

Scattering function of a ring polymer with fixed knot:

An exact expression in the θ condition and that of the correlation function

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We show an analytic expression for scattering function $g_K(q)$ of a ring polymer with fixed knot K in the theta condition. We discuss its asymptotic behavior, which suggests nontrivial topological entropic effects. We derive $g_K(q)$ via an empirical formula for the probability distribution of distance between two nodes in random polygon of knot K consistent with simulations.

シータ温度溶液中でトポロジ的拘束条件下にある環状高分子鎖の散乱関数と2点相関関数を表す解析的表式を数値シミュレーションの結果を援用して導出した。相関関数はある解析関数の積分の形に表される。散乱関数の高波数極限などは、数値的な取り扱いが微妙で困難である。しかし、この解析的方法により厳密に調べられる。その結果、興味深いクロスオーバーが示唆される。

1 Introduction and Conclusion

Ring polymers have attracted much interest in polymer physics, and their various properties have been studied not only theoretically but also experimentally such as using circular DNAs. [1] Recently ring polymers under topological constraints have been studied extensively. [2, 3] According to des Cloizeaux, a topological constraint should lead to an effective repulsion among segments of ring polymers, which has been numerically confirmed. [3]

Let us denote by $f(r; \lambda, N)$ the probability distribution of distance r between two nodes in a random polygon of N nodes having fixed knot type K . [4] For a given pair of nodes, say, j and k , out of the N nodes, we define parameter λ by the fraction n/N , if the two arcs between them have segments n and $N-n$ where $n \leq N-n$. Here $\mathbf{r}$ denotes the difference of the position vectors: $\mathbf{r} = \mathbf{R}_j - \mathbf{R}_k$, and $r = |\mathbf{r}|$. We propose the following formula for $f_K(r; \lambda, N)$:

$$f_K(r; \lambda, N) = C_K r^{2+\theta_K} \exp \left[\frac{-3r^2}{2N\sigma_K^2} \right] \quad (1)$$

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

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

The parameters α_K , β_K and b_K depend on the knot K and the number of nodes, N .

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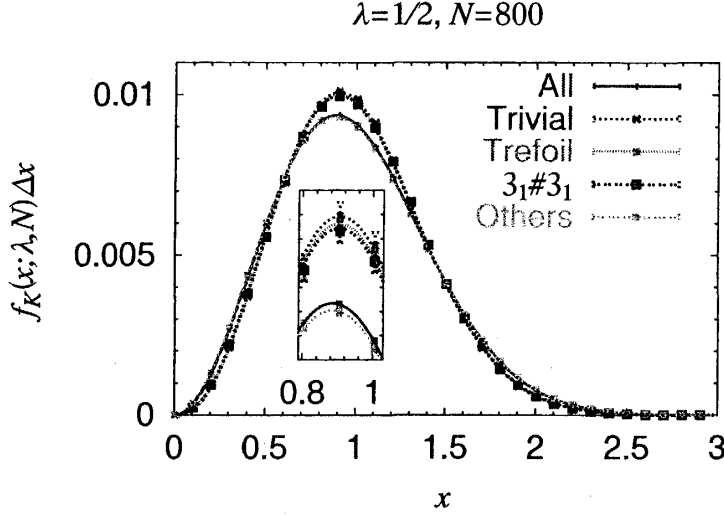


Figure 1: The normalized probability distribution $\tilde{f}_K(x; \lambda, N)$ for $\lambda = 1/2$ and $N = 800$, where $x = r/r_K$ for the average distance r_K . For knots, 0, 3_1 , $3_1\#3_1$, *others* and *all*, θ_K are estimated by 0.454 ± 0.005 , 0.413 ± 0.006 , 0.389 ± 0.005 , -0.033 ± 0.0005 and 0.002 ± 0.003 , respectively. In the inset, the peaks are given by 0, 3_1 , $3_1\#3_1$, *all* and *others*, respectively, in decreasing order.

The model function (1) of $f_K(r; \lambda, N)$ is consistent with simulation data as shown in Fig. 1. [6] The function (1) leads to an analytic expression of scattering function $g_K(q)$, which is consistent with that evaluated in recent simulation [5]. Moreover, for $q = |\vec{q}| \gg 1$ we have

$$\frac{g_K(q)}{N} = 2 \int_0^{1/2} \frac{\sqrt{2} \sin(\pi\theta_K(\lambda) + \pi/4)}{\Gamma(\{3 + \theta_K(\lambda)\}/2)/(\sqrt{\pi}/2)} \left(\frac{Nq^2}{6} \sigma_K^2 \right)^{\theta_K(\lambda)} \exp\left(-\frac{Nq^2}{6} \sigma_K^2\right) d\lambda + O(1/A) \quad (3)$$

where $A = Nq^2/12$ and we have a slow asymptotic expansion with $\beta_K \approx 0.5$:

$$\frac{g_K(q)}{N} = \frac{1}{A} \left(1 + O(A^{-\beta_K}) \right). \quad (4)$$

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