Effects of Thermal Fluctuations on Thin-Sheet Materials

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Questions and Motivations

Want to use materials like graphene in beyond-silicon electronics

How do thermal fluctuations affect mechanical properties?

When do we need to take thermal fluctuations into account?

Background

Explored triangle lattices with different geometries, and bond strengths.

Thermal fluctuations become relevant at length scale l_{th} [1]
$$l_{th} \sim \kappa_0 / \sqrt{(3k_B T Y_0)}$$

Mechanical Properties characterized by elastic constants: κ_0 (Bending Rigidity) and Y_0 (Young's Modulus)

Both κ_0 and Y_0 change (renormalize) with temperature in a non-trivial way: $\kappa_0 \rightarrow \kappa_R$, and $Y_0 \rightarrow Y_R$.

Elastic Constant Behavior for Isotropic Flat-Sheets

Both κ_0 and Y_0 renormalize with system size ($q \sim 1/l$) according to: [1, 2]

$$\kappa_R(l) \sim \kappa_0 \qquad l \ll l_{th} \qquad \rightarrow \qquad \kappa_R(q) \sim \kappa_0 \qquad q \gg q_{th}$$
$$\kappa_R(l) \sim \kappa_0(l/l_{th})^\eta \qquad l \gg l_{th} \qquad \kappa_R(q) \sim \kappa_0(q/q_{th})^{-\eta} \qquad q \ll q_{th} \quad (\eta \sim 0.8)$$

$$Y_R(l) \sim Y_0 \qquad l \ll l_{th}$$
$$Y_R(l) \sim Y_0(l/l_{th})^{-\eta u} \qquad l \gg l_{th} \quad (\eta u \sim 0.38)$$

Analyze height fluctuations in momentum space via Fourier transformation $h(\mathbf{x}) \rightarrow h(\mathbf{q})$. Height fluctuations are related to κ_R by:
$$\langle h(\mathbf{q})h(-\mathbf{q})\rangle \sim 1/\kappa_R(q)q^4$$

Slope of log-log plot gives η; a change in η means κ_R changes. Similarly for ηu, a change in slope for log-log plot of $Y_R(l) \sim Y_0(l/l_{th})^{-\eta u}$ means a change in Y_R.

References

(1) M. J. Bowick, A. Košmrlj, D. R. Nelson, and Ratsko Sknepnek, PRB 95, 104109 (2017)
(2) A. Košmrlj, and D. R. Nelson, PRB 93, 125431 (2016)

