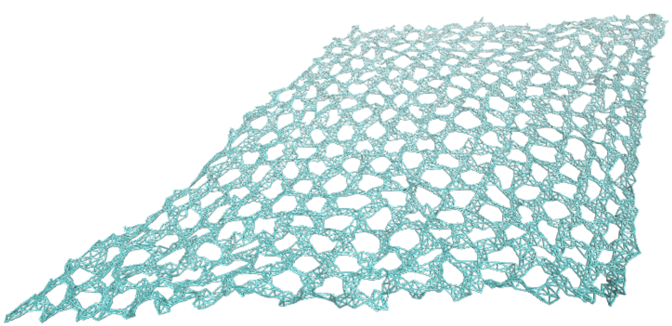
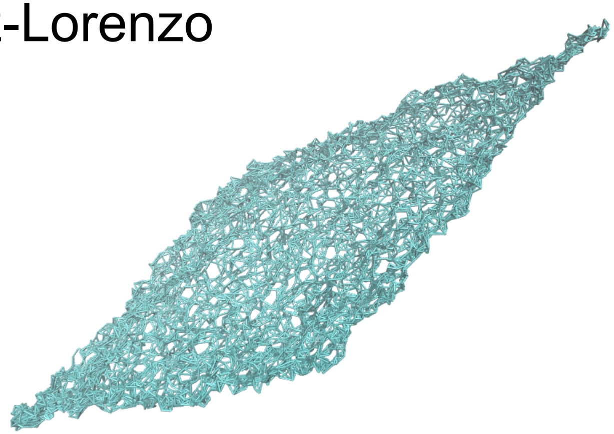
Crumpling Transition and Low Temperatures Properties of Crystalline Membranes with Perforation Patterns

A. Gordillo-Guerrero, and J. J. Ruiz-Lorenzo

mailto: anto@unex.es





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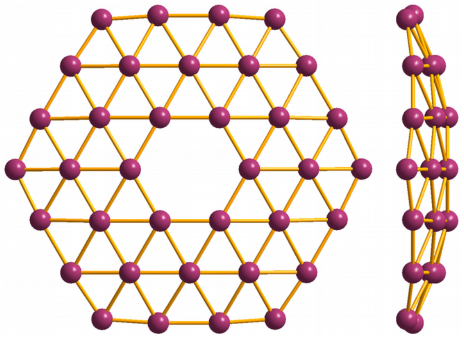
Overview

Motivation

- We can define two main types of membranes:
  - Fluid membranes: variable topology.
  - Crystalline membranes: fixed connectivity.
- Characteristics
  - Transition between plane and crumpled phases
  - Negative Poisson module
- Examples:
  - Red blood cells skeleton
  - Graphite oxide thin sheets
  - Some 2D materials

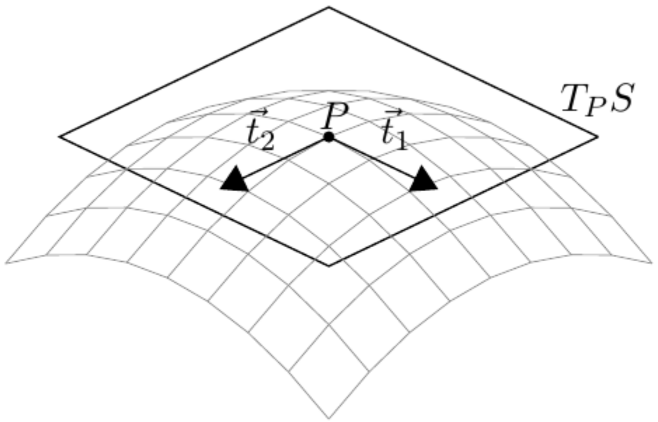


Overview

Order parameter

- From the tangent vectors

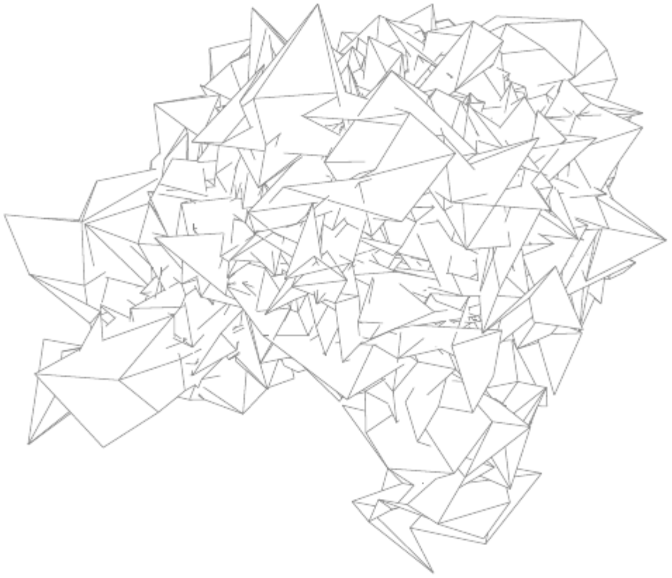
  we can define the order parameter.



- Plane phase:

$$\langle \vec{t}_\alpha \rangle \neq 0$$

- Crumpled phase:



$$\langle \vec{t}_\alpha \rangle = 0$$

Free energy definition

- By imposing:
  - Locality, translational invariance.
  - Rotational and translational symmetry.
  - Self avoidance.

we can define the free energy as a sum of three terms:

$$F[\vec{t}_\alpha(\mathbf{x}), T] = F_E[\vec{t}_\alpha(\mathbf{x}), T] + F_C[\vec{t}_\alpha(\mathbf{x}), T] + F_b[\vec{t}_\alpha(\mathbf{x}), T]$$

with:

$$F_E[\vec{t}_\alpha(\mathbf{x}), T] = \int d^2\mathbf{s} \left[\frac{t}{2}(\vec{t}_\alpha \cdot \vec{t}^\alpha) + u(\vec{t}_\alpha \cdot \vec{t}_\beta)(\vec{t}^\alpha \cdot \vec{t}^\beta) + v(\vec{t}_\alpha \cdot \vec{t}^\alpha)(\vec{t}_\beta \cdot \vec{t}^\beta) \right]$$

$$F_C[\vec{t}_\alpha(\mathbf{x}), T] = \frac{\kappa}{2} \int d^2\mathbf{s}\ \partial_\alpha \vec{t}^\alpha \cdot \partial^\beta \vec{t}_\beta$$

$$F_b[\vec{t}_\alpha(\mathbf{x}), T] = \frac{b}{2} \int d^2\mathbf{x} d^2\mathbf{x}' \delta^2(\vec{r}(\mathbf{x}) - \vec{r}(\mathbf{x}'))$$

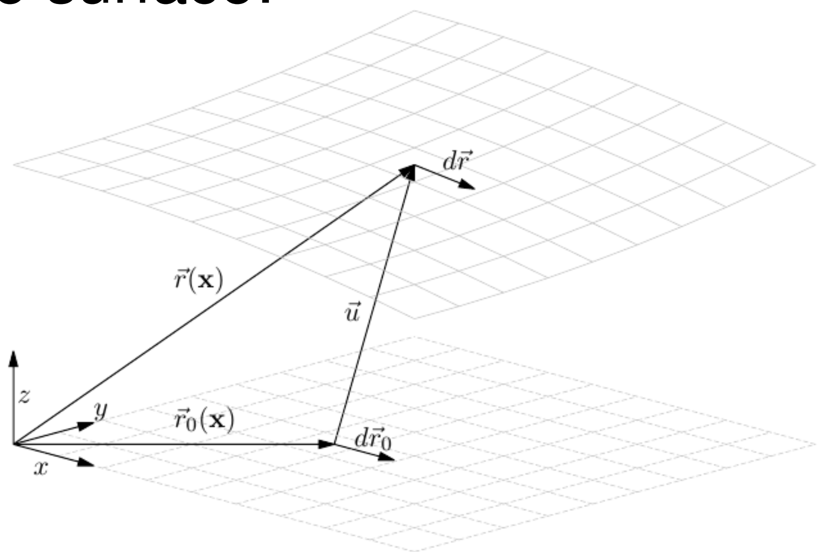
← *Not present if we use phantom surfaces*

