Title: Phase behavior of long worm-like chain confined in a cavity

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Abstract:

Free energy, density profile and segmental orientation of a long semiflexible polymer confined in a cavity

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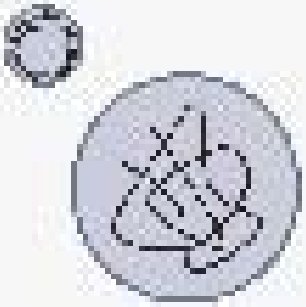
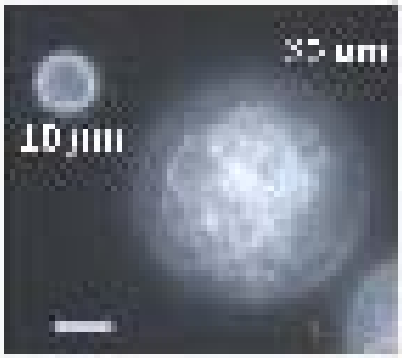
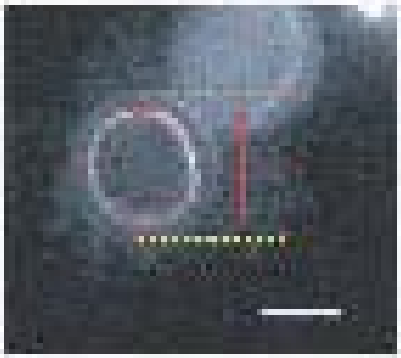
2013 Waterloo Soft Matter Theory

Wormlike chain in a cavity

Semiflexible polymers confined in droplets



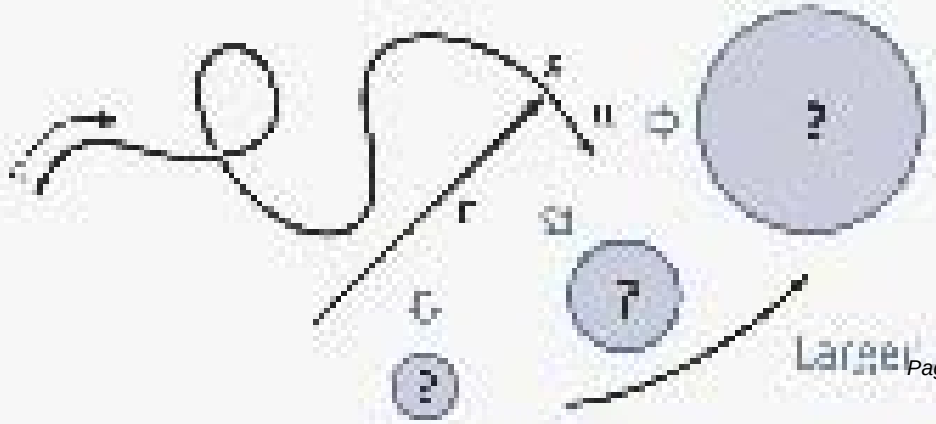




M. Chaumont, Nov. Phys., 2006
M. Chaumont, Nov. Mater., 2006

WLC in a sphere of radius R

? Entropy penalty
? Scaling laws
? Density distribution



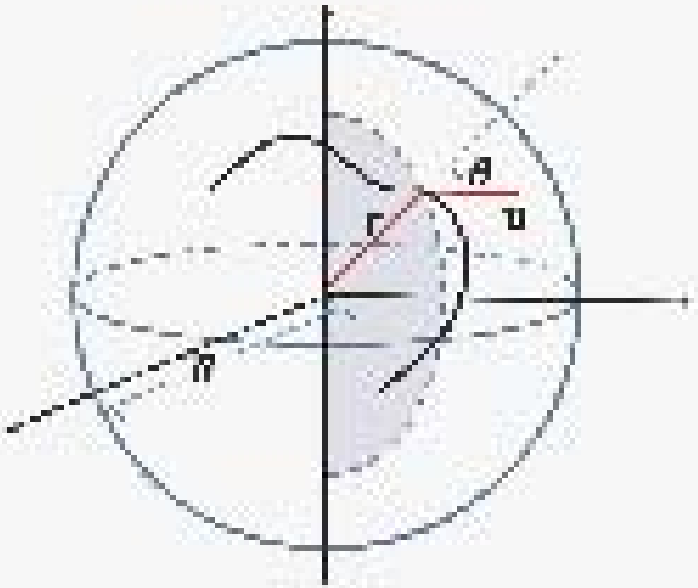
Ground-state dominance

Probability density

$$P[u(s)] \propto \exp\left[-\int_0^L ds \frac{\lambda}{2}\left(\frac{du(s)}{ds}\right)^2\right]$$

