DNA and Knots

A. Mohamad and Tsukasa Yashiro

University of Nizwa, Sultan Qaboos University

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Brief History of Knot Theory

In 19th century mathematical study on knots began. Gauss defined the linking number with integral:

$$\mathrm{lk}(K_1, K_2) = \frac{1}{4\pi} \int_{K_1} \int_{K_2} \frac{\mathbf{k}_1 - \mathbf{k}_2}{|\mathbf{k}_1 - \mathbf{k}_2|^3} \cdot (d\mathbf{k}_1 \times d\mathbf{k}_2).$$

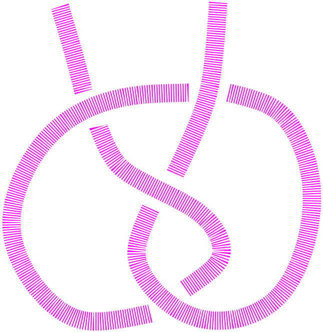
At the time most scientists believed the universe was filled with **ether** and in 1860s, Lord Kelvin proposed that atoms were knots and scientists wanted to study knots. However, as the atomic theory was accepted, scientists lost their interests in knots.

Brief History of Knot Theory

Dveloping the theory of knots was continued by mathematicians. In the early 20th century M. Dehn, J. W. Alexander and others studied knots using knot group. Alexander defined the **Alexander polynomial**.
From late of 1970's to the 1980s the development of the study was boosted. **Jones polynomial** was discovered by V. Jones.
1990s to the present, Knot Theory has been applied to other sciences such as statistical mechanics, biology, etc.

Introduction to Knots

A knot is a tangled string with connected ends. If a knot does not bound a disc in its complement, then it is called a **non-trivial knot**.



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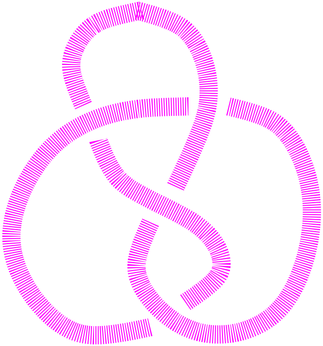
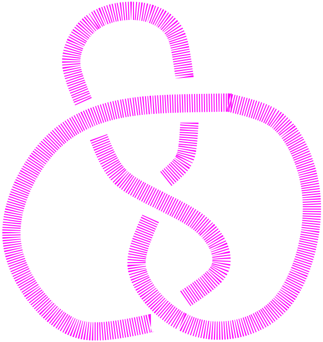


Introduction to knots

If there is a continuous move with the ambient space so that the knot is untied (trivial), then the knot is called a **trivial knot**.



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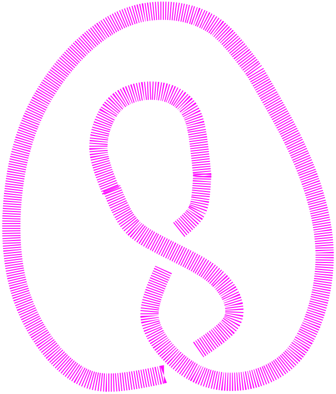

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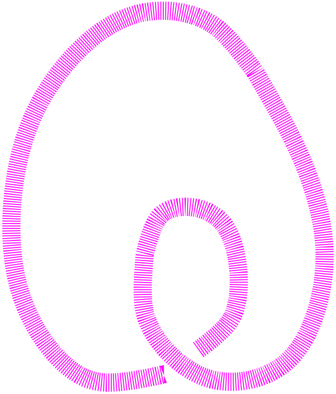

Introduction to knots

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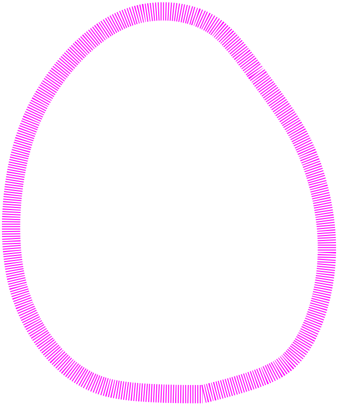
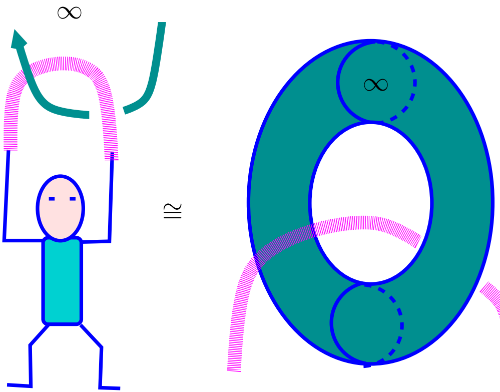


