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Intrinsic viscosity of knots in solution evaluated through the 
Brownian Dynamics

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Abstract: We have evaluated the intrinsic viscosity of the solution of ring polymers 
of a knot type K by the Brownian dynamics with both hydrodynamic and excluded 
volume effects. Due to recent development of experiments, we expect that knotted 
ring polymers will be synthesized near future. It is thus important to formulate 
empirical equations for describing the intrinsic viscosity in terms of K. They should 
be useful for separating knot species in solution. We found that the ratio of the 
intrinsic viscosity of a knot to that of the trefoil knot is independent of the number 
of segments N in the investigated range. We also found that it is expressed by a 
quadratic function of the average crossing number of the ideal knot of K \((ACN(K))\).

Introduction

In this work, we have investigated the intrinsic viscosity of the solution of knotted 
ring-polymers through the Brownian dynamics with hydrodynamic and excluded 
volume effects. In recent experiments, ring polymers of high purity have been 
synthesized with small dispersion \(^{[1]}\). We thus expect that knotted ring polymers 
will be synthesized near future. It is then important to express the intrinsic 
viscosity of the solution of knotted ring polymers with the same knot type K in 
terms of knot K. We formulate an empirical equation of the ratio of the intrinsic 
viscosity of a nontrivial knot to that of the trefoil knot expressed in terms of the 
average crossing number of ideal knot of knot K \((ACN(K))\). Here we remark that the 
ideal knot should play a fundamental role in the dynamics of knots in solution. In 
fact we have found in the previous study that the ratio of the diffusion constant of a 
nontrivial knot to that of a linear polymer is almost independent of the number of 
segments N, and also that it is given by a linear function of \(ACN(K)\) \(^{[2]}\).
2. Result

Fig. 1 shows the $N$-dependence of the intrinsic viscosity $[\eta]/[\eta]_0$ for the trefoil knot in the case of $N=20, 27$ and $36$ (here $[\eta]_0$ is the zero-shear viscosity for the Rouse model). The intrinsic viscosity at shear rate $\gamma$ depends on the number of segments $N$. However, in Fig. 2 we find that the intrinsic viscosity divided by $N^{0.8}$ is independent of $N$. For other knots such as the $4_1$ knot and the $5_1$ knot, the intrinsic viscosity divided by $N^{0.8}$ is almost independent of $N$. In our numerical simulation, we have $[\eta]_K = a(K) [\eta]_0 N^{0.8}$ for any given knot type $K$, where the coefficient $a(K)$ depends on the shear rate $\gamma$. Therefore, the ratio of the intrinsic viscosity of a nontrivial knot to that of the trefoil knot is given by $[\eta]_K/[\eta]_3 = a(K)/a(3_1)$.

We have found that the ratio $[\eta]_K/[\eta]_3$ is expressed as a quadratic function of $\text{ACN}(N)$ and shear rate $\gamma$. In the case of high shear rate, we have

$$[\eta]_K/[\eta]_3 = -0.00045 \gamma ((\text{ACN}(K) - \text{ACN}(3_1))^2 + 460 \gamma^2 (\text{ACN}(K) - \text{ACN}(3_1))) + 1.0$$

In the case of low shear rate, we have

$$[\eta]_K/[\eta]_3 = 0.0028 \gamma^2 (\text{ACN}(K) - \text{ACN}(3_1))^2 - 37 \gamma (\text{ACN}(K) - \text{ACN}(3_1)) + 1.0$$

These empirical equations should be independent of $N$ in the investigated range.

3. Conclusion

The ratio of intrinsic viscosities $[\eta]_K/[\eta]_3$ is almost independent of $N$. This ratio is expressed as the quadratic function of $\text{ACN}(K)$. Furthermore we suggest that the ideal knot should be a fundamental concept in the dynamics of knots in solution.

References
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