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Globule-coil Transition in Models of Linear Magnetic Polymers

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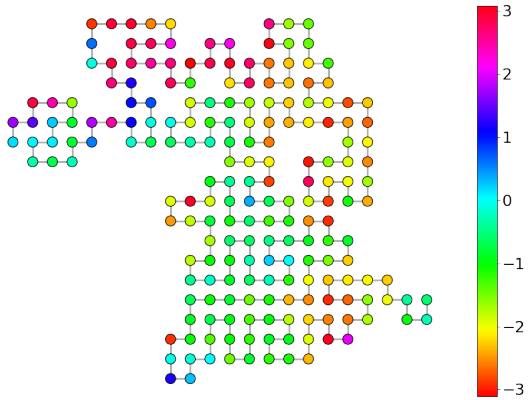
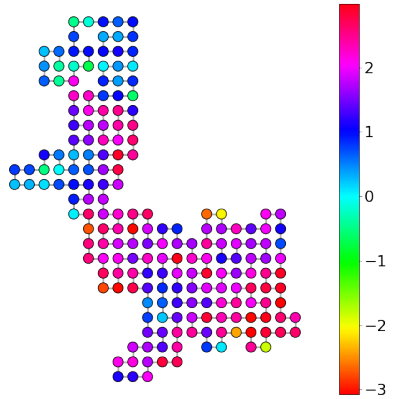
XY model on self-avoiding walks (SAWs)

- Magnetic polymer is a sequence of N monomers
- Conformation is a self-avoiding walk
- Each node represents a spin-like variable s_i associated with angle $\theta_i \in [-\pi; \pi]$

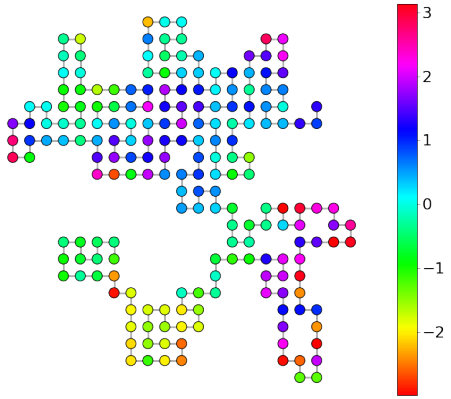




XY model on self-avoiding walks (SAWs)

- Hamiltonian in lack of an external field:

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

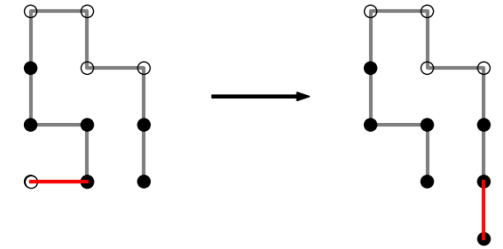


Partition function:

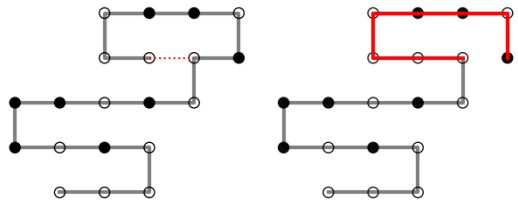
$$Z(J) = \sum_{u\in U_N} \int_{-\pi}^{\pi} \frac{1}{(2\pi)^N} d\theta_1 d\theta_2 \dots d\theta_N e^{J\cos(\theta_1-\theta_2)} e^{J\cos(\theta_2-\theta_3)} \dots e^{J\cos(\theta_{N-1}-\theta_N)}$$

