Topological Invariants of Links and Application to Random Knots

(`Perspectives of Soliton Physics', Koshiba Hall, Feb. 16-17, 2007)

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- **Link polynomials: Invariants of knots and links**
- **Random knots: a model of knotted ring polymers**
- **We can study**
  Topological entanglement effects among polymers
  and DNA topology

through simulation using knot invariants.

Knots and Links

- A knot is a closed curve in three dimensions with no self-intersection.

  ex. A circle gives a trivial knot.

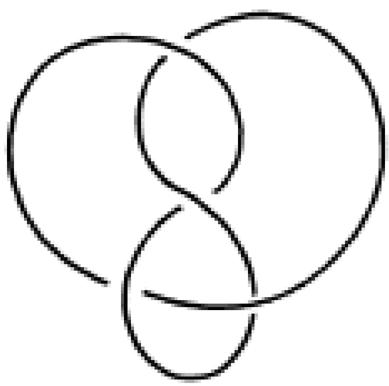


Fig. 2. A knot.

Fig. 3. A link.

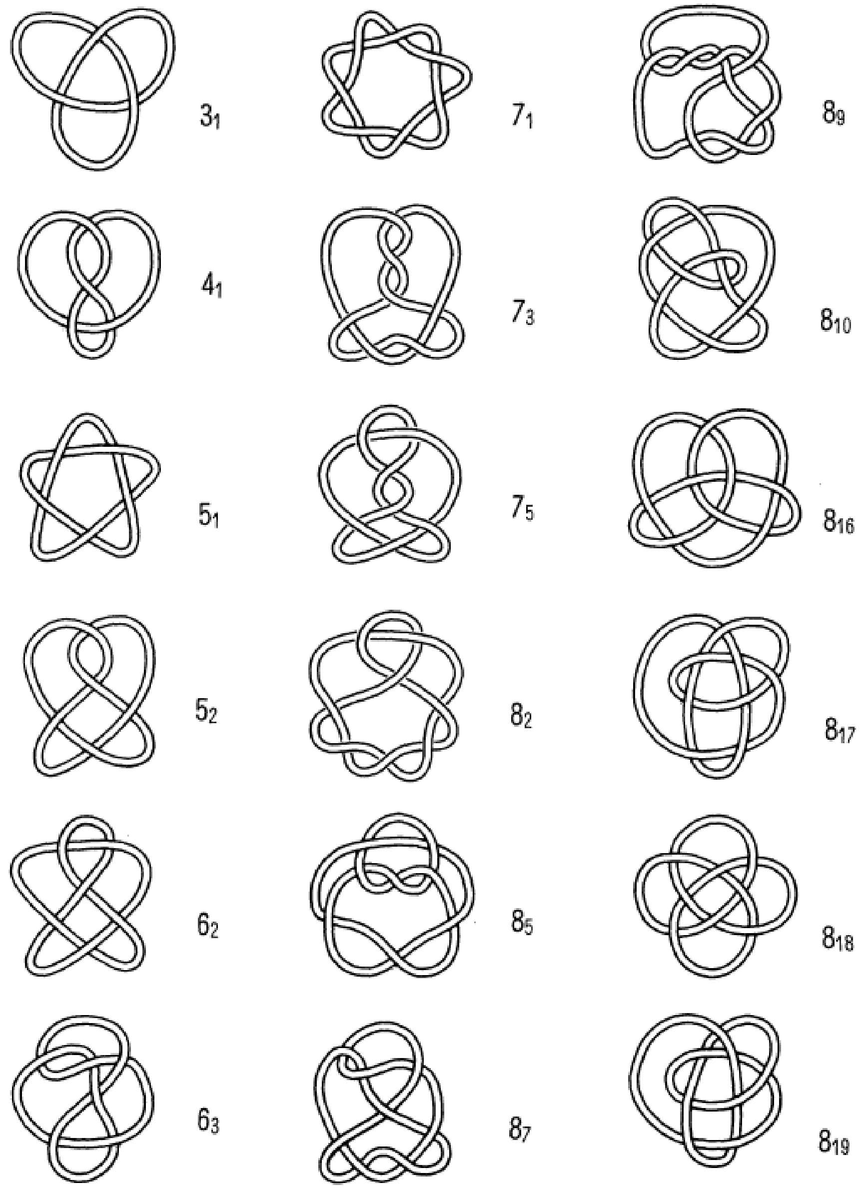
- A link is a set of closed curves in three dimensions. => Links generalize knots.

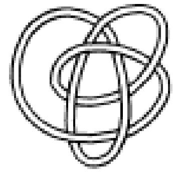
Link diagrams

- We express links by projections on a plane where upper curves and lower curves are distinguished at all crossing points.

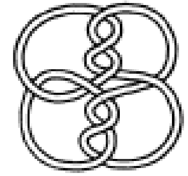
- We call such projections *link diagrams*.

Nontrivial knots (closed 3-braids)

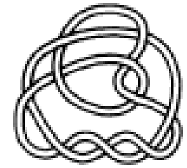




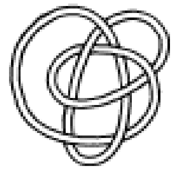
8_{20}



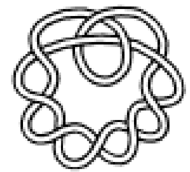
9_{16}



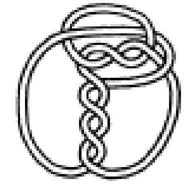
10_{47}



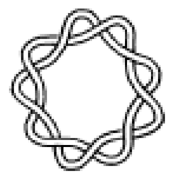
8_{21}



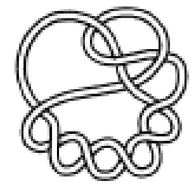
10_{2}



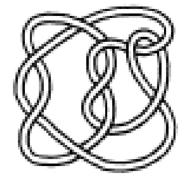
10_{48}



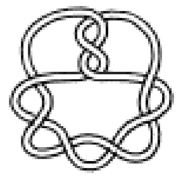
9_{1}



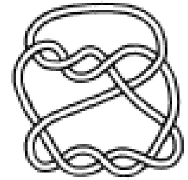
10_{5}



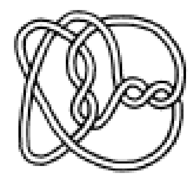
10_{62}



9_{3}



10_{9}



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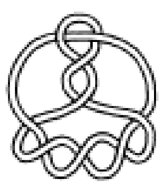
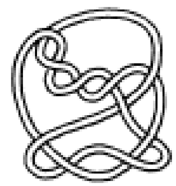
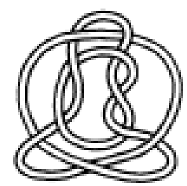


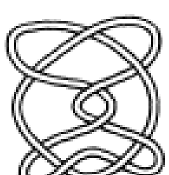
9_{6}



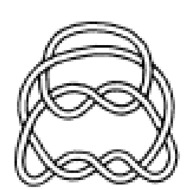
10_{17}



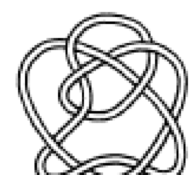
10_{79}



9_{9}



10_{46}



10_{82}

Reidemeister moves on a link diagram does not change the topology.

