Winding angle distributions of interacting polymers

Arturo Narros[†], Aleks Owczarek[‡], and Thomas Prellberg[†]

† School of Mathematical Sciences, Queen Mary University of London
‡ School of Mathematics and Statistics, The University of Melbourne

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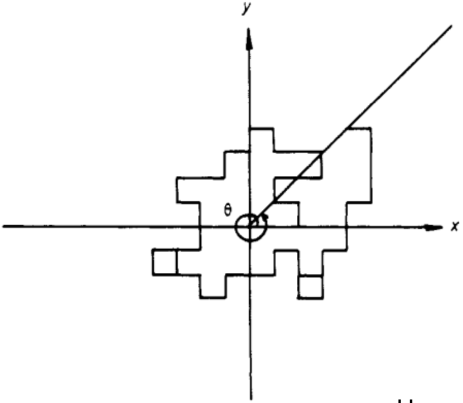
Topic Outline

1. Theory
2. Simulations
   - FlatPERM
   - Simulations of ISAW
   - Simulations of ISAT

Random walks

Winding of N-step random walk about origin



Hu and Rudnick, 1987

Winding angle θ measured with respect to direction of first step

Brownian motion

Winding of Brownian path of length N about origin

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Swollen polymers

Winding angle distribution is Gaussian

$$P(x = \theta/\sqrt{\log N}) \sim \exp(-x^2/(2C))$$

and the scaling variable has changed from $\theta/\log N$ to $\theta/\sqrt{\log N}$

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- Law-of-large-numbers implies Gaussian distribution

The constant C is universal

Prediction from Coulomb Gas methods (Duplantier and Saleur, 1988)

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with

$$C = \begin{cases} 2 & \text{swollen phase} \\ 24/7 & \text{critical state} \\ 4 & \text{dense phase} \end{cases}$$

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Also derivable from SLE (Gherardi, 2015, private communication)

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  - number of contacts m (energy $E = -mJ$)
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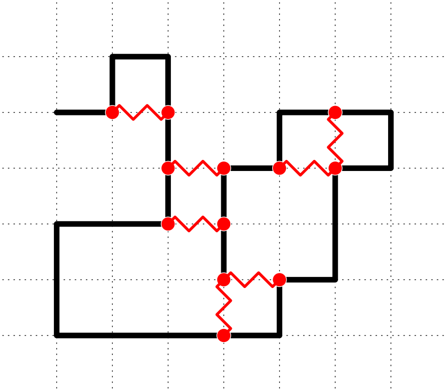
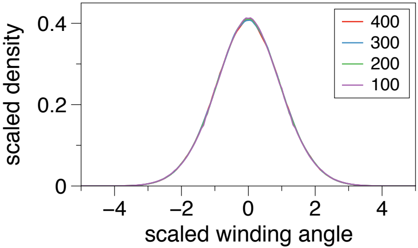
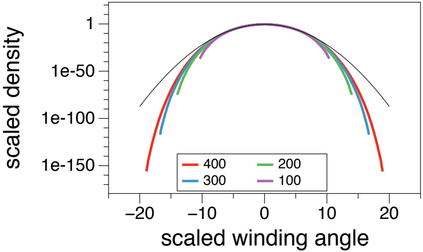
- Winding angle θ is not discrete $\implies$ binning

Interacting Self-avoiding Walk (ISAW)

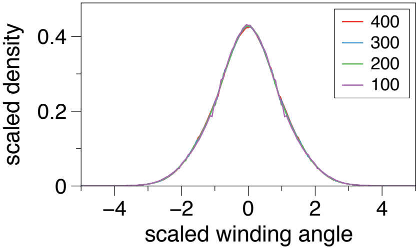


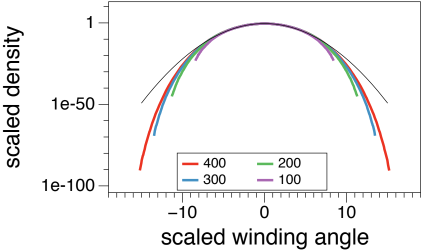
Self-avoiding walk (ISAW for $\beta = 0$)