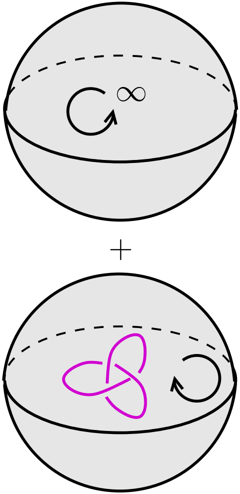
Introduction to knots

The ambient space of a trivial knot in $\mathbb{S}^3 \cong \mathbb{R}^3 \cup \{\infty\}$ is homeomorphic to a solid torus.



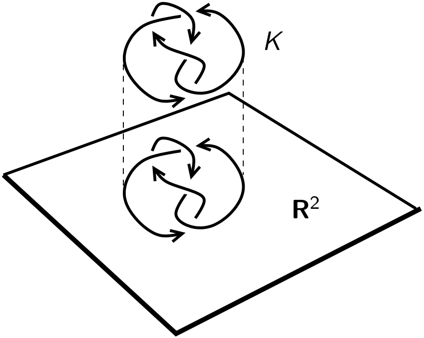
Knots

A **knot** is an embedded finite plygonal circle embedded in $\mathbb{R}^3$ (or $\mathbb{S}^3$). A **link** is a disjoint union of knots.



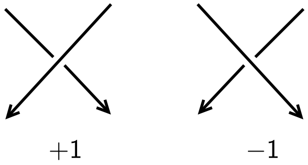
Knots

A **knot diagram** is a projected image of a knot into $\mathbb{R}^2$ with crossing information. We denote it by D_K.



Linking Number

Let D_K be a diagram of L. Add a signnature $\varepsilon(d)$ to each crossing of D as follows.



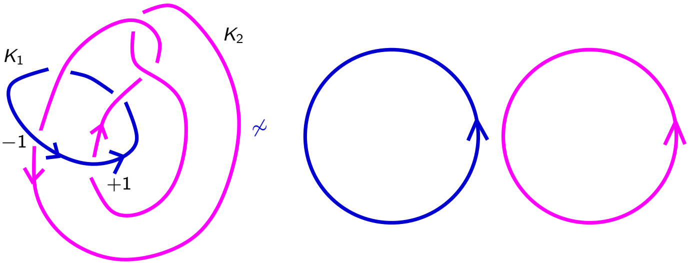
Let $L = K_1 \cup K_2$ be an oriented two-component link. Then we define a function $\mathrm{lk}(K_1, K_2)$ by

$$\frac{1}{2}\sum_{i=1}^{n} \varepsilon(d_i),$$

where $d_1, \ldots, d_n$ are crossings between D_{K_1} and D_{K_2}.

Splittable links

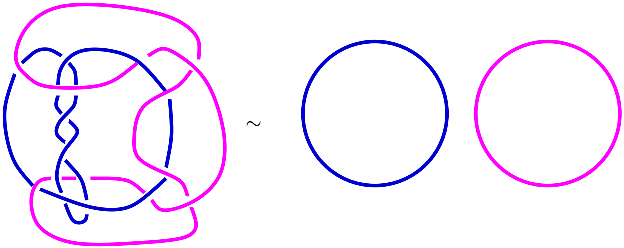
In the following $\mathrm{lk}(K_1, K_2) = +1 - 1 = 0$



The linking number does not tell us if it is splittable or not.

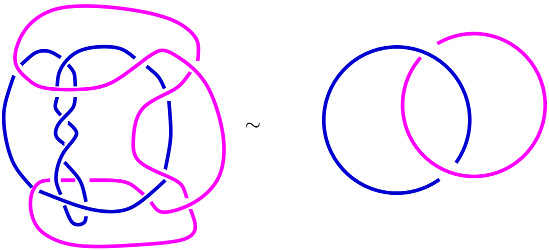
Splittable links

Some link diagrams look very complicated but it is splittable.