Markov chain Monte-Carlo

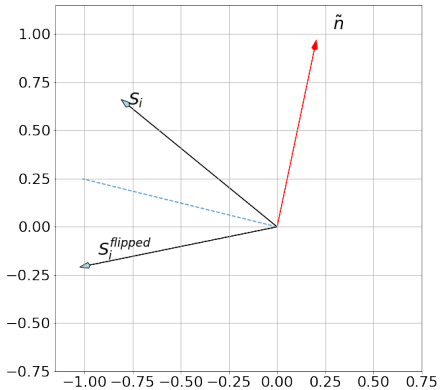
- Snake-like algorithm

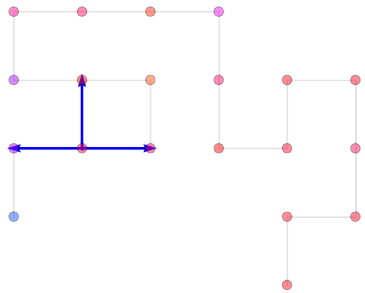


- Reconnect



- Wolff cluster update



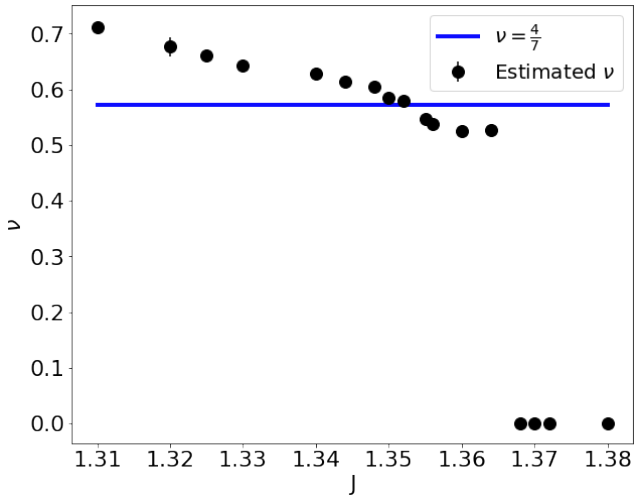


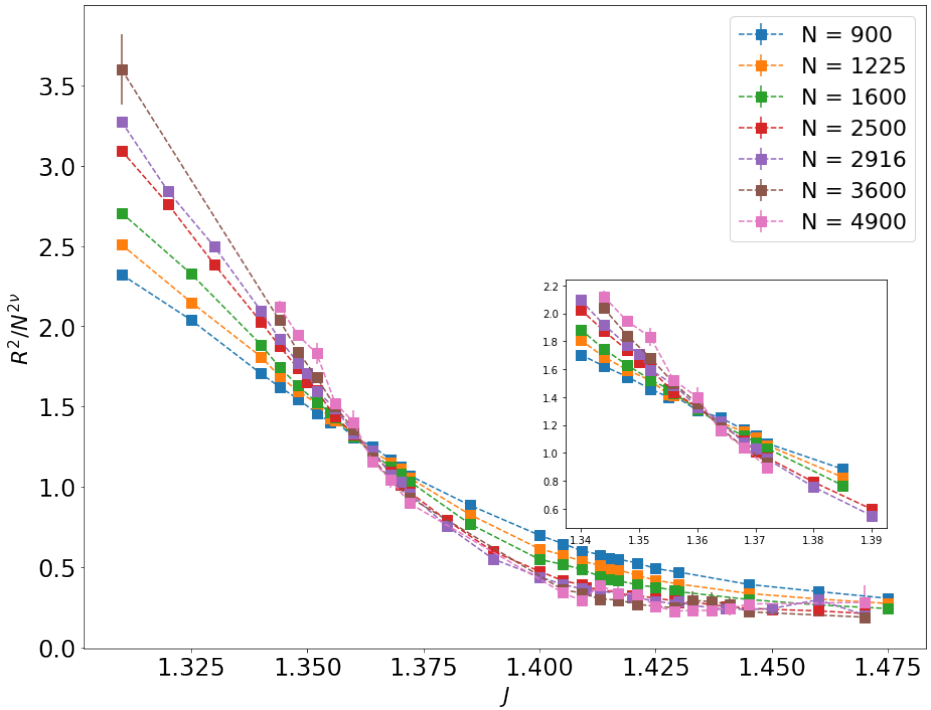
Phase transition, 2D

Structural transtition

- $\langle R_N^2 \rangle_x \sim N^{2\nu(x)}$