Plane phase

- From the Monge representation of the surface:

$$\vec{r}(\mathbf{x}) = (\mathbf{x} + \mathbf{u}(\mathbf{x}), h(\mathbf{x}))$$

$$(d\vec{r})^2 = (d\vec{r}_0)^2 + 2u_{\alpha\beta}dx^\alpha dx^\beta$$



being $u_{\alpha\beta}$ the deformation tensor:

$$u_{\alpha\beta} = \frac{1}{2}(\vec{t}_\alpha \cdot \vec{t}_\beta - \delta_{\alpha\beta}) \;\Rightarrow \vec{t}_\alpha \cdot \vec{t}_\beta = \delta_{\alpha\beta} + 2u_{\alpha\beta}$$

- Therefore:

$$F_E[u_{\alpha\beta}, T] = \int d^2\mathbf{x} \left[\mu u_{\alpha\beta}u^{\alpha\beta} + \frac{\lambda}{2}u_\alpha{}^\alpha u^\beta{}_\beta\right],$$

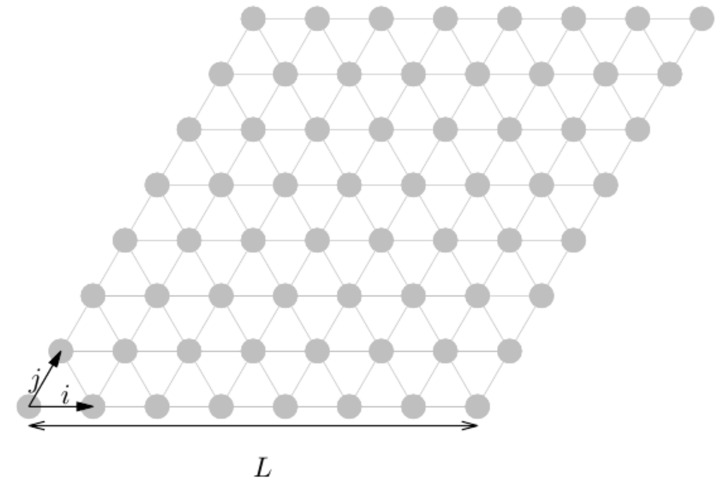
$$F_C[\mathbf{y}, T] \simeq \frac{\kappa}{2}\int d^2\mathbf{y} K_\alpha{}^\beta K^\alpha{}_\beta \simeq \frac{1}{2}\hat{\kappa}\int d^2\mathbf{y}\, H^2$$

Curvature tensor

Overview

Discrete Pure Model

- 2D triangular lattice with $N{=}L^2$ points “living” in a 3D space
- Free boundary conditions
- Effective hamiltonian:



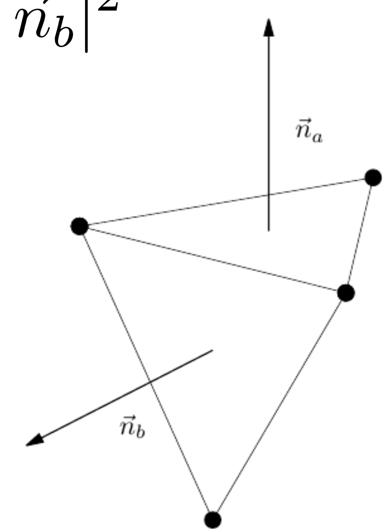
$$\mathcal{H} = \mathcal{H}_E + \mathcal{H}_C$$

with:

$$\mathcal{H}_E = \frac{1}{2}\sum_{\langle ij\rangle} |\vec{r}_i - \vec{r}_j|^2 \qquad \mathcal{H}_C = \frac{\kappa}{2}\sum_{\langle ab\rangle} |\vec{n}_a - \vec{n}_b|^2$$

Elastic energy

Curvature energy



Reproduce the previous free energy in the continuous limit

Update Algorithm (Metropolis)

- For a fixed value of κ

1) Choose a point i

2) Set $\vec{r}_i \to \vec{r}_i + \vec{\epsilon}$, with $\vec{\epsilon}$ randomly chosen on a box of size δ (chosen dynamically for acceptance ~ 50%)

3) If $\Delta\mathcal{H} = \mathcal{H}_{NEW} - \mathcal{H}_{OLD} < 0$, accept the new position.

4) If $\Delta\mathcal{H} > 0$, accept the new position with probability $e^{-\Delta\mathcal{H}}$.

5) Repeat step 1 for every point in the lattice.

After enough iterations (thermalization): $P(\vec{r}_i) \propto e^{-\mathcal{H}(\kappa)}$

Overview

Possible observable to extract

- Specific heat:

$$C_V = \frac{3(N-1)}{2} + \frac{\kappa^2}{N}(\langle E_C^2\rangle - \langle E_C\rangle^2)$$

- Square of the gyration ratio

$$R_g^2 = \frac{1}{3N}\left\langle \sum_i \vec{R}_i \cdot \vec{R}_i \right\rangle = \frac{1}{3N}(\langle \vec{R}^2\rangle - \langle \vec{R}\rangle^2), \quad \text{with} \quad \vec{R}_i = \vec{r}_{CM} - \vec{r}_i$$

- Gyration ratio kappa-derivative

$$\frac{\partial R_g^2}{\partial \kappa} = \langle R_g^2 E_C\rangle - \langle R_G^2\rangle\langle E_C\rangle \equiv \langle R_g^2 E_C\rangle_c = N\langle R_g^2 e_C\rangle_c,$$

- Poisson Module

Compression and shear modules

Induced metric tensor

$$g_{\alpha\beta} = \vec{t}_\alpha \cdot \vec{t}_\beta$$

$$\sigma = -\frac{\delta x^2/x^2}{\delta x^1/x^1}$$

$$\sigma = \frac{K-\mu}{K+\mu} = -\frac{\langle u_{11}u_{22}\rangle_c}{\langle u_{22}^2\rangle_c} = -\frac{\langle g_{11}g_{22}\rangle_c}{\langle g_{22}^2\rangle_c}$$

Finite Size Scaling and kappa extrapolations

- We can obtain critical exponents via standard FSS with κ playing the role of (inverse) temperature.

