1 Models

1.1 XY model on SAWs

A molecular conformation of the length N is represented by a self-avoiding walk (SAW) on a regular lattice with $N-1$ edges and N nodes. Each ith node represents a spin-like variable s_i which is associated with angle $\theta_i \in [-\pi;\pi]$. The Hamiltonian for sequence of spins s and conformation u is defined as the sum over all non-repeating neighbor pairs $\langle i,j \rangle$ in conformation:

$$H(u,s) = -J\sum_{\langle i,j \rangle} cos(\theta_i - \theta_j) - h\sum_i cos(\theta_i) \tag{1.1}$$

In case of the free boundary conditions, the partition function for the chain of the length N has the following form:

$$Z(J) = \int_{-\pi}^{\pi} d\theta_1 d\theta_2 \ldots d\theta_N e^{J(cos\theta_1 - \theta_2)} e^{J(cos\theta_2 - \theta_3)} e^{J(cos\theta_{N-1} - \theta_N)} \tag{1.2}$$

The mean magnetization is defined as a vector:

$$\langle m \rangle = \frac{1}{N} \langle (\sum_{i=1}^{N} cos\theta_i, \sum_{i=1}^{N} sin\theta_i) \rangle \tag{1.3}$$

The second moment of magnetization is a square of the norm:

$$\langle m^2 \rangle = \frac{1}{N^2} \langle (\sum_{i=1}^{N} cos\theta_i)^2 + (\sum_{i=1}^{N} sin\theta_i)^2 \rangle \tag{1.4}$$

From measurements of the average magnetization per spin $\langle m \rangle (J)$, we can obtain the value of the magnetic cumulant (Binder parameters) of fourth order [2], which is helpful to study magnetic phase transition:

$$U_4(J) = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2} \tag{1.5}$$

In case $J = 0$ (high-temperature regime), all states have equal probabilities:

$$Z(0) = \int_{-\pi}^{\pi} (\frac{1}{2\pi})^N d\theta_1 d\theta_2 \ldots d\theta_N \tag{1.6}$$

To calculate the exact value of $\langle m^2 \rangle (J=0)$ we use following results:

$$\int_{-\pi}^{\pi} \frac{1}{2\pi} sin^2\theta d\theta = \int_{-\pi}^{\pi} \frac{1}{2\pi} cos^2\theta d\theta = \frac{1}{2}$$

$$\int_{-\pi}^{\pi} \frac{1}{2\pi} sin\theta d\theta = \int_{-\pi}^{\pi} \frac{1}{2\pi} cos\theta d\theta = 0$$

After some calculation, only integration results for N times $sin^2\theta_i$ and N times $cos^2\theta_i$ survive:

$$\langle m^2 \rangle (J=0) = \frac{1}{N^2} \int_{-\pi}^{\pi} (\frac{1}{2\pi})^N \left((\sum_{i=1}^{N} cos\theta_i)^2 + (\sum_{i=1}^{N} sin\theta_i)^2 \right) d\theta_1 d\theta_2 \ldots d\theta_N = \frac{1}{N^2} (\frac{1}{2}N + \frac{1}{2}N) = \frac{1}{N} \tag{1.7}$$

Next, to calculate $\langle m^4 \rangle (J=0)$ we use following facts:

$$\langle m^4 \rangle (J=0) = \frac{1}{N^4} \int_{-\pi}^{\pi} (\frac{1}{2\pi})^N \left((\sum_{i=1}^{N} cos\theta_i)^2 + (\sum_{i=1}^{N} sin\theta_i)^2 \right)^2 d\theta_1 d\theta_2 \ldots d\theta_N$$

$$\left((\sum_{i=1}^{N} cos\theta_i)^2 + (\sum_{i=1}^{N} sin\theta_i)^2 \right)^2 = (\sum_{i=1}^{N} cos\theta_i)^4 + (\sum_{i=1}^{N} sin\theta_i)^4 + 2(\sum_{i=1}^{N} cos\theta_i)^2 (\sum_{i=1}^{N} sin\theta_i)^2$$

$\int_{-\pi}^{\pi} \frac{1}{2\pi} sin^4\theta d\theta = \int_{-\pi}^{\pi} \frac{1}{2\pi} cos^4\theta d\theta = \frac{3}{8}$ (We have N times $sin^4\theta_i$-term and N times $cos^4\theta_i$-term what results in $2 \times \frac{3}{8} \times N$).