- iSAW: $\nu_\theta = \frac{4}{7}$

$$\log(R_N^2 + k_1) = 2\nu \log(N + k_2) + b$$



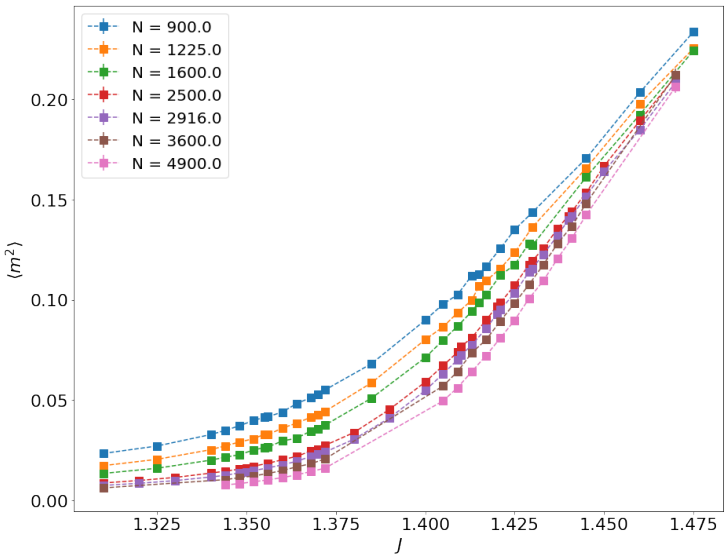


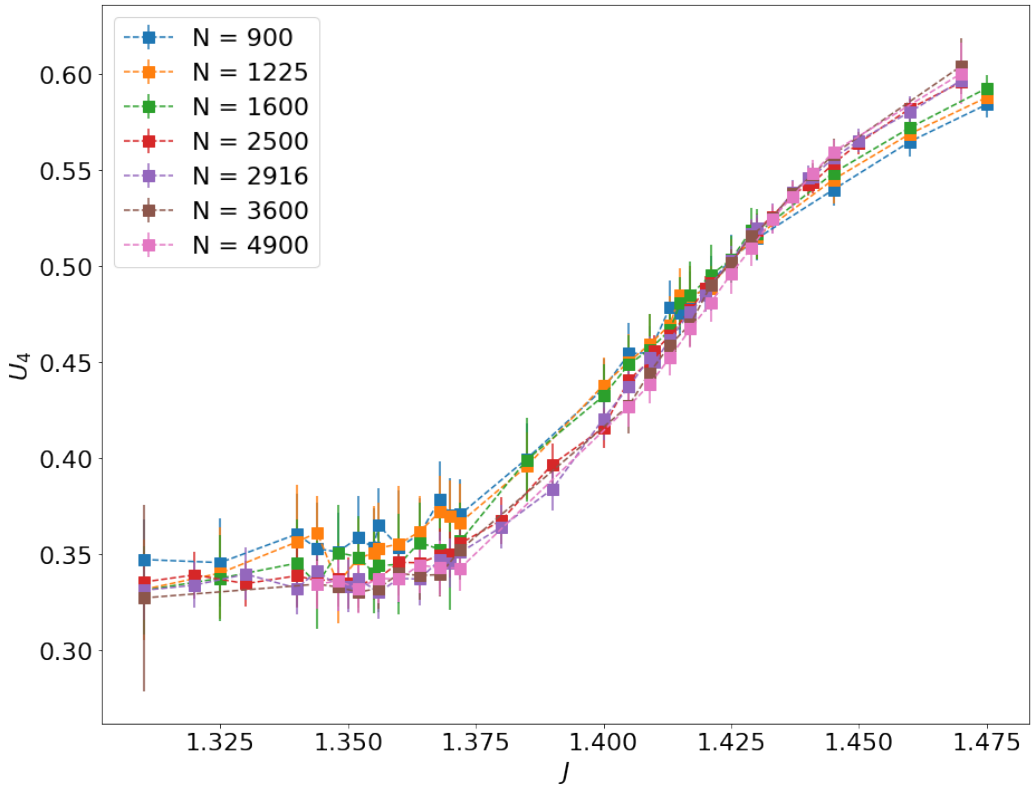
Phase transition, 2D

Magnetic transtition

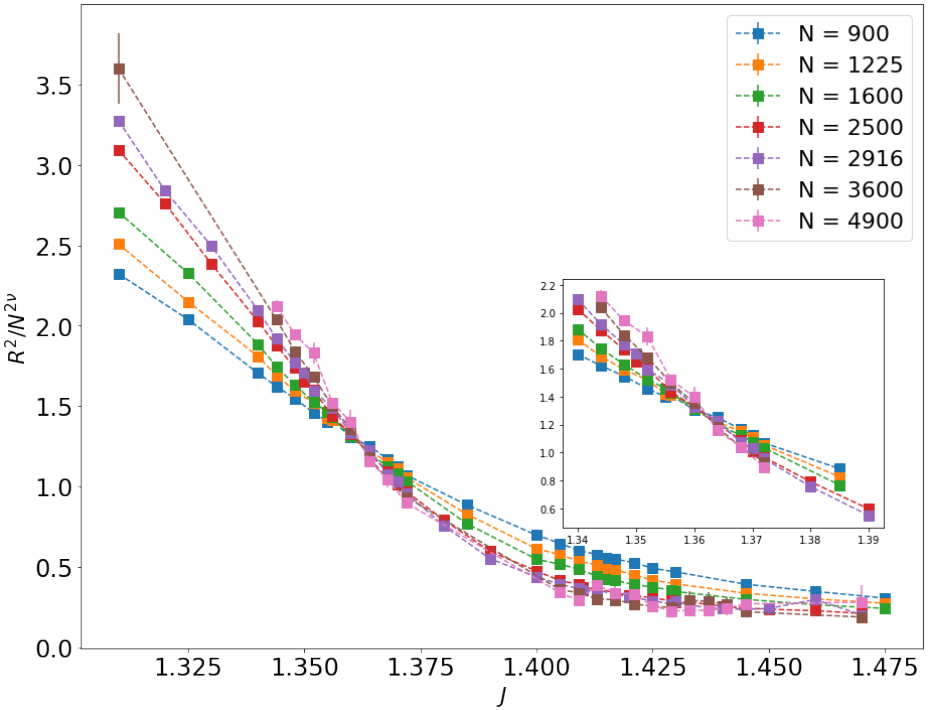
$$U_4(J) = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}$$

