Mean-field theories of curvature sensing and generation of isotropic and anisotropic curvature-inducing proteins

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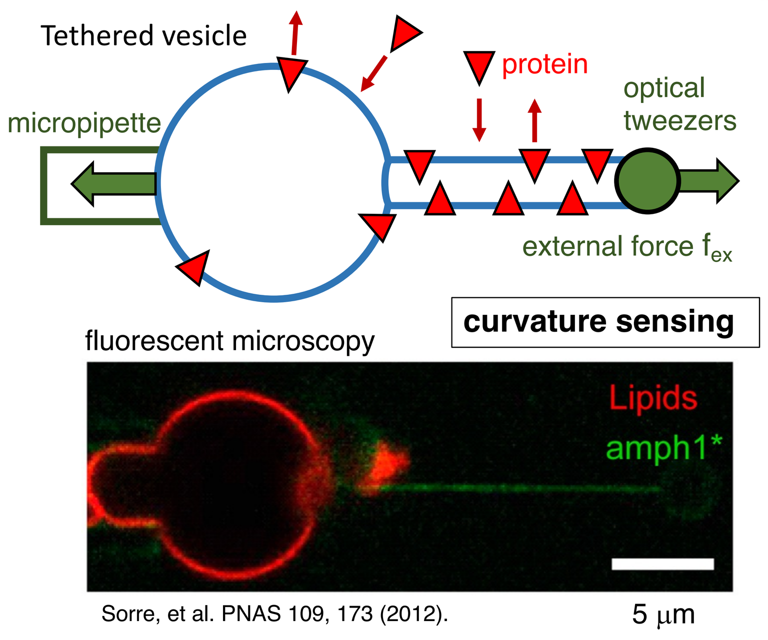
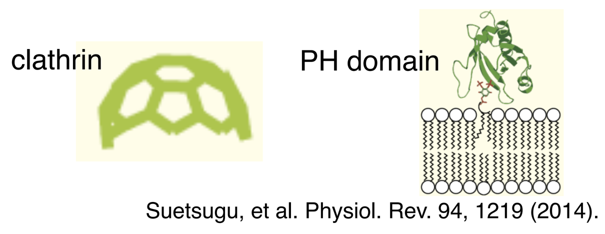
Isotropic curvature-inducing proteins generate spherical buds, and anisotropic curvature-inducing proteins (BAR etc.) generate tubules. These proteins bind more to membranes of their preferred curvatures. Here, we report mean-field theories of these protein bindings [1-4].



isotropic proteins



Free energy

$$F = F_{\rm cv} + \int {\rm d}A \left\{ -\frac{\mu}{a_{\rm p}}\phi + b\phi^2 + \frac{k_{\rm B}T}{a_{\rm p}}[\phi\ln(\phi) + (1-\phi)\ln(1-\phi)] \right\}$$

protein density; inter-protein interaction; mixing entropy

bending energy

$$F_{\rm cv} = 4\pi\bar{\kappa}_{\rm d}(1-g_{\rm ves}) + \int {\rm d}A \left\{ 2\kappa_{\rm d}H^2(1-\phi) + \frac{\kappa_{\rm p}}{2}(2H - C_0)^2\phi + (\bar{\kappa}_{\rm p} - \bar{\kappa}_{\rm d})K\phi \right\}$$