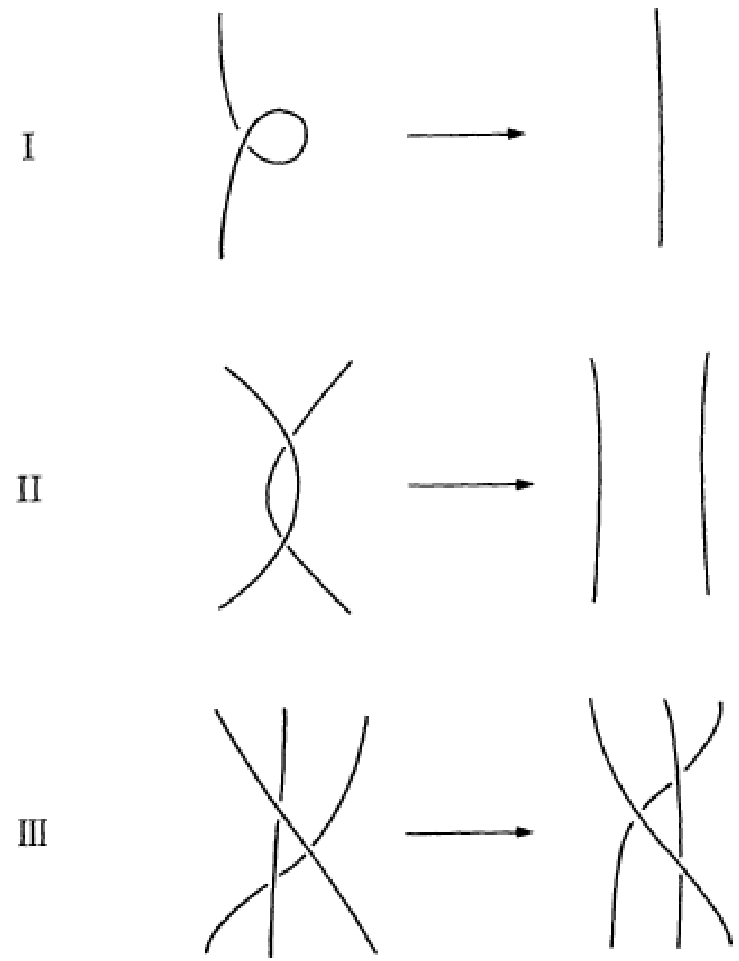


Fig. 17. Reidemeister moves I, II and III.

Topological invariants of knots and links

- Two link diagrams express the same link if and only if there exists a finite sequence of Reidemeister moves which connects one to the other.

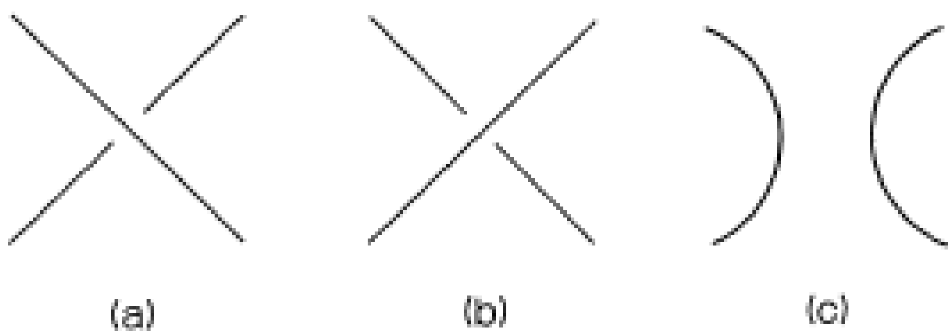
- A link invariant is such a quantity defined on link diagrams that is invariant under Reidemeister moves.

Skein diagrams

Suppose that D_-, D_+, and D_0 are link diagrams which are the same except at one crossing point.

We call them skein diagrams.

(a) minus - ; (b) plus + ; (c) zero 0



The Alexander-Conway polynomial

We assume that the Alexander-Conway polynomial for the trivial knot is equal to 1.

We calculate it through the following recursive relation with respect to the number of crossing points:

$$\nabla_{D_+}(z) - \nabla_{D_-}(z) = z\nabla_{D_0}(z)$$

J.W. Alexander (1928); J. Conway (1970)

The Jones polynomial

We assume that the Jones polynomial for the trivial knot is equal to 1.

We calculate it through the following recursive relation with respect to the number of crossing points:

$$t^{-1}V_{D_+}(t) - tV_{D_-}(t) = \left(\sqrt{t} - \frac{1}{\sqrt{t}}\right)V_{D_0}(t)$$

V.F.R. Jones (1985); cf. the Temperley-Lieb-Jones algebra

The HOMFLY polynomial

We assume that the HOMFLY polynomial for the trivial knot is equal to 1.

We calculate it through the following recursive relation with respect to the number of crossing points:

$$v^{-1} P_{D_+}(v,z) - v V_{D_-}(v,z) = z P_{D_0}(v,z)$$

P.Freyd, D. Yetter, J. Hoste, W.B.R. Lickorish, K.C. Millett, and A. Ocneanu (1985); J.H. Przytycki and P. Traczyk (1987)

The Kauffman polynomial

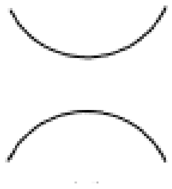
We assume that the Kauffman polynomial for the trivial knot is equal to 1.

We calculate it through the 3rd order recursive relation with respect to the number of crossing points:

$$L_{D_+}(a,z)+L_{D_-}(a,z)=z\left(L_{D_0}(a,z)+L_{D_\infty}(a,z)\right)$$

L.H. Kauffman (1987)

creation-annihilation diagram



The HOMFLY-PT polynomial
(the skein polynomial)

- The HOMFLY-PT polynomial of a link gives a two-variable polynomial and generalizes both the Alexander polynomial and the Jones polynomial.

- However, there exists another generalization to the Jones polynomial.

Link polynomials generalizing the Jones polynomial are derived from the solvable N-state vertex models (fusion hierarchy)

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LETTERS

Knot Invariants and the Critical Statistical Systems

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(Received December 4, 1986)

A new invariant polynomial for knots and links is constructed from a solvable vertex model describing a critical statistical system. Various implications and the possible generalizations are discussed in connection with the recent development in the study of critical phenomena in two dimensions.

Recent development[1–7] in the study of two-dimensional statistical systems is quite exciting. The conformal bootstrap program[2] revealed rich physical and mathematical structures of the statistical systems at criticality. An

models),[11] and the self-dual Potts models,[10,12] which are exactly solvable. An important fact is that for the existence of the normalized trace associated with the algebra $A_{q,n}$ in the $n \to \infty$ limit ("thermodynamic limit"), the

A universal property of solitons:
Factorized Scattering among solitons
=> the Yang-Baxter equation

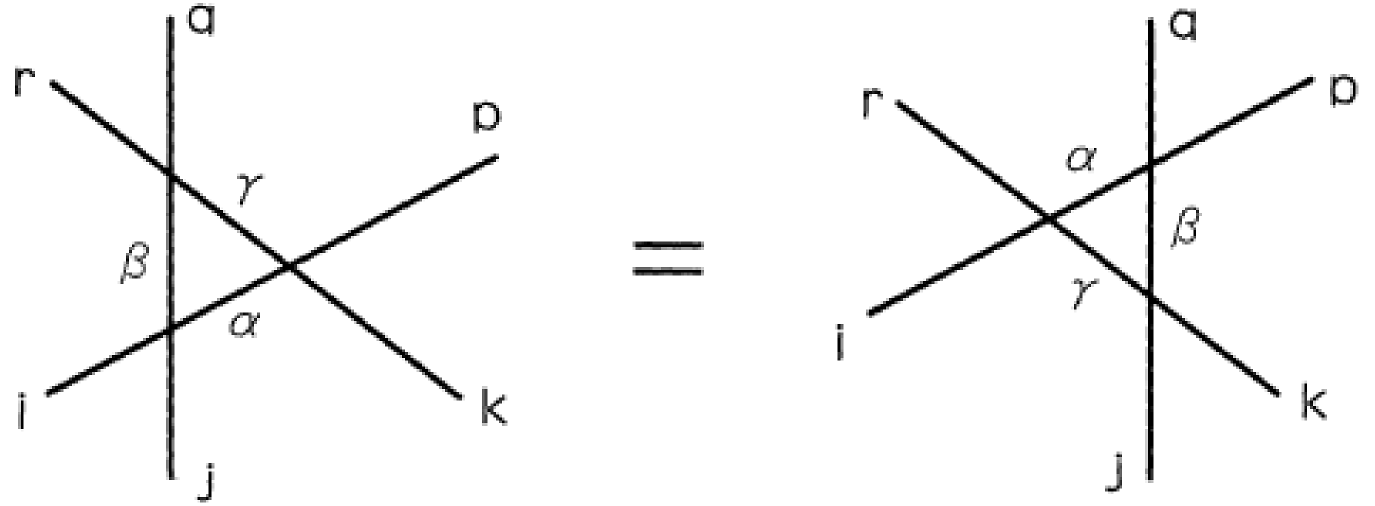


Fig. 1. Schematic explanation of the factorization equation. Time direction is upward.

