Statistical Mechanics of a polymer chain attached to the interface of a cone shpaed channel

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Thanks
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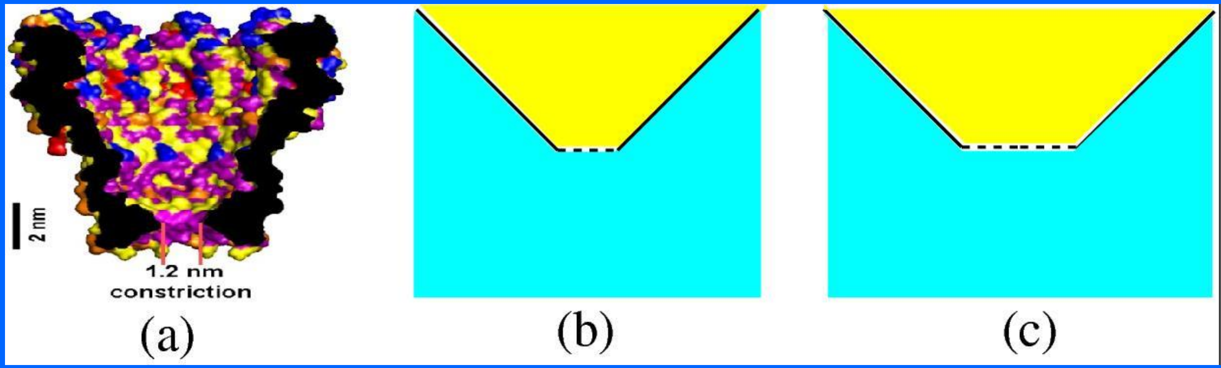
Outline

- Introduction
- Model
- Method
- Results
- Conclusions

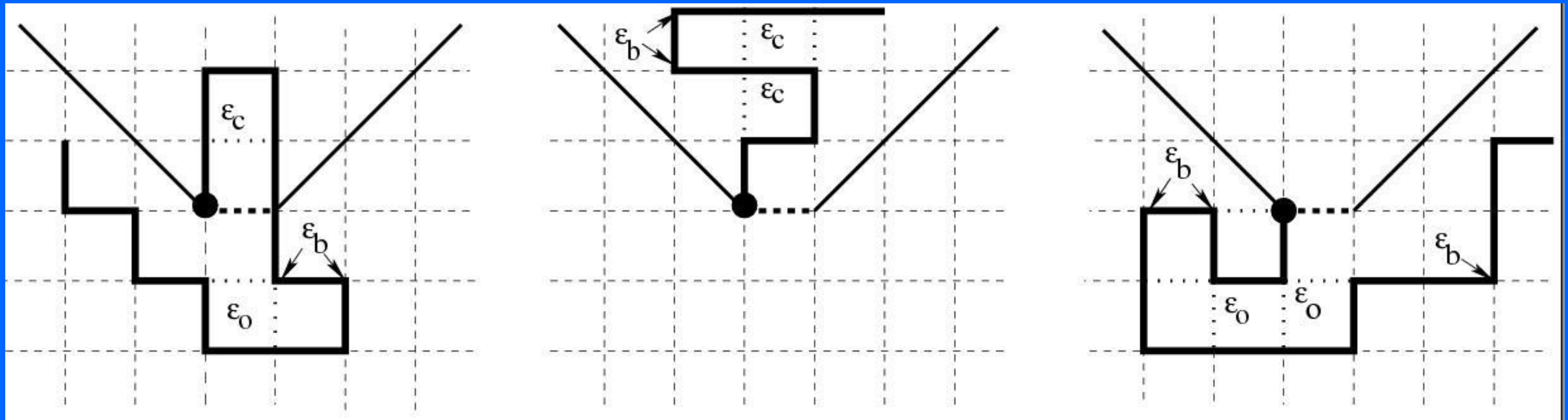
Polymer Confined in nano-scale geometry

- Translocation
- Transport of proteins from Nucleus
- Ejection of viral DNA from Capsid
- DNA sequencing
- Protein sensing etc