Ground-state dominance approximation

$$-\beta\mu\Psi_0(\vec{r},\theta,s) = \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) - \frac{a}{R}\cos\theta\frac{\partial}{\partial r} + \frac{a}{R}\frac{\sin\theta}{r}\frac{\partial}{\partial\theta}\right]\Psi_0(\vec{r},\theta,s)$$



a: Kuhn's length of the chain

✓ Free energy

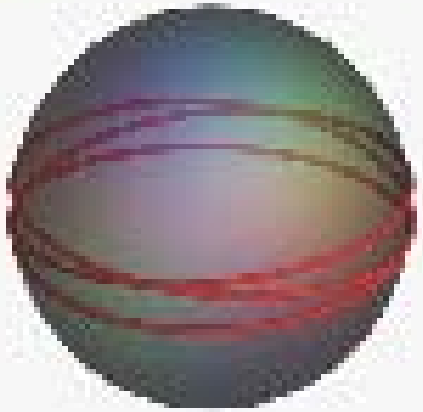
$$\beta F = (L/s)\mu + \ldots$$

✓ Density profile

$$\rho(\vec{r}) \propto \int_0^{\pi} \Psi_0(\vec{r},\theta)\Psi_0(\vec{r},\pi-\theta)\sin\theta d\theta$$