- For a given observable:

$$\mathcal{O}_L \sim L^{\frac{x_0}{\nu}} f\left[L(\kappa(L) - \kappa_c(\infty))^{\nu}\right]$$

- In the maximum of the observable:
  - We obtain the critical exponent by: $\mathcal{O}_L^{max} \sim L^{\frac{x_0}{\nu}}$
  - We can also use: $\kappa_c(L) = \kappa_c(\infty) + x_C L^{1/\nu}$

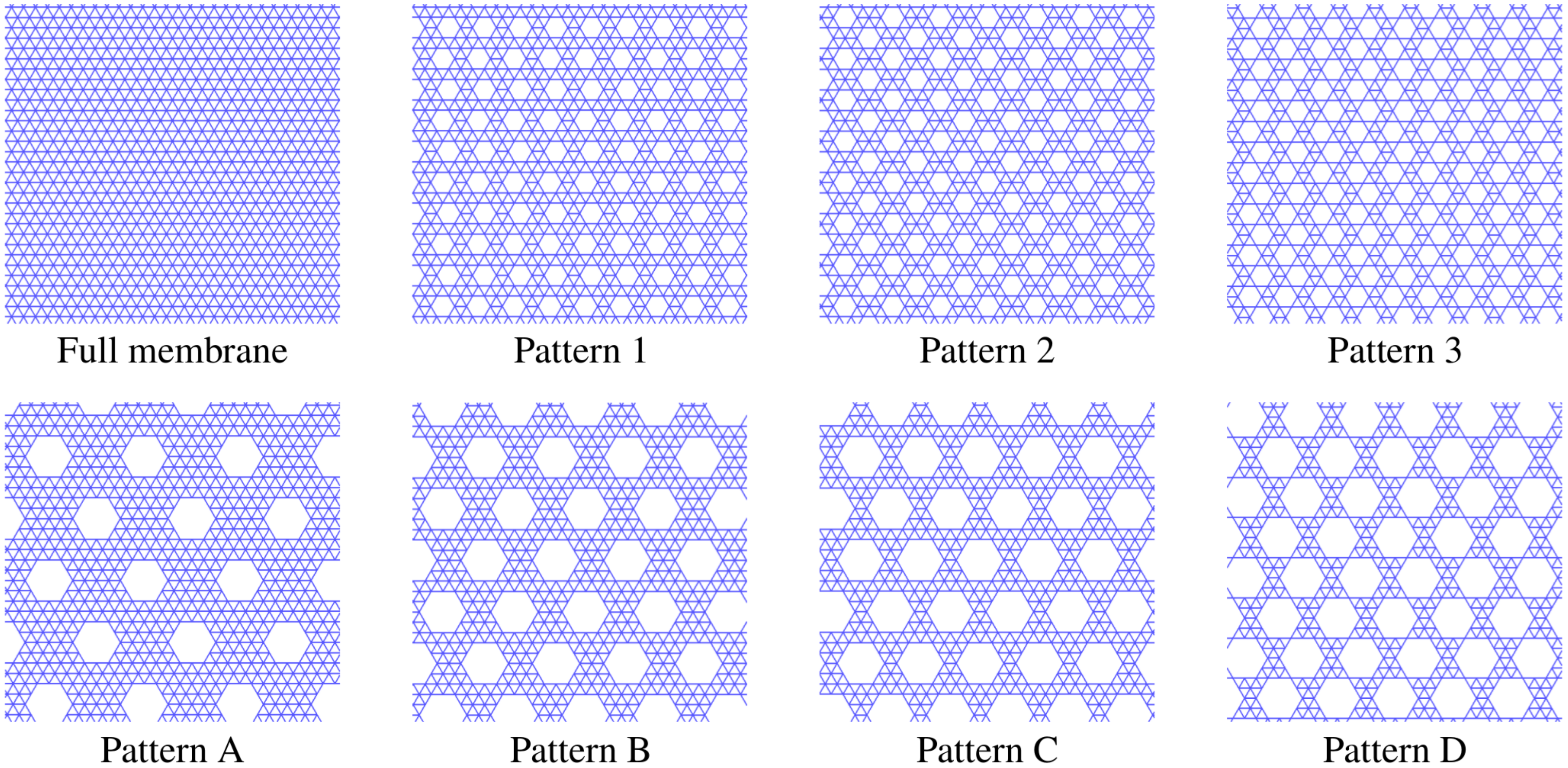
- We can locate the maximum using extrapolations in κ:

$$\langle O \rangle_{\kappa'} = \frac{\sum_E O(E) p_\kappa(E) e^{-(\kappa' - \kappa) E_c}}{\sum_E e^{-(\kappa' - \kappa) E_c}}$$

Curvature energy

What does it happen if we perforate the model?

- Following: *D. Yllanes, S. Bhabesh, D.R.Nelson & M.J. Bowick, Nature Communications 8, 1381 (2017)*
- We can define patterns of perforations spanning all the lattice.
  - Different sizes (R=1 or 2), distances, and shifts.



Overview

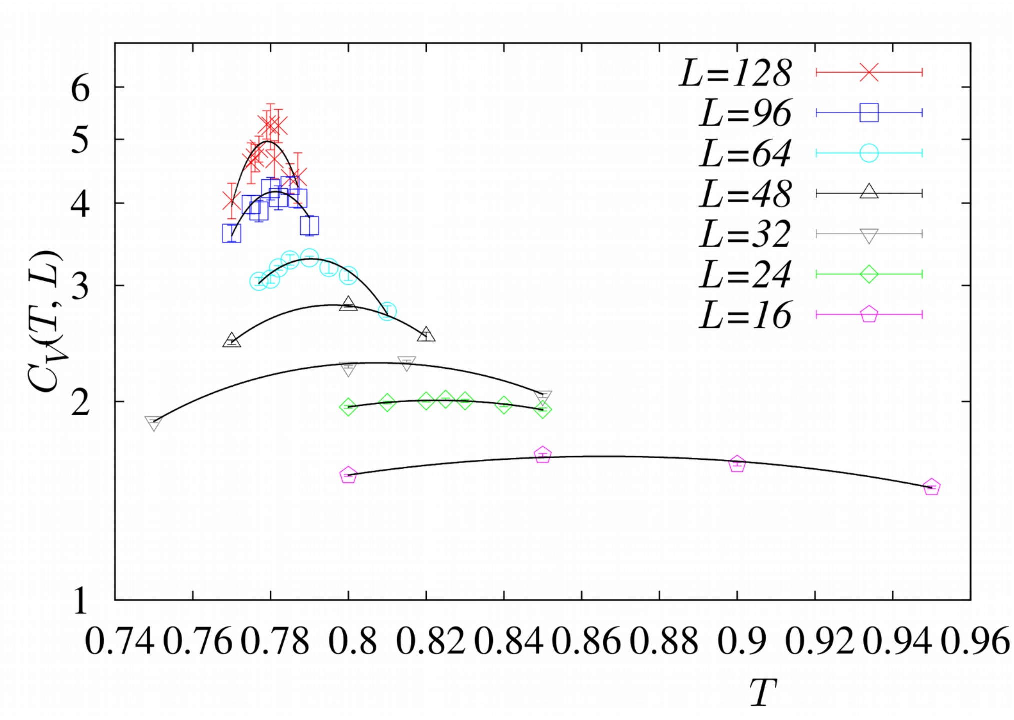
Pure model: just to remind

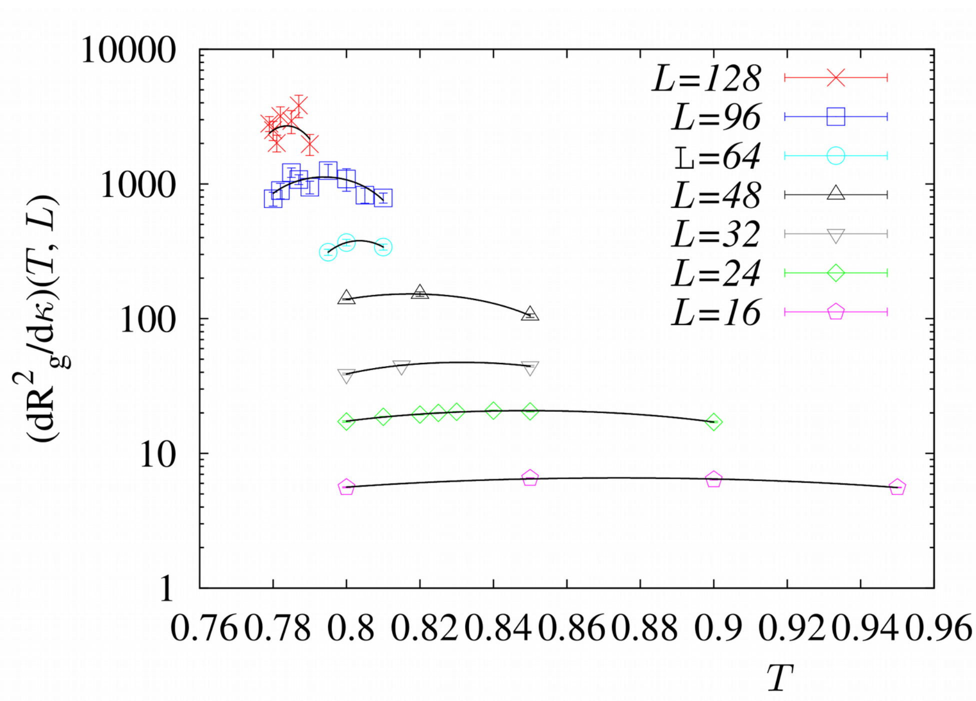
- We simulated systems with $16 \leq L \leq 128$, focusing around