Acknowledgments
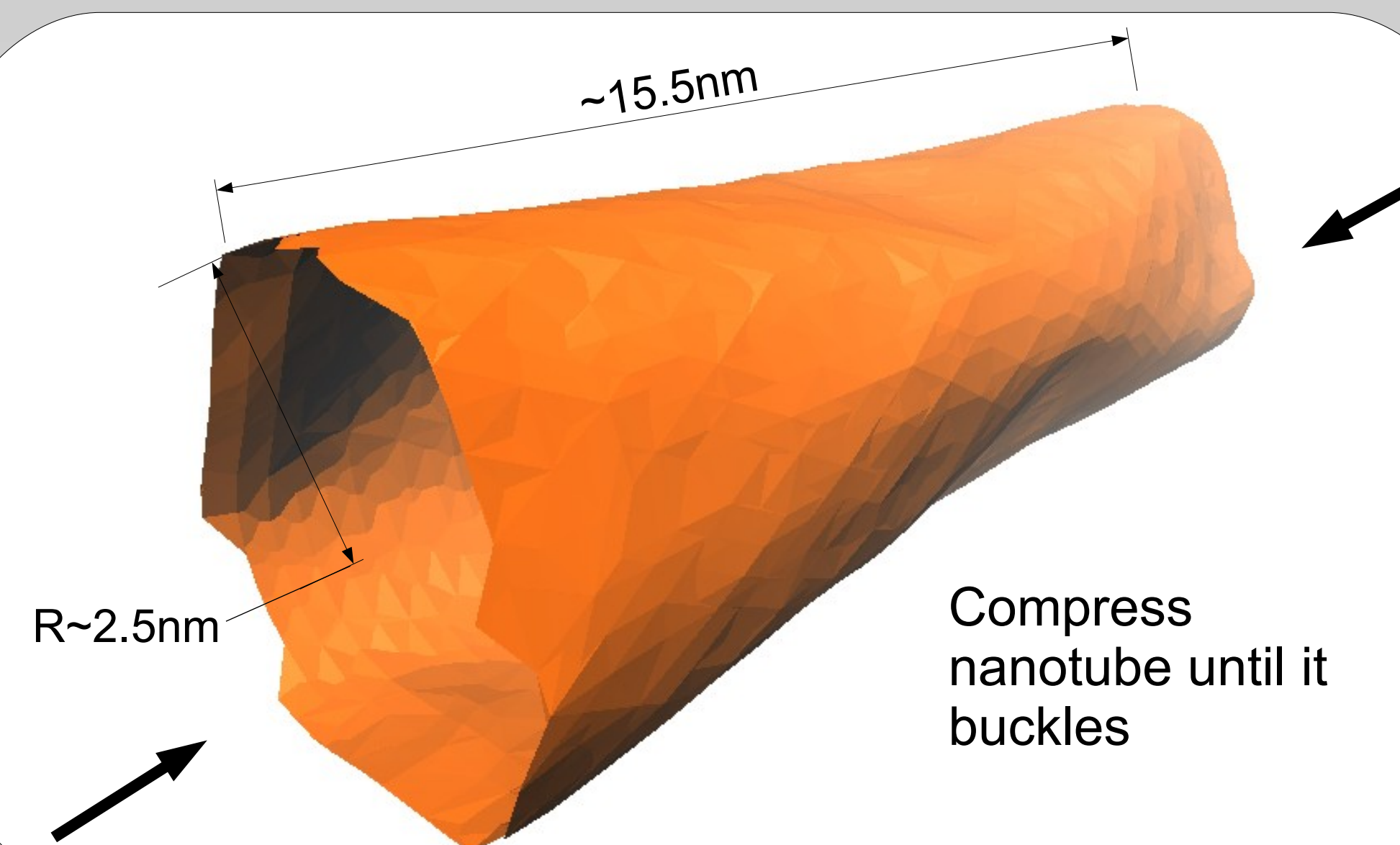