Conformational transitions in random heteropolymer models

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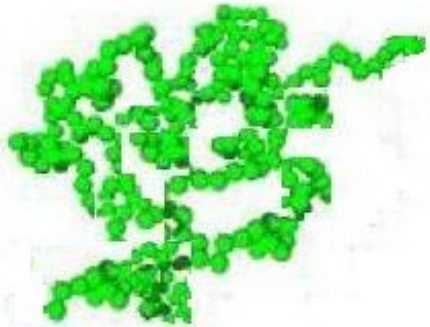
Conformations of polymer macromolecules

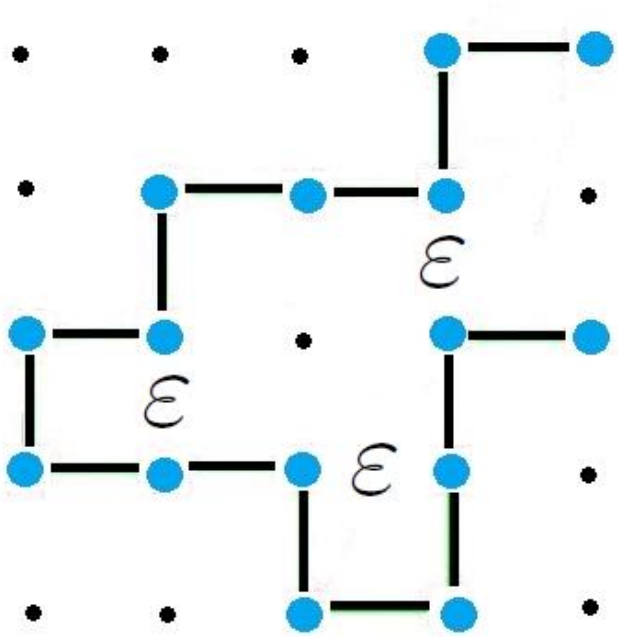


$T > T_\Theta$	$T = T_\Theta$	$T < T_\Theta$
Coil (extended state)	Θ-transition	*Globule* (compact state)

Linear size of polymer chain:

$\langle R \rangle \sim N^{0.588}$	$\langle R \rangle \sim N^{1/2}$	$\langle R \rangle \sim N^{1/3}$

Lattice model of polymer chain

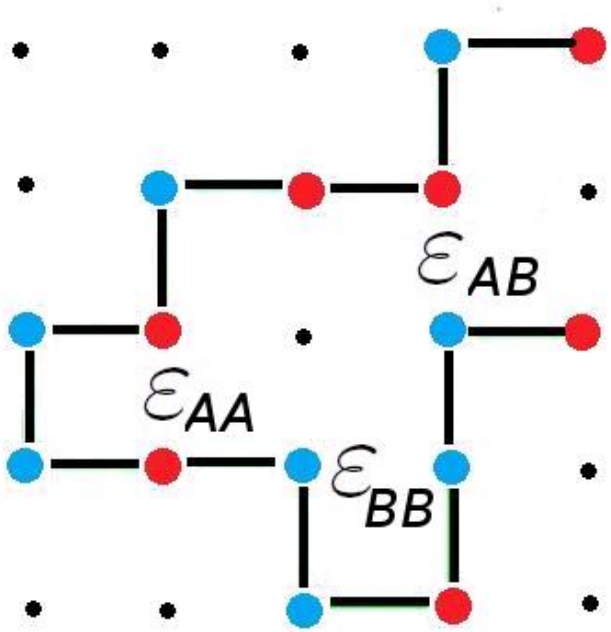


- n – number of nearest neighbour contacts
- $E_N = n \cdot \varepsilon$ – energy of a chain
- Statistical weight $W_N \sim \mathrm{e}^{\frac{-E_N}{k_B T}}$
- let us take: $k_B = 1$, $\varepsilon = -1$