$$0.5 \leq \kappa \leq 2 \qquad \kappa_c \approx 0.8$$

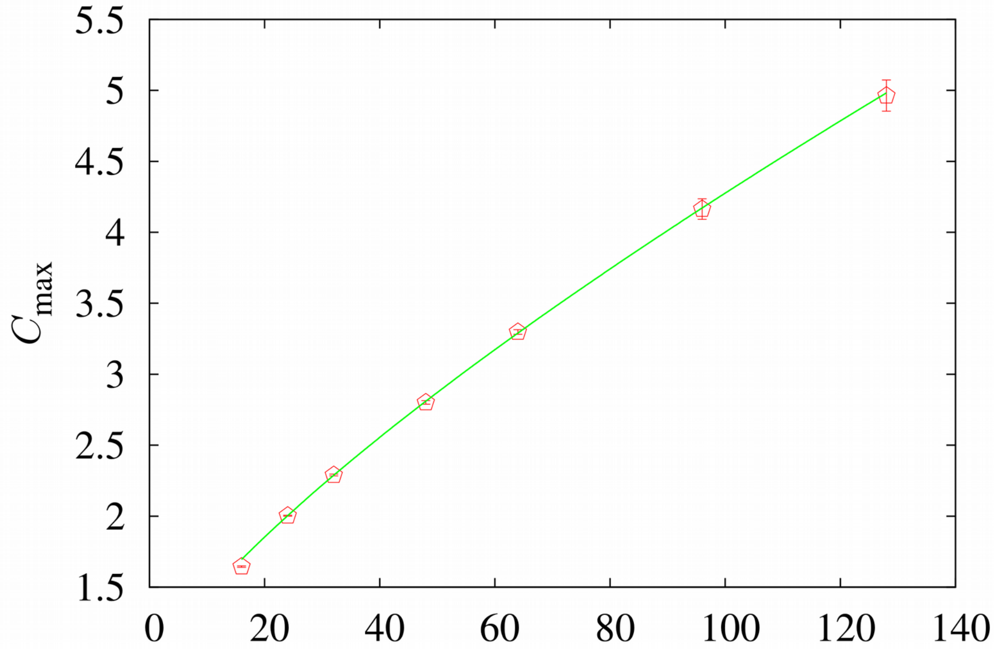
- We checked that the behavior is critical and were able to distinguish between discrepancies in previous works.

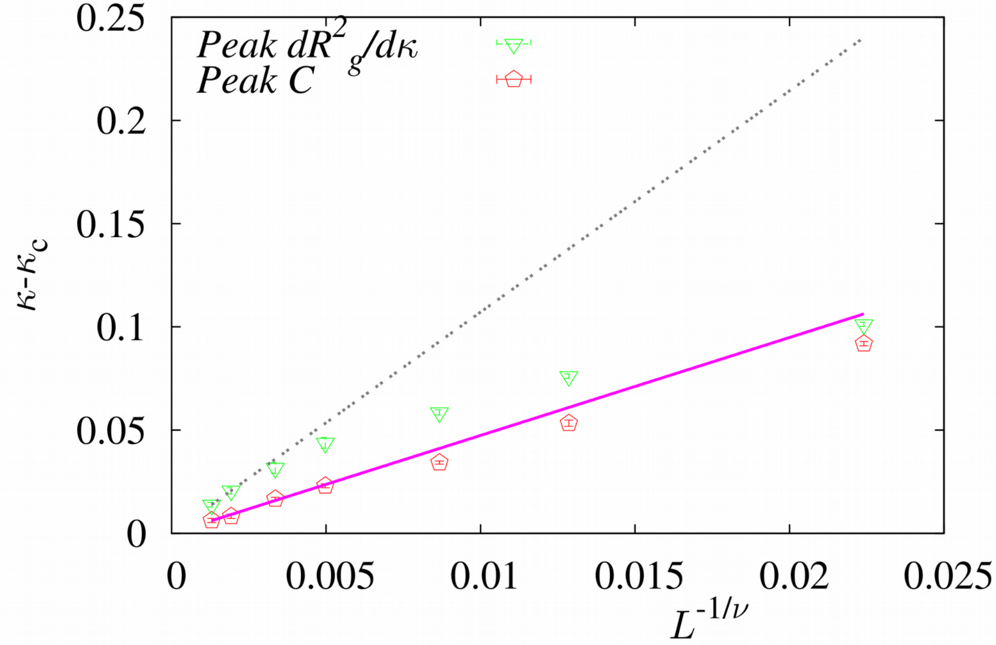
Phys. Rev. E 93, 022111 (2016). arXiv:1511.08615