Derrington et al PNAS 107, 16060 (2010)
Kumar et al EPL (Under Review)

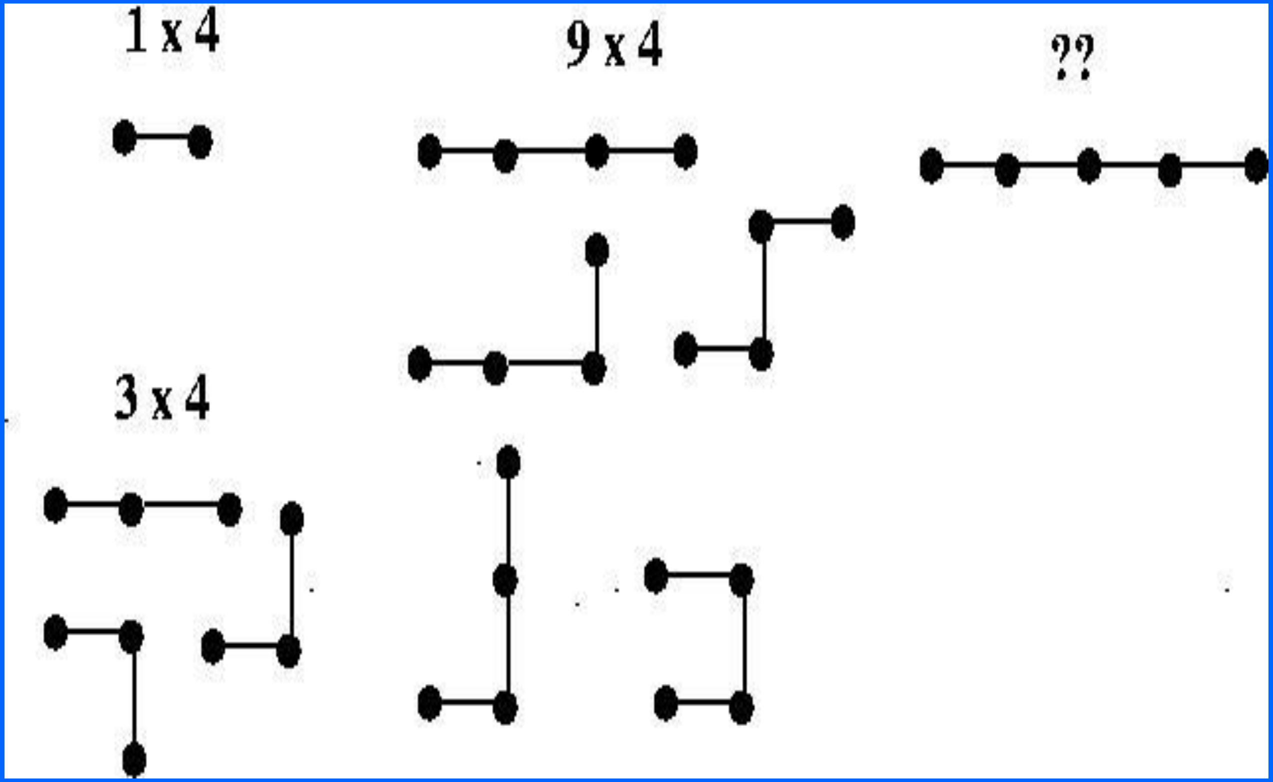
Lattice model of polymer chain in a confined channel



(a) (b) (c)

$$Z(T) = \sum_{N=0}^{\infty} C_N(N_{pc}, N_{po}, N_b,)\, u^{N_{pc}} \omega^{N_{po}} b^{N_b}$$