Small radius and large radius limits

For $R/a \ll 1$ cases



For $R/a \gg 1$ cases

Reduced free energy

$$\beta\mu = \frac{1}{4}\left(\frac{a}{R}\right)^2$$

Bending penalty dominance

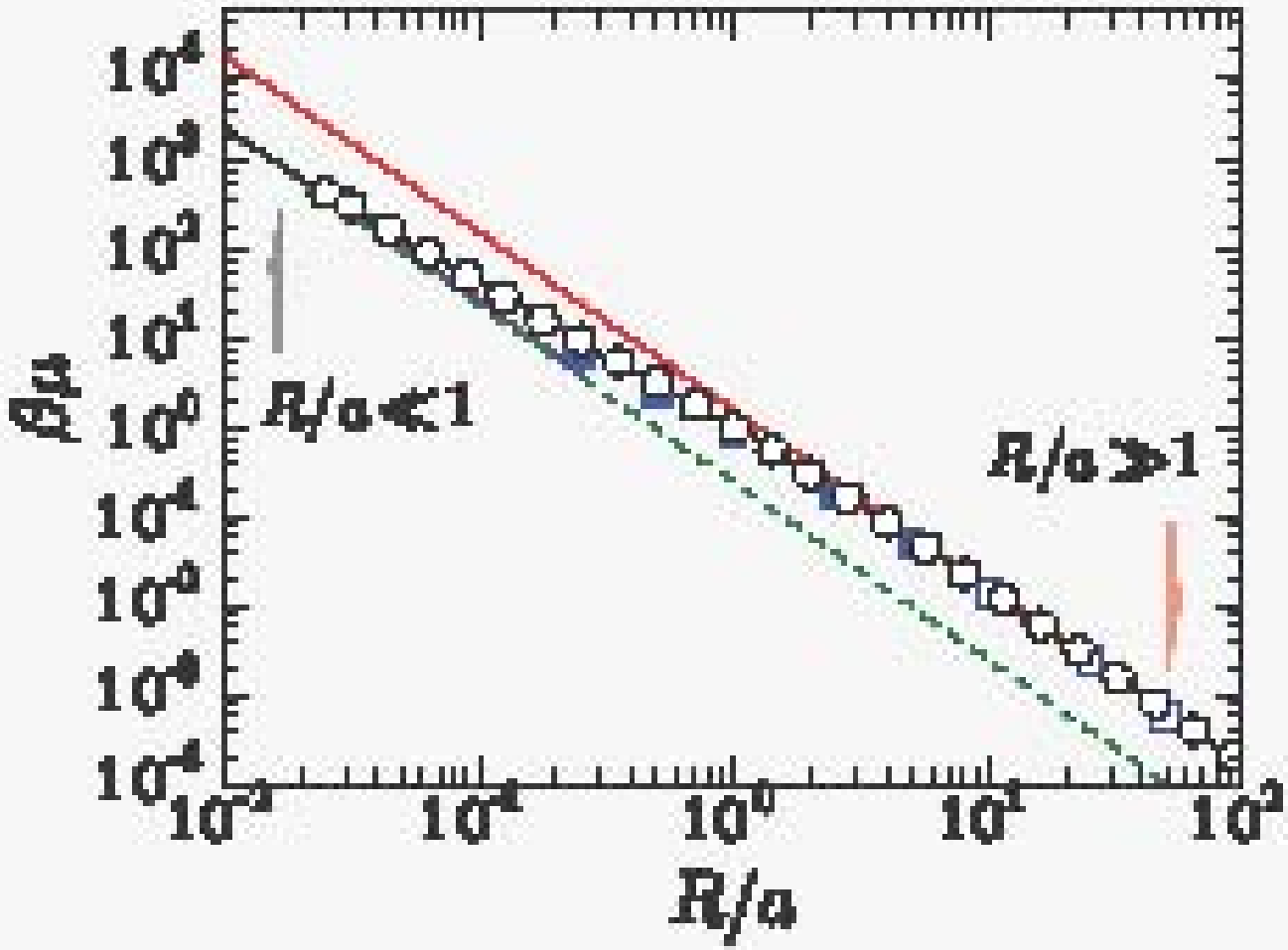
Reduced free energy

$$\beta\mu = \frac{\pi^2}{6}\left(\frac{a}{R}\right)^2$$

Back to a Gaussian chain