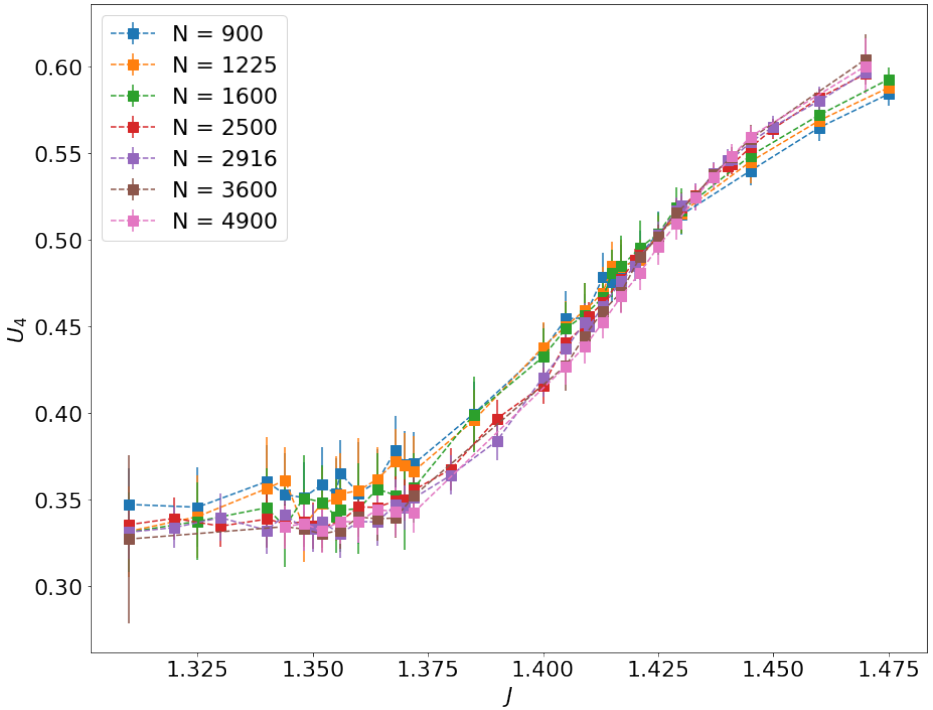
- The mean magnetization :
  $\langle \vec{m} \rangle = \frac{1}{N} \left\langle (\sum_{i=1}^{N} cos\theta_i, \sum_{i=1}^{N} sin\theta_i) \right\rangle$
- The second moment:
  $\langle m^2 \rangle = \frac{1}{N^2} \left\langle (\sum_{i=1}^{N} cos\theta_i)^2 + (\sum_{i=1}^{N} sin\theta_i)^2 \right\rangle$