Braids and the braid group

- An example of a braid

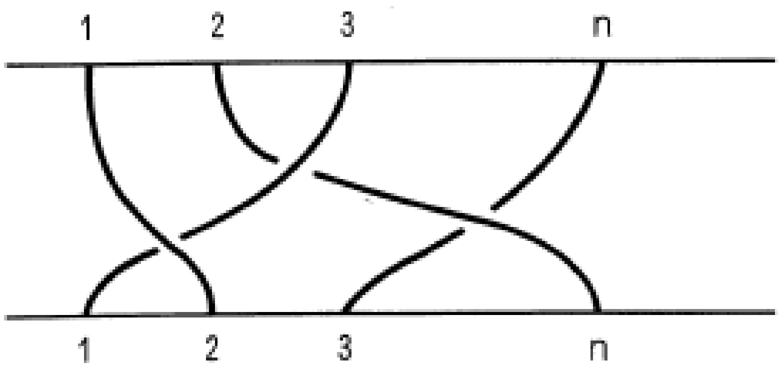


Fig. 1. An example of *n* braids.

- The braid operation

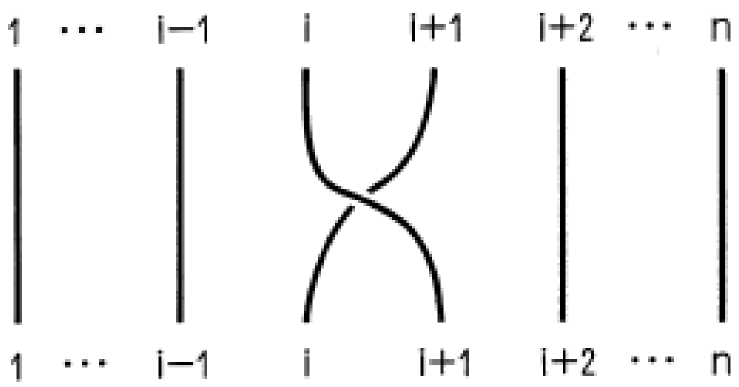
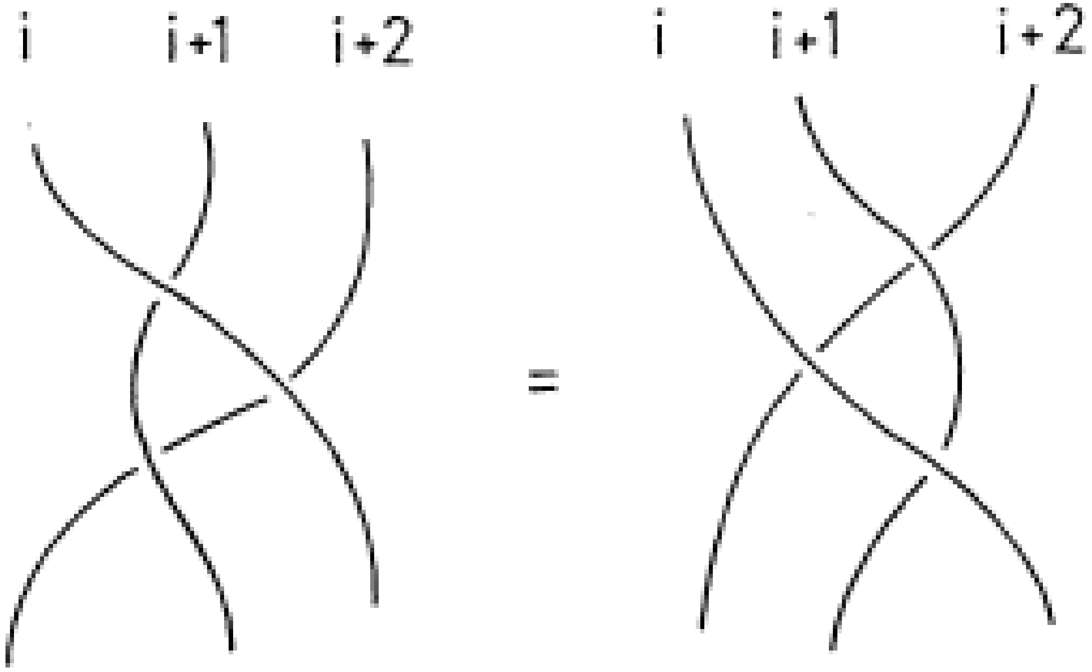


Fig. 2. Generator b_i.

The braid group relation corresponds to the Yang-Baxter equation



$b_i b_{i+1} b_i$ $\qquad$ $b_{i+1} b_i b_{i+1}$

Fig. 3. Two topologically equivalent braids.

Higher order skein relations

$N=3$

$$\alpha(L_{2+}) = t(1-t^2+t^3)\alpha(L_+) + t^2(t^2-t^3+t^5)\alpha(L_0) - t^8\alpha(L_-). \tag{5.23}$$

$N=4$

$$\alpha(L_{3+}) = t^{3/2}(1-t^3+t^5-t^6)\alpha(L_{2+}) + t^6(1-t^2+t^3+t^5-t^6+t^8)\alpha(L_+) + t^{9/2}t^8(-1+t-t^3+t^6)\alpha(L_0) - t^{20}\alpha(L_-). \tag{5.24}$$

The N=3 link polynomial distinguishes a pair of links which have the same Jones polynomial

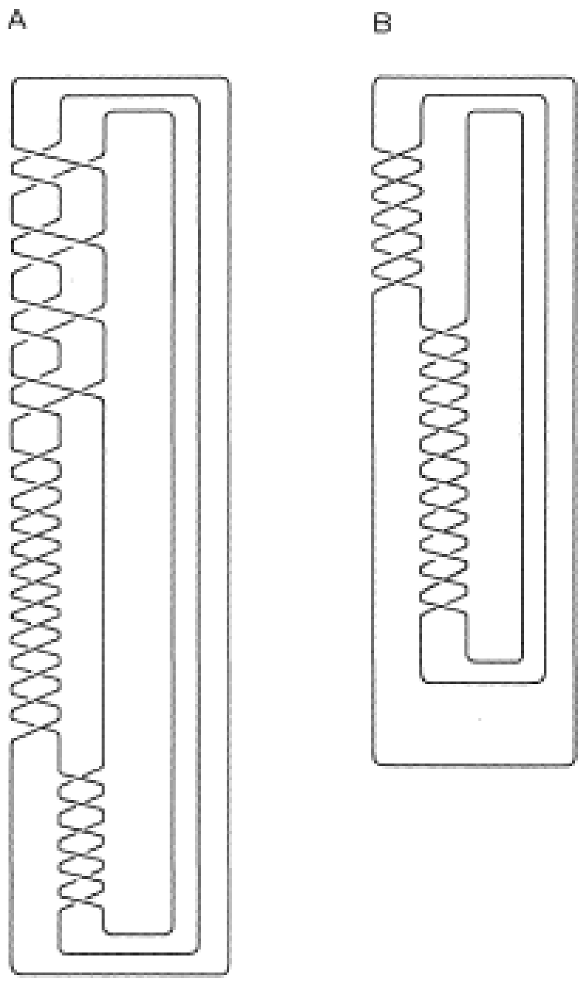


Fig. 4. Closed braids, $A=(b_1b_2b_1)^4b_1^{-12}b_2^6$ and $B=b_1^{-6}b_2^{12}$.