Splittable links

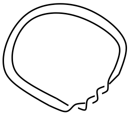
This is similar to the previous diagram but it is not splittable.

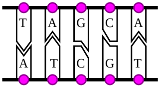


This suggests us that a small change in the diagram may change the splittability.

DNA Knots

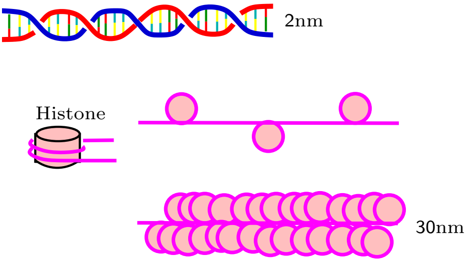
Most cellular DNA (deoxyribonucleic acid) is double-stranded (duplex) and has a sturucture that has two linear backbones alternating sugar and phosphorus. Each sugar molecule is attached by one of four nucleotide bases: A= Adenine, T = Thymine, C = Cytosine, G = Guamine.





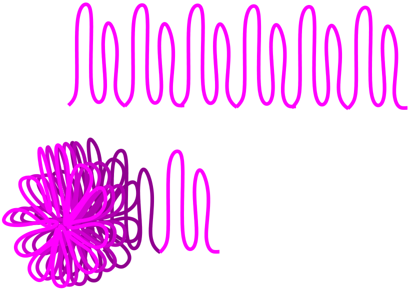
Chromosomes

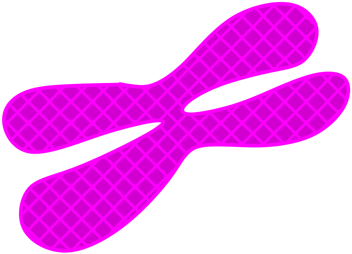
DNA is a double helix strands with the diameter 2 nm (1 nm $= 1/10^9$ metre). It forms a winding structure around histones to make a beads structure. Also it forms a 30 nm fibre.



Chromosomes

The 30 nm fibre will form a loop structure and this structure gethers and forms a chromosome.





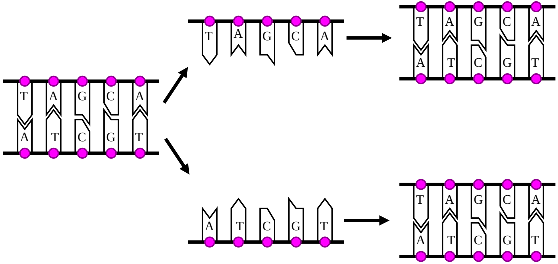
DNA Replication

DNA has the double helix structure. In eukaryotic cell, DNA is packed in the nuclear as tangled long strings. As we know a cell divides itself into two cells. Each cell has the same genetic information: the same DNA. the cell make a copy from DNA called **DNA replication**.

Semi Conservative Replication

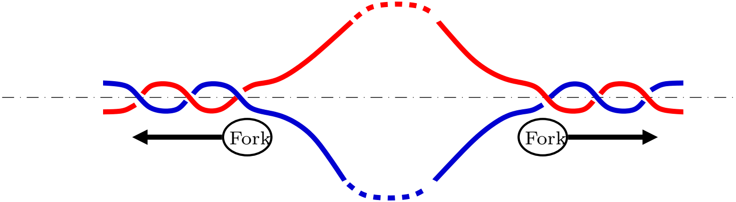
The double strands are connected by nucleotide bases: A= Adenine, T = Thymine, C = Cytosine, G = Guamine. T always joins A and G always joins C. Replication scheme is the following.

1. Locally, the double strands are separated into two chains.
2. Each chain has a sequence of bases A, T, C, G and this sequece casts its counterpart.