$T_\Theta = 3.717(3)$

P. Grassberger, Phys. Rev. E **56** *(1997)*

Lattice model of heteropolymer



- N_A monomers of type A
- $N_B = N - N_A$ monomers of type B
- Inhomogeneity ratio:

$$c \equiv \frac{N_A}{N}$$

- Energy of a chain:

$$E_N = n_{AA}\varepsilon_{AA} + n_{BB}\varepsilon_{BB} + n_{AB}\varepsilon_{AB}$$

with n_{AA} - number of AA nearest neigbour contacts

Realizations

HP model of proteins

K.F. Lau and K.A. Dill, Macromolecules **22**, *3986 (1989)*

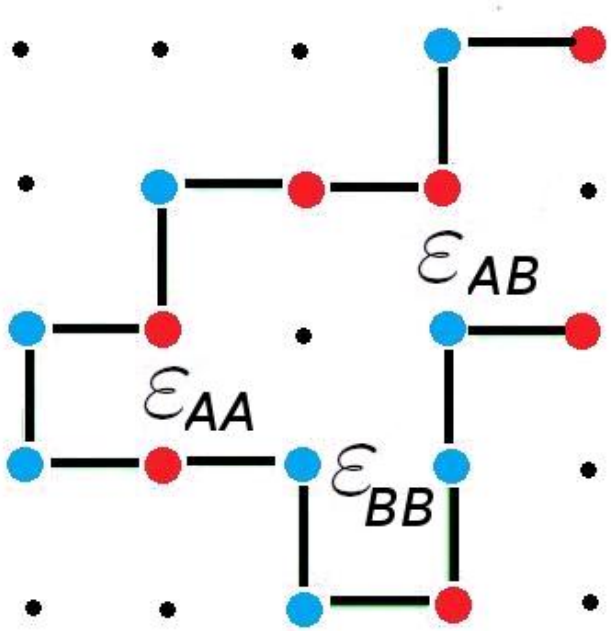
Hydrophobic (A) and polar (B) monomers:
$\varepsilon_{AA} = -1$, $\varepsilon_{BB} = \varepsilon_{AB} = 0$

Polyampholytes with strongly screened Coulomb interactions

Y. Kantor and M. Kardar, Europhys. Lett. **28**, *169 (1994)*

Positively charged (A) and negatively charged (B) monomers:
$\varepsilon_{AA} = 1$, $\varepsilon_{BB} = 1$, $\varepsilon_{AB} = -1$

Generalizations



Model 1: $\varepsilon_{AA} = \varepsilon_{BB} = 1, \varepsilon_{AB} = -1$

Model 2: $\varepsilon_{AA} = \varepsilon_{BB} = -1, \varepsilon_{AB} = 1$

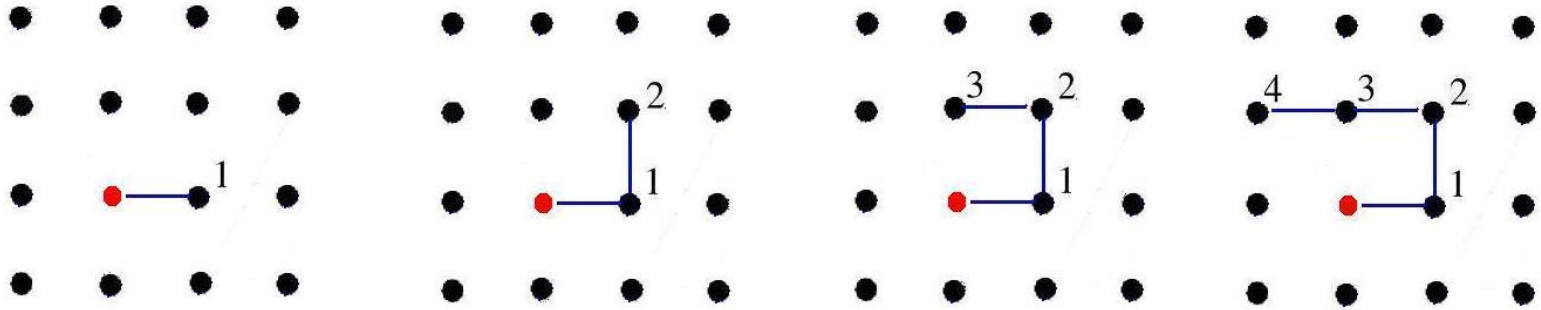
Model 3: $\varepsilon_{AA} = 1, \varepsilon_{BB} = \varepsilon_{AB} = 0$

Model 4: $\varepsilon_{AA} = -1, \varepsilon_{BB} = \varepsilon_{AB} = 0$

Model 5: $\varepsilon_{AA} = -1, \varepsilon_{BB} = 1, \varepsilon_{AB} = 0$

Conformational properties at fixed inhomogeneity ratio $c \equiv \frac{N_A}{N}$ (?)

