ON A UNIVERSALITY OF RANDOM KNOTTING

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The entropy of a knotted ring polymer has been numerically evaluated and the entanglement effect on it has been studied exactly through the computer simulation of random knotting. The peoblem is how the entropy of a knotted polymer changes with respect to the length N under the topological constraint. We show that the entropy as a function of N can be expressed by a scaling formula and also that the exponent is universal for models of random polygon.

Let us consider a random model of ring polymer of N monomers, which gives random configurations of polygons with N vertices. For example, we may take the Gaussian random polygon, or the rod-bead random polygon; the former is given by ideal chains and the latter consists of real chains with the self-avoiding parameter of bead radius r. Suppose that we have M configurations of N-noded random polygon of the random model. We define the knotting probability $P_K(N)$ for a knot K by the fraction of those configurations that have the same knot type K; If there are M_K configurations with knot K, then it is given by $P_K(N) = M_K/M$. The entropy $S_K(N)$ of an N-noded ring polymer of knot K is equivalent to the knotting probability: $S_K(N) = -k_B \log P_K(N) + const. \times N$.

The number M_K of the configurations with K can be numerically obtained by calculating knot invariants for each of the M configurations of random polygon. [1] We see that the finite-type invariants are practically useful. [1] We propose a scaling formula for knotting probability $P_K(N) = C(K)N^{m(K)} \exp(-N/N(K))$, where $m(K)$, $N(K)$ and $C(K)$ are fitting parameters. [1] Applying the formula to the numerical data of the knotting probability $P_K(N)$ with $N = 50 \sim 2000$, we see that it gives good fitting curves to the data for both the gaussian model and the rod-bead models. [1, 2, 3, 4]

From the numerical result [4] we propose that the exponent $m(K)$ is universal for each knot type K: for different models of random polygon the knotting probability for knot K is expressed by the scaling formula with the same value of the exponent $m(K)$ and that the exponent is determined only by the knot type.

References

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Model	Knot K	$m(K)$	$C(K)$	$N(K)$
Gaussian	0	0.0	1.05 ± 0.03	(3.4 ± 0.1) ×10^2
Gaussian	3_1	1.0	0.62 ± 0.02	(3.4 ± 0.3) ×10^2
Gaussian	$3_1\sharp 3_1$	2.0	0.17 ± 0.02	(3.4 ± 0.2)×10^2
$r = 0.05$	0	0.0	1.06 ± 0.03	(3.0 ± 0.3)×10^2
$r = 0.05$	3_1	1.0	0.63 ± 0.02	(3.1 ± 0.3) ×10^2
$r = 0.05$	$3_1\sharp 3_1$	2.0	0.19 ± 0.02	(3.0 ± 0.2) ×10^2
$r = 0.10$	0	0.0	1.04 ± 0.03	(4.2 ± 0.1)×10^2
$r = 0.10$	3_1	1.0	0.70 ± 0.02	(4.3 ± 0.4) ×10^2
$r = 0.10$	$3_1\sharp 3_1$	2.0	0.25 ± 0.03	(4.4 ± 0.3) ×10^2
$r = 0.15$	0	0.0	1.00 ± 0.03	(9.0 ± 0.3)×10^2
$r = 0.15$	3_1	1.0	0.82 ± 0.02	(8.8 ± 0.8)×10^2
$r = 0.15$	$3_1\sharp 3_1$	2.0	0.34 ± 0.04	(9.2 ± 0.5) ×10^2

TABLE I. The parameters $m(K)$, $N(K)$, and $C(K)$ of the fitting curves to the knotting probabilities for the Gaussian model and the rod-bead models with the three bead-radii: r=0.05, 0.10, and 0.15. Symbol $K_1\sharp K_2$ denotes the product (or the composite knot) of K_1 and K_2.