* Pictures on the left comes from: J. Gao et al., Phys. Rev. E, 2012

Crossover region: numerical results

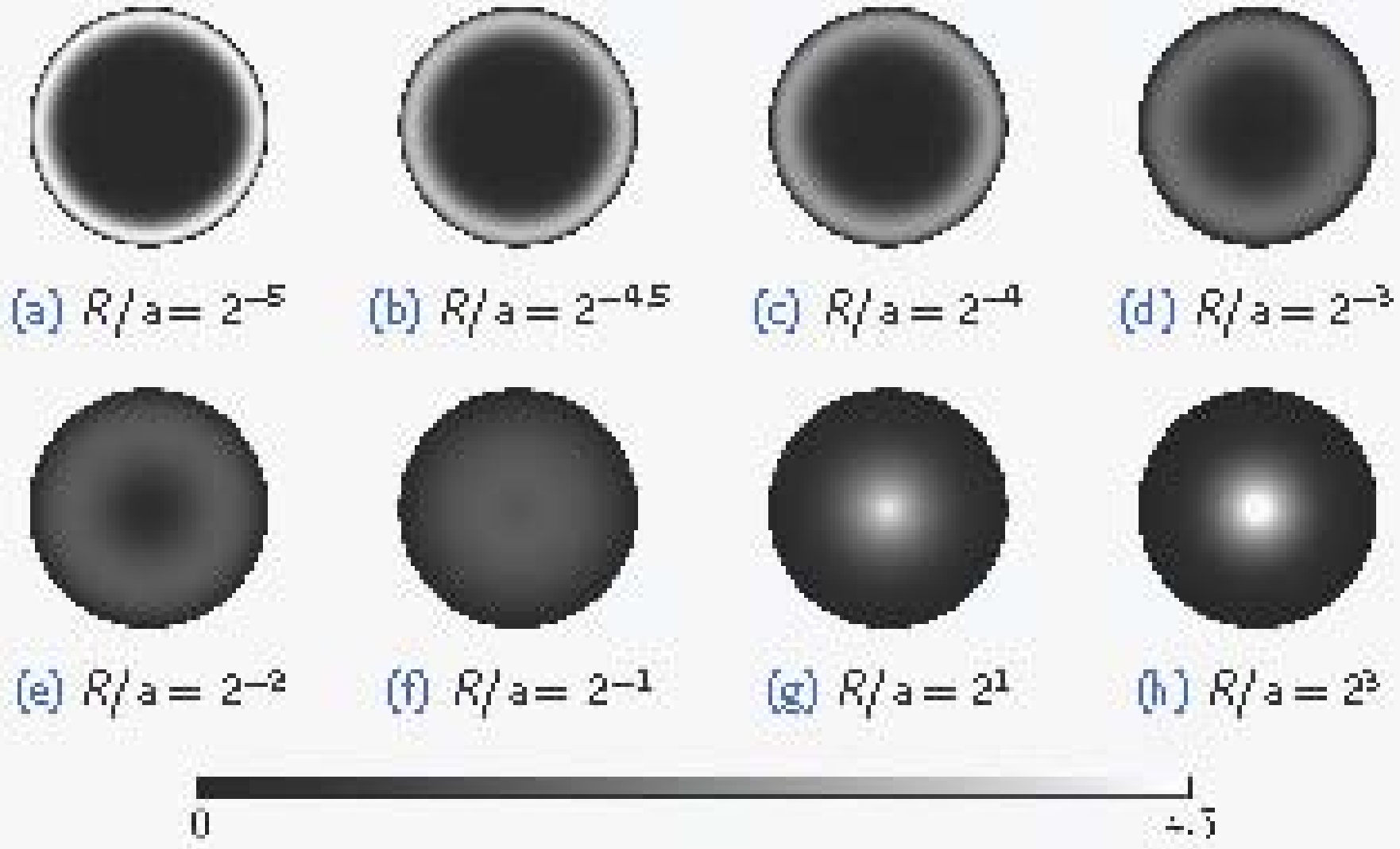


- Data by M. Smyda* using Monte Carlo
- — Analytical prediction by G. Morrison†

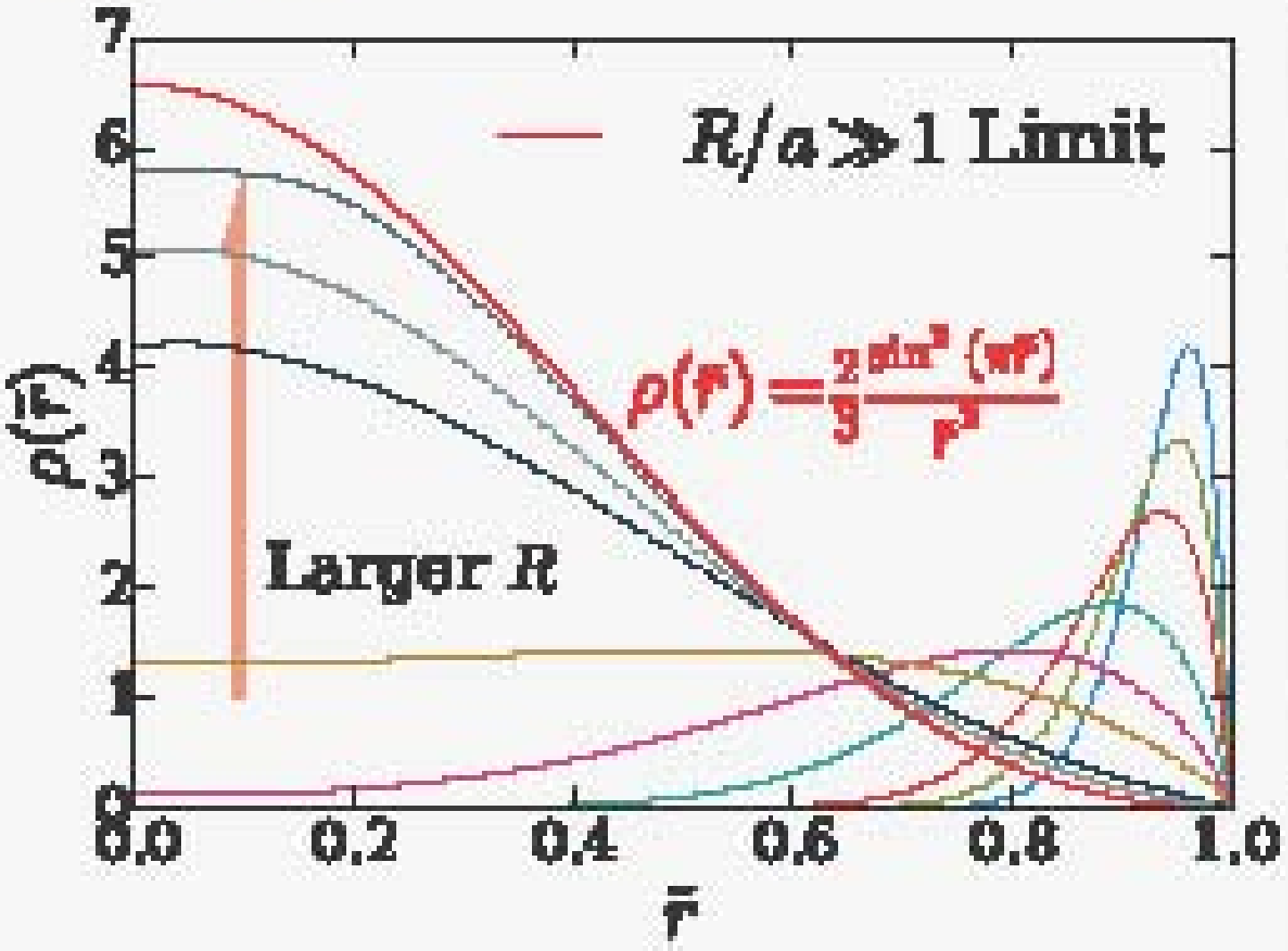
* M. Smyda et al, J. Phys. Chem. B, 2012