$$\alpha(A)=\alpha(B)$$
$$=(t^{18}-t^{17}+2t^{16}-3t^{15}+4t^{14}-5t^{13}+6t^{12}$$
$$-6t^{11}+6t^{10}-6t^{9}+6t^{8}-5t^{7}+6t^{6}-4t^{5}$$
$$+4t^{4}-3t^{3}+2t^{2}-t+1)/t^{3}. \qquad (5.3)$$

On the other hand, $\alpha(A)$ and $\alpha(B)$ are different in the $N=3$ case. We have

$$\alpha(B)=P_{-6}P_{12}=(t^{54}-t^{53}+2t^{51}-2t^{50}-t^{49}$$
$$+4t^{48}-3t^{47}-2t^{46}+6t^{45}-4t^{44}-2t^{43}$$
$$+8t^{42}-4t^{41}-4t^{40}+10t^{39}-6t^{38}-5t^{37}$$
$$+12t^{36}-7t^{35}-5t^{34}+12t^{33}-7t^{32}-5t^{31}$$
$$+13t^{30}-7t^{29}-5t^{28}+12t^{27}-7t^{26}-5t^{25}$$
$$+12t^{24}-6t^{23}-6t^{22}+12t^{21}-5t^{20}-6t^{19}$$
$$+12t^{18}-4t^{17}-6t^{16}+10t^{15}-3t^{14}-6t^{13}$$
$$+8t^{12}-2t^{11}-5t^{10}+6t^{9}-t^{8}-3t^{7}+4t^{6}$$
$$-2t^{4}+2t^{3}-t+1)/t^{12}. \qquad (5.4)$$

We may evaluate $\alpha(A)$ as follows. Using formula (3.7b) and the generalized Alexander-Conway relation (2.15), we have

$$\alpha(A)=\alpha(\Delta^4b_1^{-12}b_2^6)=\alpha(b_1b_2^3b_1b_2^{-9}b_1b_2^6)$$
$$=a\alpha(b_1b_2^3b_1b_2^{-9}b_1b_2^{-9})$$
$$+b\alpha(b_1b_2b_1b_2^{-9}b_1b_2^6)$$
$$+c\alpha(b_1^3b_2^{-9}b_1b_2^6). \qquad (5.5)$$

Each term in (5.5) may be calculated as

Various approaches to the fusion hierarchy

- The fusion hierarchy of link polynomials introduced by Akutsu and Wadati (1987) are reconstructed as quantum invariants of higher spin representations of the quantum group *Uq(sl(2)).* (Kirillov-Reshetikhin, 1989)

- Related works: invariants of parallel links (J. Murakami, 1989); invariants of spatial graphs (S. Yamada, 1989)

- The Chern-Simons quantum field theory with su(2). (Witten 1989)

- They are also called the colored Jones polynomials in knot theory (Cf. Melvin-Morton (1995) `The colored Jones function').

Several Advantages of the fusion hierarchy

- The link polynomials in the hierarchy can be *systematically and explicitly calculated*.

  (Many useful tools such as *q*-analogues of 3*j* and 6*j* symbols)

- At roots of unity, it leads to *invariants of three-dimensional manifolds.*

  (Turaev-Reshetikhin, Turaev-Viro, Kohno)

- It is one of the most useful families of link polynomials for studying knots and links. (Cf. Melvin-Morton (1995))

Physical applications of knot invariants:

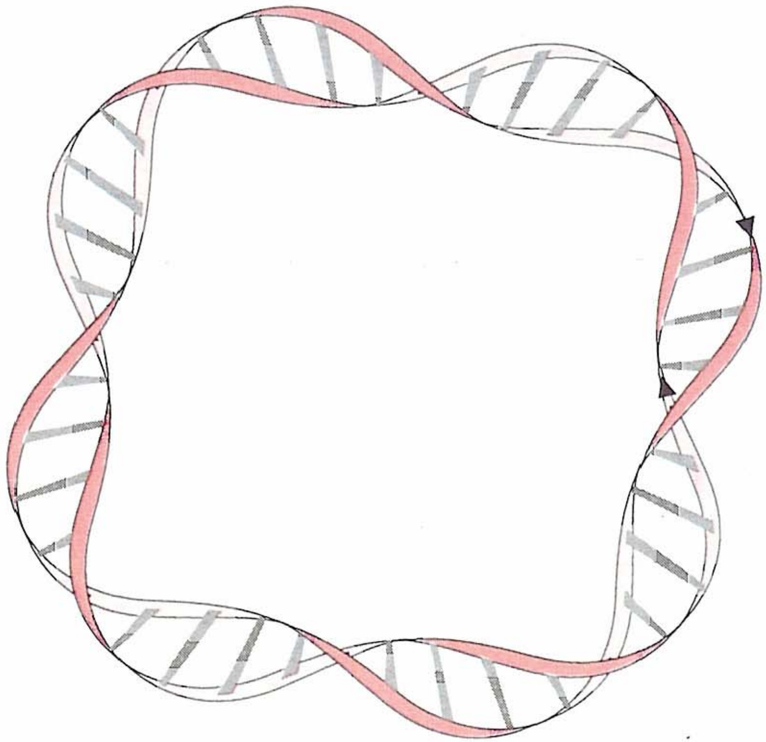
Topological entanglement effects

- Consider polymers in solution or polymer networks consisting of polymer chains.
- Ring polymers and polymer networks have fixed topology under thermal fluctuations.
- Topological constraints may lead to nontrivial statistical and dynamical properties of polymers, such as topological entropic repulsion.
- We study such topological effects through computer simulations using invariants of knots and links.

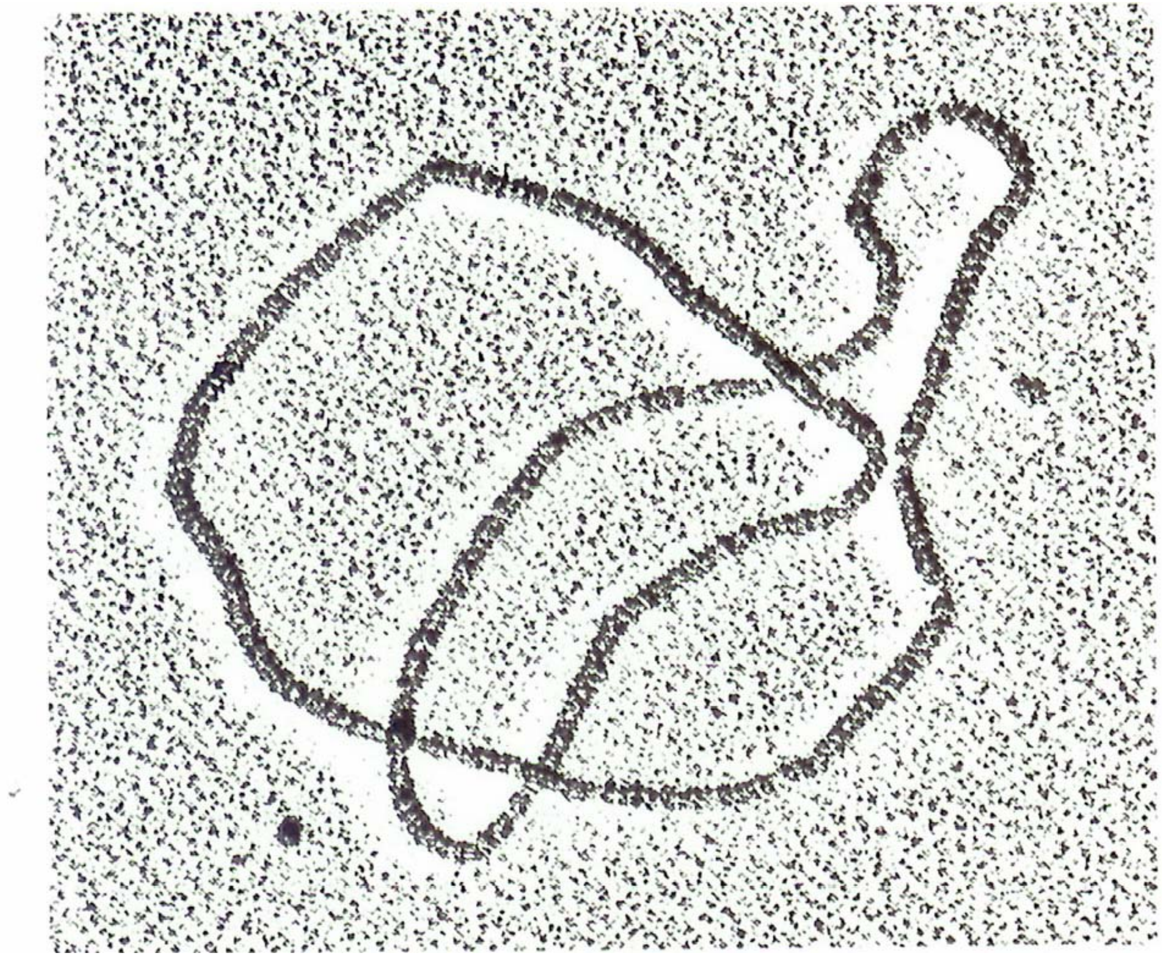
  (random knots or random links)