Pruned-enriched Rosenbluth method (PERM)



$m_1 = 4$ $m_2 = 3$ $m_3 = 3$ $m_4 = 2$

Weight of Nth step: $W_N = \prod_{l=1}^{N} w_l e^{\frac{-(E_N)}{k_B T}}$

Control parameters: W_n^{max} W_n^{min} *(P. Grassberger, Phys. Rev. E* **56** *(1997))*

- $W_n < W_n^{min}$ – pruning with probability $1/2$, $W_n = 2W_n$
- $W_n > W_n^{max}$ – enrichment, $W_n = W_n/2$

Observables averaging

The configurational averaging is performed over an ensemble of possible conformations of a macromolecule with a fixed sequence of A and B monomers at fixed inhomogeneity ratio c:

$$\langle O \rangle = \frac{\sum_{\text{conf}} W_N^{\text{conf}} O}{\sum_{\text{conf}} W_N^{\text{conf}}}, \tag{1}$$

The quenched sequence averaging is carried out over different random sequences of A and B monomers at fixed c value:

$$\overline{\langle O \rangle} = \frac{1}{M} \sum_{i=1}^{M} \langle O \rangle_i. \tag{2}$$

Energy of heteropolymer chain

p – averaged number of nearest neigbours per monomer

- Number of AA contacts:

$$n_{AA}=\frac{1}{2}N_A pc=\frac{1}{2}Npc^2$$

- Number of BB contacts:

$$n_{BB}=\frac{1}{2}N_B p(1-c)=\frac{1}{2}Np(1-c)^2$$

- Number of AB contacts:

$$n_{AB}=N_A p(1-c)=Npc(1-c)$$

Simple SAWs: p=0.31596(3)
D. MacDonald et al., J. Stat. Phys. **33**, *5973 (2000)*

$$E_N = n_{AA}\varepsilon_{AA} + n_{BB}\varepsilon_{BB} + n_{AB}\varepsilon_{AB}$$

$$E_N^{\text{Model 1}}=2Np\left(c^2-c+\frac{1}{4}\right)$$

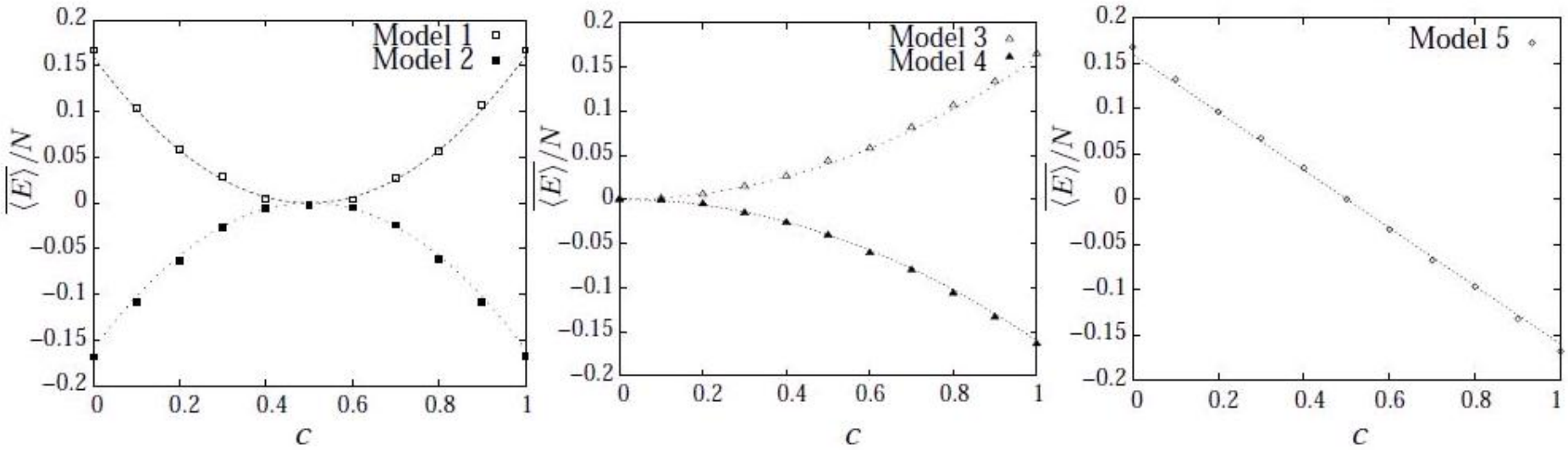
$$E_N^{\text{Model 2}}=-2Np\left(c^2-c+\frac{1}{4}\right)$$