Transition, 2D



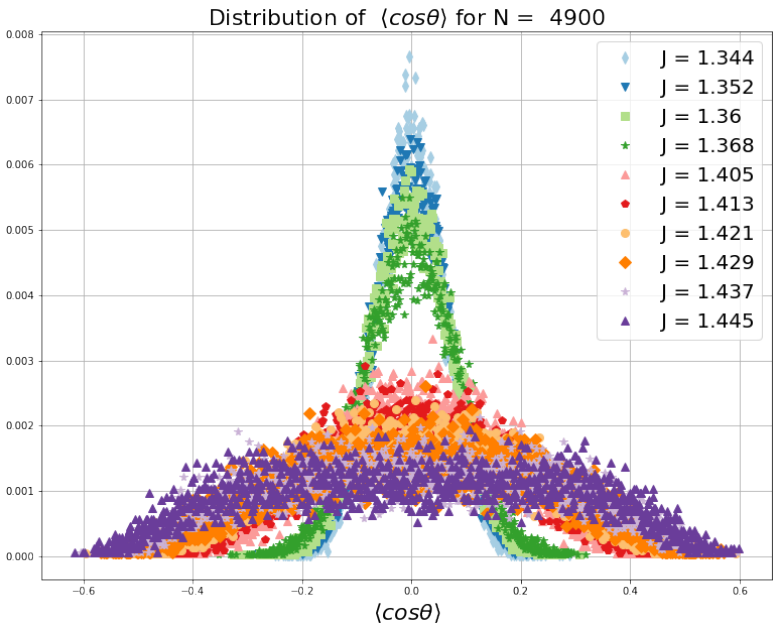


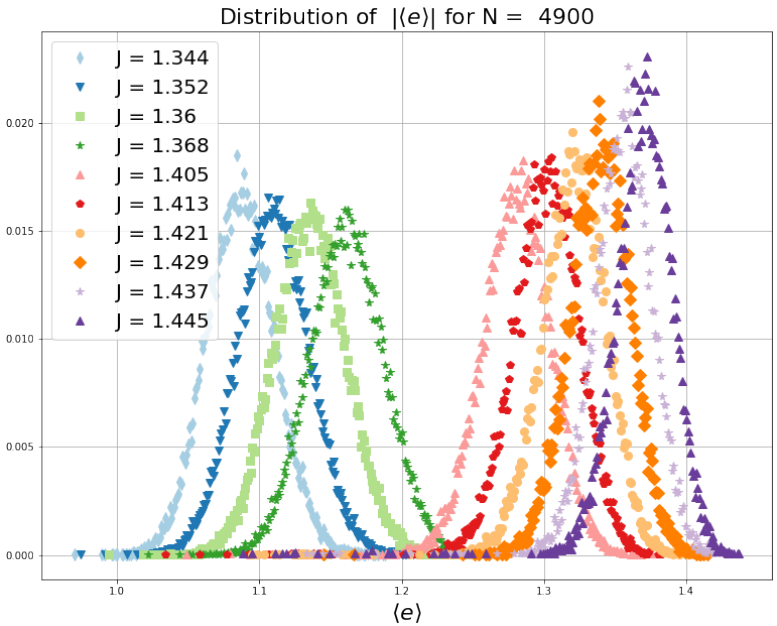
$$J_{\theta}^{3600} \approx 1.36(1)$$

$$J_{cr}^{3600} \approx 1.43(1)$$

Transition, 2D

Distributions





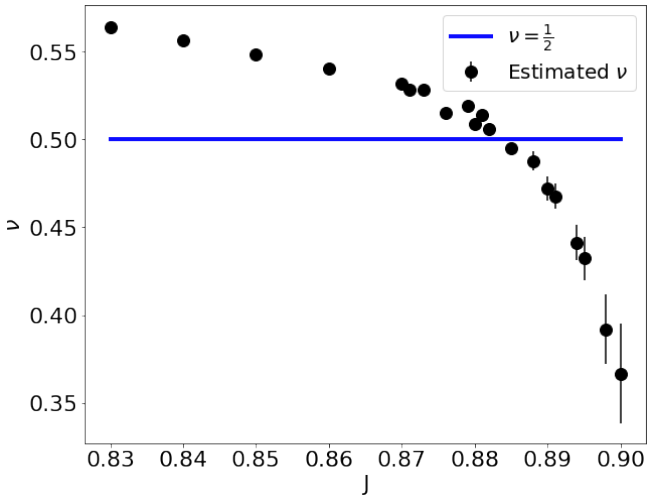
No bimodal energy, no signs of first-order transition

