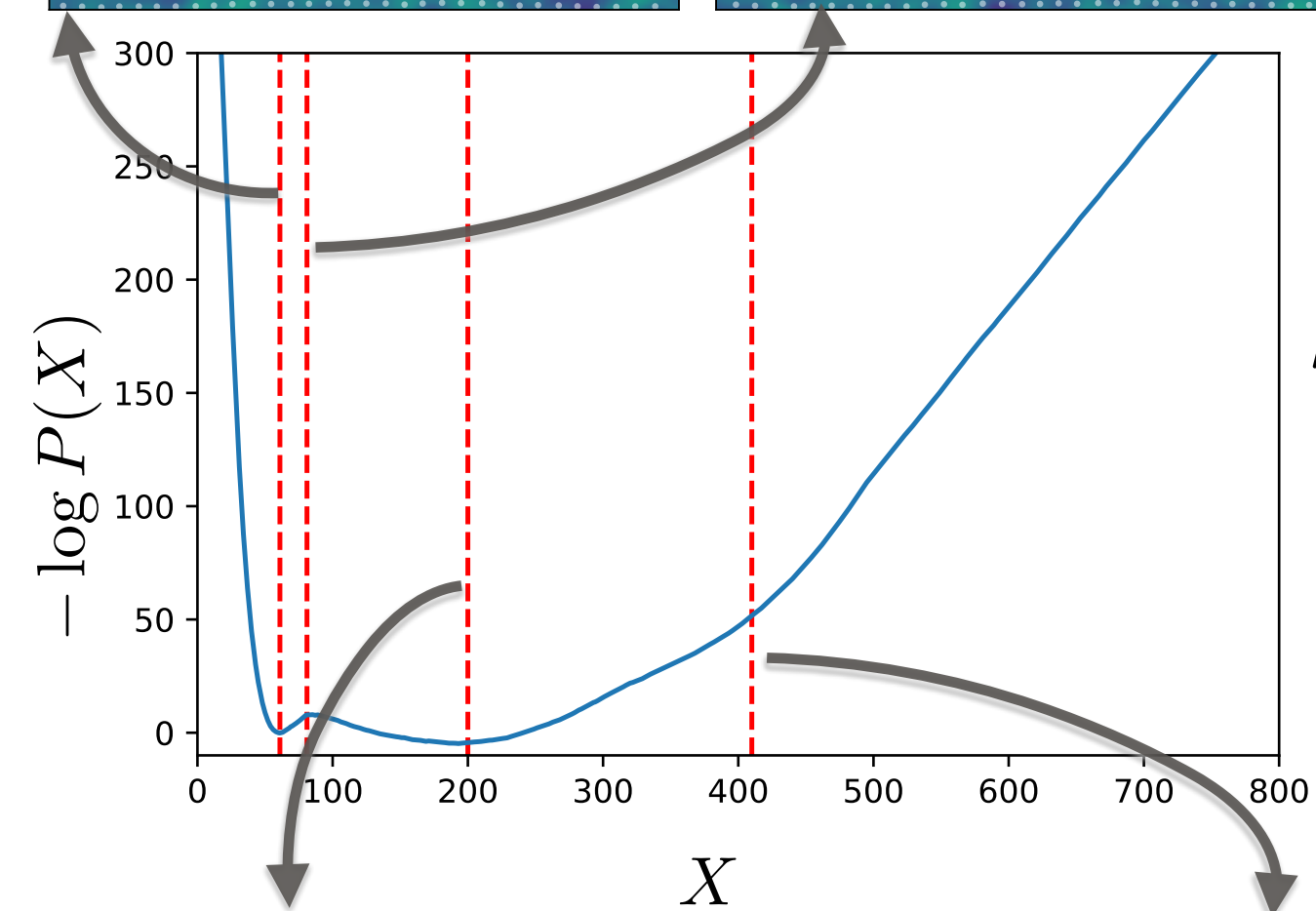
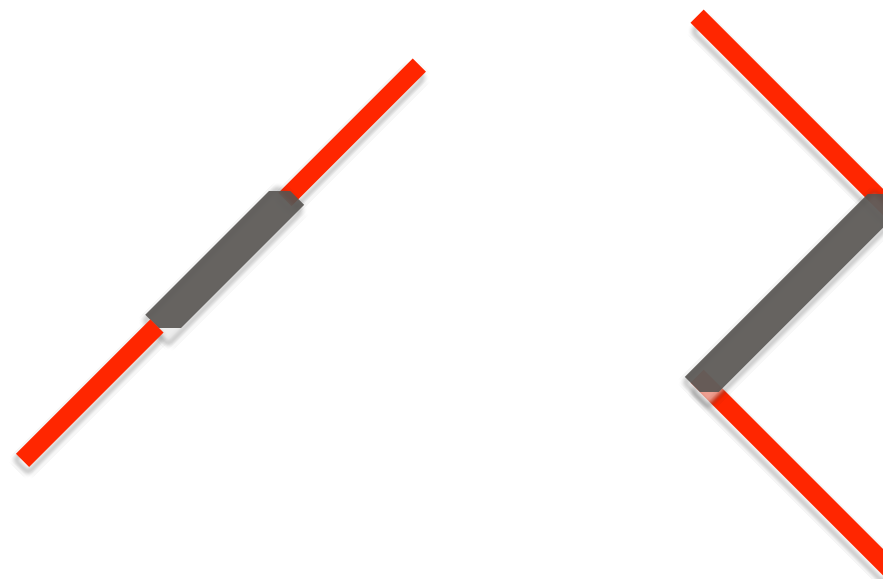
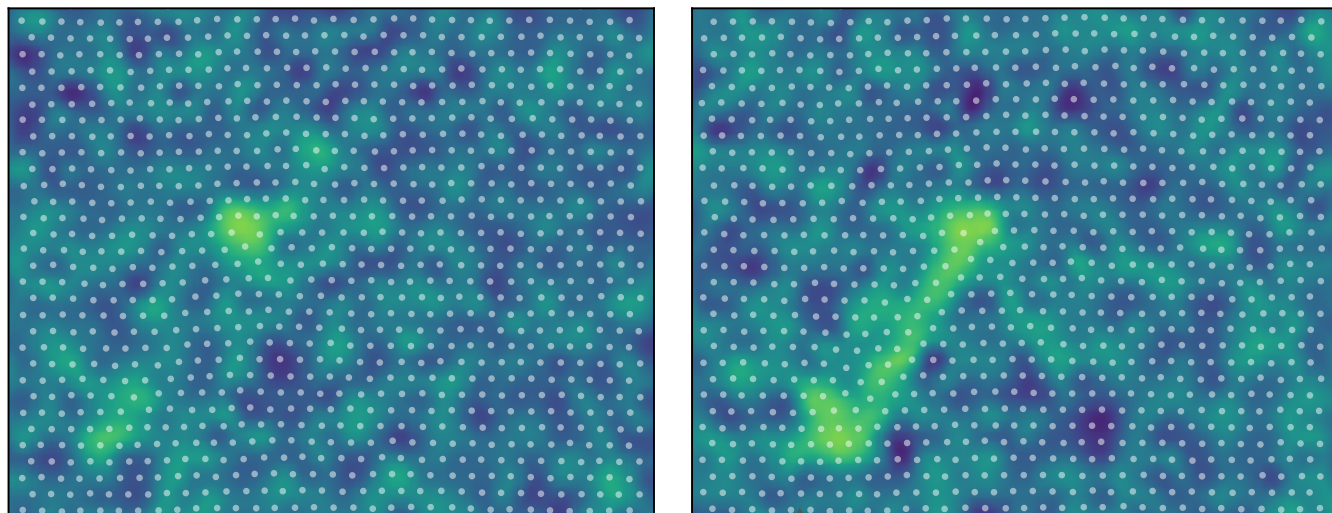