$$E_N^{\text{Model 3}}=\frac{1}{2}Npc^2$$

$$E_N^{\text{Model 4}}=-\frac{1}{2}Npc^2$$

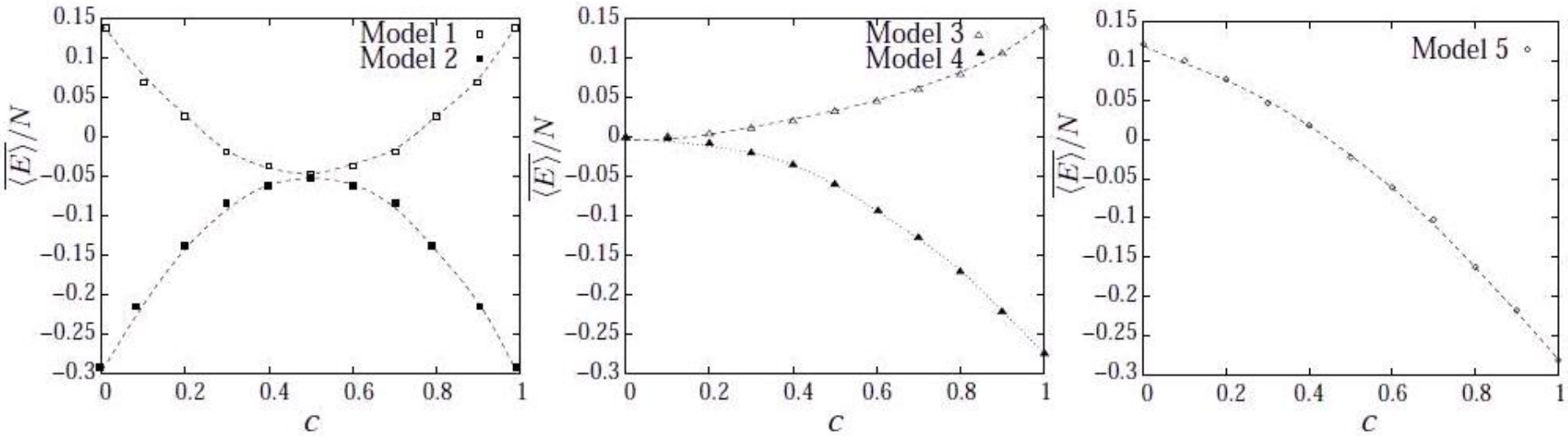
$$E_N^{\text{Model 5}}=Np\left(\frac{1}{2}-c\right)$$

Energy of heteropolymer chain



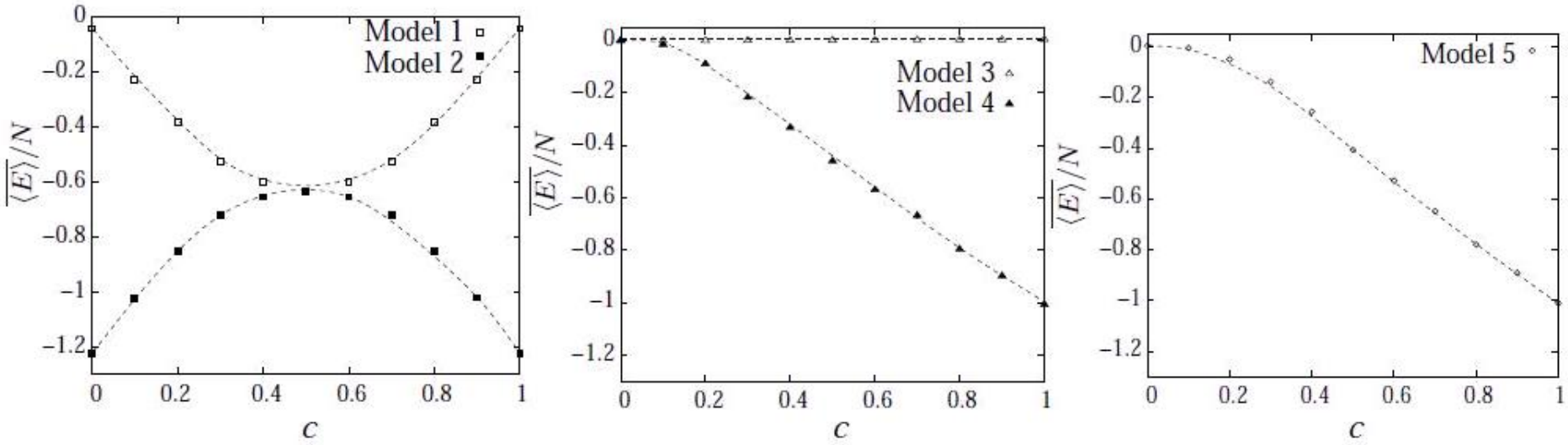
The averaged energy per monomer of an $N = 100$-monomer heterogeneous chain as function of c at $T = 10.0$