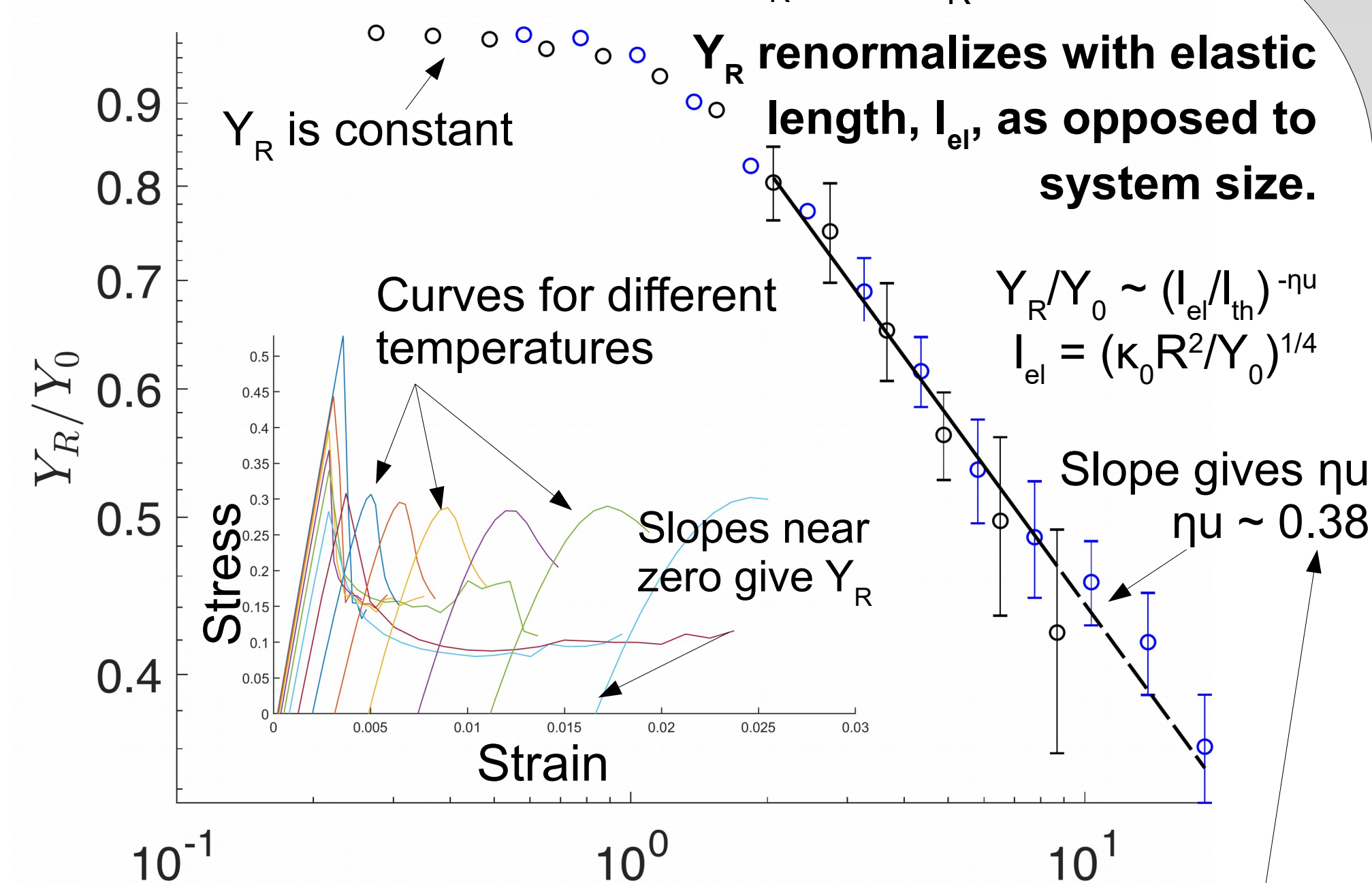
Nanotubes