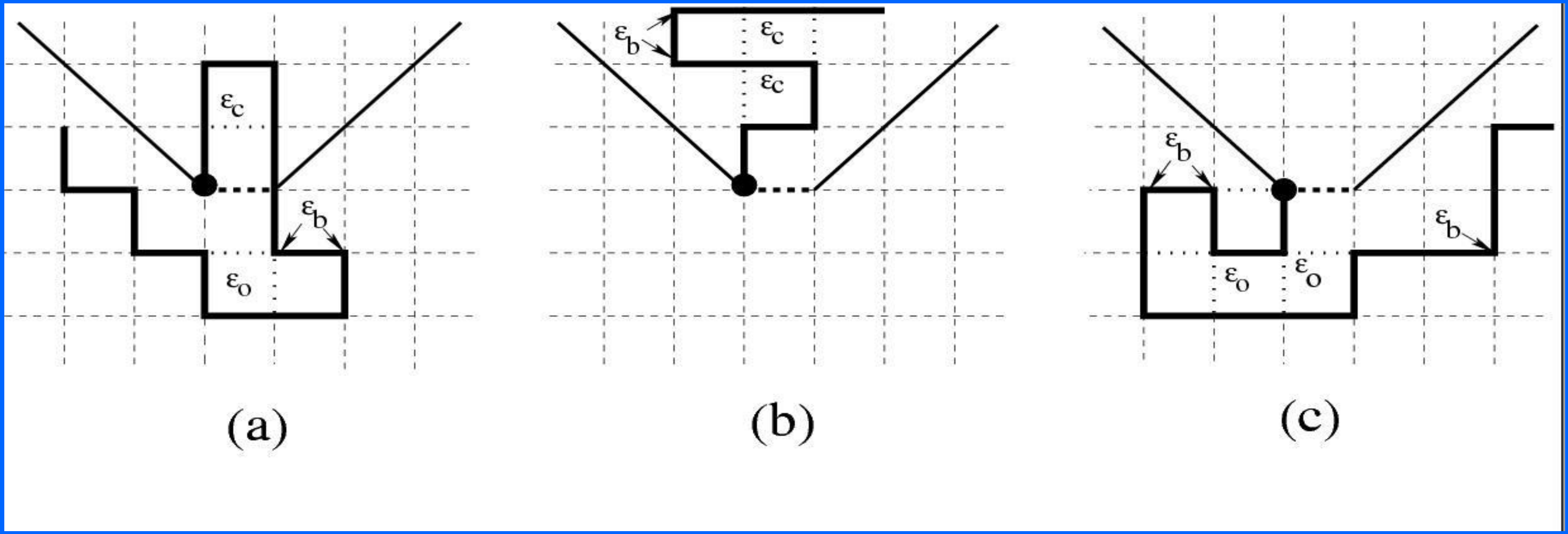
Exact Enumeration technique:



$$C_N = \mu^N N^{\gamma - 1}$$

Phase transition and Critical Phenomena,Vol.3 &13 Guttmann (1989)

Observables:



$$< N_{pc} > = \sum_{N=0}^{N} N_{pc} C_N(N_{pc}, N_{po}, N_b)\, u^{N_{pc}} \omega^{N_{po}} b^{N_b}$$

$$< N_{pc}^2 > = \sum_{N=0}^{N} N_{pc}^2 C_N(N_{pc}, N_{po}, N_b)\, u^{N_{pc}} \omega^{N_{po}} b^{N_b}$$