mean curvature; Gaussian curvature

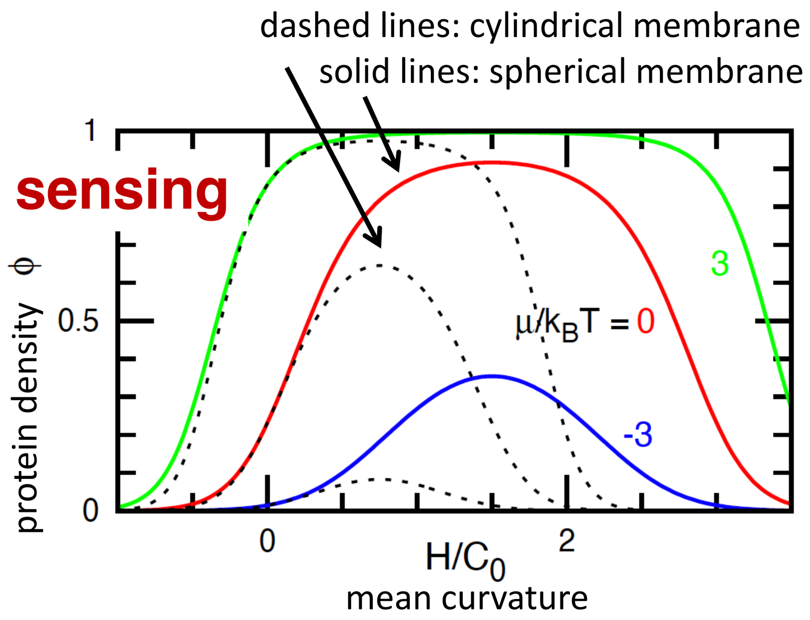
Protein binding

$$\phi = \frac{1}{1+\exp(w_{\rm b})}$$

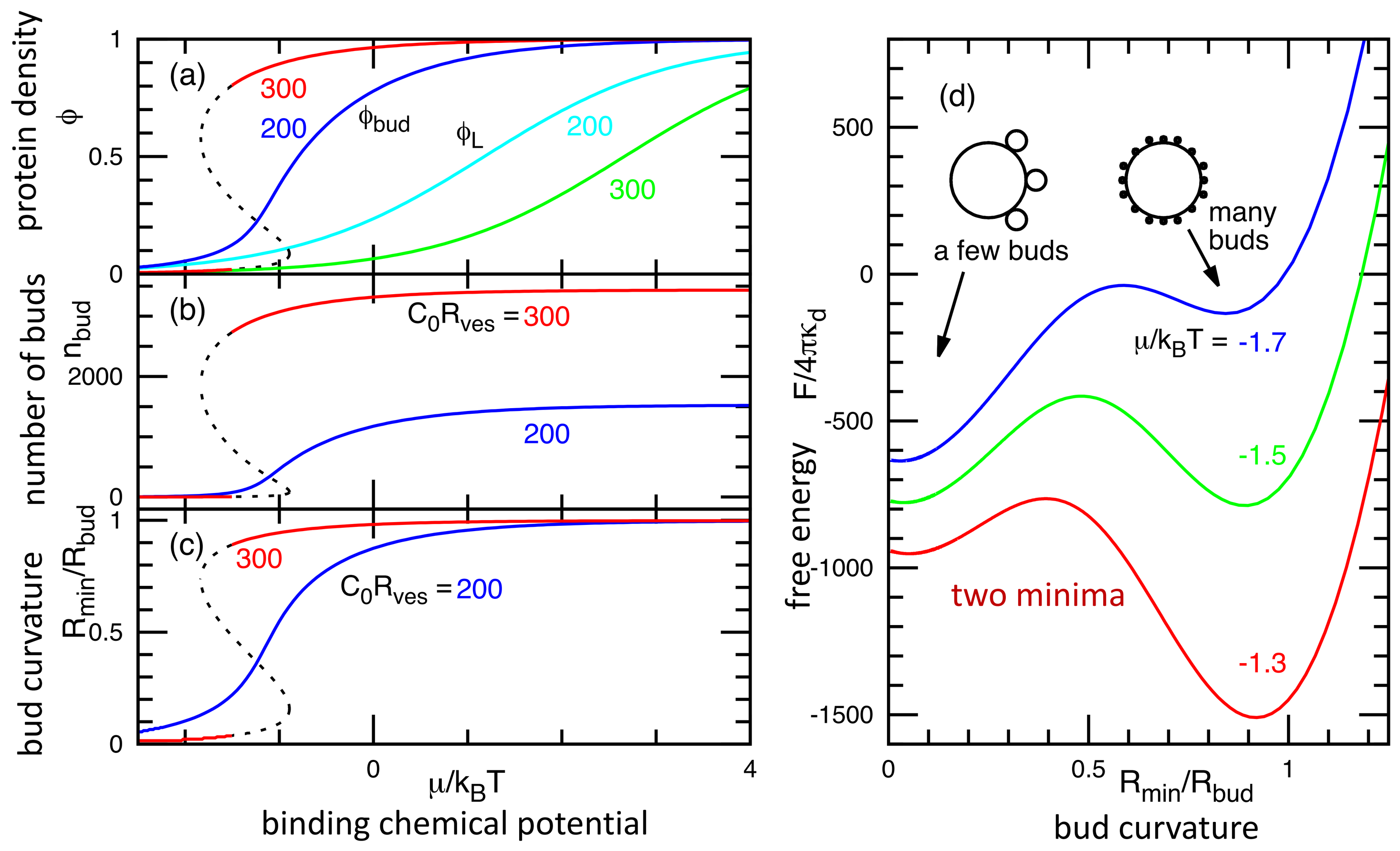
$$w_{\rm b} = -\frac{\mu}{k_{\rm B}T} + \frac{a_{\rm p}}{k_{\rm B}T}\Big[2(\kappa_{\rm p} - \kappa_{\rm d})H^2 + (\bar{\kappa}_{\rm p} - \bar{\kappa}_{\rm d})K - 2\kappa_{\rm p}C_0H + \frac{\kappa_{\rm p}C_0^2}{2}\Big]$$