~15.5nm

R~2.5nm

Compress nanotube until it buckles

Renormalization of κ_R and Y_R

Y_R is constant

Y_R renormalizes with elastic length, l_{el}, as opposed to system size.

$$Y_R/Y_0 \sim (l_{el}/l_{th})^{-\eta u}$$
$$l_{el} = (\kappa_0 R^2/Y_0)^{1/4}$$

Curves for different temperatures

Slopes near zero give Y_R

Slope gives ηu
$\eta u \sim 0.38$

Stress vs Strain (inset plot)

same values for isotropic flat-sheets!

Y_R along the longitudinal direction decreases.

$\eta \sim 0.8$

q_{el}/q_{th}

$\left(\frac{q_\varphi}{q_{th}}\right)^{-3.2}$

$\langle|h(\mathbf{q})|^2\rangle A q_{th}^4 \kappa_0/(k_B T)$

Radial Fluctuations

κ_R renormalizes with elastic length, l_{el}, as opposed to system size:

$$\kappa_R(q_\varphi) \sim \kappa_0(q_\varphi/q_{th})^{-\eta}$$
$$q_{el} \sim 1/l_{el}$$

Slopes give $\eta - 4$

Curves for different temperatures

$\left(\frac{q_\varphi}{q_{th}}\right)^{-4}$
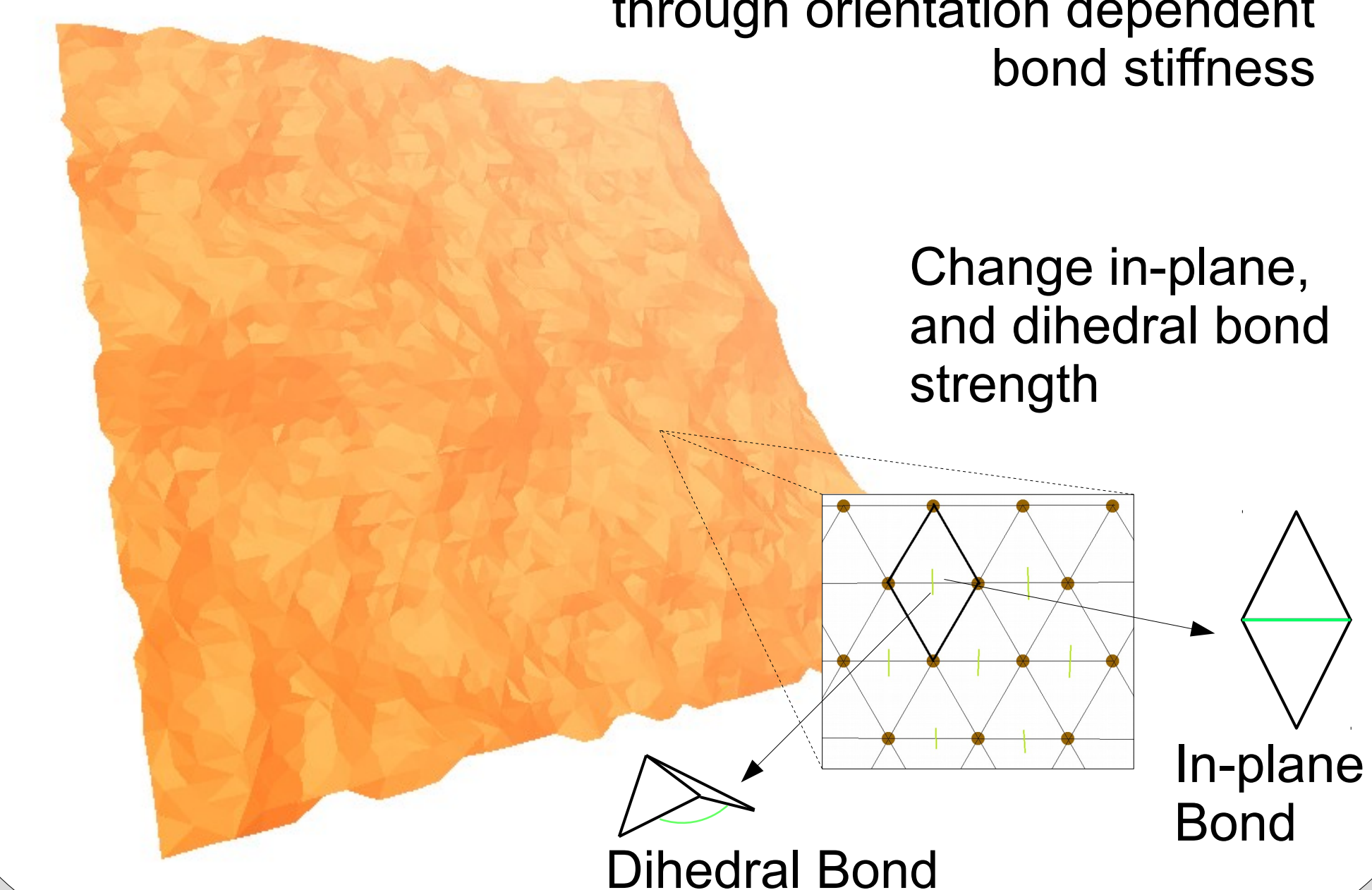
$\eta \sim 0$