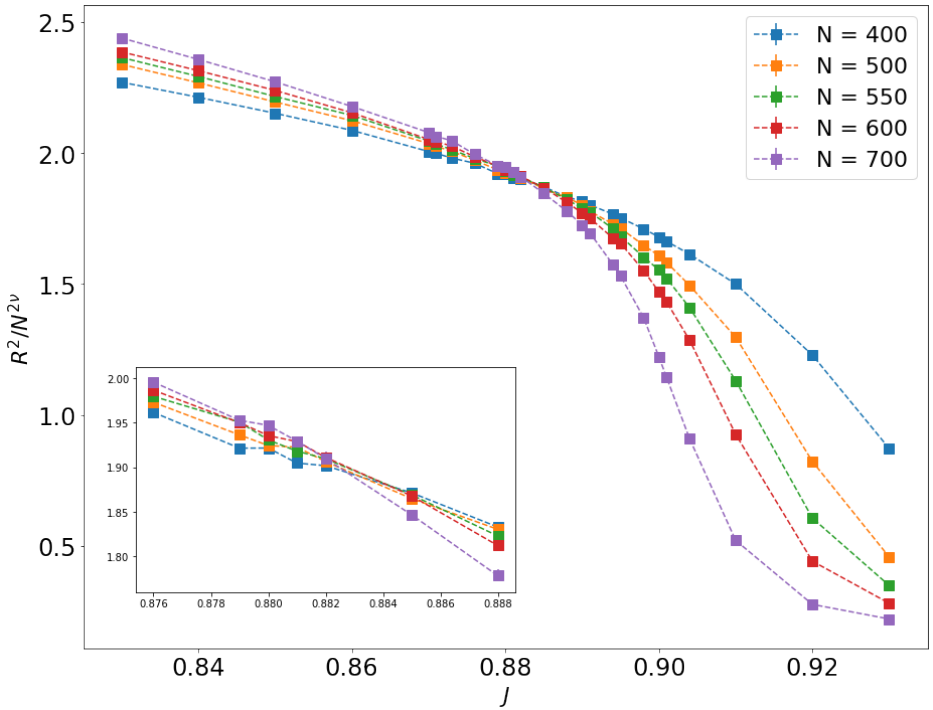
Phase transition, 3D

Structural transtition

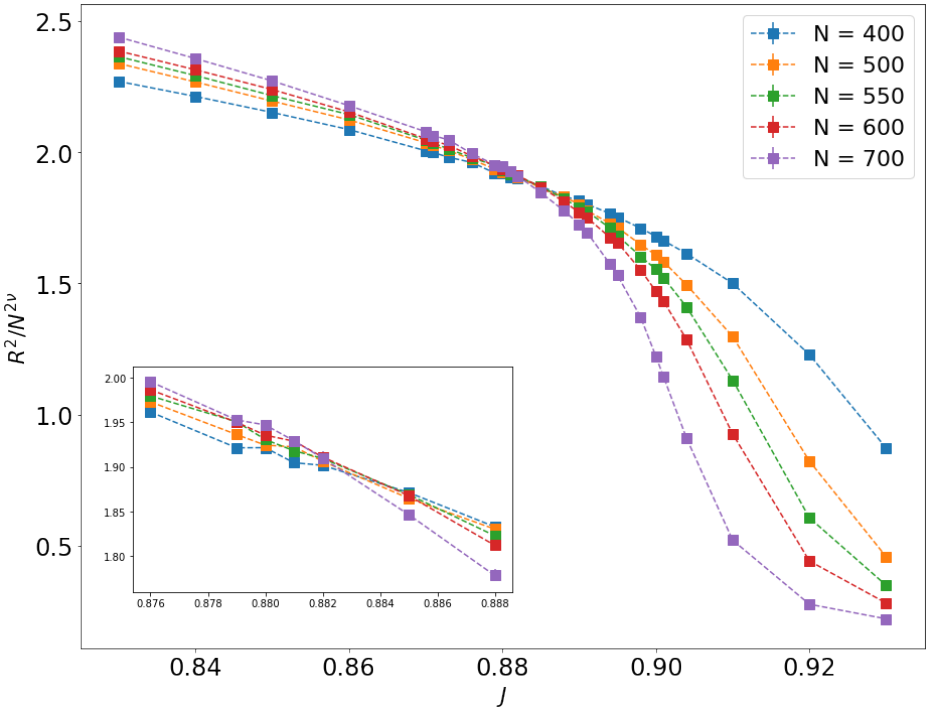
- $\langle R_N^2 \rangle_x \sim N^{2\nu(x)}$