Energy of heteropolymer chain



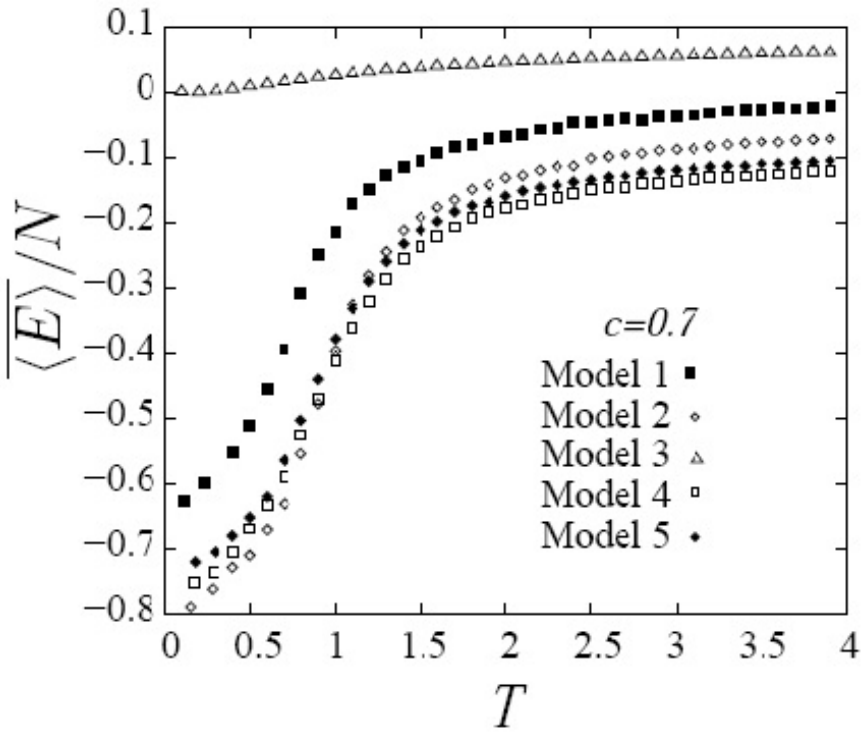
The averaged energy per monomer of an $N = 100$-monomer heterogeneous chain as function of c at $T = 4.0$

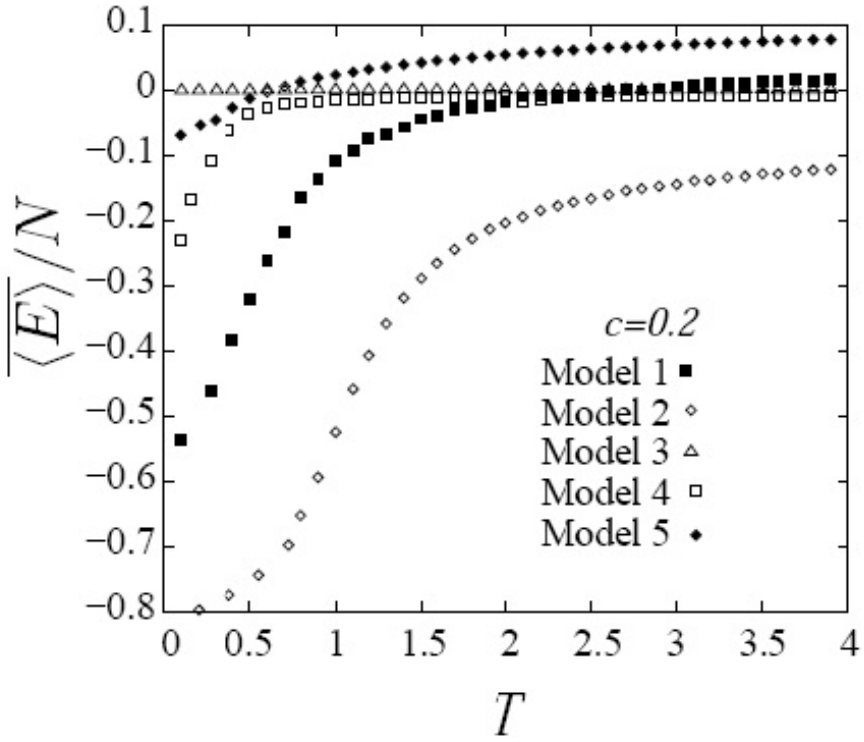
Energy of heteropolymer chain



The averaged energy per monomer of an $N = 100$-monomer heterogeneous chain as function of c at $T = 0.6$

