On the criticality of random knots at the θ temperature: A preliminary report (Knots and soft-matter physics: Topology of polymers and related topics in physics, mathematics and biology)

Author(s): Deguchi, Tetsuo; Akita, Yoko; Yao, Akihisa

Citation: 物性研究 (2009), 92(1): 131-134

Issue Date: 2009-04-20

URL: http://hdl.handle.net/2433/169099

Type: Departmental Bulletin Paper

Textversion: publisher

Kyoto University
On the criticality of random knots at the $\theta$ temperature
— A preliminary report —

Tetsuo Deguchi†, Yoko Akita‡ and Akihisa Yaat
† Department of Physics, Graduate School of Humanities and Sciences, Ochanomizu University,
2-1-1 Ohtsuka, Bunkyo-ku, Tokyo 112-8610, Japan
‡ Internal Audit Division, Mizuho Corporate Bank, Ltd.,
Yaesu 1-2-16, Chuo-ku, Tokyo 103-0028, Japan

Abstract: Through simulation using knot invariants we suggest that random polygons under a topological constraint (i.e. random knots) should have novel critical behavior. We recall that the mean-square radius of gyration of random knots with $N$ nodes increases with respect to $N$ almost as that of the self-avoiding polygons, as was pointed out by many authors previously. We find that the two-point correlation function is well approximated by a function close to the Gaussian one. Furthermore, our preliminary data analysis for $N = 1000$ also suggest the similar result. However, the Gaussian behavior is not consistent with the criticality of the self-avoiding walk. We thus suggest that random knots should have nontrivial and new critical behavior.

1 Introduction

Recently, an important statistical property of ring polymers with fixed topology in a $\theta$ solvent has been studied [1, 2, 3, 4, 5, 6, 7, 8, 9]. Under a topological constraint, the average size of ring polymers with zero or very small excluded volume can be much larger than that of no topological constraint. We call this phenomenon topological swelling. Hereafter we call random polygons with fixed knot and zero excluded volume random knots. They correspond to ring polymers with fixed topology in a $\theta$ solvent.

---

1E-mail: deguchi@phys.ocha.ac.jp
Let us consider a random polygon (RP) or self-avoiding polygon (SAP) consisting of \( N \) nodes and having a fixed knot type \( K \). We define the mean square radius of gyration by

\[
R^2_{g,K} = \frac{1}{2N^2} \sum_{j=1}^{N} \sum_{k=1}^{N} \langle (R_j - R_k)^2 \rangle_K.
\]

Here the symbol \( \langle \cdot \rangle_K \) denotes the ensemble average over all configurations of the RP or SAP with fixed knot \( K \). We denote by \( \langle \cdot \rangle_{\text{all}} \) the ensemble average over all configurations under no topological constraint.

For ring polymers a topological constraint should lead to entropic repulsions among segments, as was first pointed by des Cloizeaux [1]. Topological swelling was observed in simulation of random knots: \( R_{g,K} > R_{g,\text{all}} \) if \( N \) is large enough such as \( N = 1000 \) or \( 2000 \) [2, 4, 5, 6, 7]. We also observe topological swelling for SAPs with very small excluded volume [8, 9]. It was suggested that due to topological entropic repulsions, we should have \( R_{g,K} \propto N^{\nu_{\text{SAW}}} \) for very large \( N \), where \( \nu_{\text{SAW}} \) is the exponent of self-avoiding walks (SAW) [3, 5, 6, 7].

Let us now consider the end-to-end distance distribution, \( f_{\text{ete}}(r) \), for SAWs. It has the large-\( N \) behavior such as \( f_{\text{ete}}(r) \propto \exp(-r^4) \) with \( \delta = 1/(1 - \nu_{\text{SAW}}) \) for \( r \gg 1 \) [10]. For the case of random polygons we introduce the distribution function of distance between two nodes [11]. We select the \( j \)th and \( k \)th nodes out of the \( N \) nodes, and consider the distance between them, \( r = |r| \), with \( r = R_j - R_k \) where \( R_m \) denote the position vectors of the \( m \)th node for \( m = 1, 2, \ldots, N \). When the two arcs between them have segments \( n \) and \( N - n \), respectively, and \( n \leq N - n \), we define parameter \( \lambda \) by fraction \( n/N \). We denote by \( f_{\text{all}}(r; \lambda, N) \) the probability distribution of distance \( r \) between the two nodes under no topological constraint. For RPs under a topological constraint of \( K \), we denote it by \( f_K(r; \lambda, N) \). The asymptotic behavior of \( f_K(r; \lambda, N) \) should play a similar role as that of \( f_{\text{ete}}(r) \). In fact, integrating \( f_{\text{all}}(r; \lambda, N) \) over \( \lambda \), we have the monomer-monomer distribution function, which has the same large \( N \) behavior as \( f_{\text{ete}}(r) \) [12].

## 2 Numerical result and the model function

The following formula was proposed for describing the distance distribution \( f_K(r; \lambda, N) \) under the topological constraint of a given knot type \( K \) [13, 14]:

\[
f_K(r; \lambda, N) = C_K(\lambda, N) r^{2+\theta_K(\lambda)} \exp \left[ \frac{-3r^2}{2N\sigma_K(\lambda)^2} \right]
\]

where the normalization \( C_K(\lambda, N) \) is given by

\[
C_K(\lambda, N) = \left( \frac{3}{2N\sigma_K^2} \right)^{\frac{3+\theta_K}{2}} \frac{2}{\Gamma\left(\frac{3+\theta_K}{2}\right)}.
\]
Figure 1: The probability distribution $f_K(x; \lambda, N)$ for $\lambda = 1/2$ and $N = 300$ [13, 14]. For topological conditions, 0, 3, 3_1#3_1, others and all, the $\chi^2$ per datum are given by 3.19, 1.30, 0.31, 2.85 and 0.17, respectively; the estimates of $\theta_K$ are given by $0.300 \pm 0.004$, $0.225 \pm 0.003$, $0.169 \pm 0.003$, $-0.164 \pm 0.003$ and $0.0007 \pm 0.0005$, respectively.

The constants $\theta_K$ and $\sigma_K$ are functions of variable $z = \lambda(1 - \lambda)$ as

$$\sigma_K(z; N) = z^{1/2} \exp(\alpha_K z), \quad \theta_K(z; N) = b_K z^{\beta_K}$$

The parameters $\alpha_K$, $\beta_K$ and $b_K$ depend on the knot $K$ and the number of nodes, $N$.

It has been shown [13, 14] that the distance distribution is consistent with the function (2) close to the Gaussian for the cases of $N = 100, 300$ and 800. Figure 1 is reproduced from Ref. [14]. Furthermore, as far as our preliminary data analysis is concerned, the distance distribution is consistent with (2) even for $N = 1000$.

3 Conclusion

We suggest that the distance distribution of random knots should be well approximated by model function (2) even for $N > 1000$. Therefore, the critical behavior of random knots should be different from that of self-avoiding walks. Furthermore, combining the known result that the mean-square radius of gyration of random knots with $N$ nodes increases with respect to $N$ almost as that of the self-avoiding polygons, we suggest that the criticality of random knots should be nontrivial.
Acknowledgment

The present study is partially supported by KAKENHI (Grant-in-Aid for Scientific Research) on Priority Area “Soft Matter Physics” from the Ministry of Education, Culture, Sports, Science and Technology of Japan, 19031007.

References