curvature sensing

analytically determined at b = 0



Formation of many buds in vesicle



First-order transition from a few buds of large radius to many buds of small radius

Binding onto membrane tube

force along tube axis

$$f_{\rm ex} = \left\{ \left[\left(\frac{\kappa_{\rm p}}{\kappa_{\rm d}} - 1\right)\phi + 1 \right] \left(\frac{1}{R_{\rm cy}C_{\rm s}} - 1 \right) + 1 \right\} f_{\rm s}$$

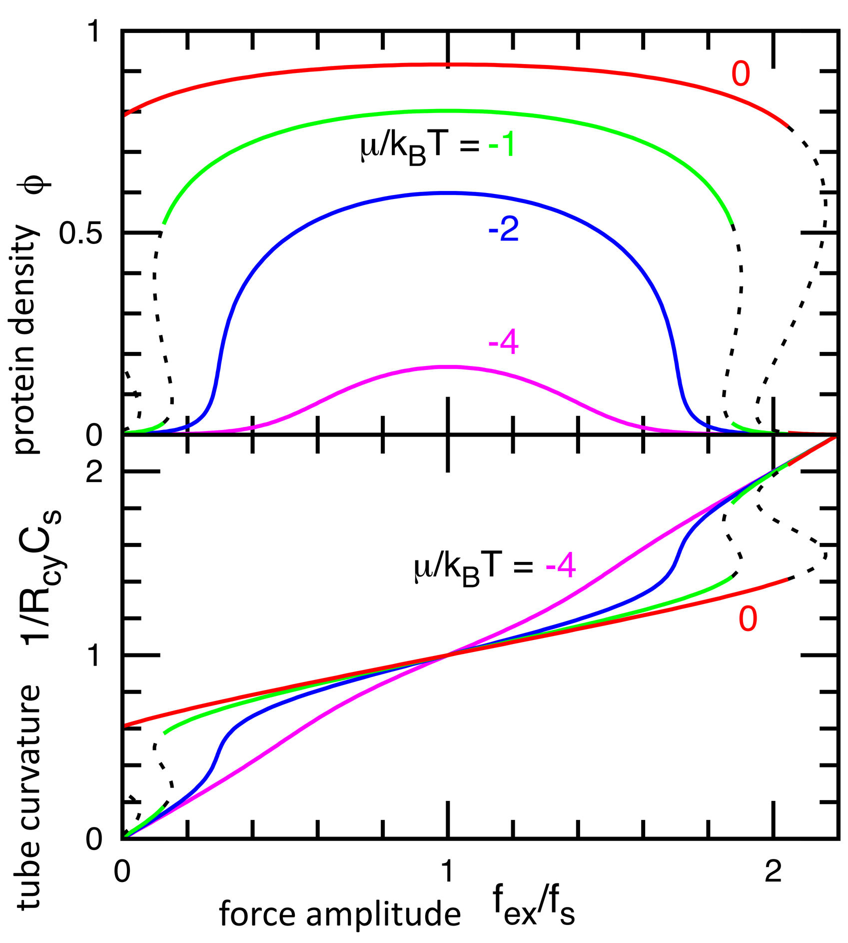
sensing curvature

$$C_{\rm s} = \kappa_{\rm p}C_0/(\kappa_{\rm p} - \kappa_{\rm d})$$

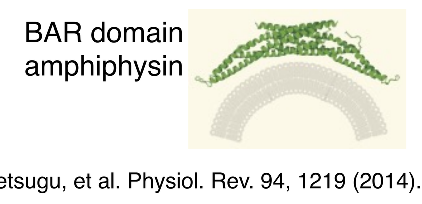
$$f_{\rm s} = 2\pi\kappa_{\rm d}C_{\rm s}$$

