

Folding of the Randomly Triangulated Surface : Review

北里大学 理学部 物理学科: 守 真太郎

2003/12/16

- Folding of Geometric Objects
- 1-dim. Case : Meander Problem
- 2-dim. Case : Polymer(ized) Membrane
- 2-dim. Case : Fluid Membrane (under construction)

1 Folding of Geometric Objects

Geometric Objects ?

- 1-D string like objects

Polymer, Flux line, Vortex line,
World line (Trajectory of Particle)

- 2-D objects

Fluid Membrane, Polymer Membrane,
World Sheet (Trajectory of String)

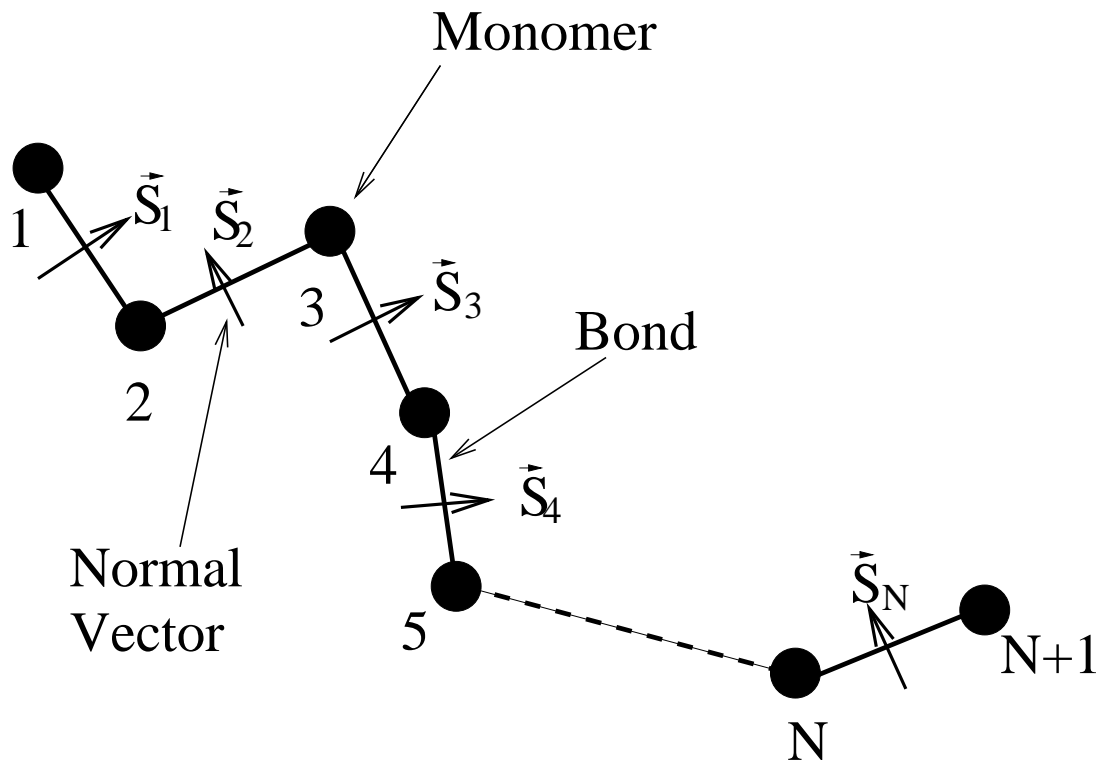
- 3-D objects

Gel

- 4-D objects

Space-Time (Universe)

Polymer ?

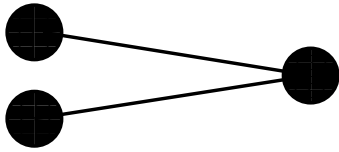


$$E = -J \sum_{i=1}^N \vec{S}_i \cdot \vec{S}_{i+1} \quad (1)$$

J : Bending Energy

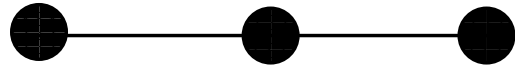
Embedded in 1-dimensional Space \rightarrow Fold or Flat