$$h_X = -5, \varepsilon = .02$$

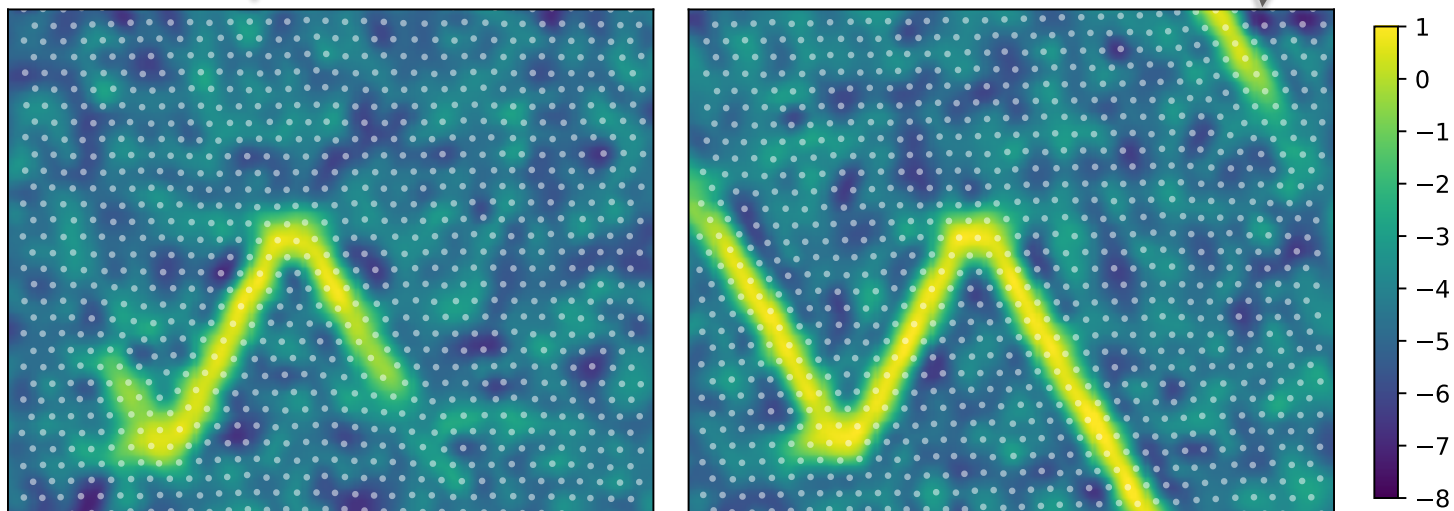
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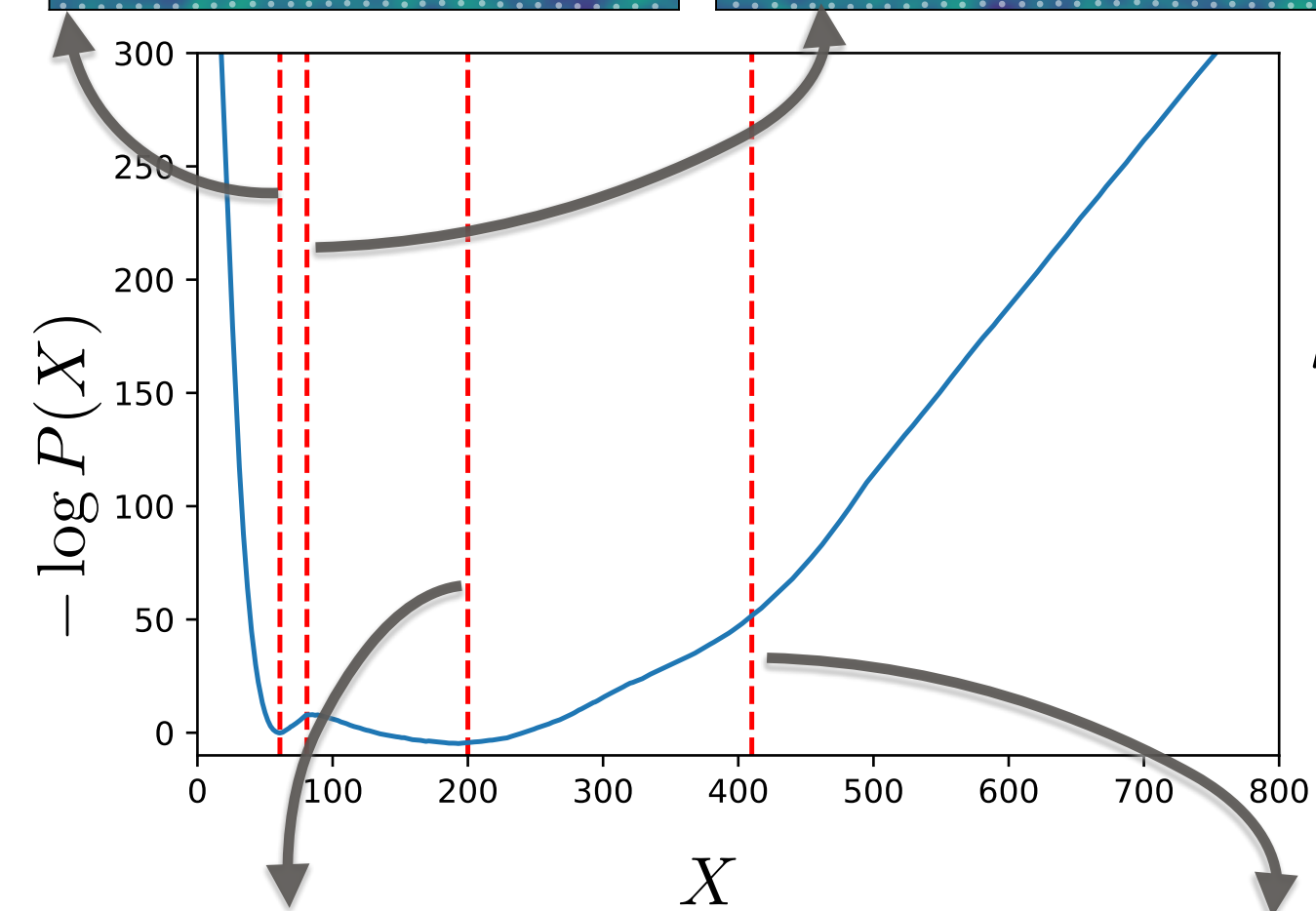
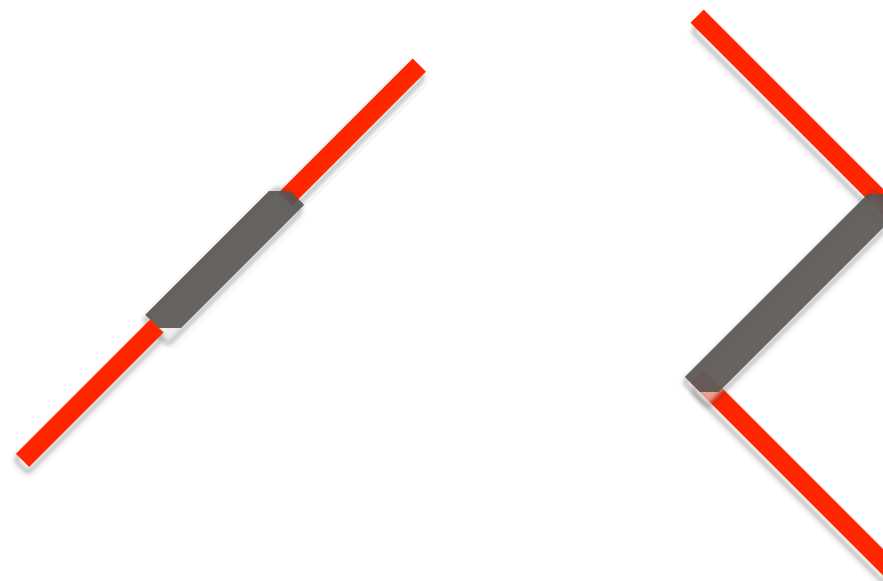
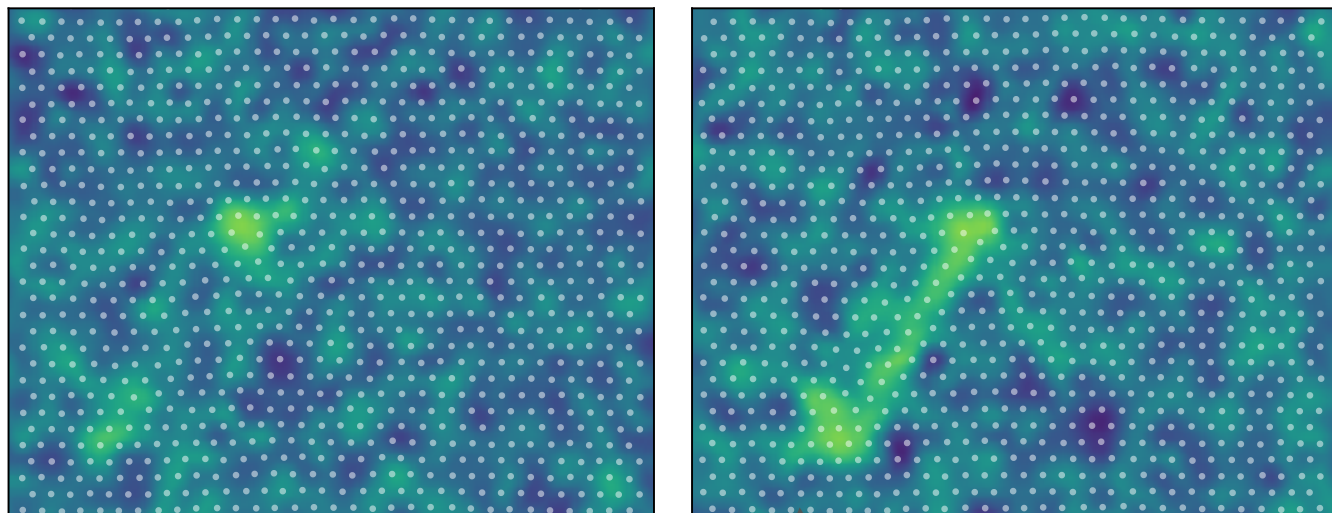