Double stranded circular DNA

(A.D. Bates and A. Maxwell, *DNA Topology*, Oxford Univ. Press, 1993)



An electron micrograph of Trefoil knot DNA
M.A. Krasnow, A. Stasiak, S.J. Spengler, F. Dean, T. Koller, and N.R. Cozzarelli, Nature 304 (1983) 559



Motivations for studying random knots and links: knotted DNAs

- Many DNA knots are derived from circular DNAs. (Circular DNAs are the key to understand replication process.)

- It is nontrivial how to keep the topology of a double stranded DNA chain during replication process. (enzymes, ‘topoisomerases’)

- To understand DNA topology, we study statistical mechanics and dynamics of (thin) knotted ring polymers.

- Topological effects are nontrivial. A topological constraint leads to entropic repulsions among polymer segments.

  (cf. topological swelling of random knots)

Approaches to topological entanglement effects

- Statistical study:

  Construct random configurations of ring polymers with fixed topology (cf. Monte Carlo methods)

  knotting probability (entropy of a random knot)

  linking probability (entropic repulsion among ring polymers,

  => anomalous osmotic pressure)

  the mean square radius of gyration (average size of ring polymers)

  two-point correlation functions

  scattering functions (static structure factors)

- Dynamical study:

  Dynamical simulation of a ring polymer with fixed topology (cf. Molecular Dynamics)

An example of simulation scheme for statistical study of random knots

Construct 1000,000 polygons of N vertices for N=100, 300 and 800

Calculate knot invariants:

the determinant of knots; the 2nd order Vassiliev invariant.

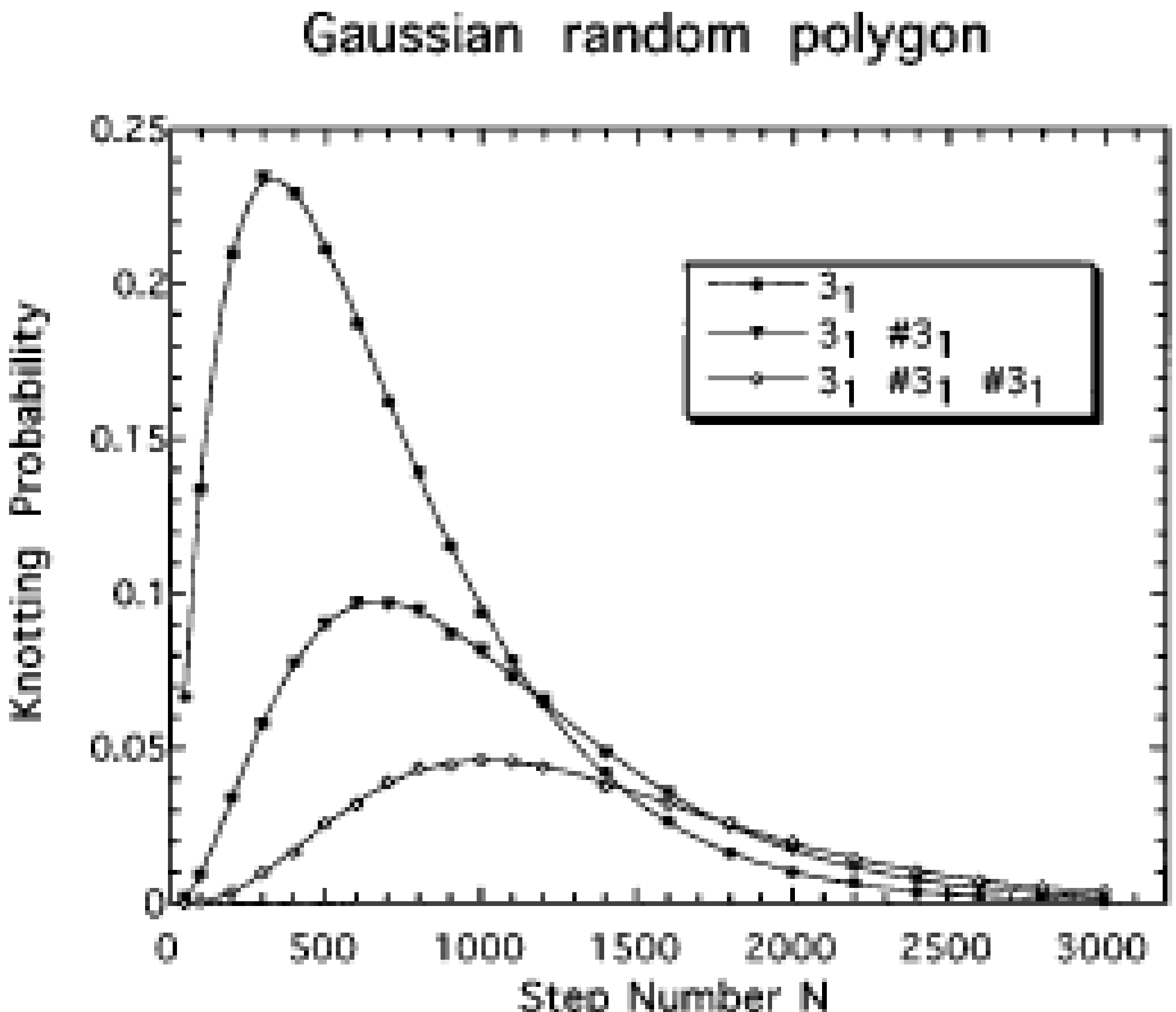
We pick up such polygons that have the same set of values of the two knot invariants.

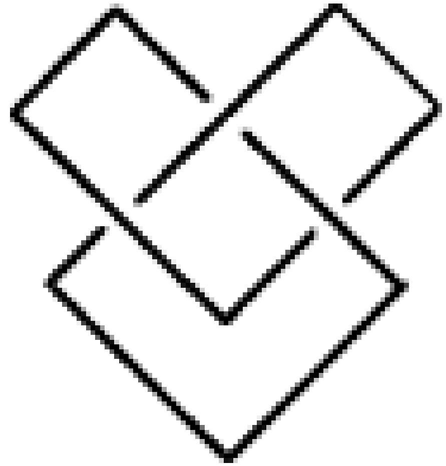
We evaluate the statistical expectation of some physical quantity taking the average over selected polygons.