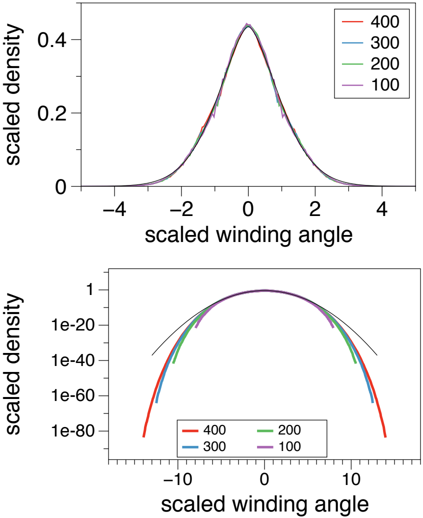


Collapsing self-avoiding walk (ISAW for $\beta = 0.6637$)

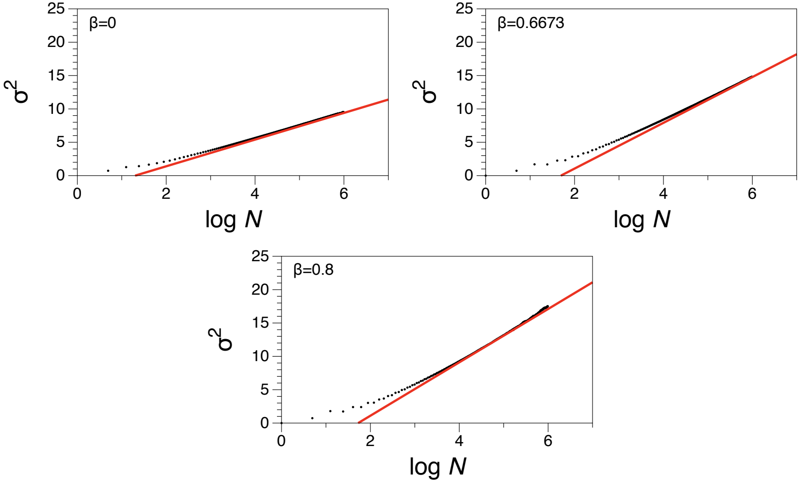




Collapsed self-avoiding walk (ISAW for $\beta = 0.8$)



Scaling of the variance



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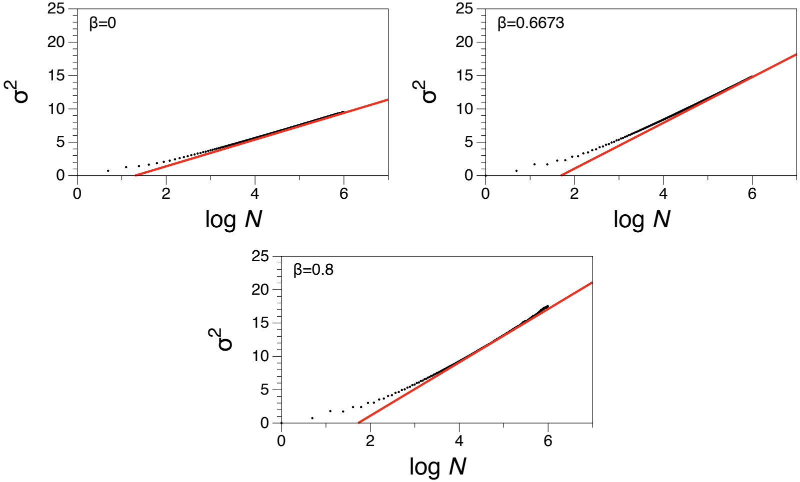
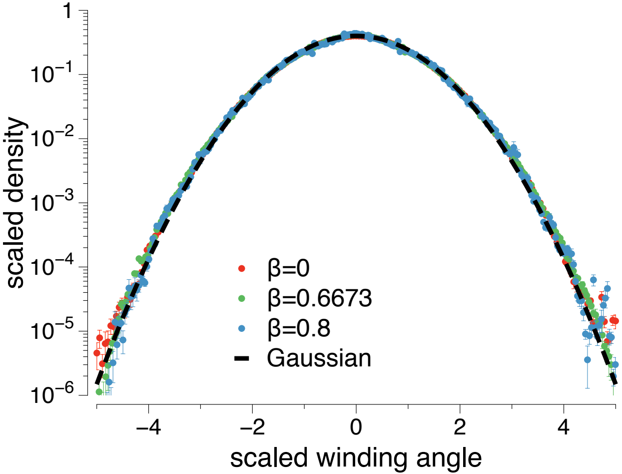