$\int_{-\pi}^{\pi} \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{2\pi} sin^2\theta_i sin^2\theta_j d\theta_i d\theta_j = \int_{-\pi}^{\pi} \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{2\pi} cos^2\theta_i cos^2\theta_j d\theta_i d\theta_j = \frac{1}{4}$ (We have $6N(N-1)\frac{1}{2}$ times sin-term and $6N(N-1)\frac{1}{2}$ times cos-term what results in $6 \times \frac{1}{4} \times N(N-1)$).

$\int_{-\pi}^{\pi} \frac{1}{2\pi} sin^2\theta cos^2\theta d\theta = \frac{1}{8}$ (We have this term $2N$ times what results in $2 \times \frac{1}{8} \times N$).

$\int_{-\pi}^{\pi} \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{2\pi} cos^2\theta_i sin^2\theta_j d\theta_i d\theta_j = \frac{1}{4}$ (We have $2N(N-1)\frac{1}{2}$ times what results in $2 \times \frac{1}{4} \times N(N-1)$).

All other terms with odd power of sin of cos function are equals zero after integration over period.

$$\langle m^4 \rangle (J=0) = \frac{1}{N^4} \left(2 \times \frac{3}{8} \times N + 6 \times \frac{1}{4} \times N(N-1) + 2 \times \frac{1}{8} \times N + 2 \times \frac{1}{4} \times N(N-1) \right) = \frac{2N-1}{N^3}$$

$$U_4(J=0) = 1 - \frac{\frac{2N-1}{N^3}}{3\frac{1}{N^2}} = 1 - \frac{2N-1}{3N} \tag{1.8}$$

1.2 Structural properties

To study structural phase transition, we use the mean square end-to-end distance of self-avoiding-walks which is defined as the sum over all configurations:

$$\langle R_N^2 \rangle = \frac{1}{Z_N} \sum_{|u|=N} |u|^2 e^{-E_u}, \tag{1.9}$$

where $|u|$ is the Euclidean distance between the endpoints of conformation u, and Z_N is partition function in the canonical assemble (1.2). As $N \to \infty$, the mean norm of SAWs is believed to scale as

$$\langle R_N^2 \rangle \sim N^{2\nu}. \tag{1.10}$$

Here ν is the critical exponent. In two dimensions, the exact value for non-interacting SAWs [5]

$$\nu = \frac{3}{4}. \tag{1.11}$$

The case of non-interacting SAWs is equivalent to case $J = 0$ for XY model on polymers or Ising model on polymers [4]. Consider collapsing self-avoiding walks, or classical homopolymer model (see chapter 9 in Ref.[6]. For thermodynamic limit $N \to \infty$, ν is believed to have the form of a step function of interaction energy J. For finite systems, this effect is rounded [7]. At low $J < J_\theta$, the system is equivalent to SAW without interaction. At the theta-point, ν_θ is obtained via Coulomb-gas approximations [3]:

$$\nu_\theta = \frac{4}{7}. \tag{1.12}$$

For the globular regime ($J > J_\theta$) in 2D case:

$$\nu = \frac{1}{2}. \tag{1.13}$$

2 Results

2.1 XY model on SAWs, 2D

2.1.1 Tests for validation simulations

To test our Monte-Carlo (M) simulation, we compare results obtained using MC and Sampling + Exact Enumeration. For short chains ($N = 5, N = 8$), we generate all set of self-avoiding walks and sample spin configurations by uniform distribution $U(-\pi, \pi)$. As this is resource-consuming procedure, we sample spin configurations only 600 times (so, 600 sequences of spins applied to each conformation) and repeat this 10 times. Figure 2.1 shows obtained results. This method is not reliable, but it helps to make approximate checks. For $J = 0$, the second moment of magnetization are close to exact values (1.7) and the mean energy starts at $\langle e \rangle = 0$.