Pure model: critical behavior





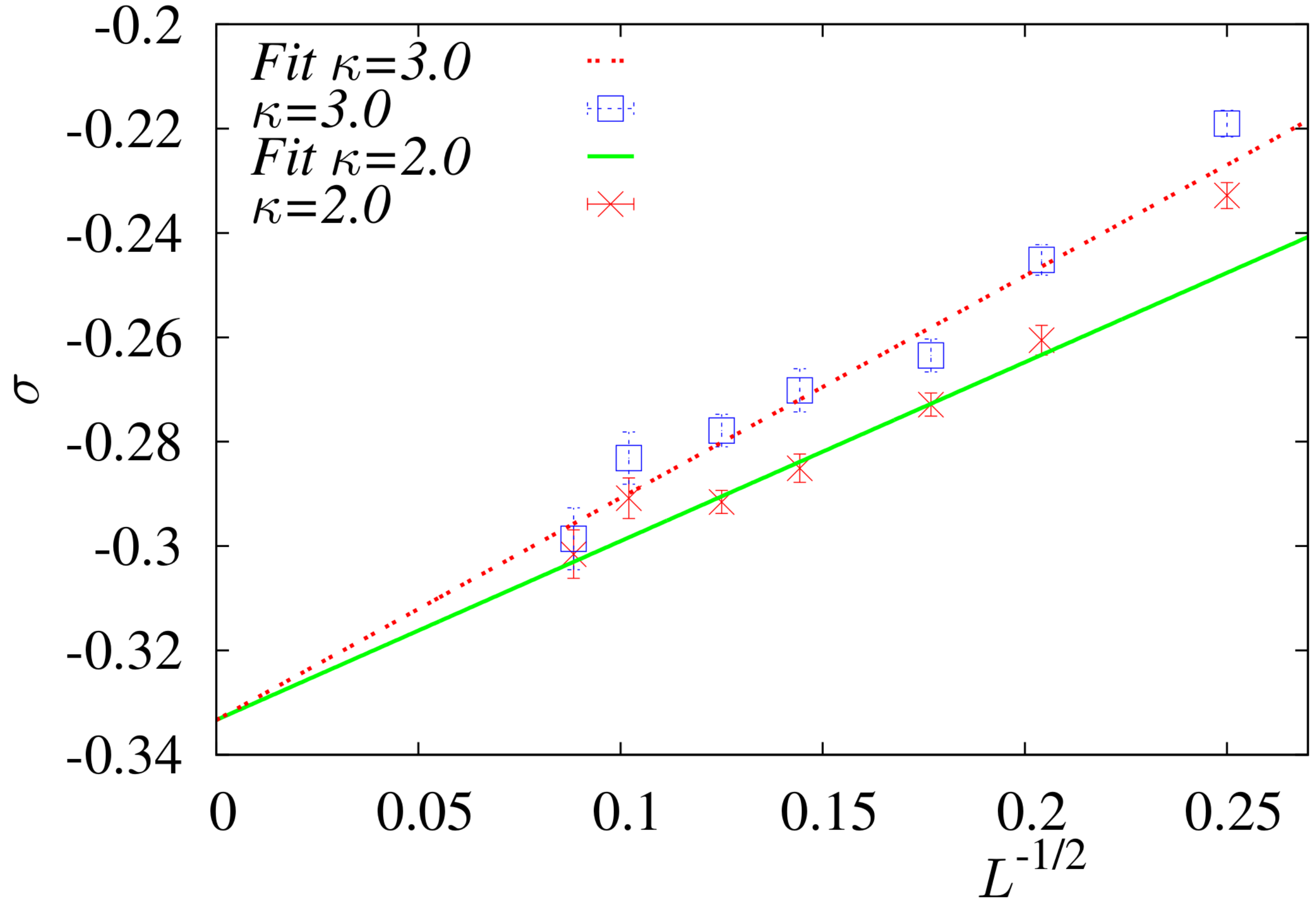
$$\kappa_c(L) = \kappa_c(\infty) + C_0 L^{-1/\nu}, \qquad \kappa_c(\infty) = 0.777(3)(3)$$

Coeficients/Critical Exponents	Results
c_0	0.7702(36)
c_1	0.1098(95)
$c_2 = \alpha/\nu$	0.76(18)
α	0.55(18)
ν	0.72(4)
χ^2_c/ndf	0.38/2
$P(\chi^2 > \chi^2_c)$	0.8257

Quite precise compared with previous estimations

Good agreement with previous estimations

Pure model: Poisson module at low temperature (flat phase)

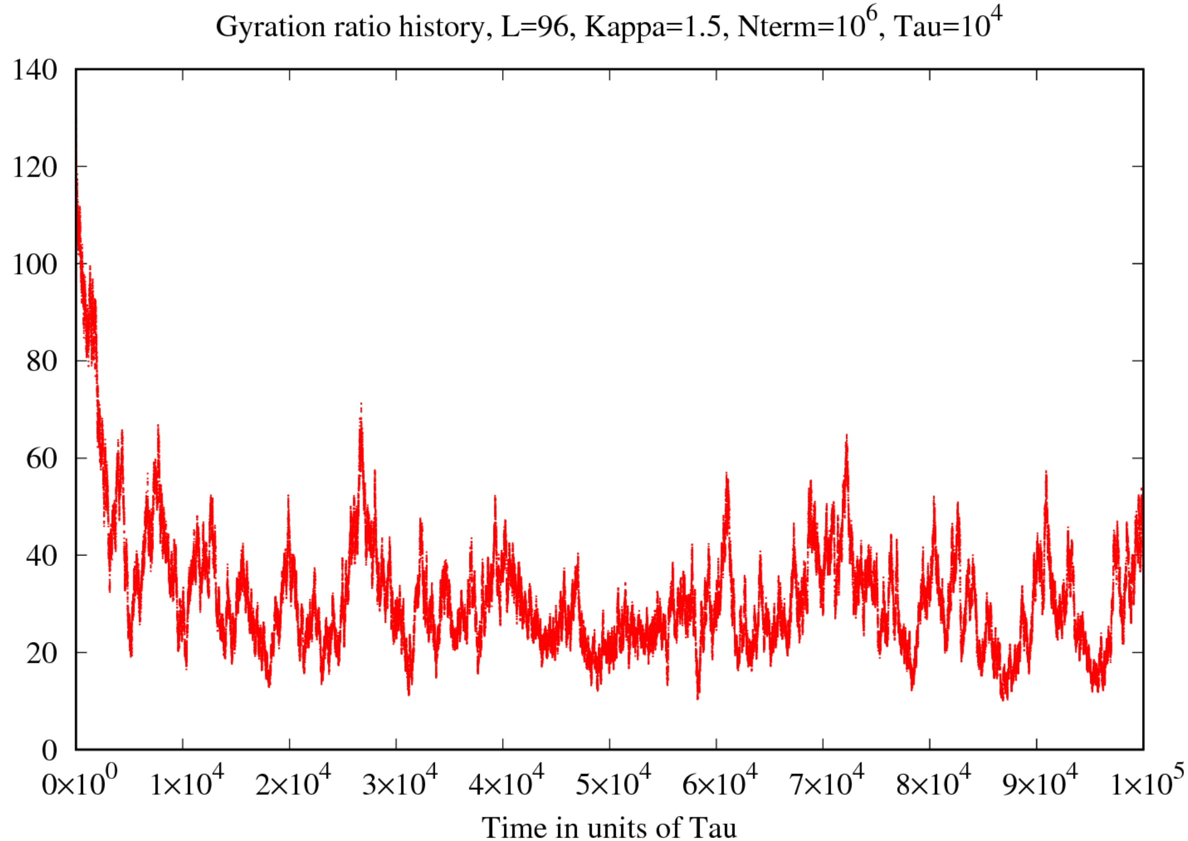


Both s1 and s2 extrapolate well to the analytical value -0.33, with the expected power law.

Overview

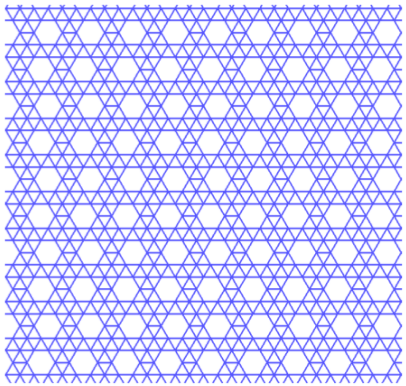
Thermalization

- These surfaces can have a more slow behavior and longer correlation times.
- Take care with thermalization steps and frequency of measures (we use 10^7 and 10^5 MC full sweeps, respectively).