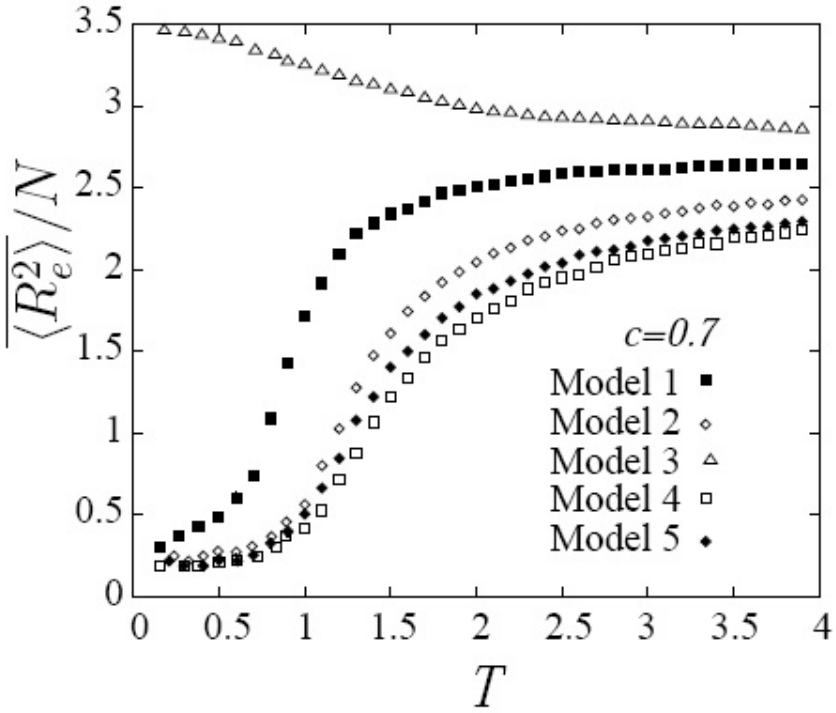
Energy of heteropolymer chain

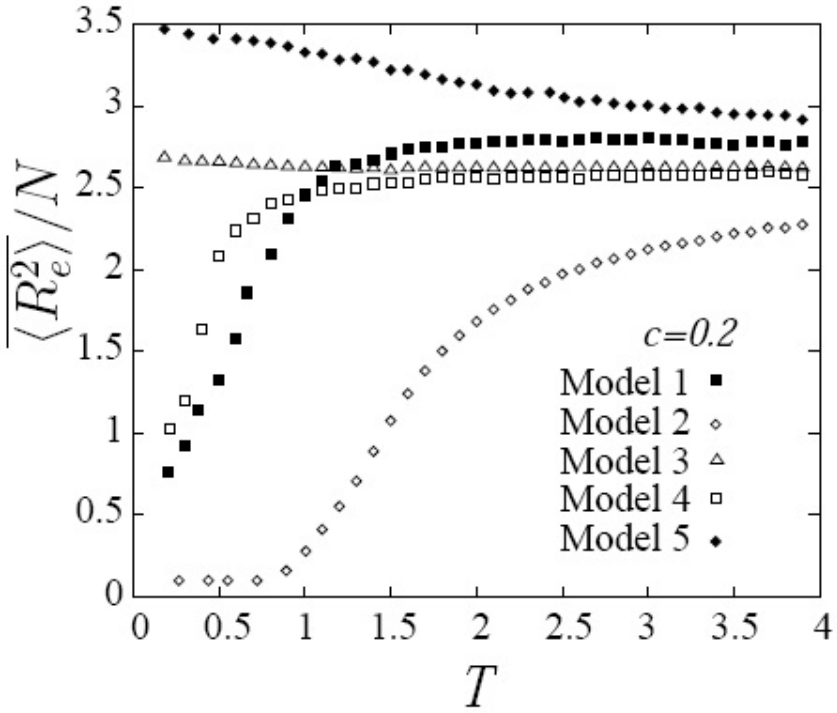




Averaged energy per one monomer of the heterogeneous polymer chain with various types of monomer-monomer interactions as function of temperature at fixed inhomogeneity ratio $c = 0.7$ and $c = 0.2$.