Knotting Probability:

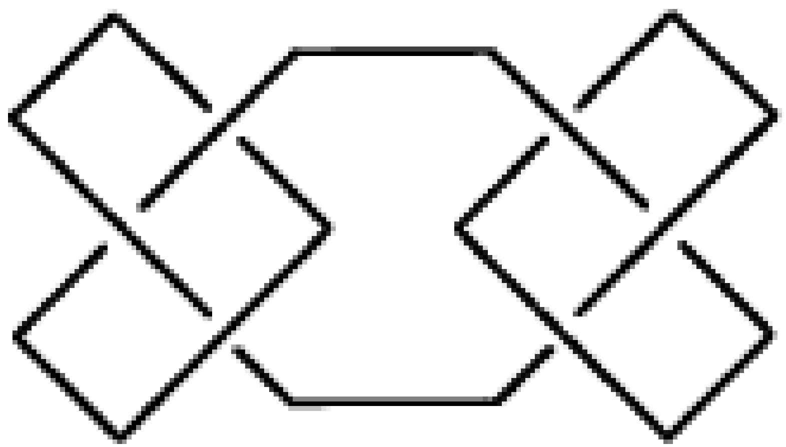
Probability of a random polygon being a given knot

T.D. and K. Tsurusaki, PRE 55 (1997)





(a)



(b)

FIG. 1. (a) A diagram of prime knot 3_1 with 3 crossing points. (b) A diagram of composite knot $3_1 \# 3_1$.

Fitting function of the knotting probability

- Let $P(K,N)$ denotes the probability of random polygon with N-vertices having knot type K

- $P(K,N) = C(K)\, N^{\,m(K)} \exp(-\,N/N_0\,)$

- Scaling concepts of polymers explain the N -dependence of knotting probability.

  (Criticality at infinite N)

Knotting probability can be compared with DNA experiment (Cf. A. Vologodskii, to appear)

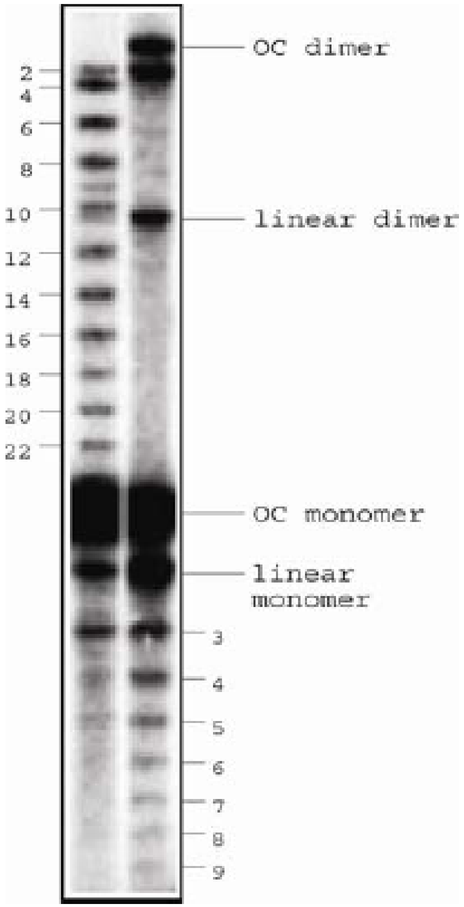


Figure 5. Electrophoretic separation of knotted (right lane) and linked (left lane) DNA molecules 4363 bp length. Each band corresponds to a knot or link with a specific number of intersections in the standard form. These numbers are shown next to eacl band. All links belong to the torus family. OC dimer is open circular DNA molecule o: double length. (Illustration provided by E. M. Shekhtman and D. E. Adams.)

The average size

The mean square radius of gyration of a ring polymer with fixed knot *K.*

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

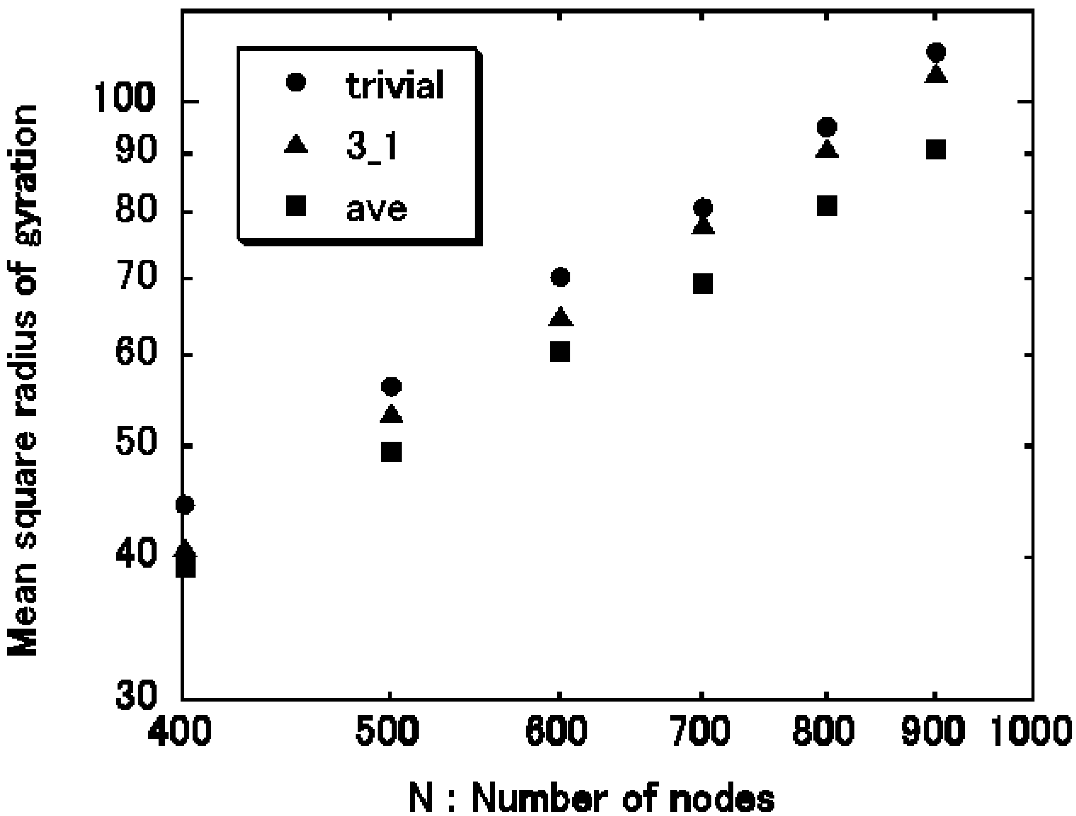
We take the average over all configurations of the ring polymer with fixed knot type.