$$u = \exp(-\varepsilon_c / KT)$$

$$\omega = \exp(-\varepsilon_o / KT)$$

$$b = \exp(-\varepsilon_b / KT)$$

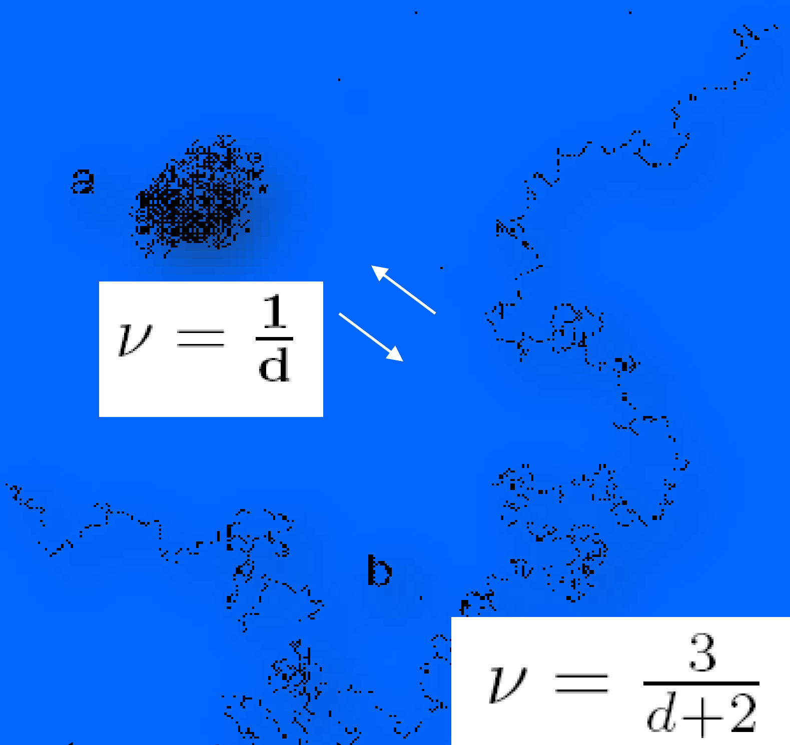
$$\chi = < N_{pc}^2 > - < N_{pc} >^2$$

Coil-Globule transition

A polymer chain in a solvent may always remain in swollen (coil) form or may undergo a transition from coil to globule.

- The solvent in which polymer chain always remains in coil state is known as Good Solvent

- A solvent in which the polymer chain undergoes coil-globule transition is Poor Solvent