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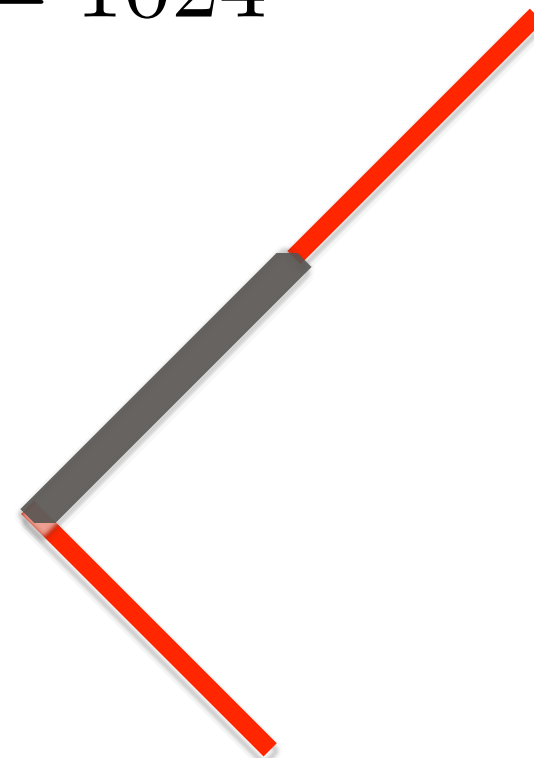
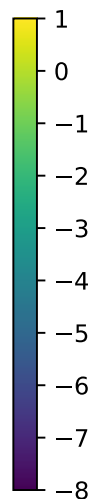
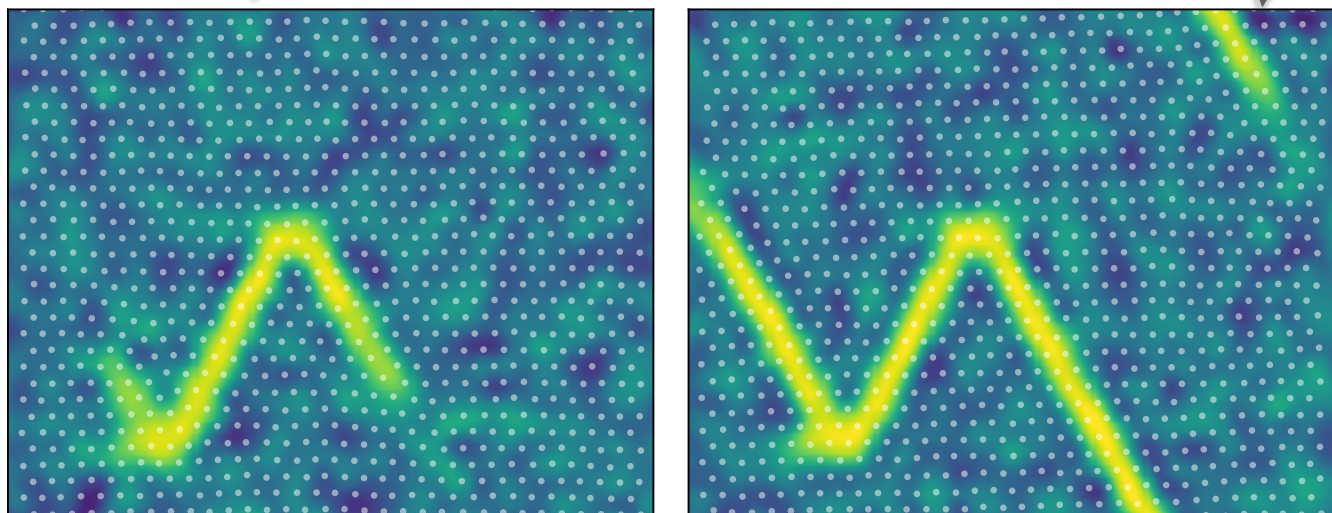