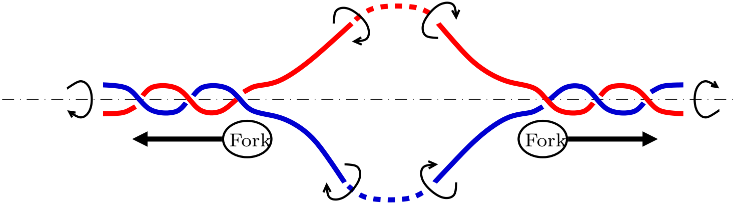
DNA Replication

The replication starts at a special site on the DNA starands called **Ori**. There are mainly two types of replications: Bidirectional and Unidirectional replications. Either case, at the *ori* DNA helix is relaxed and forms a site where the replication is done called **fork**.



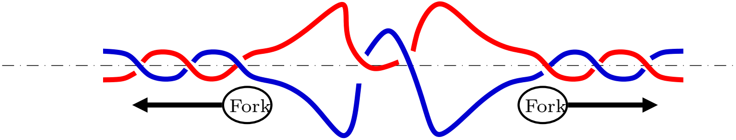
DNA Replication

We propose the follwoing mechanism for the fork moving. As the forks move away from the ori, the starand rotates as below.



Topological Problems

When a replication is done in the nuclear of a cell, there is a topological problem. If the site **replication eye** (replication bubble) is twisted, then the resulting copies are linked (catenated):



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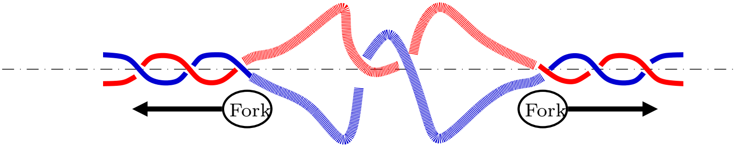
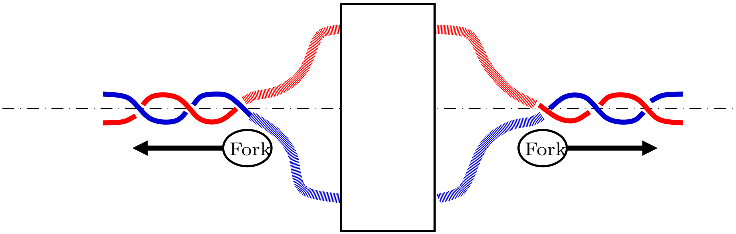


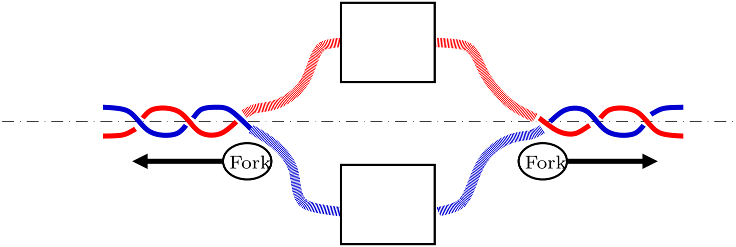
Topological Problems

It is said that a catenated DNA is decatenated by action of enzymes.
We propose the model that has a mechanism to avoid creating the catenated DNA in the site of replication. The mechanism is placed in the box.



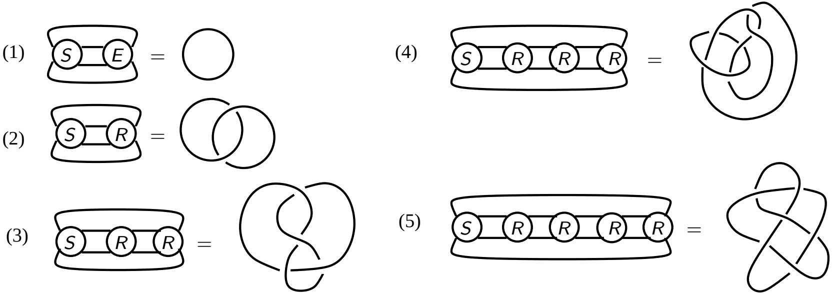
Topological Problems

In order to separate the doughter DNA, there may be two mechamisms on each daughter DNA. Each box may have a widing mechanism to form a chromosome.



DNA and Enzymes

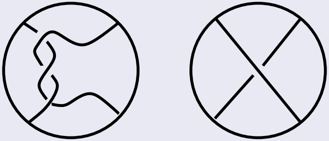
For the following tangle equations, (2)-(5) have solutions but for (1), E is not determined.