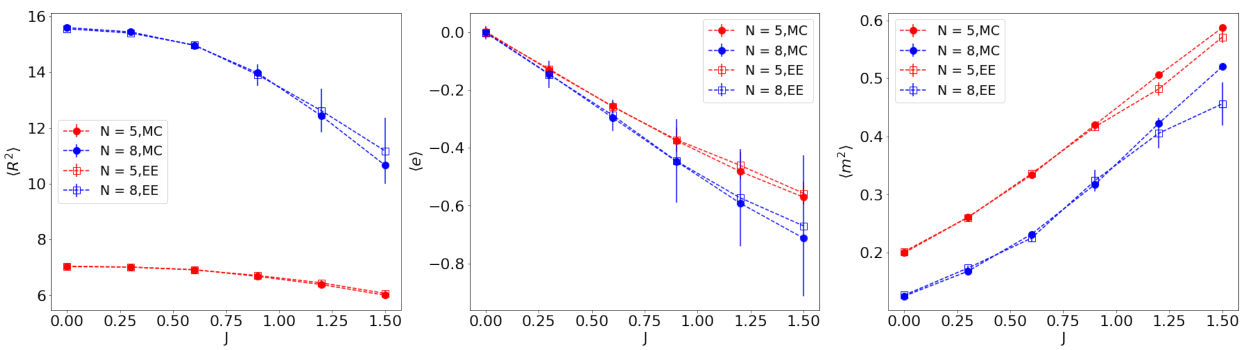

Figure 2.1: $h = 0$. Mean Radius (1.9), mean energy (1.1) and second moment of magnetization (1.4).

2.1.2 Thermodynamics and structural properties, short chains

To perform MC simulations for short chains from $N = 100$ to $N = 1000$, we run 4×10^8 MC steps for achieving equilibrium and at least 2.1×10^9 MC steps for measuring properties of the model.

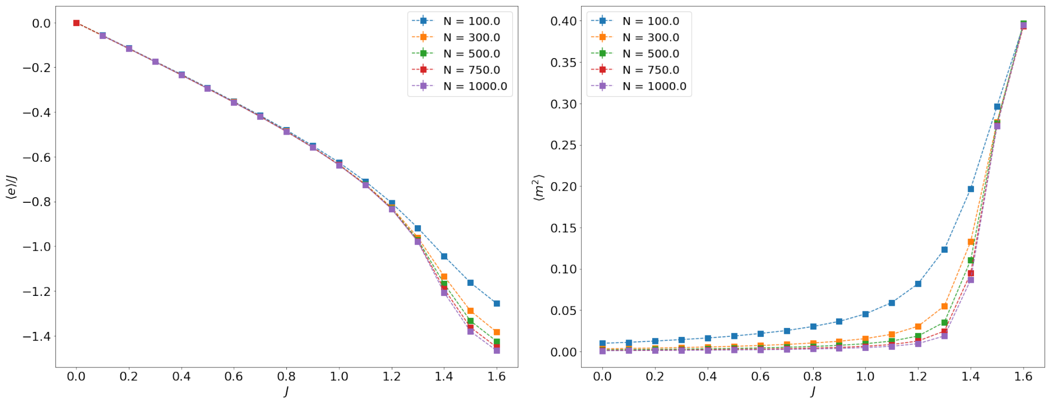

Figure 2.2: $h = 0$. Mean energy (1.1) and second moment of magnetization (1.4) for short chains. $> 4 \times 10^9$ MC steps in each simulations with two types of updates: snake-like and reconnect.

Figure 2.2 illustrates obtained results for Mean energy (1.1) and second moment of magnetization (1.4) for short chains. The system tends to order as interaction energy J gets larger.

Next, we estimate critical exponent ν. We use following ansatz [1]:

$$\log(R_N^2 + k_1) = 2\nu \log(N + k_2) + b. \tag{2.1}$$

Here $k_1 = k_2 = 1$ are phenomenological parameters.

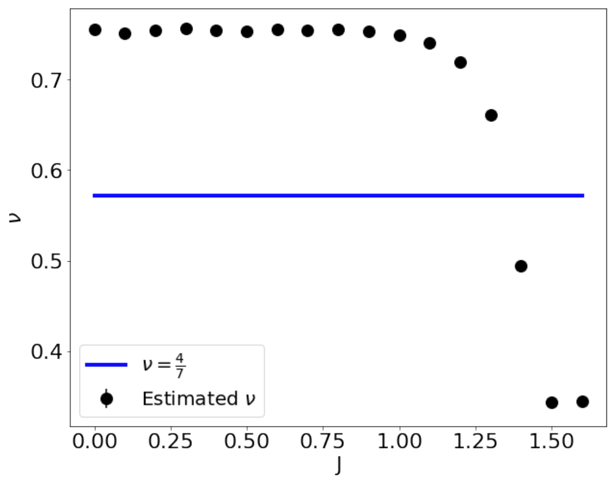

Figure 2.3: $h = 0$. Estimations with errorbars of critical exponent ν .