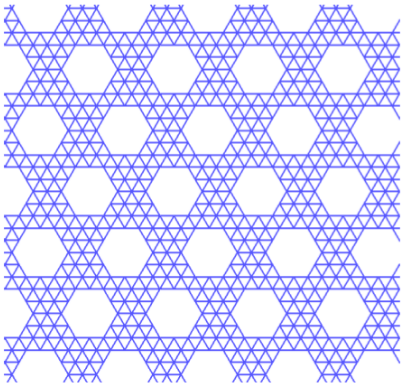
Perforated models: critical behavior

- We have checked it with the patterns:

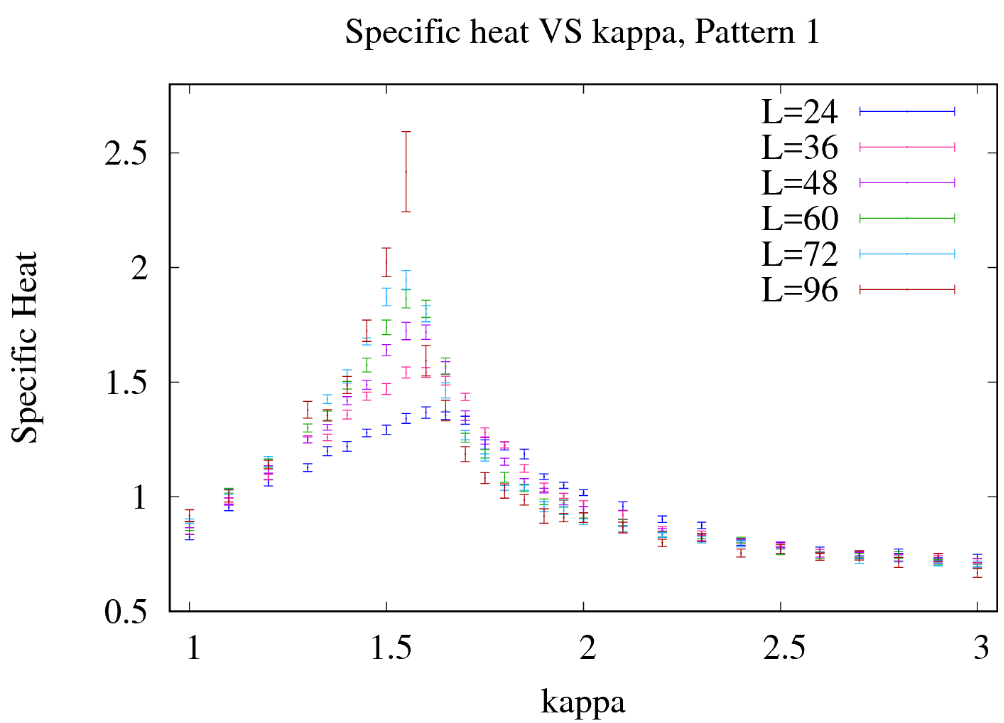


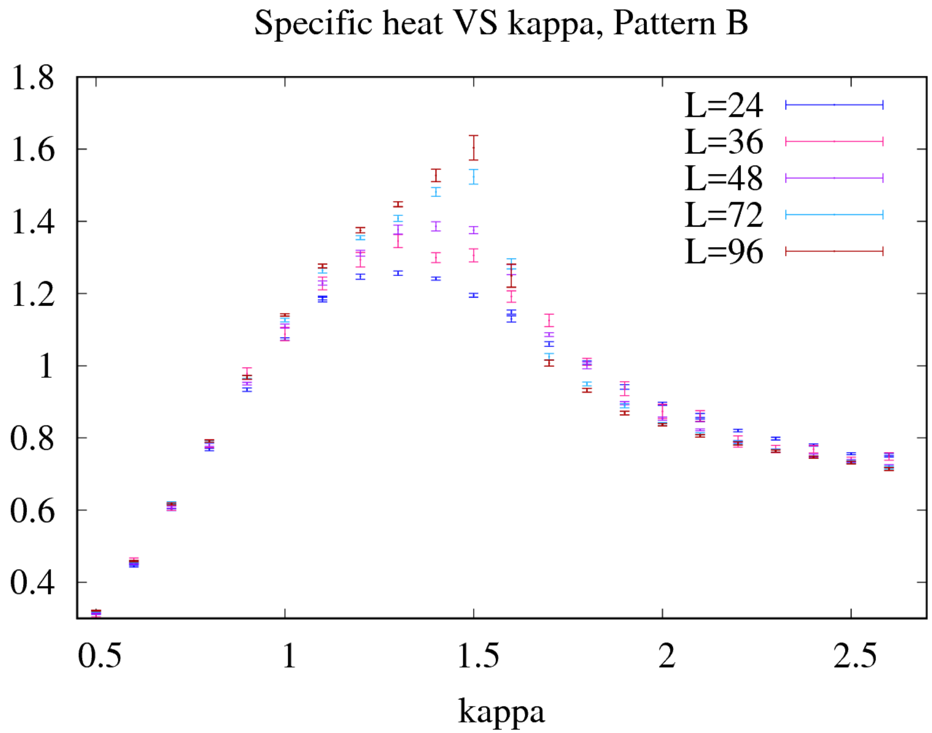
Pattern 1

They have very similar K_c



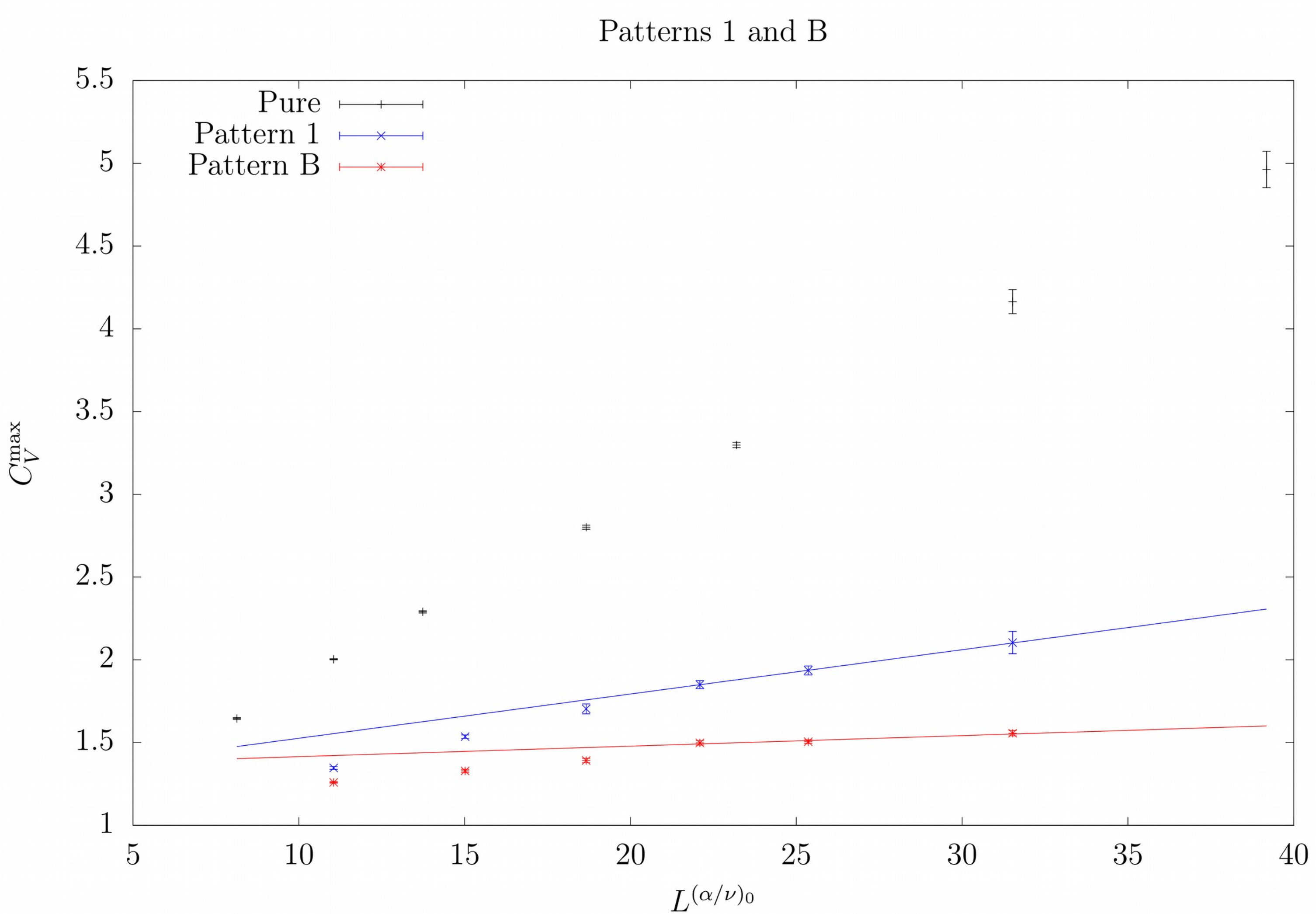
Pattern B





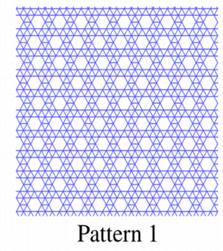
Perforated models: critical behavior

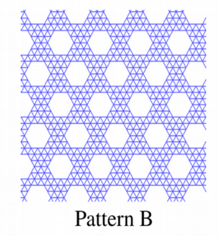
- We can check with both signals good compatibility with the critical exponents of the pure model .