Symmetric with respect to $f_{ex} = f_0$

Two first-order transitions



anisotropic proteins



Free energy

$$F_{\rm p} = \int {\rm d}A \frac{\phi k_{\rm B}T}{a_{\rm p}} \left[\ln(\phi) + \frac{S\Psi}{2} - \ln\left(\int_{-\pi}^{\pi} w(\theta_{\rm ps})\,{\rm d}\theta_{\rm ps} \right) \right]$$

$$w(\theta_{\rm ps}) = g\exp[\Psi s_{\rm p}(\theta_{\rm ps}) + \bar{\Psi}\sin(\theta_{\rm ps})\cos(\theta_{\rm ps}) - U_{\rm p}/k_{\rm B}T]\Theta(g)$$

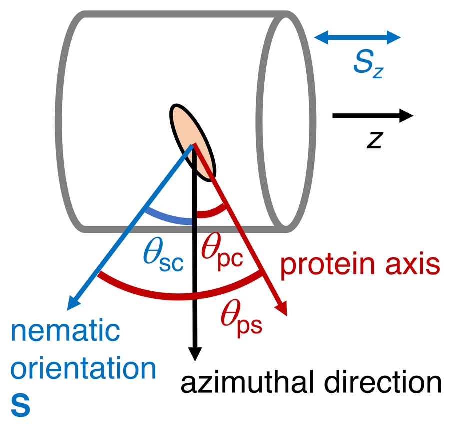
excluded-area term

$$g = 1 - \phi(b_0 - b_2Ss_{\rm p}(\theta_{\rm ps}))$$

orientational order

$$S = 2\langle s_{\rm p}(\theta_{\rm ps})\rangle$$

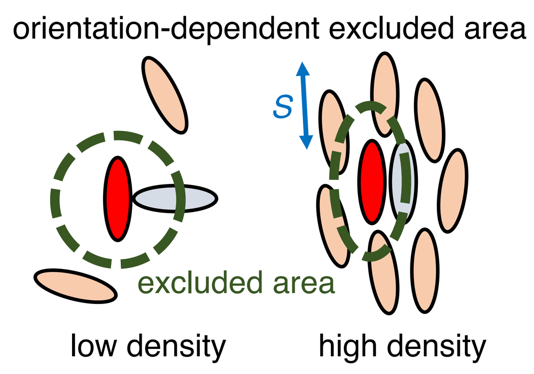
$$s_{\rm p}(\theta_{\rm ps}) = \cos^2(\theta_{\rm ps}) - 1/2$$