† G. Morrison et al, Phys. Rev. E, 2009

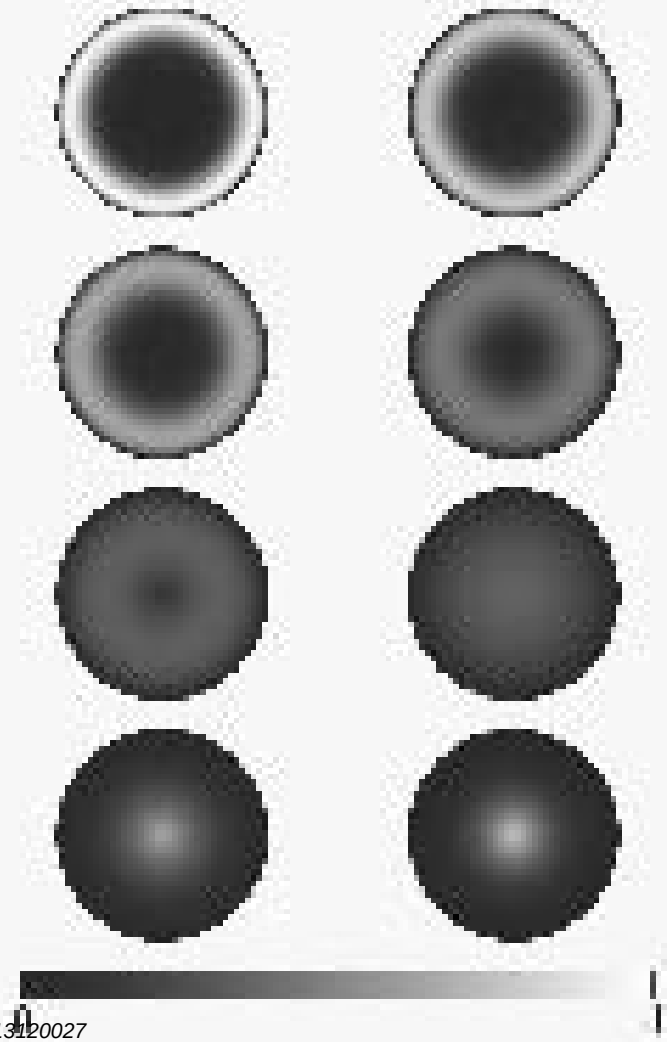
Density profiles

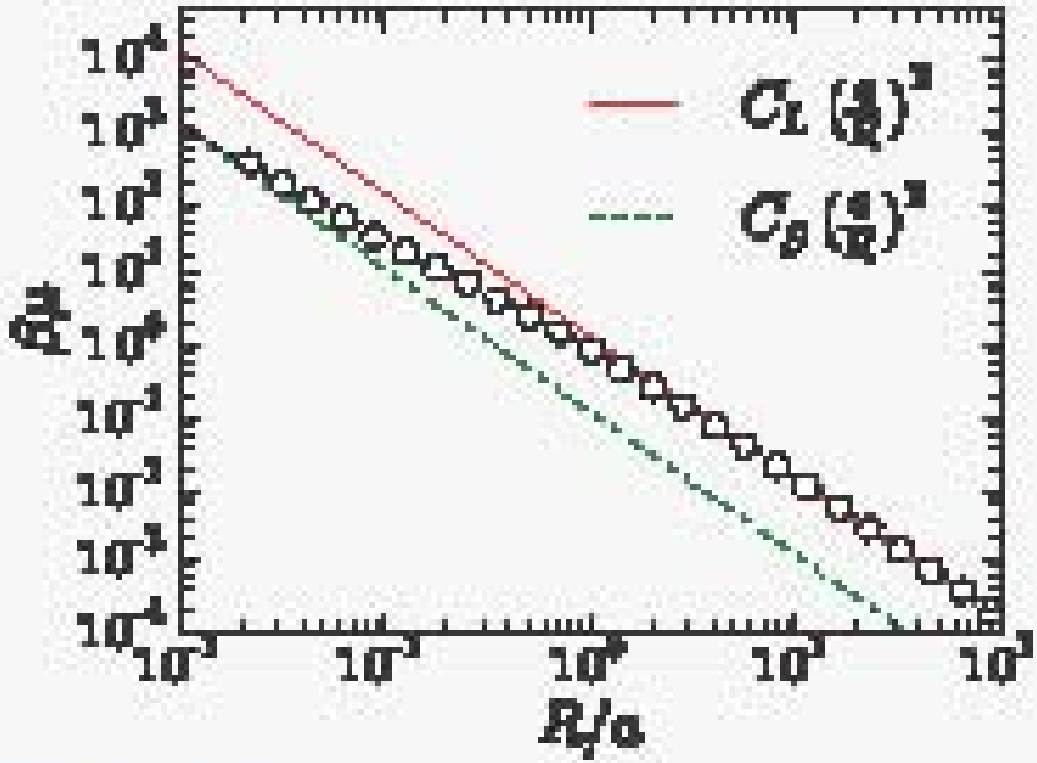


Density profiles



WLC in 2D circular confinement





$R/a \gg 1$ limit

$$C_L = 1.44590\ldots$$

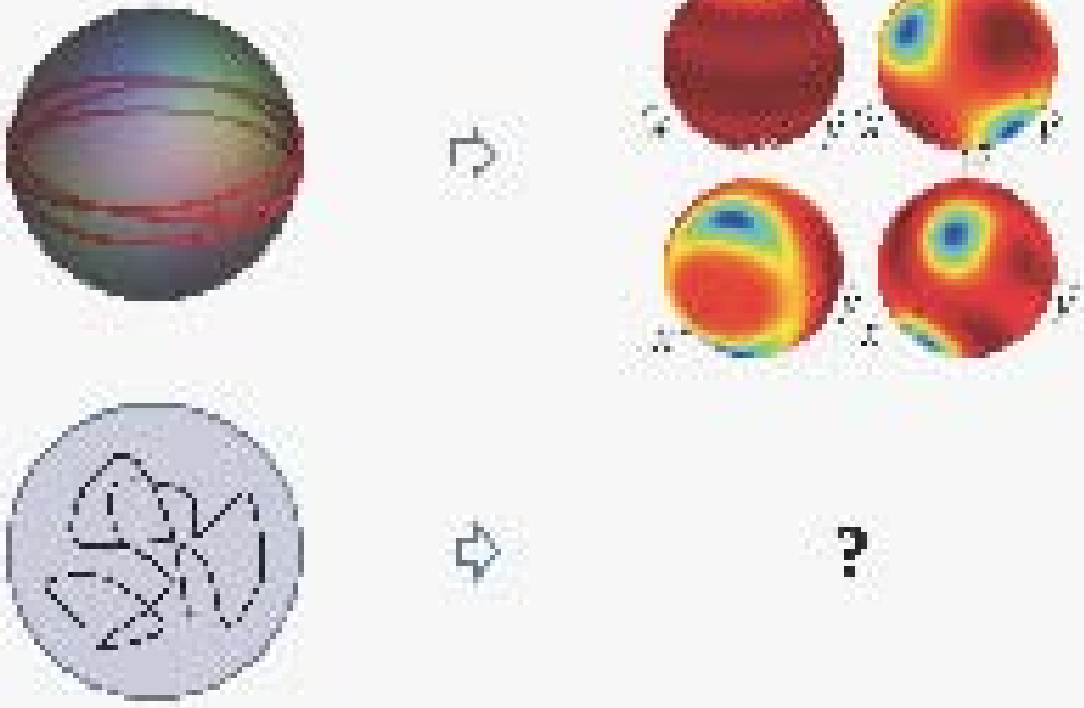
$R/a \ll 1$ limit

$$C_S = 1/8$$

Outlook

Excluded-volumn

$$P[u(s), w] \propto \exp\left[-\int_0^L ds\, w(r(s), u(s))\right] \times \exp\left[-\int_0^L ds \frac{\lambda}{2}\left(\frac{du(s)}{ds}\right)^2\right]$$



Acknowledgements

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Publications:

- J. Gao *et al.*, *Soft Matter* 7, 5208 (2011)
- J. Gao *et al.*, *Soft Matter* 9, 69 (2013)
- J. Gao , P. Tang and Jeff Z. Y. Chen (*In preparation*)

Thanks for your attention.

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