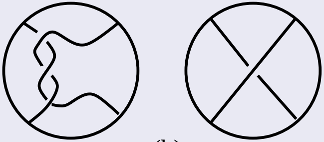
DNA and Enzymes

Theorem

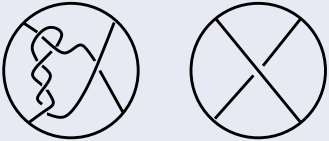
The sloutions S anr R for (2), (3), (4) *are only one of the following four cases.*



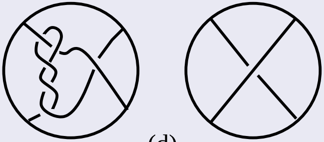
(a)



(b)



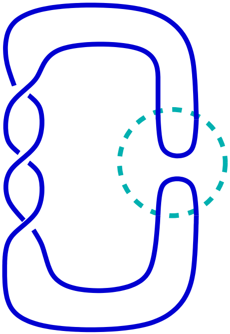
(c)



(d)

Site Specific Recombinations

An enzyme that acts in site-specific recombination is called a **recombinaze**. A recombination site is a short segment of duplex DNA which is recognized by the recombinase.



DNA Molecule Subtrate

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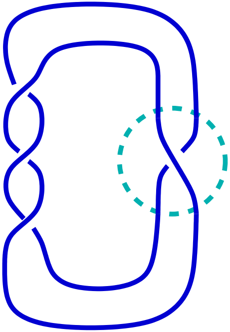


DNA Molecule Product

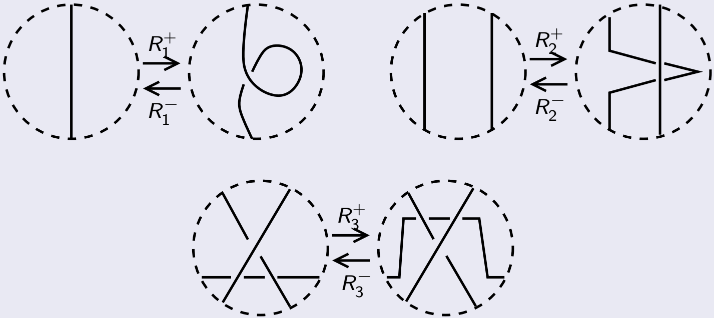
Elementary Moves

We define the elementary moves as follows.
Exchange an edge P_iP_{i+1} of K with two edges $P_iP' \cup P'P_{i+1}$ of a triangle $\triangle P_iP_{i+1}P'$. Also $\triangle P_iP_{i+1}P' \cap K = P_iP_{i+1}$.
Knots K and K' are equivalent if there exists a finite sequence of elementary moves such that it deforms K into K'.
We denote $K \sim K'$.
The relation $\sim$ is an equivalent relation.
Let $f : \mathbb{S}^3 \to \mathbb{S}^3$ be an orientation preserving homeomorphism, then $K \sim f(K)$.

Reidemeister Moves

Theorem

If $K \sim K'$, then $D_{K'}$ is obtained from D_K by applying a finite sequence of the following three moves to $D_{K'}$.

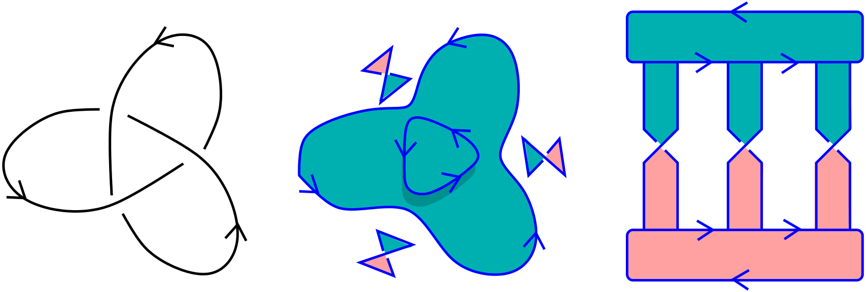


Knot Invariants

Given two knots K and K', how can we distinguish them?
Let $\mathcal{K}$ be the set of all knots (or links). Let W be some algebraic structures. A mapping $\rho : \mathcal{K} \to W$ is a knot invariant if $K \sim K'$ implies that $\rho(K) = \rho(K')$.