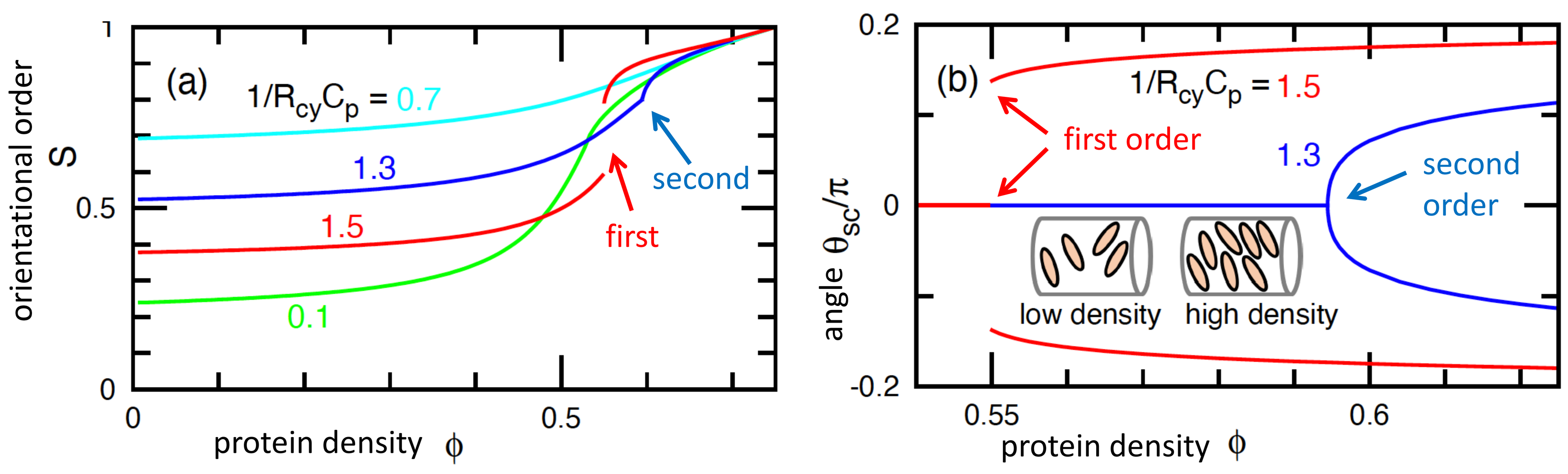
Anisotropic bending energy

$$U_{\rm p} = \frac{\kappa_{\rm pm}a_{\rm p}}{2}(C_{\ell 1} - C_{\rm p})^2$$

$$C_{\ell 1} = C_1\cos^2(\theta_{\rm pc}) + C_2\sin^2(\theta_{\rm pc})$$



Nematic transition in narrow tubes



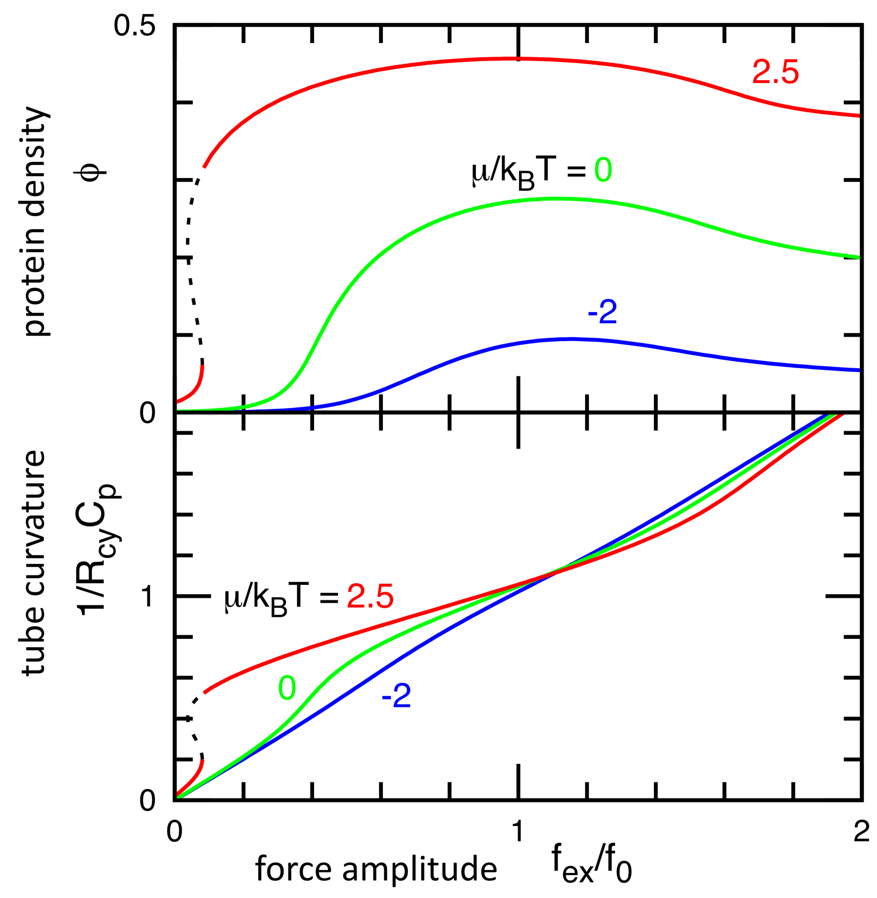
First- and second-order transitions

Binding onto membrane tube

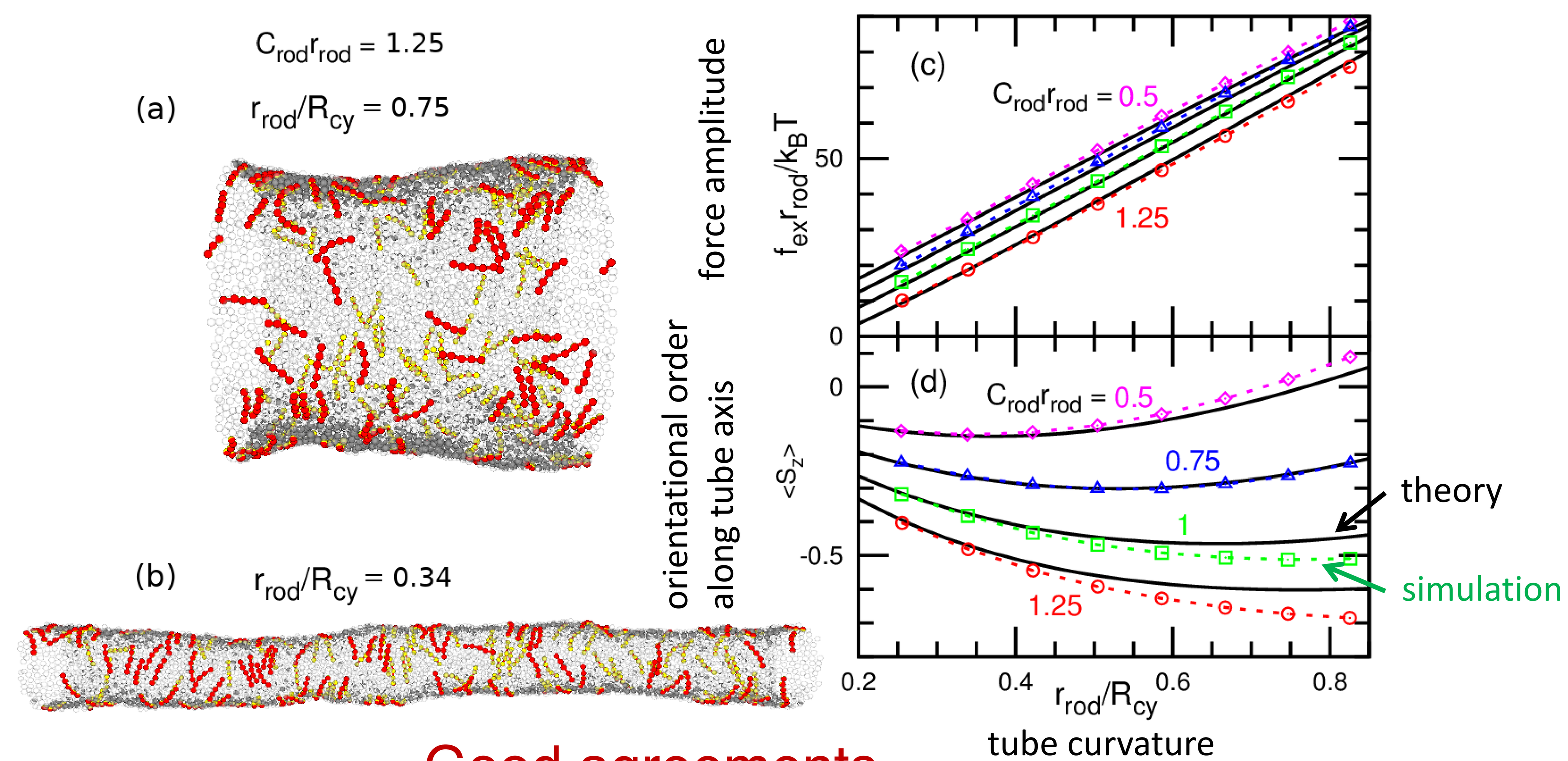
Non-symmetric

One first-order transition

Sensing curvature depending on chemical potential



Comparison with meshless simulations



Good agreements

[1] H. Noguchi, Phys. Rev. E. **104**, 014410 (2021).
[2] H. Noguchi, Soft Matter **17**, 10469 (2021).
[3] H. Noguchi, C. Tozzi, and M. Arroyo, Soft Matter **18**, 3384 (2022).
[4] H. Noguchi, Int. J. Mod. Phys. B **36**, 2230002 (2022).