Folded



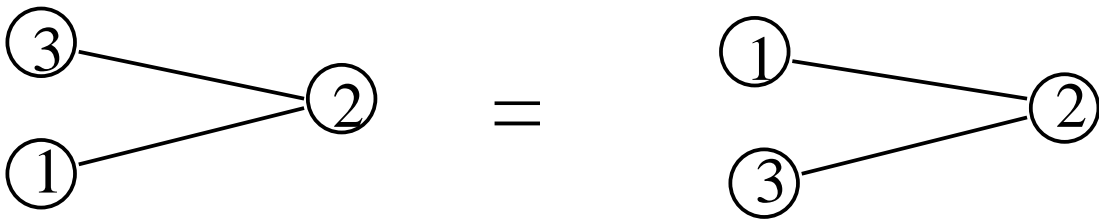
J

Flat



-J

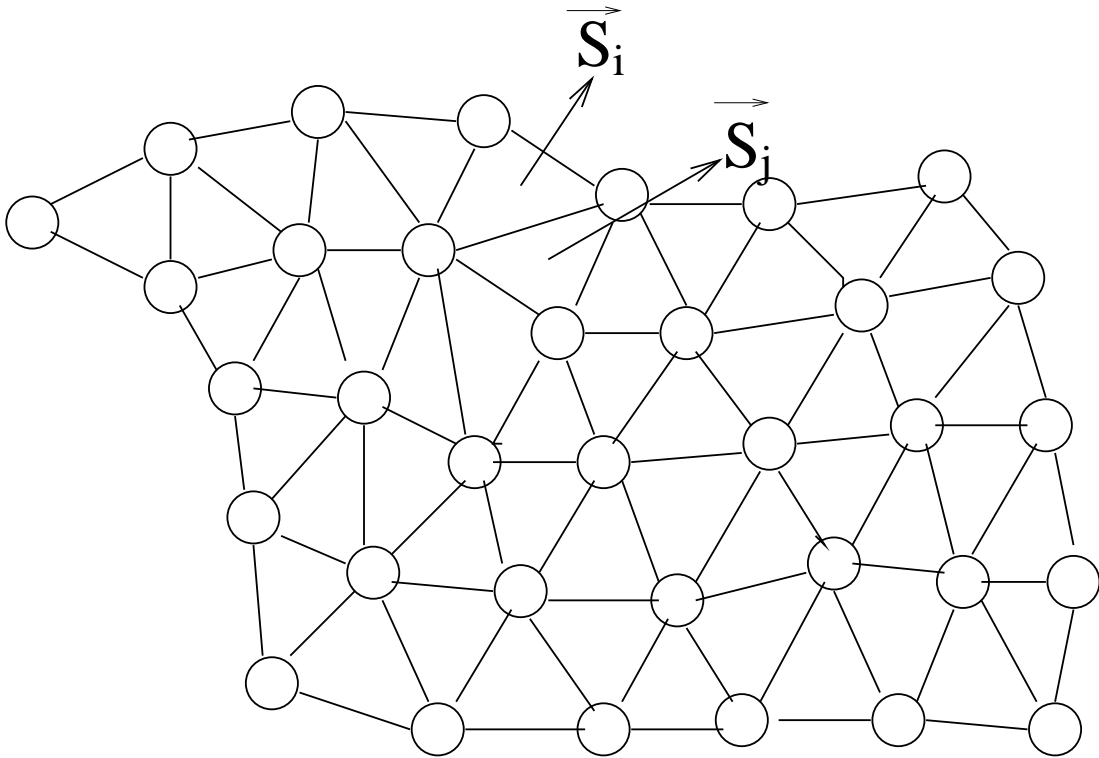
Phantom Case is very Simple !



$$E = -J \sum_{i=1}^N S_i S_{i+1} \quad (2)$$

Self-Avoiding Case is Difficult. \rightarrow Meander Problem

Membrane ?