- iSAW: $\nu_\theta = \frac{1}{2}$

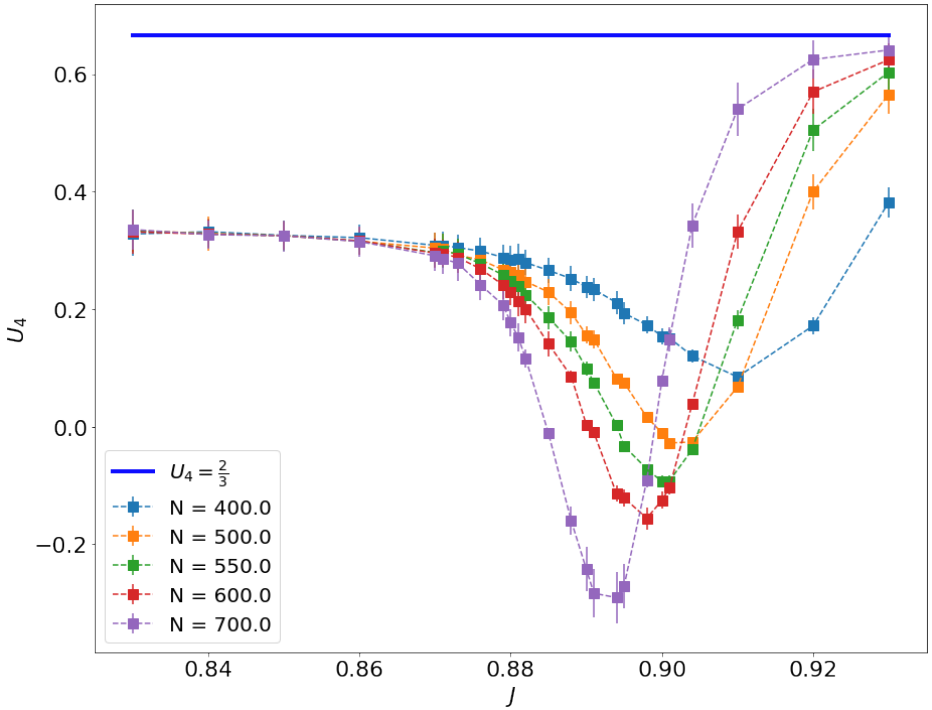
$$\log(R_N^2 + k_1) = 2\nu \log(N + k_2) + b$$