Linear size of heteropolymer chain





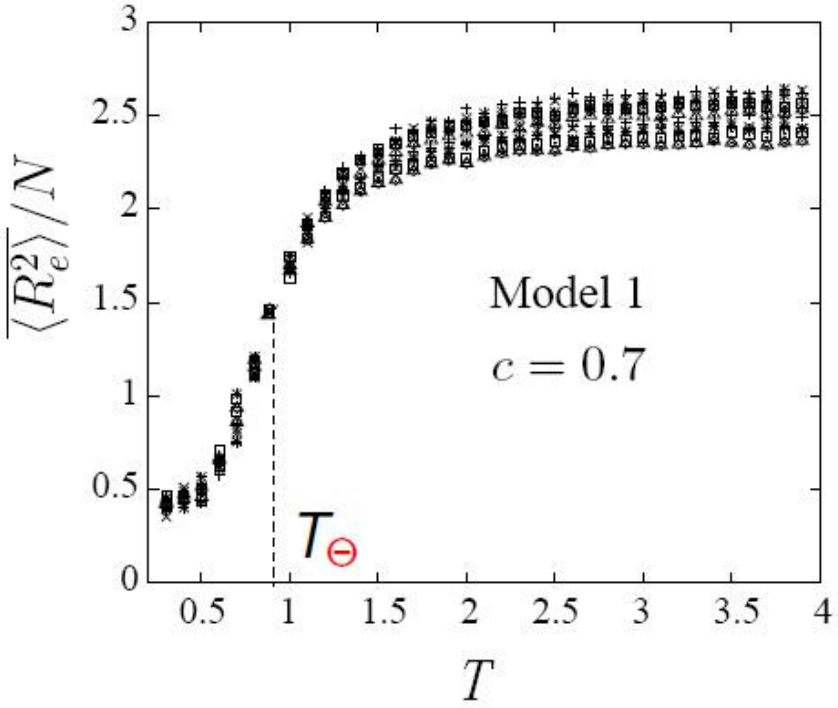
Averaged end-to-end distance of the heterogeneous polymer chain with various types of monomer-monomer interactions as function of temperature at fixed inhomogeneity ratio $c = 0.7$ and $c = 0.2$.

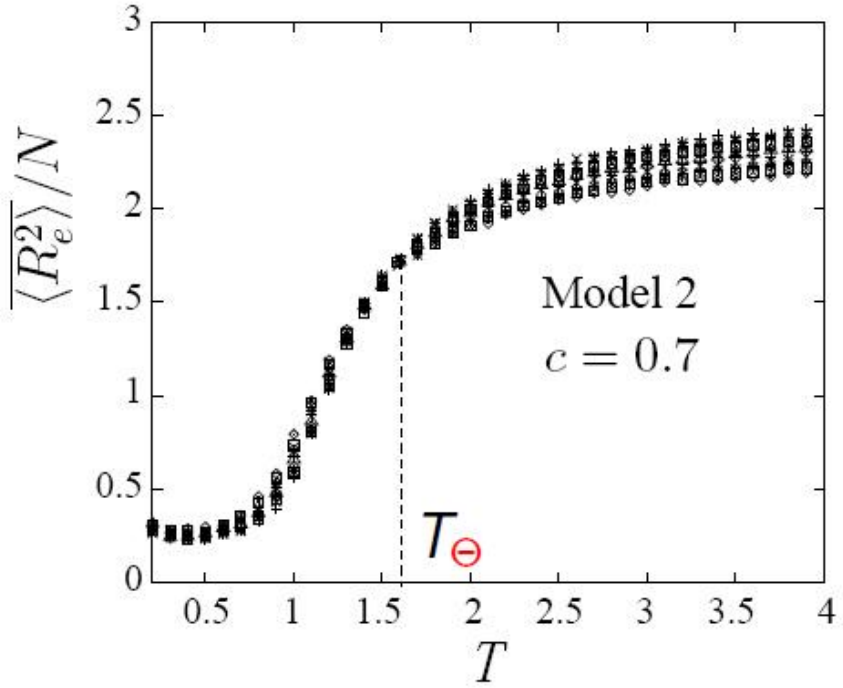
Estimation of transition temperature T_Θ