Topological swelling of thin ring polymers

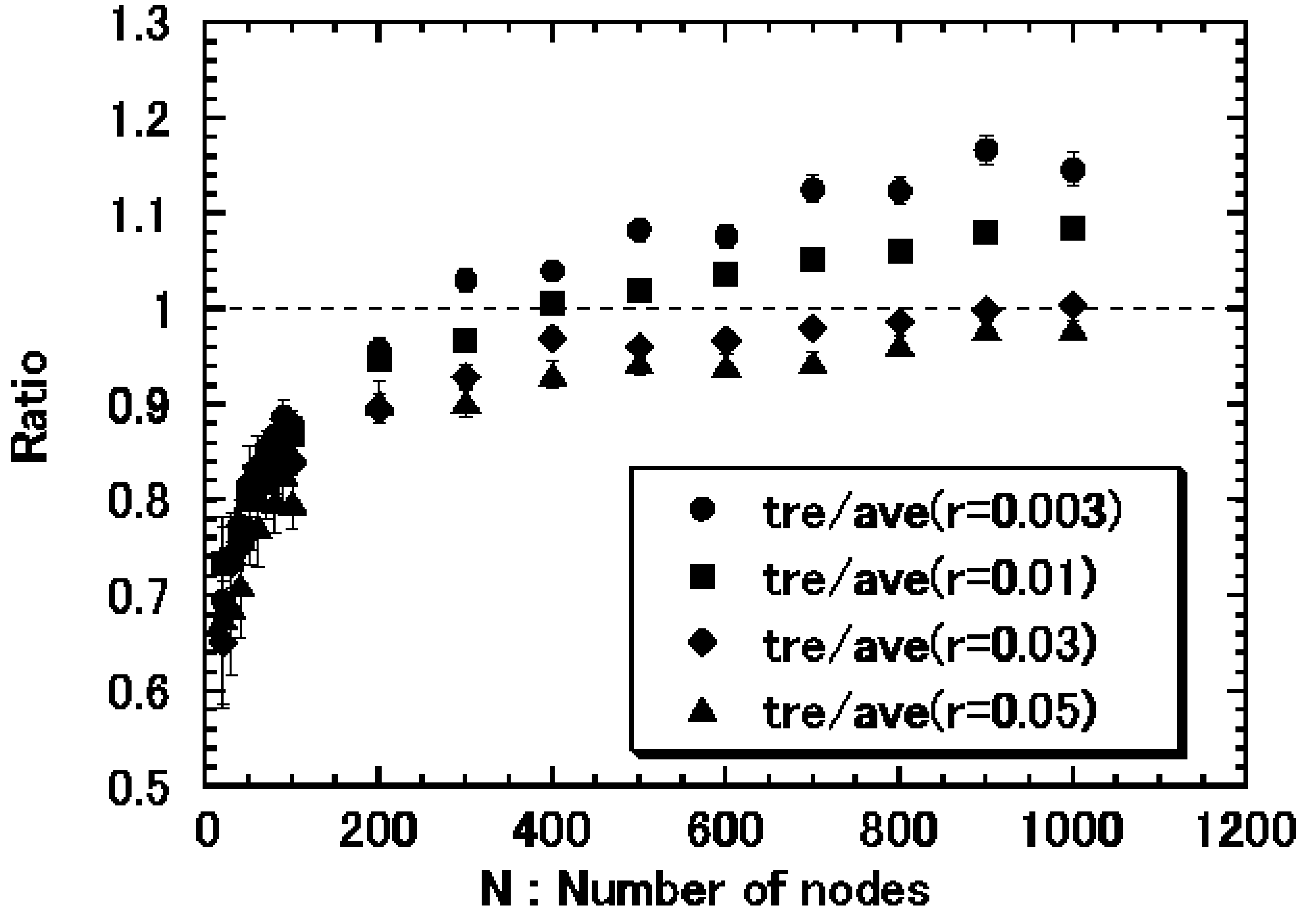
for cylindrical segments with r = 0.003)

Average size versus N:

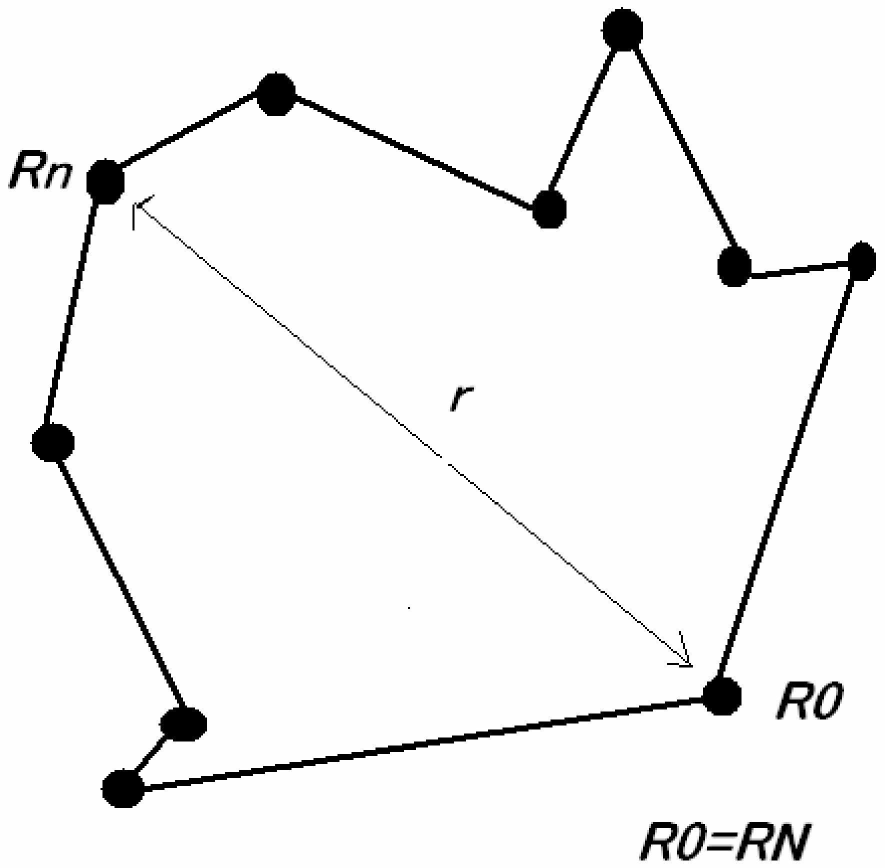
Miyuki.K. Shimamura et al., Phys. Rev. E Vol. 65, 051802 (2002)



Topological swelling occurs for SAP consisting of cylinders with small radius (the ratios of the average sizes)



Two vertices with Arc length ***n/N*** and Distance ***r***



Two-point correlation function: Probability distribution of distance *r* between two fixed vertices

$$f_K(r; n/N, N)$$

- We denote by the symbol the probability distribution of distance *r* between two vertices with parameter *n/N* of random polygon with fixed knot *K*

- We call it *Distance distribution*, briefly.

Cf. A.Yao et al, J. Phys. A **37**, (2004) 7993-8006.

Scattering function $g_K(q)$ *(static structure factor)*

- Scattering function is given by the Fourier transform of the correlation function.

$$g(\boldsymbol{q}) = \int d\boldsymbol{r} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} g(\boldsymbol{r})$$

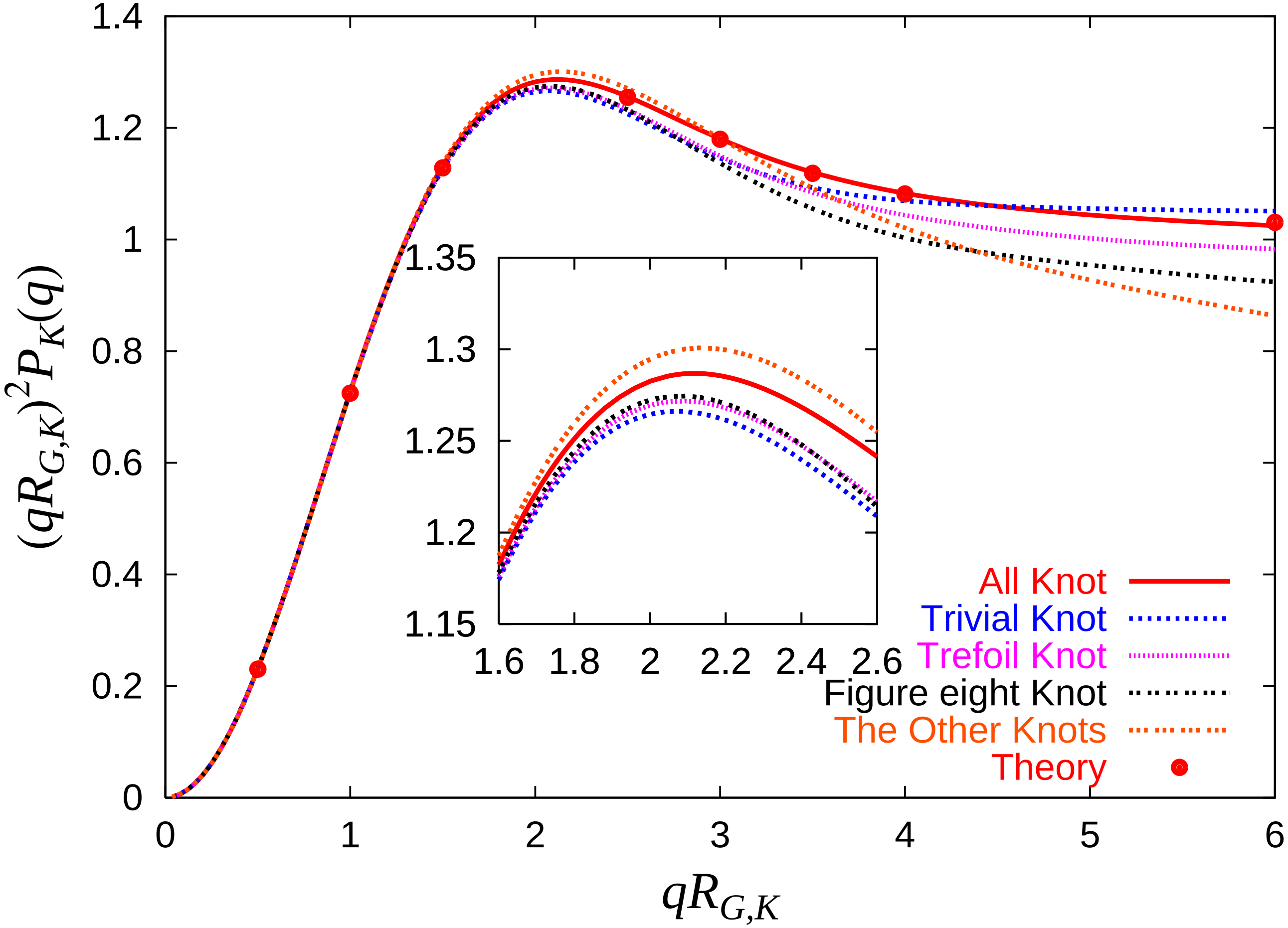
$$g_K(\boldsymbol{q}) = 2N \int_0^\infty \int_0^{1/2} f_K(r;\lambda,N)\, d\lambda \frac{\sin qr}{qr} dr$$