Transition, 3D

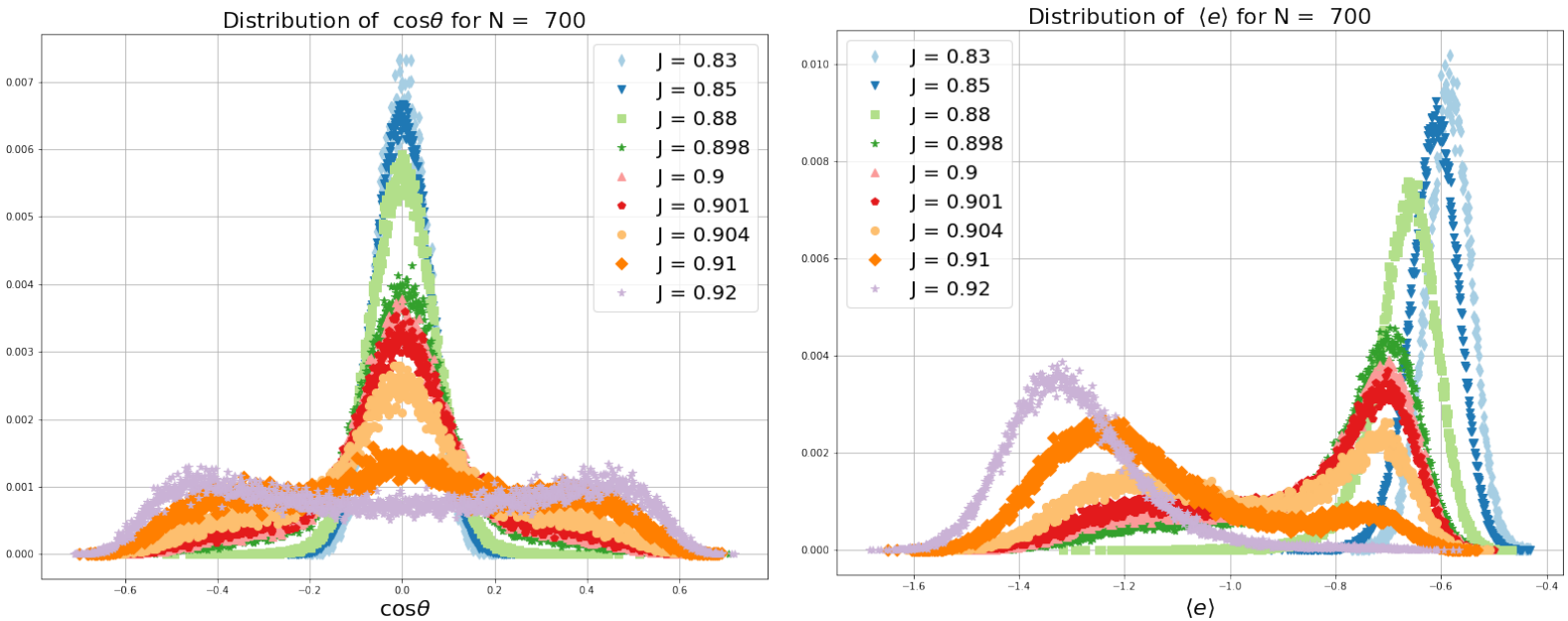




$$J_\theta^{700} \approx 0.876(5)$$

Transition, 3D

Distributions



Bimodal energy, signs of first-order transition

Conclusions and outlook

- For 3D case, MC data indicates first-order transition
- For 2D case, MC data is inconclusive, whether the transitions occur simultaneously or at distinct values of the coupling constant J. More work is needed to conclusively rule out one of possibilities.