Consistent with slopes 2, $24/7$, and 4

Gaussian nature and universality predictions confirmed



$N = 1000$

Interacting Self-avoiding Trail (ISAT)

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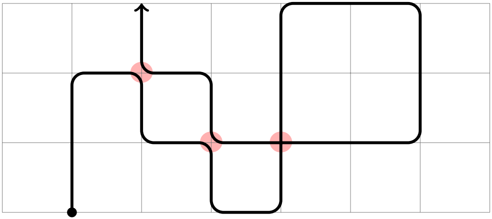

Interacting Self-avoiding Trail (ISAT)

- Canonical model: interacting self-avoiding walks (ISAW) vertex avoidance and nearest-neighbor interaction
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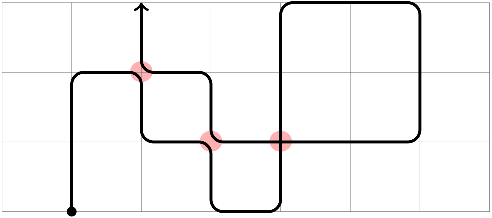
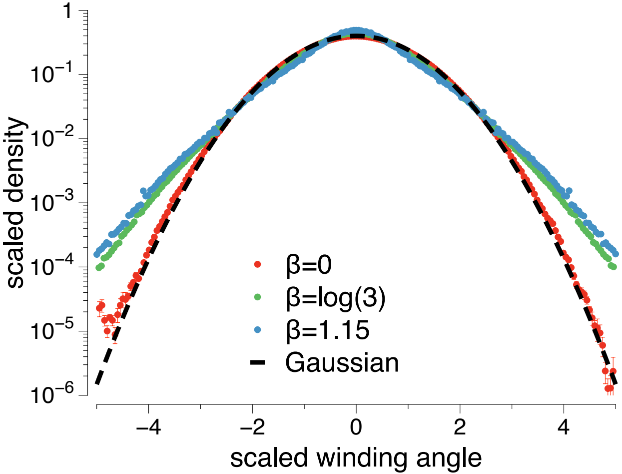


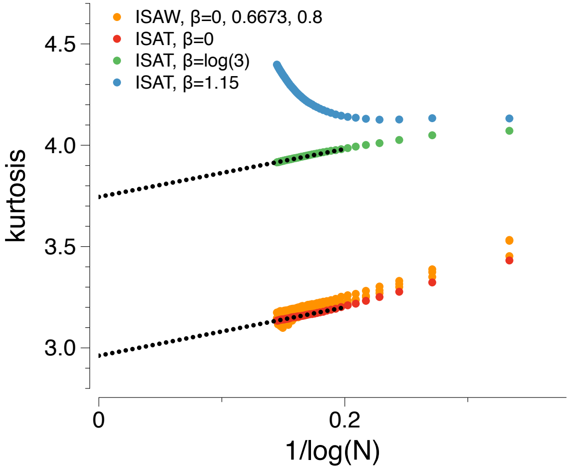
Critical temperature for ISAT is known exactly: $\beta = \log 3$