From figure 2.3, we can assume that XY model on SAWs also has value $\nu = 4/7$ (1.12) at the point os structural phase transition. We use this value to obtain collapsing plots.

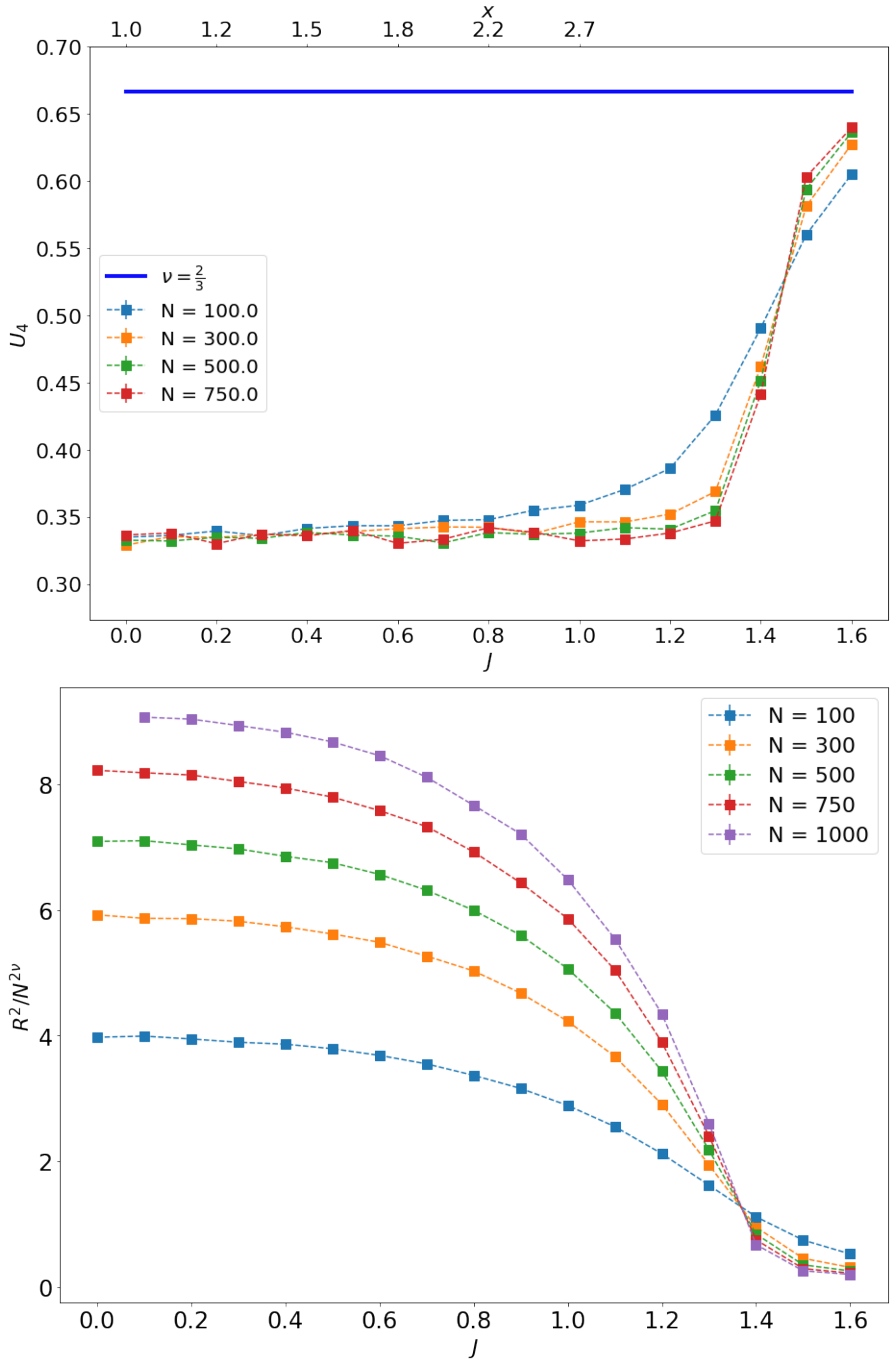

Figure 2.4: $h = 0$. Binder cumulants (1.5) and mean radius (1.9) for short chains. $> 4 \times 10^9$ MC steps in each simulations with two types of updates: snake-like and reconnect.

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