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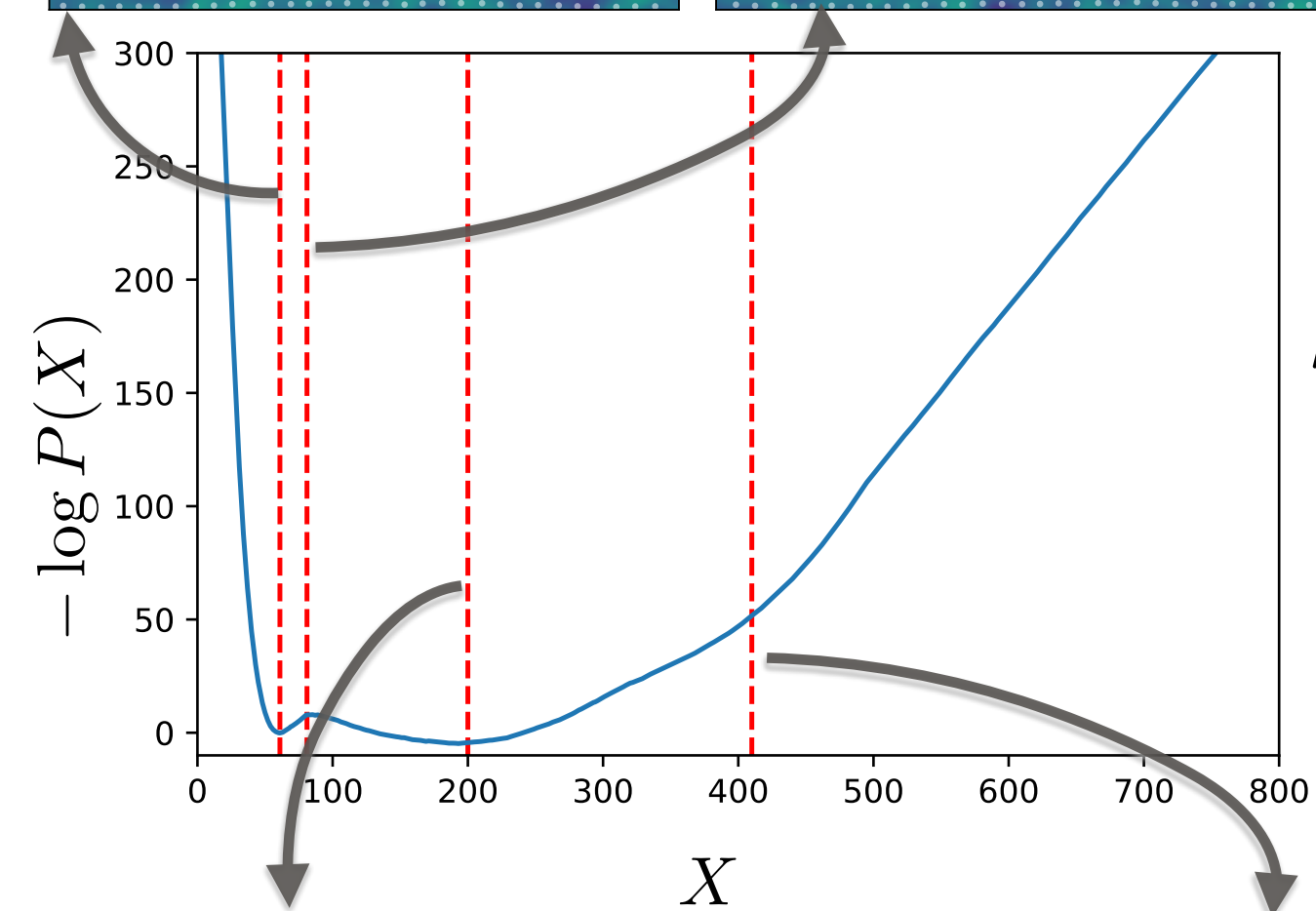
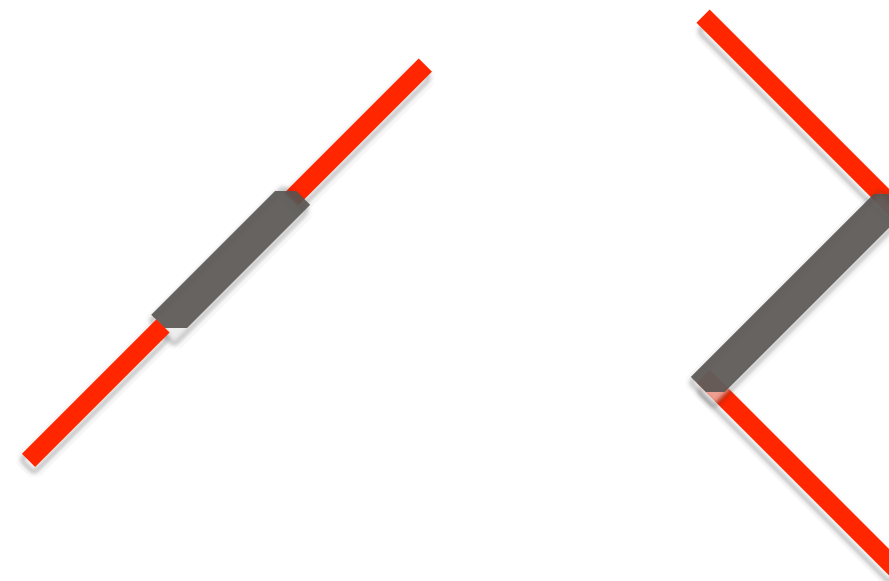
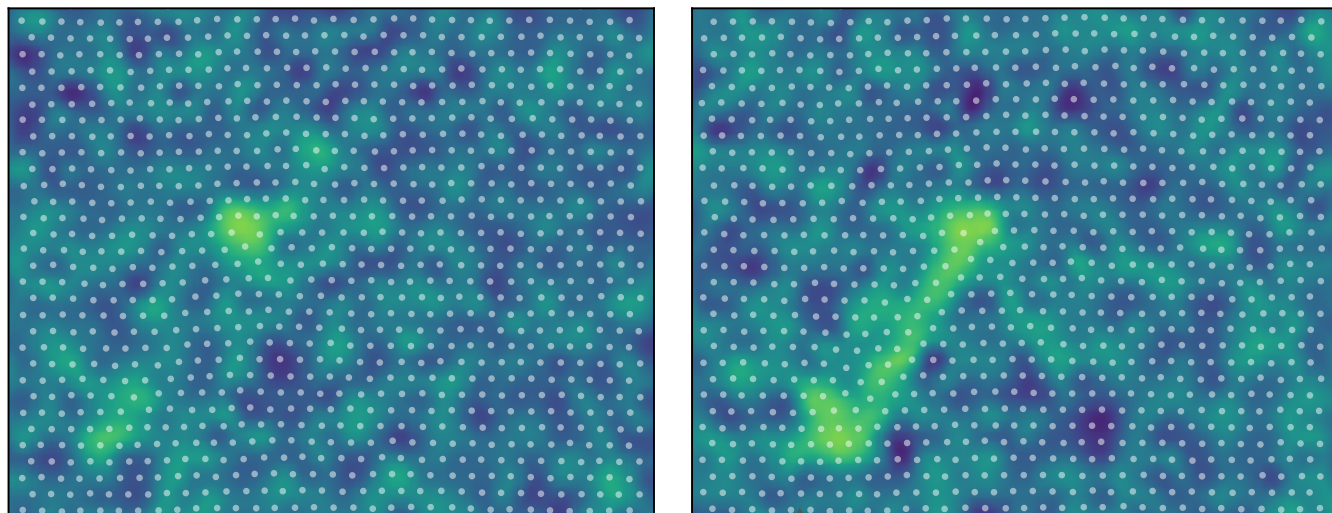