q_φ/q_{th}

Bending rigidity along the azimuthal direction increases.
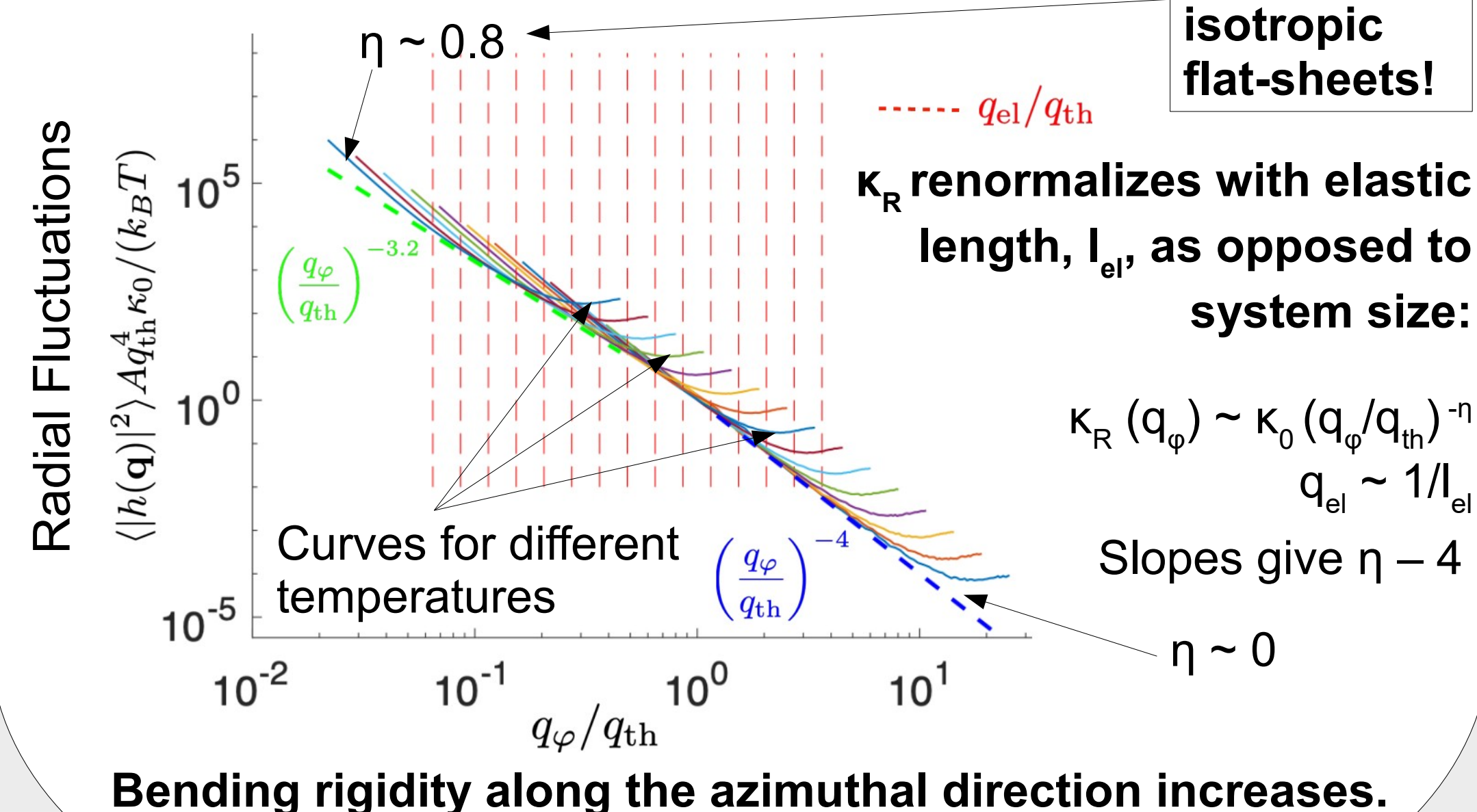
Flat-Sheets

Investigate anisoptropic flat-sheet through orientation dependent bond stiffness

Change in-plane, and dihedral bond strength

Dihedral Bond

In-plane Bond

Renormalization of κ_R

$A\kappa_0\langle|h(q)|^2\rangle q_{th}^4/(k_B T)$

Height Fluctuations

Theorized anisoptropic behavior

in-plane bond strength ratio: 1 to 20

$\eta \sim 0.8$

$\eta \sim 0$

Bending rigidity increases isotropically at higher temperatures

q/q_{th}

$A\kappa_0\langle|h(q)|^2\rangle q_{th}^4/(k_B T)$

$\eta \sim 0.8$

dihedral bond strength ratio: 1 to 10

Bending rigidity increases at higher temperatures

$\eta \sim 0$

q/q_{th}