- Here *q* denotes to the wave number.

Scattering function $P_K(q)$ of a knotted ring polymer

(M.K. Shimamura et al., Phys. Rev. E **72**, 041804 (2005))

- The Kratky plots: $q^2 \, P_K(q)$ *versus* q ($N=200$)



Exact model function of distance distribution **(A. Yao and T.D, in prep.)**

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

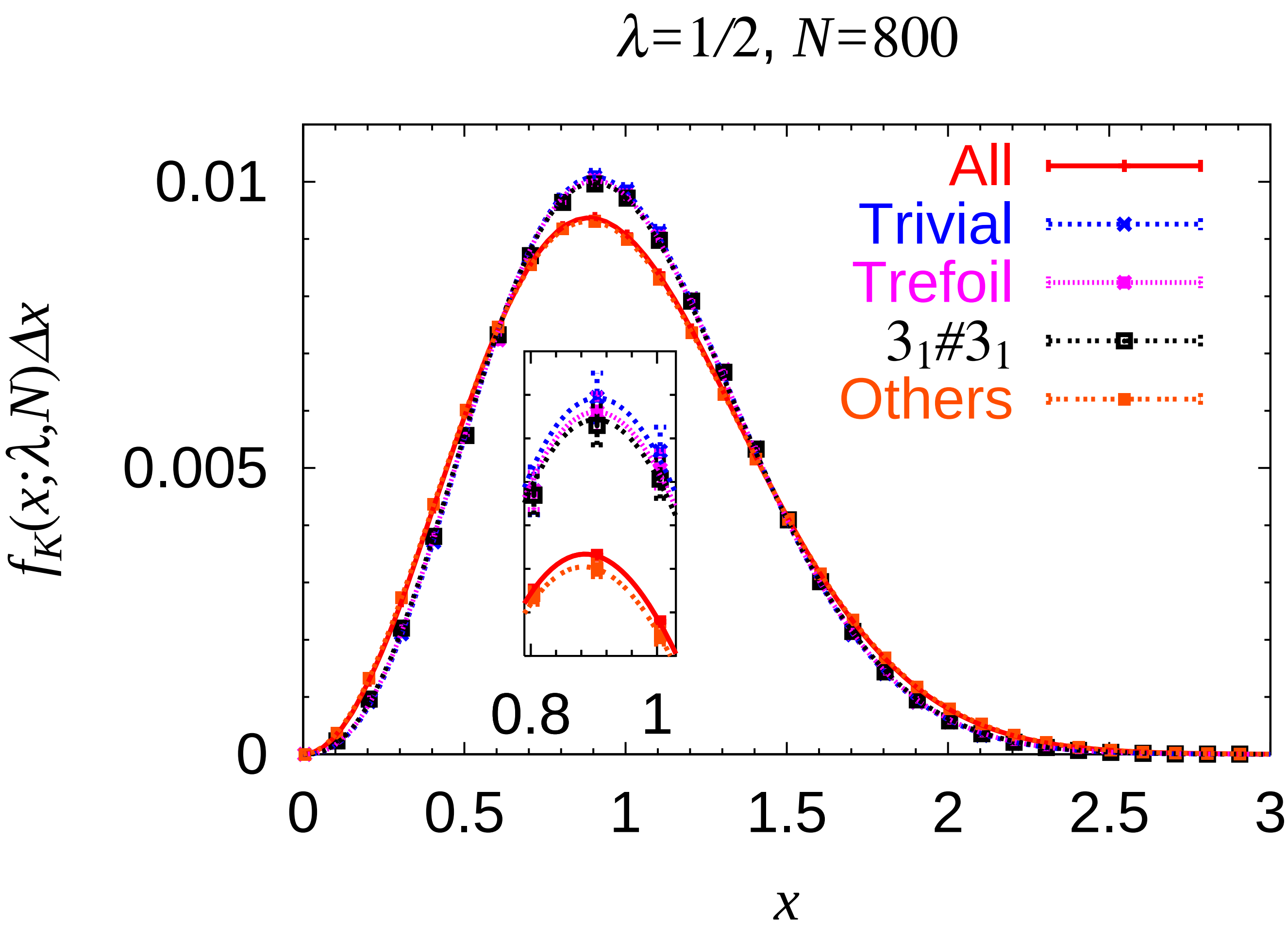
$$\sigma_K(z;N) \;=\; \sqrt{z}\,\exp(\alpha_K\, z)$$

$$\theta_K(z;N) \;=\; b_K z^{\beta_K}$$

$$z \;=\; \lambda(1-\lambda)\,, \qquad \lambda = \frac{n}{N}$$

- Here ***z*** is given by ***z=(1-n/N) n/N***

Distance distribution (n/N=1/2, N=800) **(A. Yao and T.D, in prep.)**



Analytic expression of $g_K(q)$

A. Yao and T.D. in prep. (T.D and A. Yao, to appear)

$$g_K(q) \;=\; 2N\int_0^{1/2} \frac{2}{a\Gamma((3+\theta_K(\lambda))/2)}\,d\lambda$$

$$\times \int_0^{\infty} y^{1+\theta_K(\lambda)}\,\exp(-y^2)\,\sin(ay)\,dy$$

where a is given by

$$a = \sqrt{\frac{2N}{3}}\sigma_K\,q$$

Conclusions:

Part I.

(1) We reviewed some fundamental link polynomials, in particular, the fusion hierachy of link polynomials.

(2) They were first derived by Akutsu and Wadati as a consequence of the factorized scattering of solitons.

(3) They correspond to quantum invariants of higher spin reps of *Uq(sl(2)).*

Part II.

(1) Topological entanglement effects are systematically studied through simulations using invariants of knots and links.

(2) We can evaluate knotting probability, linking probability, topological swelling, scattering functions, etc., explicitly.

(3) They are useful in studying DNA topology. Furthermore, they are to be tested in experiments of ring polymers in solution, near future.

Thank you very much.

Finally, I would like to thank Prof. Miki Wadati for his fruitful research results and continuous encouragement to many students.