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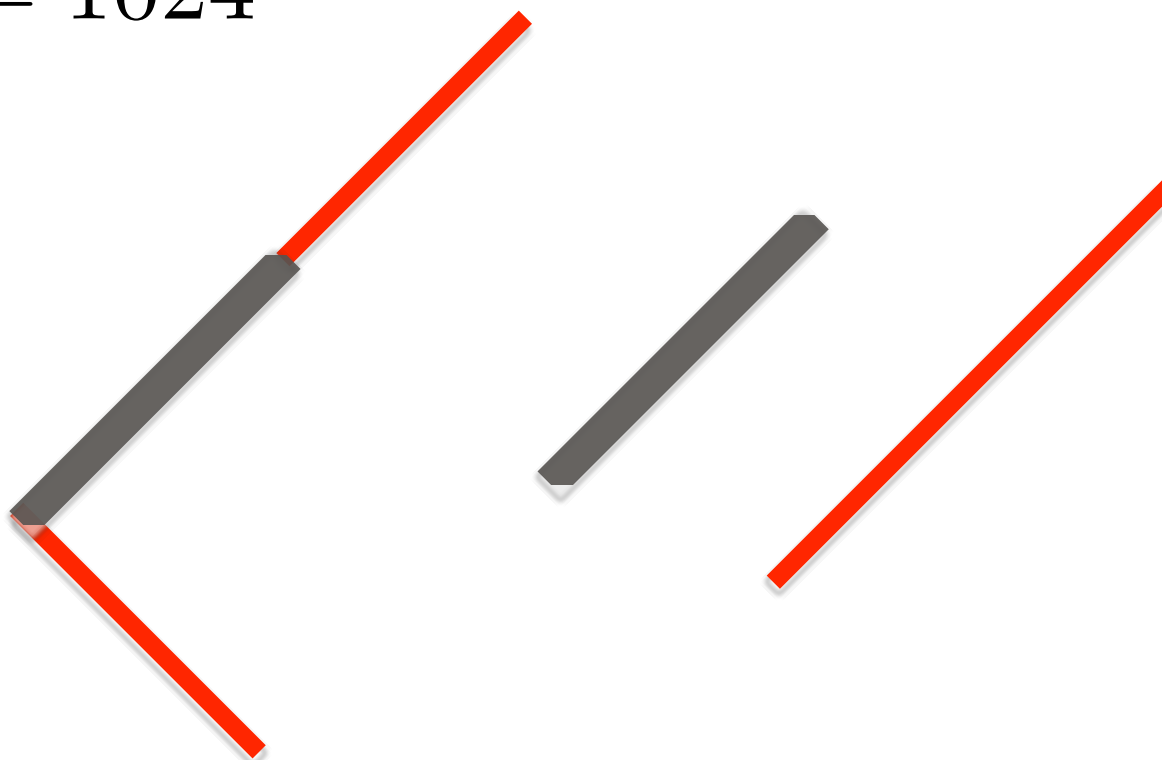
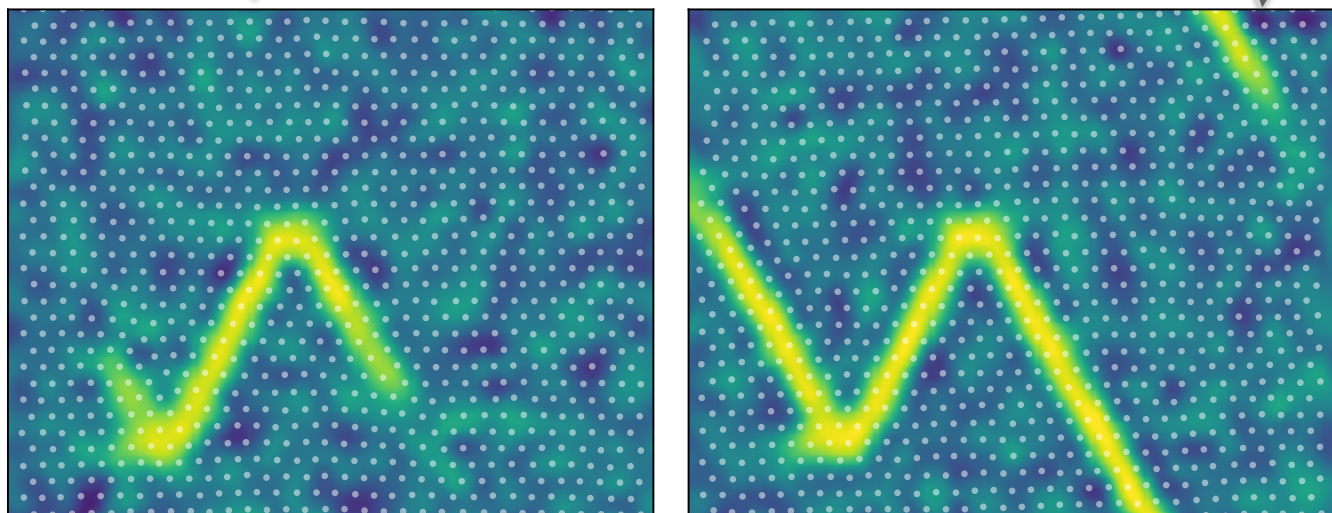
$$N = 1024$$