Coil (extended state) $\overline{\langle R_e^2 \rangle} \sim N^{1.176}$

Θ-transition $\overline{\langle R_e^2 \rangle} \sim N$

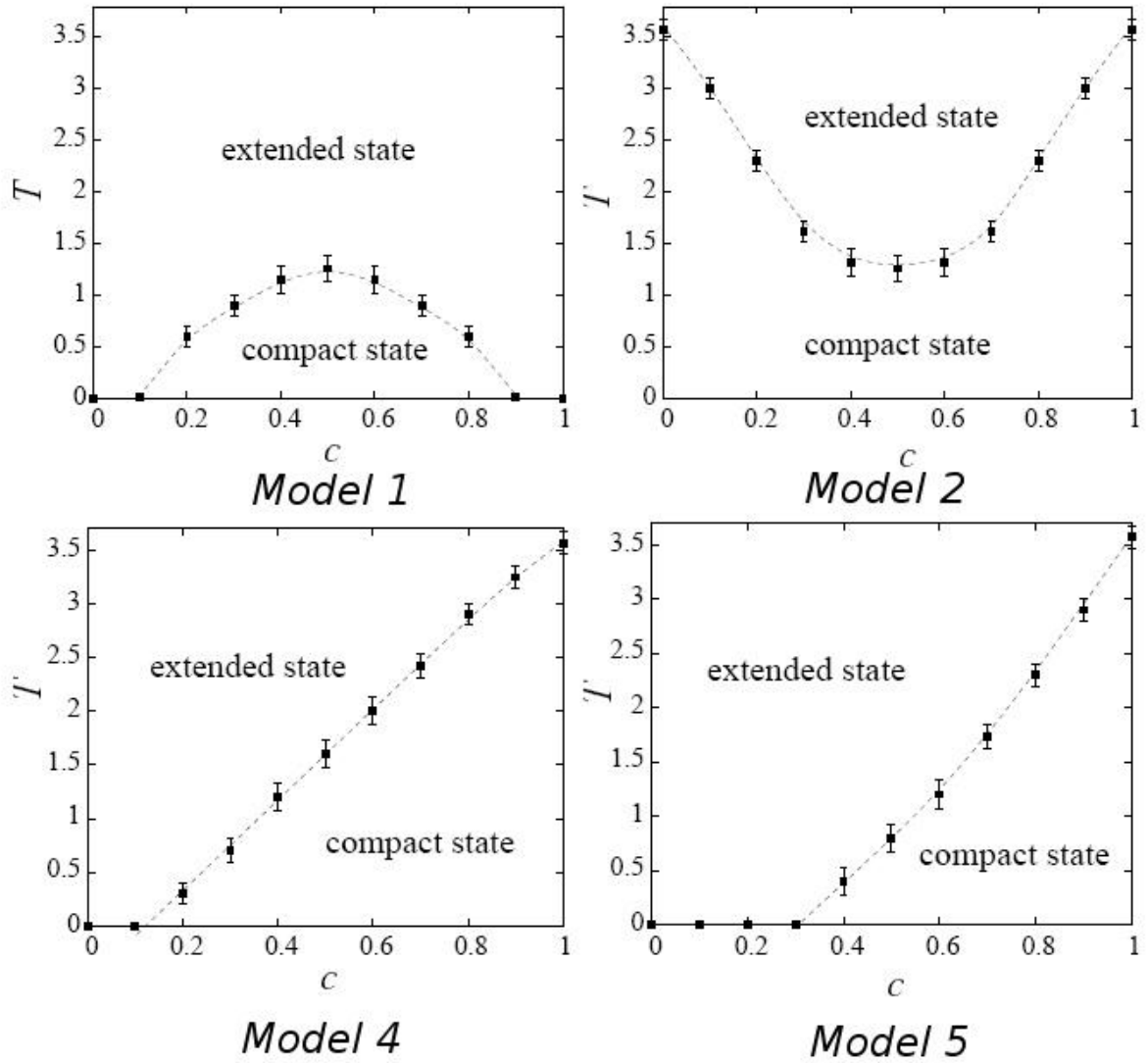
Globule (compact state) $\overline{\langle R_e^2 \rangle} \sim N^{2/3}$





The end-to end distance of a heterogeneous polymer chain divided by number of monomers as function of temperature at inhomogeneity ratio $c = 0.7$ at various values of N from 68 up to 100.

Phase diagrams of random heteropolymers in T-c plane



Conclusions

- We studied the conformational properties of heteropolymers within the frames of a lattice model containing N_A monomers of type A and $N_B = N - N_A$ monomers of type B in $d = 3$ dimensions. Restricting ourselves only to short-range interactions between any pair of monomers residing on neighboring lattice sites that are not connected by a covalent bond, we consider various generalizations of this model.
- Applying the pruned-enriched Rosenbluth algorithm we analyze numerically the peculiarities of transitions from extended into compact state as function of inhomogeneity ratio $c \equiv N_A/N$ for all the heteropolymer chain models.