$$E = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \quad (3)$$

- Polymer(ized) Membrane

Triangulated Surface with Fixed Connectivity

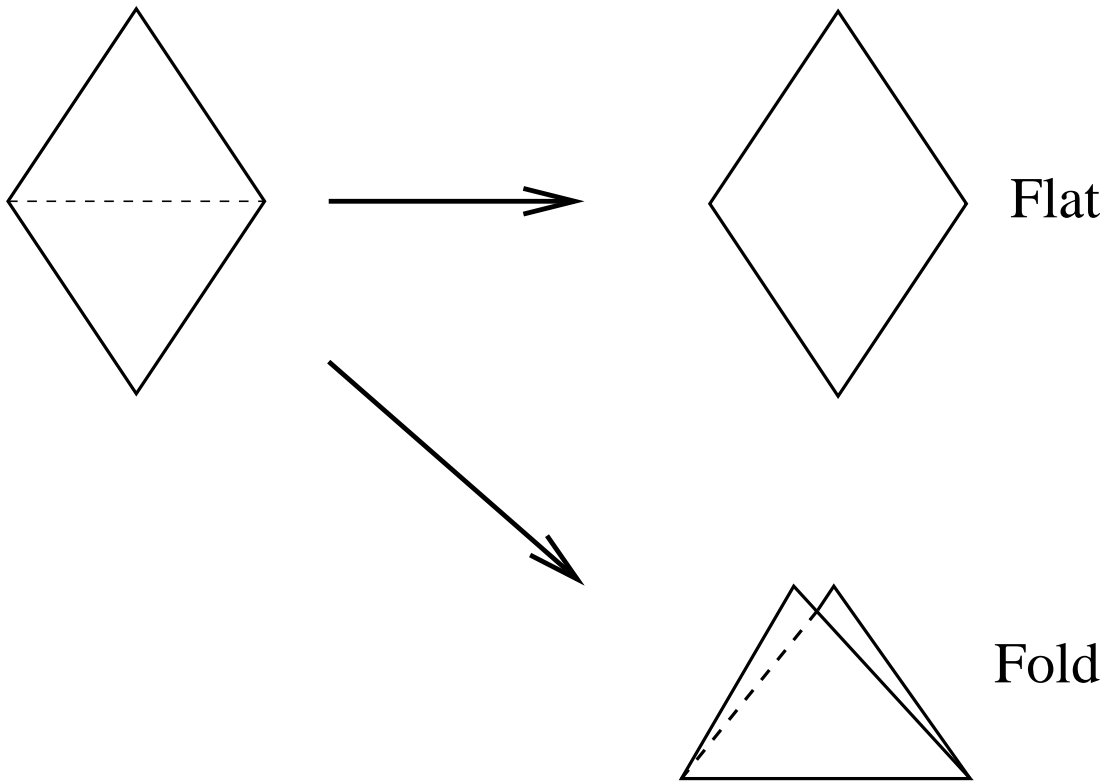
- Regular Triangular Lattice
- Randomly Polymerized Membrane (Quenched Randomly Triangulated Surface)

- Fluid Membrane

Triangulated Surface with Random Connectivity

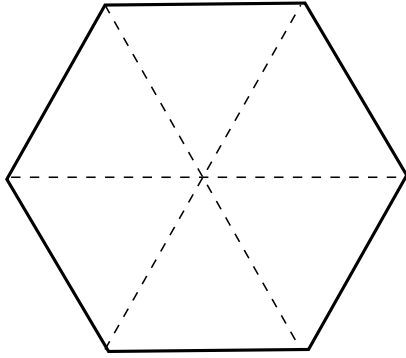
Randomly Triangulated Surface

Embedded in 2-dimensional Space \rightarrow Fold or Flat



Even Phantom Case is not Simple !

Folding of Elementary Hexagon:



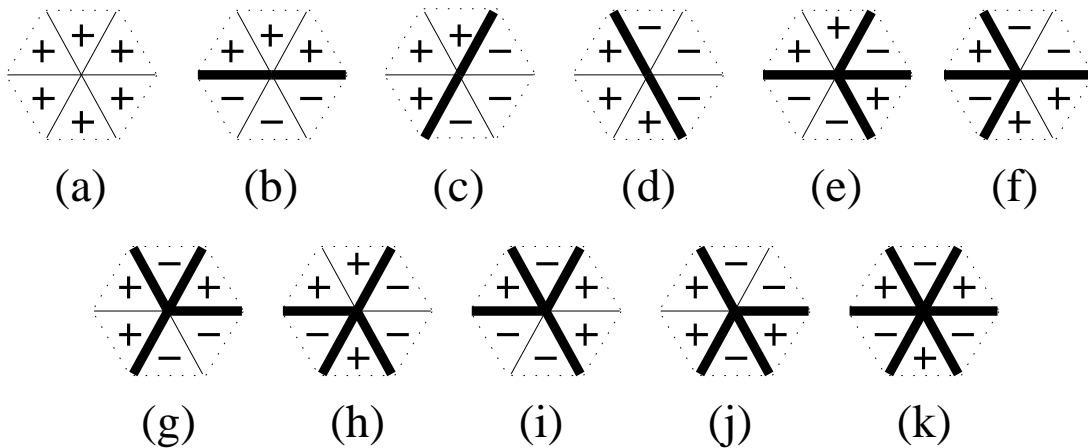
6 Bonds ----> 64 States ?