Knot Complements

Let K be a knot in $\mathbb{S}^3$. It is known that every knot K bounds an orientable surface F in $\mathbb{S}^3$, called a Seifert surface.



The Alexander Polynomial

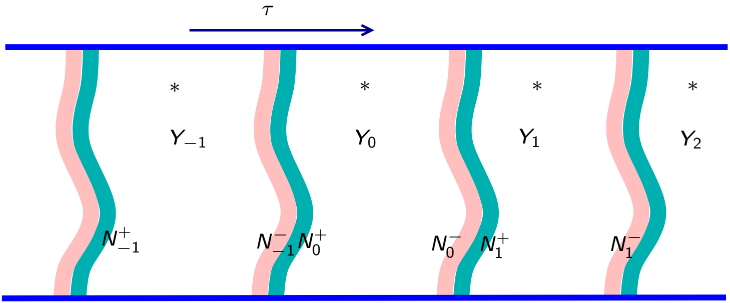
Let Λ be the ring of (finite) Laurent polynomials with integer coefficients.

$$\Lambda = \mathbb{Z}[t, t^{-1}].$$

The Alexander polynomial of a knot is the determinant of a presentation matrix for the first homology as the Λ-module of the infinite covering space over the knot complement.

Examples

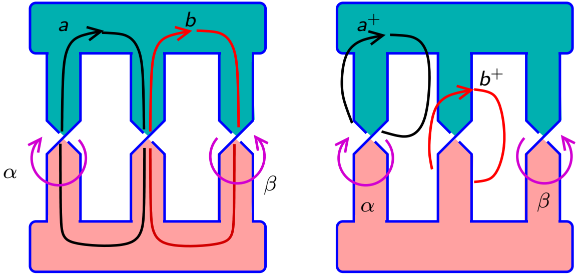
Let $\{Y_i\}_{i\in\mathbb{Z}}$ be indexed copies of $Y = X - F$. Glue Y_{i-1} and Y_i using $N_i \cong F \times (-1, 1)$ to obtain an infinite cyclic covering space over X.



Let $X = \mathbb{S}^3 - K$. Let $\widetilde{X}$ be the infinite cyclic covering space over X. Let $\tau : \widetilde{X} \to \widetilde{X}$ be a generator of the group of the covering

Examples

At the Seifert surface F, we push off the generators a and b for $H_1(F)$ into the $+$ side of F denoted by a^+ and b^+. Similarly, a^- and b^- are obtained.



Examples

Then we have the relations

$$\begin{array}{cc} a^{+} = -\alpha & b^{+} = \alpha - \beta \\ a^{-} = \beta - \alpha & b^{-} = -\beta \end{array}$$

In each neighbhourhood N_i $(i \in \mathbb{Z})$, we obtain the following relations

$$\begin{aligned} t^{i-1}(\beta - \alpha) &= -t^{i}\alpha, \\ -t^{i-1}\beta &= t^{i}(\alpha - \beta), \ i \in \mathbb{Z}. \end{aligned}$$

Thus as Λ-module (the Alexander module)

$$H_1(\widetilde{X}) \cong \langle \alpha, \beta \,; \beta - \alpha = -t\alpha, -\beta = t(\alpha - \beta) \rangle$$

Examples

The Alexander matrix is

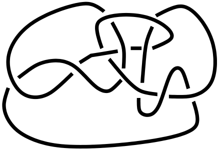
$$\begin{bmatrix} t-1 & 1 \\ t & 1-t \end{bmatrix}.$$

Thus the Alexander polynomial of K is:

$$\Delta_K(t) = -t^2 + t - 1.$$

Some Properties of $\Delta(t)$

If a knot K is trivial, then $\Delta_K(t) = 1$. However the converse is not true.



Kinoshita-Terasaka Knot

Some Properties of $\Delta(t)$

Proposition

For every Laurent polynomial $P(t)$ such that $P(1) = \pm 1$ and $P(t) = P(t^{-1})$, there exists a tame knot K in $\mathbb{S}^3$ whose Alexander polynomial is P.

