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On the criticality of random knots at the θ temperature

— A preliminary report —

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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 simialr 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 crtical behavior.

結び目不変量を用いた数値シミュレーションに基づいて、一定の結び目型を持つランダムポリゴン（ランダム結び目）の頂点数 N に関する漸近的な振る舞いは、新しく顕著な臨界現象に対応するという予想を提案する。これまでに多くの研究者によって、ランダム結び目の慣性半径は N に関して排除体積鎖と同じ指数 $\nu_{SAW} = 0.588$ のべき的振る舞いが指摘されている。一方、ランダム結び目に対して分布関数を求めるとガウス的な振る舞いを示す。予備的段階ではあるが、現在、頂点数 $N = 1000$ の場合でも同様な結果が示された。この結果は指数 $\nu_{SAW} = 0.588$ と矛盾する。

1 Introduction

Recently, an important statistical property of ring polymers with fixed topology in a θ 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 θ solvent.

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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

$$R_{g,K}^2 = \frac{1}{2N^2} \sum_{j=1}^{N} \sum_{k=1}^{N} \langle (\boldsymbol{R}_j - \boldsymbol{R}_k)^2 \rangle_K \,. \tag{1}$$

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 $\langle \cdot \rangle_{all}$ 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: $R_{g,K} > R_{g,all}$ 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 $R_{g,K} \propto N^{\nu_{\rm SAW}}$ for very large N, where $\nu_{\rm SAW}$ is the exponent of self-avoiding walks (SAW) [3, 5, 6, 7].

Let us now consider the end-to-end distance distribution, $f_{\rm ete}(r)$, for SAWs. It has the large-N behavior such as $f_{\rm ete}(r) \propto \exp(-r^{\delta})$ with $\delta = 1/(1-\nu_{\rm SAW})$ 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 jth and kth nodes out of the N nodes, and consider the distance between them, $r = |\boldsymbol{r}|$, with $\boldsymbol{r} = \boldsymbol{R}_j - \boldsymbol{R}_k$ where $\boldsymbol{R}_m$ denote the position vectors of the mth node for $m = 1, 2, \ldots, N$. When the two arcs between them have segments n and $N-n$, respectively, and $n \le N-n$, we define parameter λ by fraction n/N. We denote by $f_{all}(r; \lambda, N)$ 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 $f_{\rm ete}(r)$. In fact, integrating $f_{all}(r; \lambda, N)$ over λ, we have the monomer-monomer distribution function, which has the same large N behavior as $f_{\rm ete}(r)$ [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]:

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

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

$$C_K(\lambda, N) = \left(\frac{3}{2N{\sigma_K}^2}\right)^{\frac{3+\theta_K}{2}} \frac{2}{\Gamma\left(\frac{3+\theta_K}{2}\right)}.$$

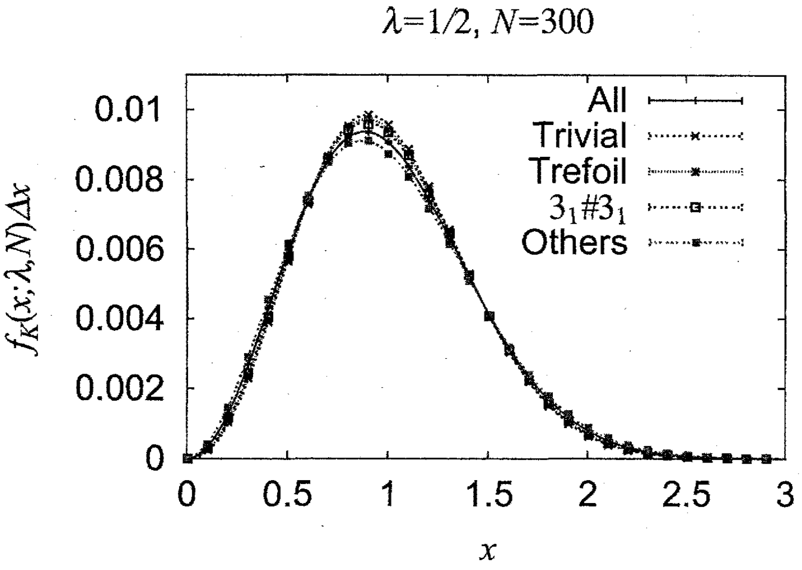

Figure 1: The probability distribution $\tilde{f}_K(x;\lambda,N)$ for $\lambda = 1/2$ and $N = 300$ [13, 14]. For topological conditions, 0, 3_1, $3_1\#3_1$, *others* and *all*, the χ^2 per datum are given by 3.19, 1.30, 0.31, 2.85 and 0.17, respectively; the estimates of θ_K are given by 0.300 ± 0.004, 0.225 ± 0.003, 0.169 ± 0.003, -0.164 ± 0.003 and 0.0007 ± 0.0005, respectively.

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

$$\sigma_K(z;N) = z^{\frac{1}{2}} \exp(\alpha_K\, z)\,, \qquad \theta_K(z;N) = b_K z^{\beta_K} \tag{3}$$

The parameters α_K, β_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.

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