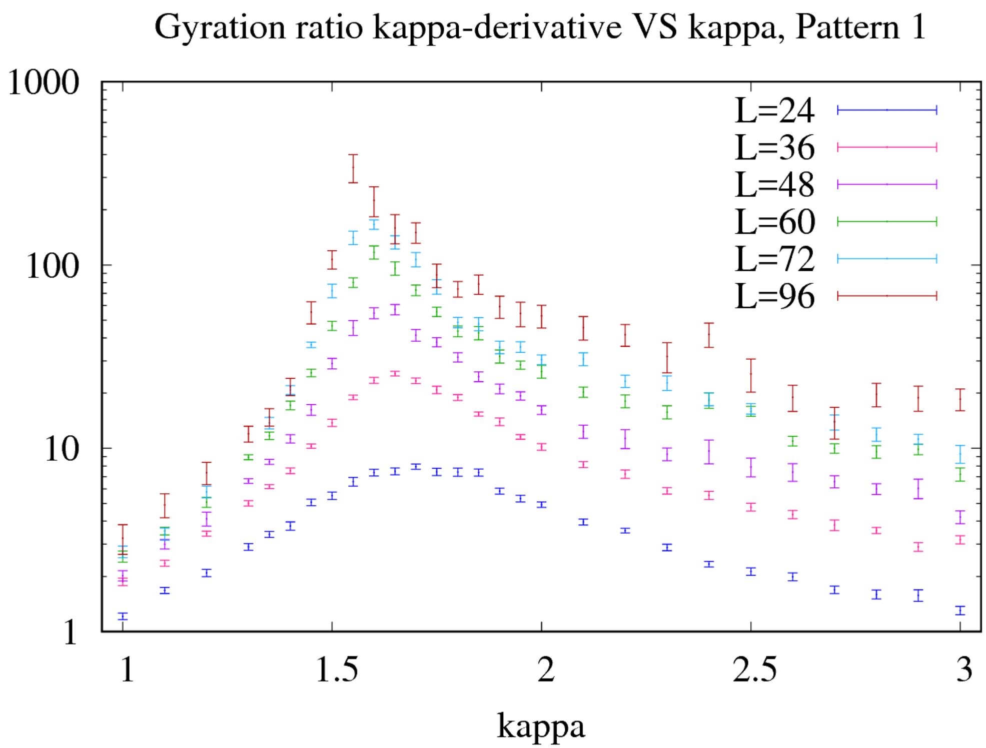


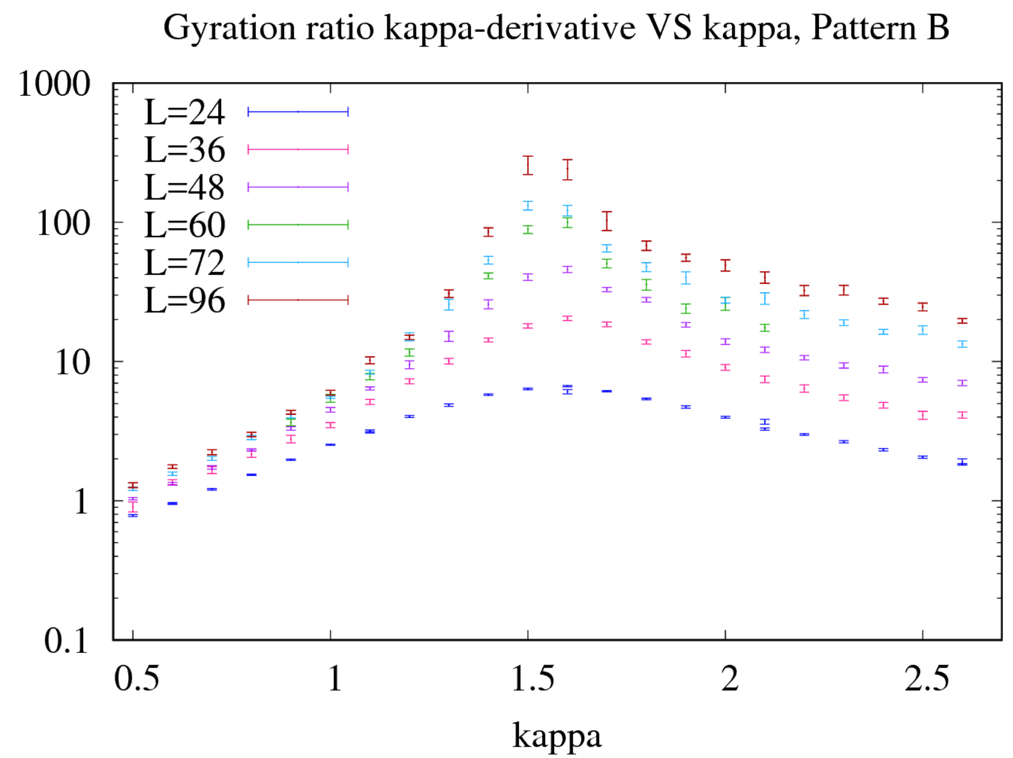
Perforated models: critical behavior

- We can also use the signal from the gyration ratio kappa-derivative:



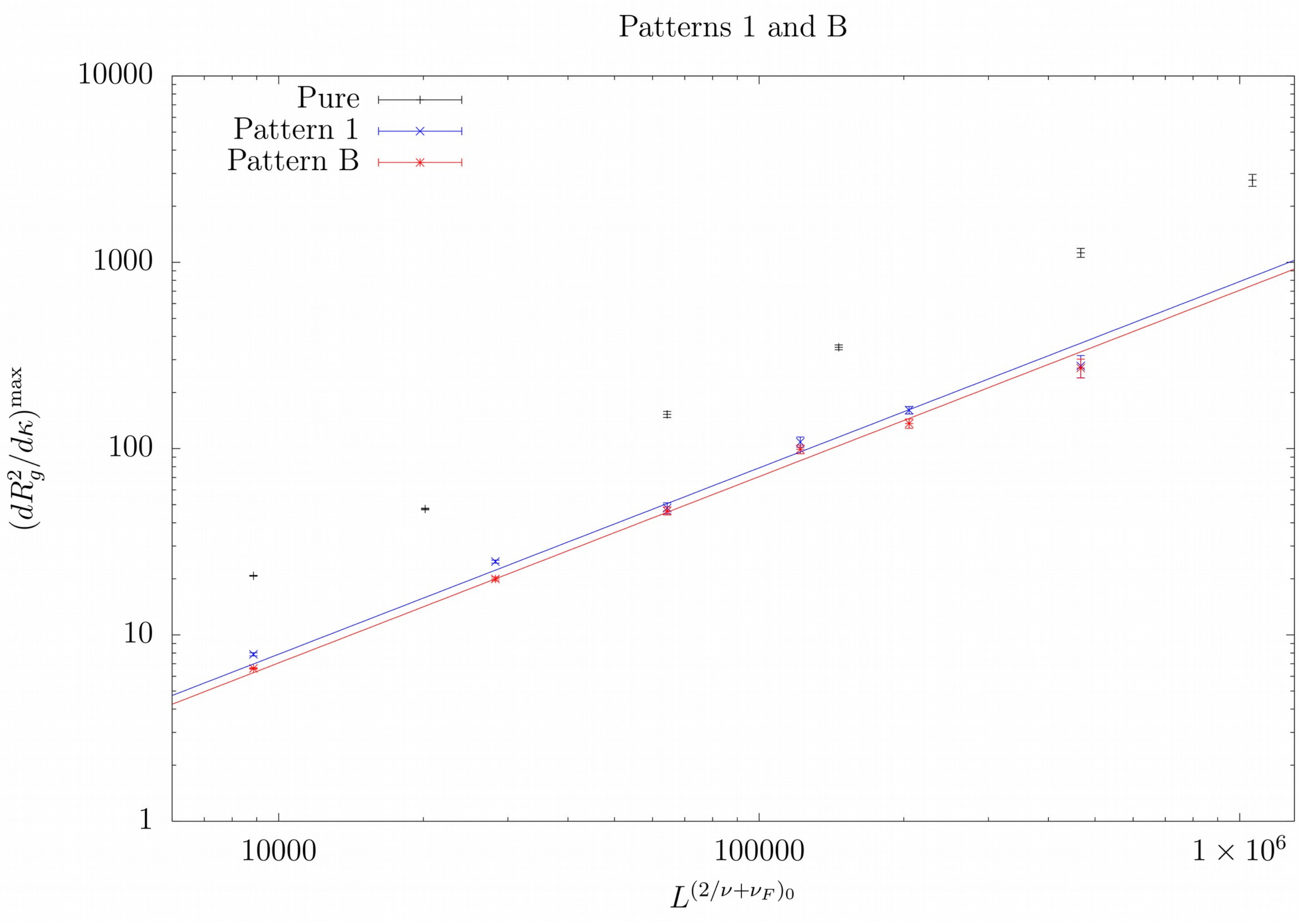






Perforated models: critical behavior

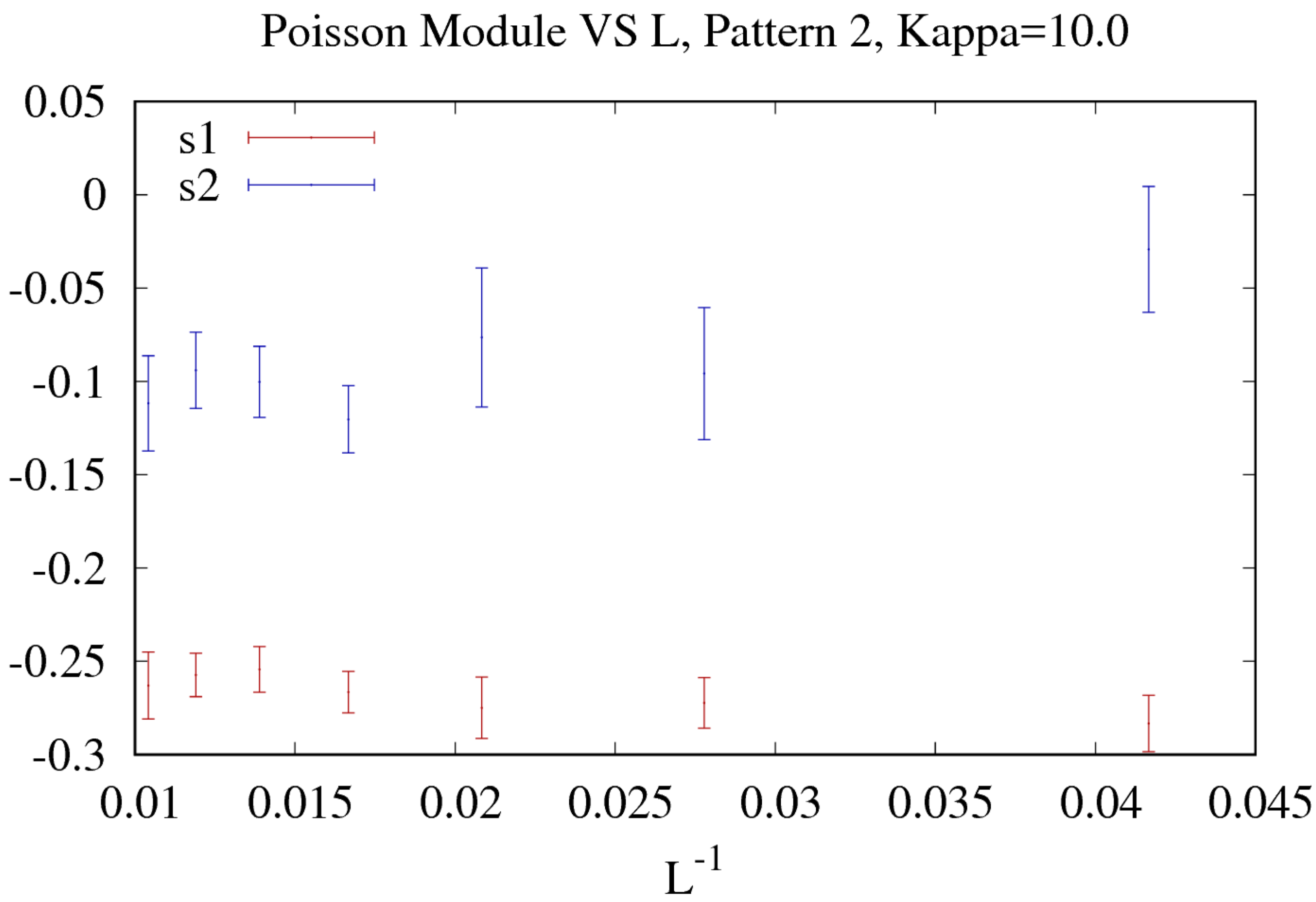
- Again, we can check with both signals the compatibility with the critical exponents of the pure model .

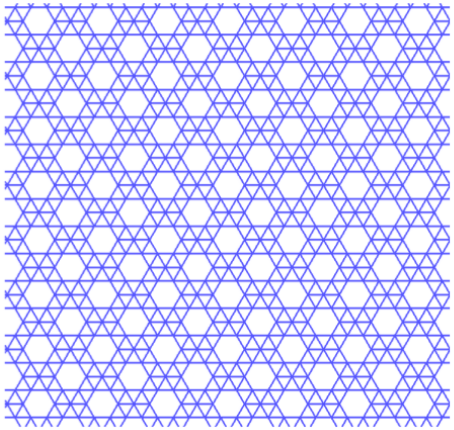


Overview

Perforated models: flat phase elasticity

- In the perforated cases, we have now anisotropy, which is also evidenced by the differences in s1 and s2





Pattern 2

Overview

Conclusions

- Following D. Yllanes, et al. (*Nature Communications 8, 1381 (2017)*), we are studying crystalline membranes using MC simulations with different patterns of perforations.
- Good agreement with the pure model for critical exponents. Disagreement with the Poisson Module (anisotropy).
- There is still quite room for numerical improvement.
- Model easily tunable. Possible next steps:
  - insert a fixed substrate and look the adhesion properties
  - insert another neighbor surface and interactions
  - simulate tubes instead of plane surfaces...

Thank you for your attention.