Theorem

Suppose $K_1 \# K_2$ is the connected sum of two knots (or links) K_1 and K_2. Then

$$\Delta_{K_1 \# K_2}(t) = \Delta_{K_1} \Delta_{K_2}.$$

Some Properties of $\Delta(t)$

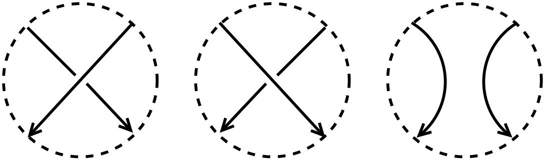
Let K be a knot and let D_K be its knot diagrm. A knot diagram D_K is called alternating diagram if you move along the diagram, at every crossing point you passes the crossing over and passes under alternatively. If a knot K has at least one alternating diagram, then K is called an **alternating knot**.

Theorem (Murasugi (1958))

Let K be an alternating knot. $\deg(\Delta_K(t)) = 2g(K)$, *where* $g(K)$ *is the genus of* K*; that is, the minimal genus of Seifert surface for* K.

The Alexander Conway Polynomial

Let D_+, D_- and D_0 denote regular diagrams of knots K_+, K_- and K_0 respectively such that these diagrams are the same except at a neighbourhood of one crossing pointi. The following local diagrams represent corresponding neighbourhoods.



D_+ D_- D_0

These diagrams D_+, D_- and D_0 are called *skein* diagrams.

The Alexander Conway Polynomial

The Conway polynomial $\nabla_K(z)$ is a Laurent polynomial defined by the following two axioms.

A1 If K is trivial, then $\nabla_K(z) = 1$.

A2 Suppose that D_+, D_-, D_0 are skein diagrams, then the following relation holds.

$$\nabla_{K_+}(z) - \nabla_{K_-}(z) = z\nabla_{K_0}(z).$$

Then the Alexander polynomial is obtained by

$$\Delta_K(t) = \nabla_K(\sqrt{t} - \frac{1}{\sqrt{t}}).$$

The Jones Plynomial

The Jones polynomial $V_K(t)$ is defined by the following two axioms.

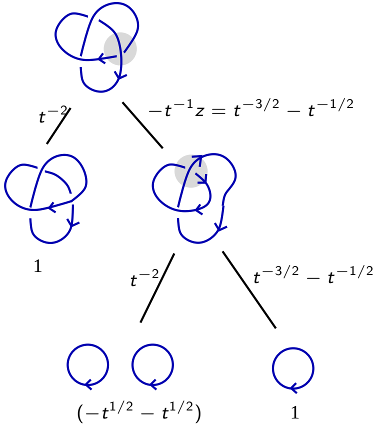
A1 If K is trivial, then $V_K(t) = 1$.

A2 Suppose that D_+, D_-, D_0 are skein diagrams, then the following relation holds.

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

Example

For example, let K be the trefoil in the figure below.



$V_K(t) = t^{-1} + t^{-3} + t^{-4}$

Statistical Mechanics

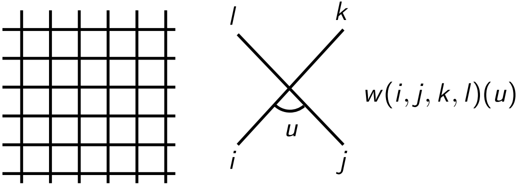
In statistical mechanics the following function is considered:

$$Z = \sum_{\sigma} \exp\left(\frac{-E(\sigma)}{kT}\right),$$

where $E(\sigma)$ is the total energy of the state σ in the particular model and T is the absolute tempature and k is the Boltzmann's constant. This function is called a partition function. If the function is concretely expressed, then the model is said to be exactly solvable.

Statistical Mechanics

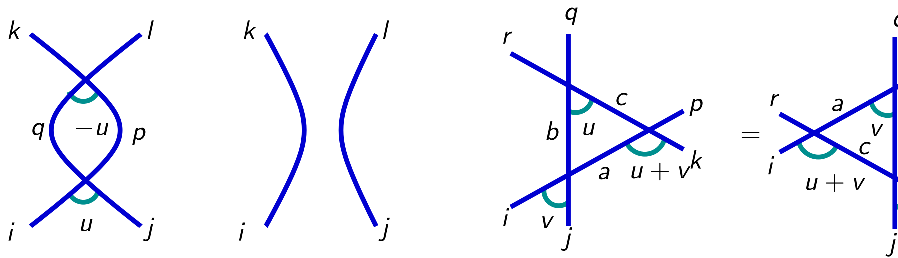
Consider the 2-dimensional lattice in which each vertex represent a state. State variables i, j, k, l are assigned to edges around a vertex.



where u is called the spectral parameter indicating the mutual interactions of the system.