$$\nu = \frac{1}{d}$$

$$\nu = \frac{3}{d+2}$$

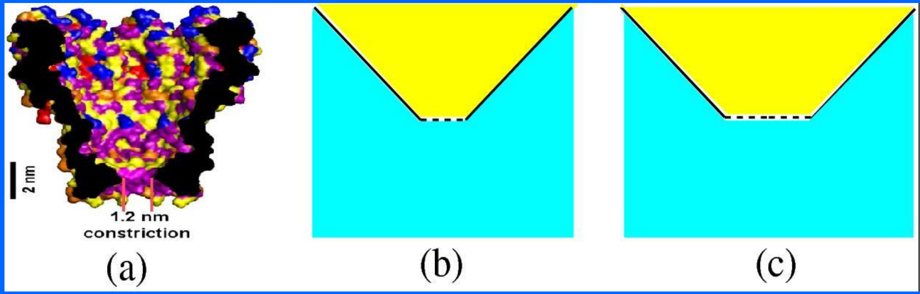
$$u = \exp(-\varepsilon_c / KT)$$

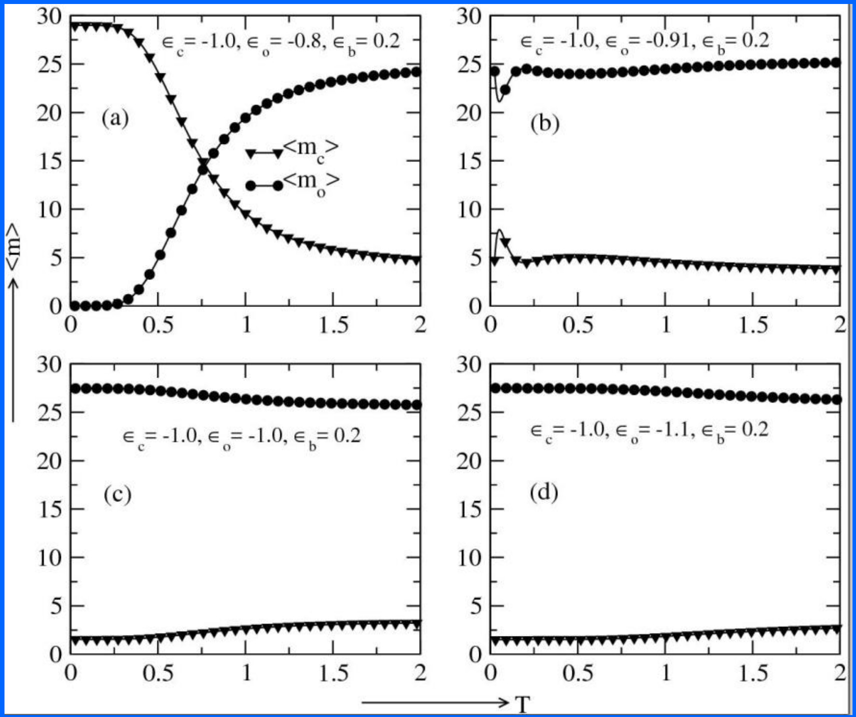
$$\omega = \exp(-\varepsilon_o / KT)$$

$$b = \exp(-\varepsilon_b / KT)$$

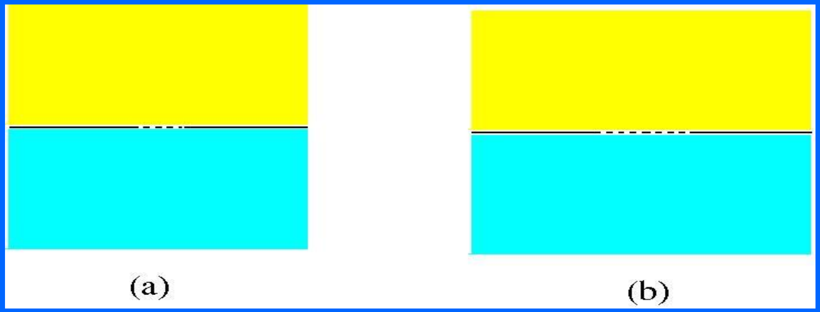
$$R_E \sim N^{\nu}$$

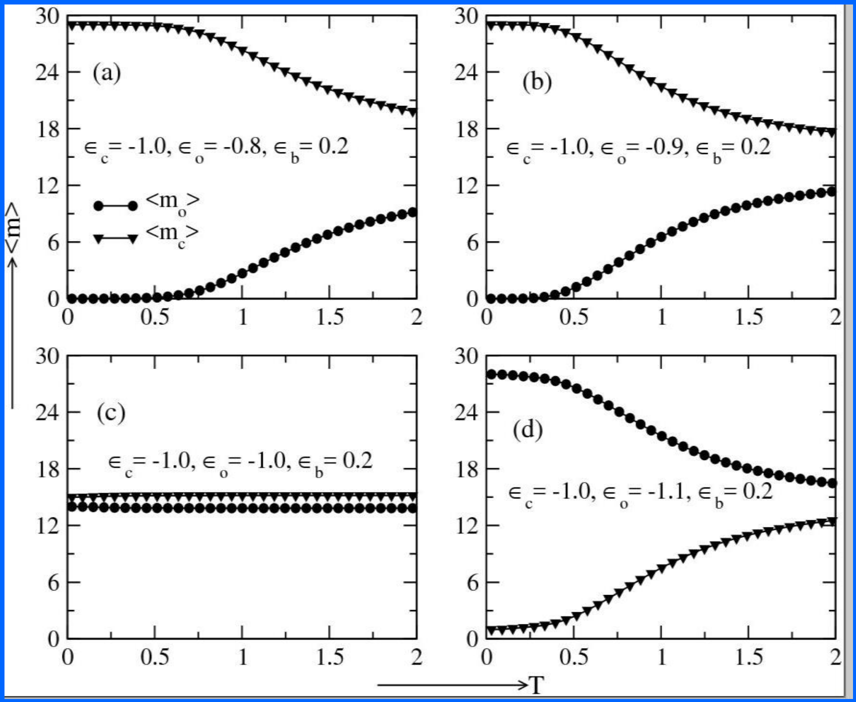
Polymer attached to a cone



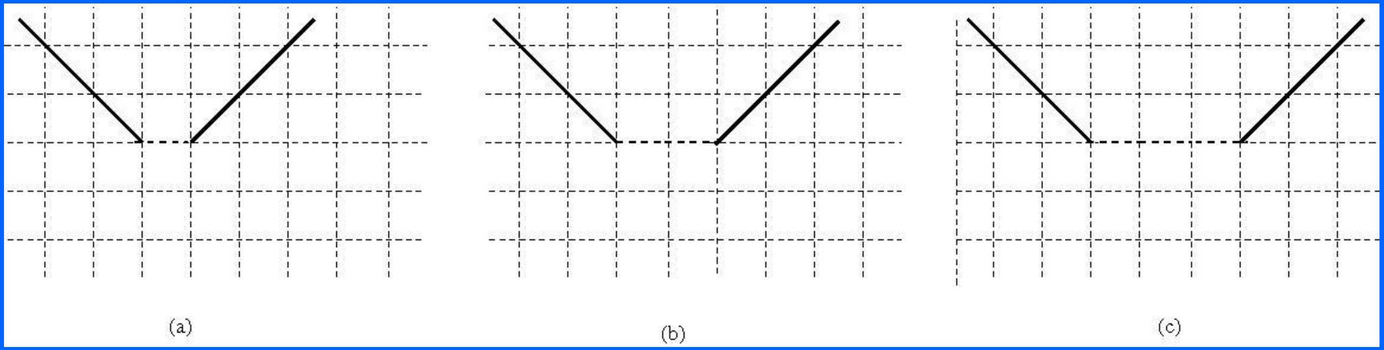


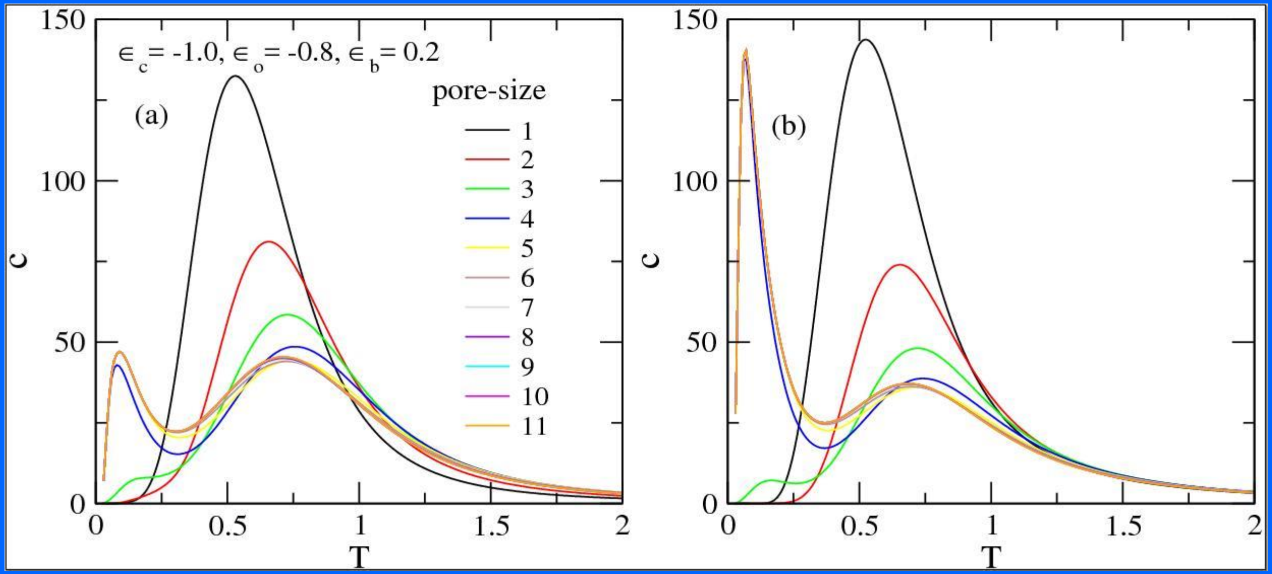
Polymer attached to a flat surface



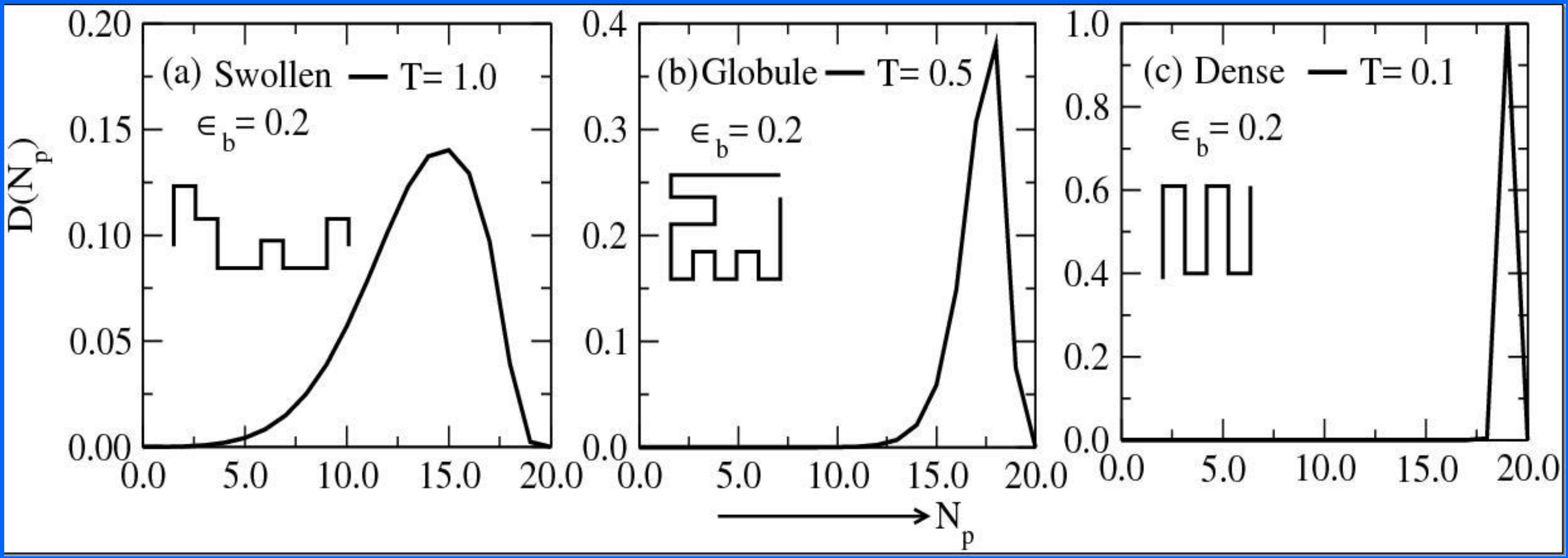


Effect of pore size





Absence of Crystalline state



Conclusions

- We developed a simple but realistic model of polymer confined in such a pore and studied the effect of asymmetry induced by the cone-shaped channel and role of the solvent quality on the equilibrium properties of a polymer chain.
- When outside and inside solvent is of similar type, polymer prefers to be outside the pore.
- When inside solvent poor than the outside, polymer stays inside the pore at low temperature.
- When inside solvent is slightly poor than outside, polymer ejects out from the pore and always remain outside. This is the important finding as in vivo, temperature of the system remains almost constant, therefore, movement of biomolecules (inside to outside and vice versa) is driven by the change in solvent quality.

These results may have applications in understanding of transport of biomolecules from the Nuclear Pore Complex (NPC) and ejection of viral DNA from the capsid.

We also report the absence of highly-dense state inside the pore below a certain pore-size, which has potential application in understanding of the existence of highly-dense state inside the viral proheads..