Deviations from Gaussian behavior

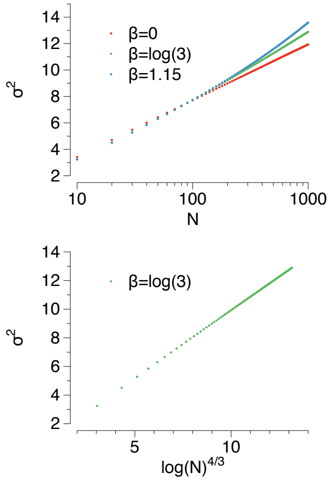


$N = 1000$

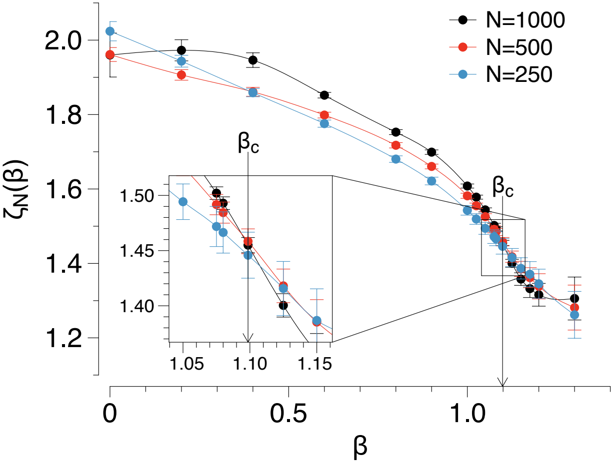
Kurtosis


ISAW, β=0, 0.6673, 0.8
ISAT, β=0
ISAT, β=log(3)
ISAT, β=1.15
kurtosis
4.5
4.0
3.5
3.0
0
0.2
1/log(N)

Scaling of the variance

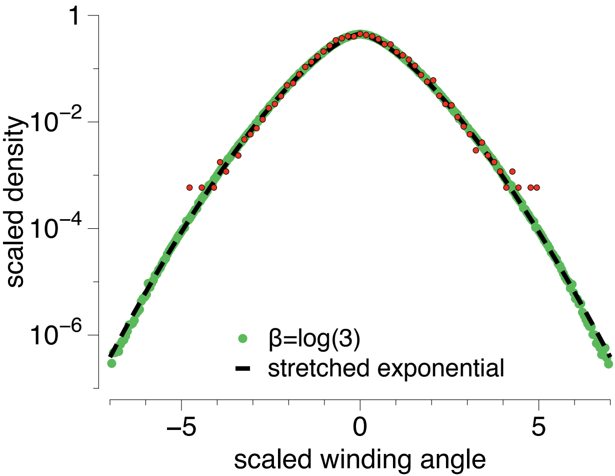


Fitting to stretched exponential



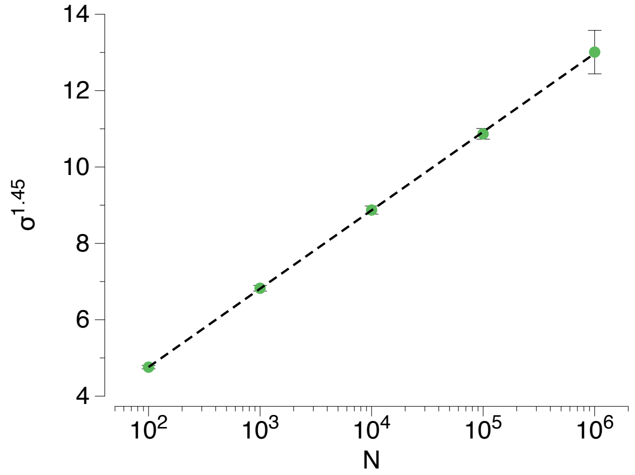
$$P(\theta) \propto \exp(-|\theta|^{\zeta}/C \log N)$$

Best fit at critical point



Fit with $\zeta = 1.45$ for $N = 1000$ (green) and $N = 1000000$ (red)

Scaling of the variance revisited



Scaling variable $x = \theta/(\log N)^{1/\zeta}$ with $\zeta = 1.45$

Conclusions

- ISAW
  - Winding angle distribution for ISAW is Gaussian at all temperatures
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  - Scaling variable

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- ISAT
  - Winding angle distribution for ISAT is not Gaussian at and below critical temperature
  - At criticality, the distribution is consistent with a stretched exponential, the scaling variable is

$$x = \theta / (\log N)^{1/\zeta} \quad \text{with} \quad \zeta = 1.45$$

  - At low temperatures, ζ seems to become smaller

A. Narros, A. L. Owczarek and T. Prellberg, "Winding angle distributions for two-dimensional collapsing polymers," J. Phys.: Conf. Ser. **686** (2016) 012007

A. Narros, A. L. Owczarek and T. Prellberg, "Anomalous polymer collapse winding angle distributions," in preparation

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