Statistical Mechanics

A model is solvable if the Yang-Baxter equation is satisfied. This equation is expressed by the diagram below.



$$\sum_{a,b,c} w_{b,c,q,r}(u) w_{a,k,p,c}(u+v) w_{i,j,a,b}(v) =$$

$$\sum_{a,b,c} w_{a,b,p,q}(v) w_{i,c,a,r}(u+v) w_{j,k,b,c}(u)$$

Statistical Mechanics

Proposition

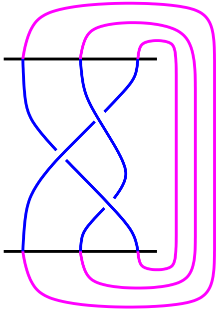
The 6-vertex model has a set of Boltzman weights $w(i, j, k, l)(u)$, defined that satisfiy the Yang-Baxter equation.

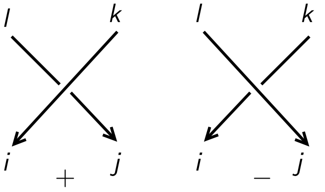
$$
\begin{aligned}
w(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2})(u) &= w(-\frac{1}{2},-\frac{1}{2},-\frac{1}{2},-\frac{1}{2})(u) = 1\\
w(\frac{1}{2},-\frac{1}{2},\frac{1}{2},-\frac{1}{2})(u) &= w(-\frac{1}{2},\frac{1}{2},-\frac{1}{2},\frac{1}{2})(u) = \frac{\sinh u}{\sinh(\lambda - u)}\\
w(\frac{1}{2},-\frac{1}{2},-\frac{1}{2},\frac{1}{2})(u) &= w(-\frac{1}{2},\frac{1}{2},\frac{1}{2},-\frac{1}{2})(u) = \frac{\sinh u}{\sinh(\lambda - u)}
\end{aligned}
$$

The diagram of Yang-Baxter equation is similar to the third Reidemeister move. Also unitary condition is epressed by a diagram change which is similar to the second Reidemeister move.

Braids

Let β be a braid of order n and let D be a regular diagram of β.





The closed braid gives a link diagram and this is a model with some boundary conditions.

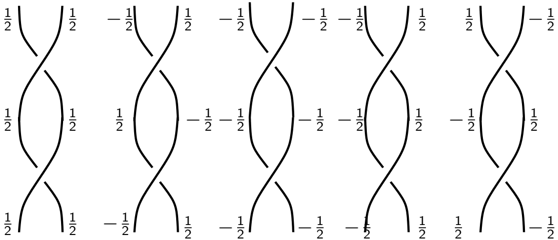
We evaluate the state S by

$$\prod_{c} \widetilde{w}_{\pm}(l,k,i,j)t^{-(a_1+\cdots+a_n)}$$

where $\widetilde{w}(l,k,i,j)(u) = \lim_{u\to\infty} e^{\frac{1}{2}(k-i-l+j)u} w(i,j,k,l)(u)$.
Take the sum for all values for all states.

$$Z_{\beta} = \sum_{S} \prod_{c} \widetilde{w}(i,j,k,l)t^{-(a_1+\cdots+a_n)}$$

If the braid $\beta = \sigma^2$, then the all states are the followings.



Then $Z_\beta = (1 + t^{-1})(1 + t^2)$.

Theorem

Suppose K is an (oriented) knot (or link) formed from a braid β and that Z_β is the partition function for β. Then

$$P_K(t) = t^{\frac{w(\beta)+1}{2}} Z_\beta$$

is an invariant of K, where $w(\beta)$ is the Tait number (writhe) of the regular diagram D of the closure of β.

If we set

$$\widetilde{P}_K(t) = \frac{P_K(t)}{1+t},$$

then this is equivalent to the Jones Polynomial of K.

Thank you!