$$h_X = -5, \varepsilon = .02$$

$$N = 1024$$



SINGLE “FROZEN-IN” DISLOCATION DIPOLE

- * Change in equilibrium phase boundary: M phase more stable.
- * Barrier height becomes 1/5th: yield threshold decreases
- * Kamer's regimes appears at much lower strain rates and spinodal regime becomes more dominant.
- * Appearance of extra minima.
- * Can already see what is expected for a glass!

WHAT IS GOING ON?

A superconductor analogy ?

- Superconductivity is associated with “gauge-symmetry breaking”.
- London equation $\mathbf{j} = -(n_s e^2 / m) \mathbf{A}$ holds only in the Coulomb gauge, namely $\nabla \cdot \mathbf{A} = 0$.
- This leads to the Meissner effect i.e. elimination of flux.
- Gauge fixing happens naturally.
- Our case is analogous.
- Choosing reference lattice and h_X “fixes” a certain indexing. Local permutation symmetry is broken.
- Artificial gauge fixing $\rightarrow$ stress Meissner effect?
- In the real world only *kinetic* effects of this phase transition is felt.

On the existence of thermodynamically stable rigid solids

Parswa Nath^{a,1}, Saswati Ganguly^{b,1}, Jürgen Horbach^b, Peter Sollich^{c,d}, Smarajit Karmakar^a, and Surajit Sengupta^{a,2}

^aCentre for Interdisciplinary Sciences, Tata Institute of Fundamental Research, Hyderabad 500107, India; ^bInstitut für Theoretische Physik II: Weiche Materie, Heinrich Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany; ^cDepartment of Mathematics, King's College London, London WC2R 2LS, United Kingdom; and ^dInstitute for Theoretical Physics, University of Göttingen, 37077 Göttingen, Germany

Edited by Andrea J. Liu, University of Pennsylvania, Philadelphia, PA, and approved March 26, 2018 (received for review January 16, 2018)

nanoscale views

A blog about condensed matter and nanoscale physics. Why should high energy and astro folks have all the fun?

Sunday, June 24, 2018

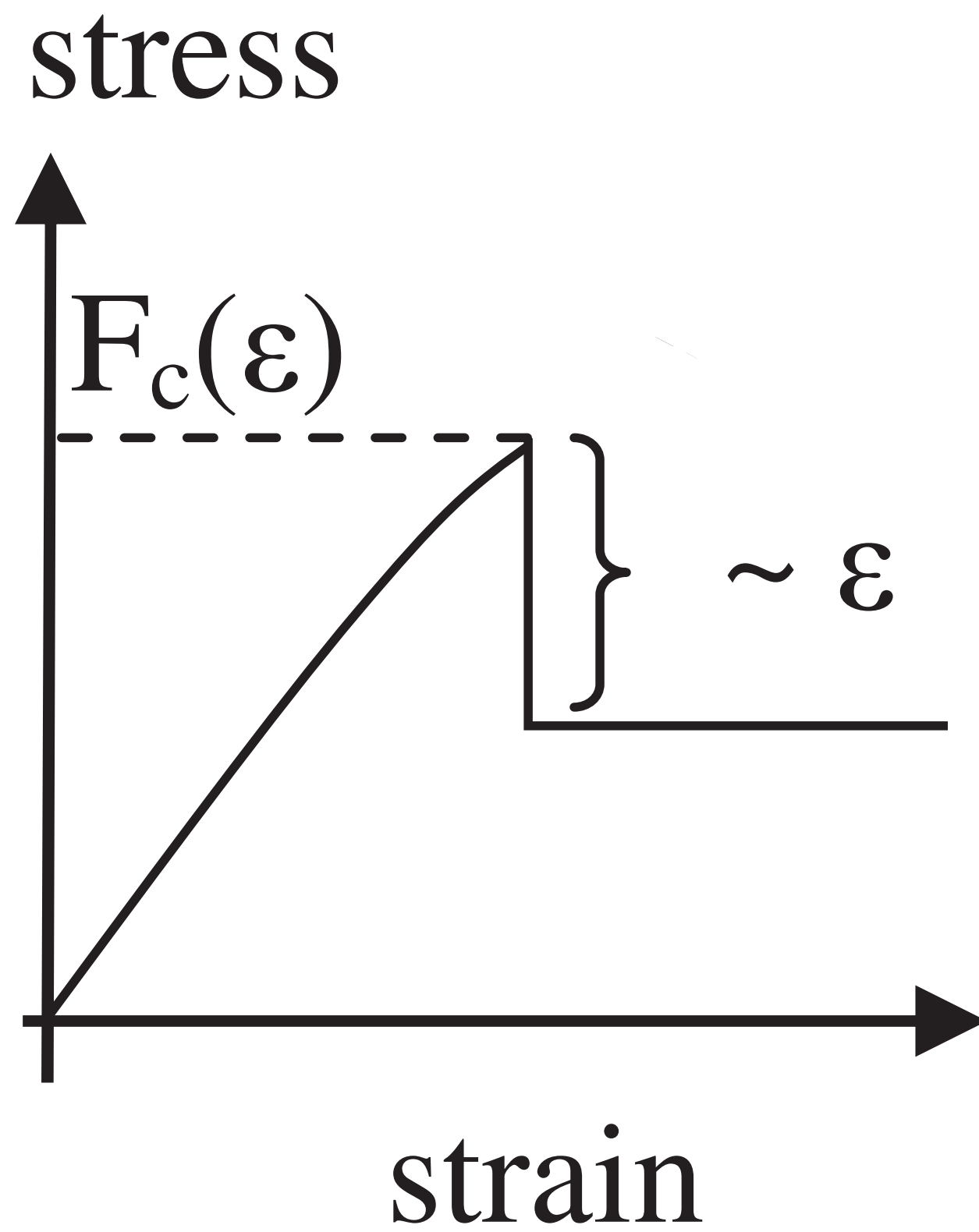
There is no such thing as a rigid solid.

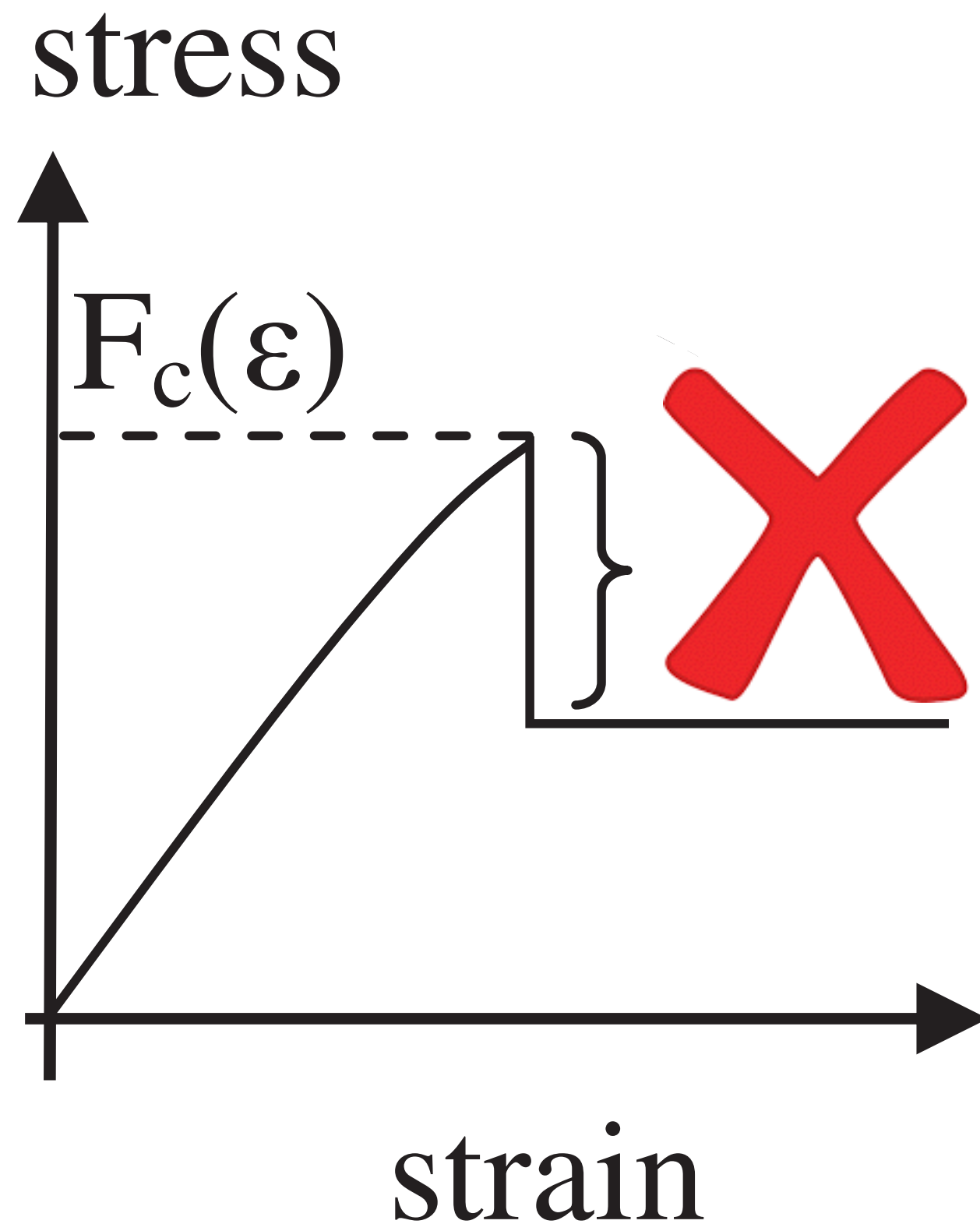
How's *that* for a provocative, click-bait headline?

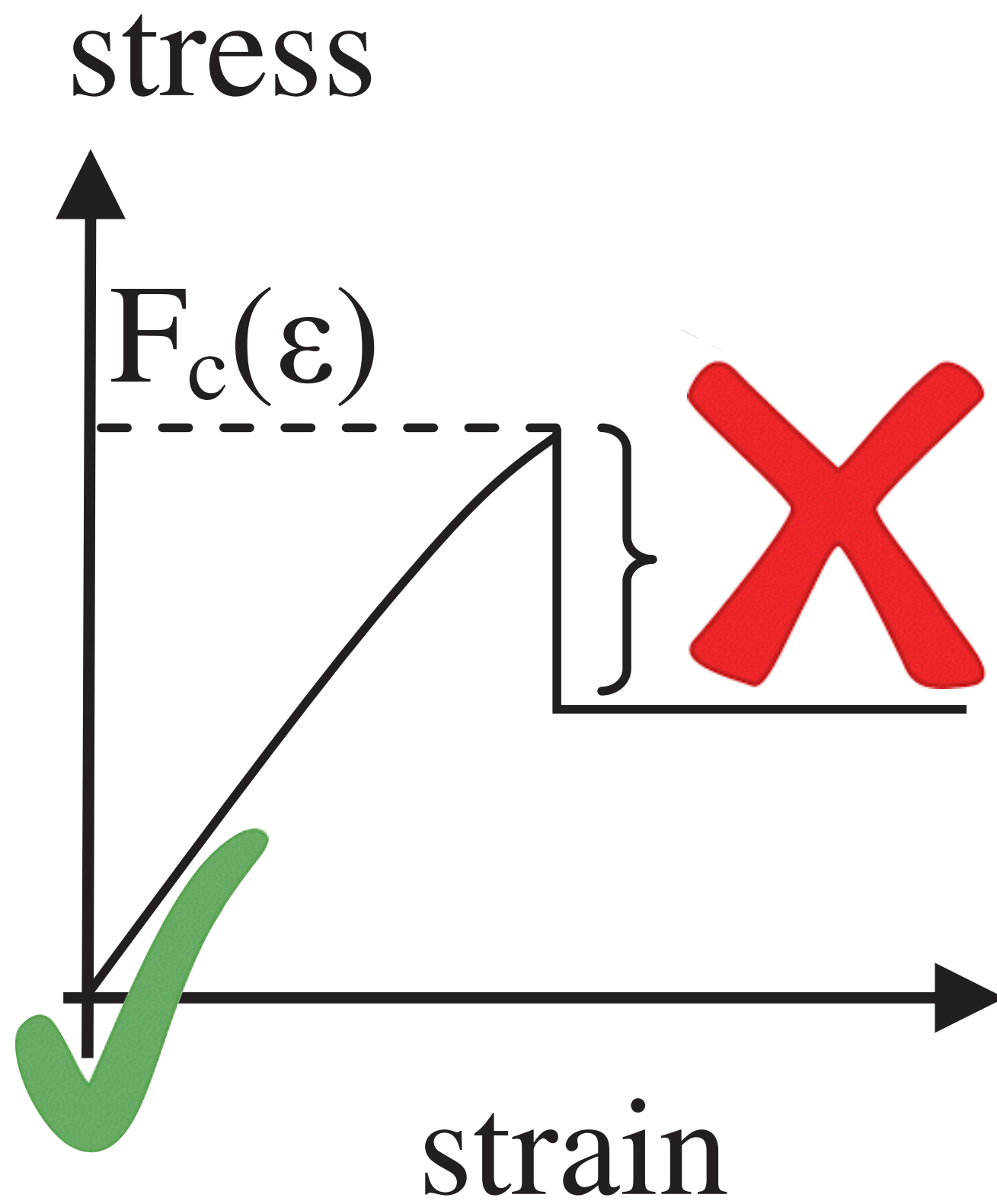
Books



<http://nanoscale.blogspot.com/2018/06/there-is-no-such-thing-as-rigid-solid.html>





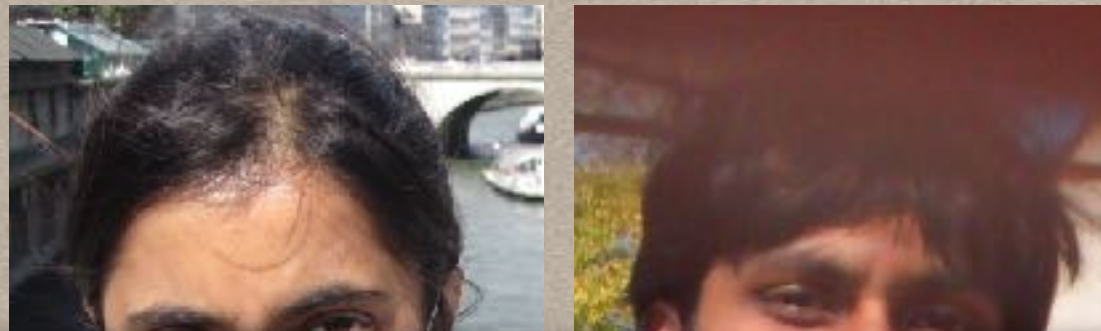


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- Colleagues: Jürgen Horbach (Düsseldorf), Peter Sollich (King's college), Smarajit Karmakar (TCIS), Madan Rao (NCBS)
- Organisations: KITP, EU FP7 collaboration DIONICOS, OIST, CSIR

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Thanks for your attention

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