Only 11 Physical States

11 local fold environments for elementary Hexagon

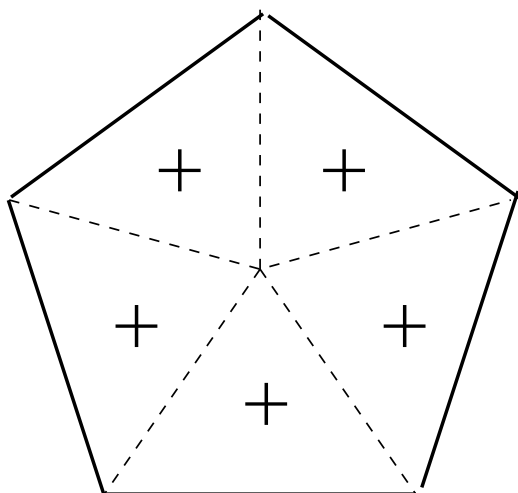
Face Up ----- > $S = +1$

Face Down ----- > $S = -1$

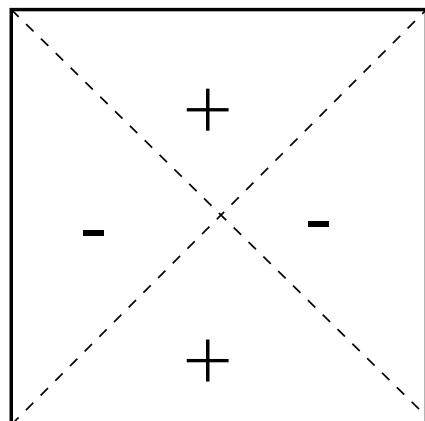


Randomly Triangulated Case:

Is It Foldable ?



Not Foldable



Foldable

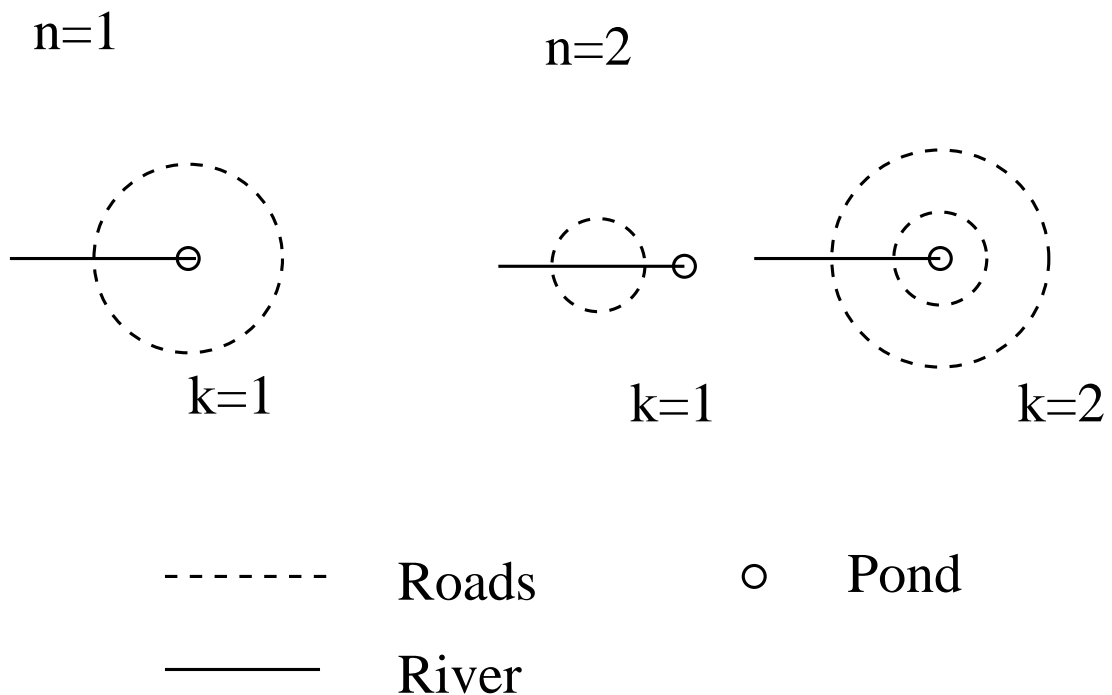
Questions :

- Foldability ?
- How to generate Foldable Randomly Triangulated Surface ?
- How to Enumerate ? Matrix Model, Decorated Tree ?

2 Meander Problem

2.1 Definition

(Semi-)Meander = Closed Non-Self-intersecting loop (road) crossing a semi-infinite line (river with a Pond) through n points (bridges).



⊠ 1: Meander with $n = 1, 2$. k is number of Connected Components.

$$M_1^1 = 1, \quad M_2^1 = 1, \quad M_2^2 = 1$$

$n=3$

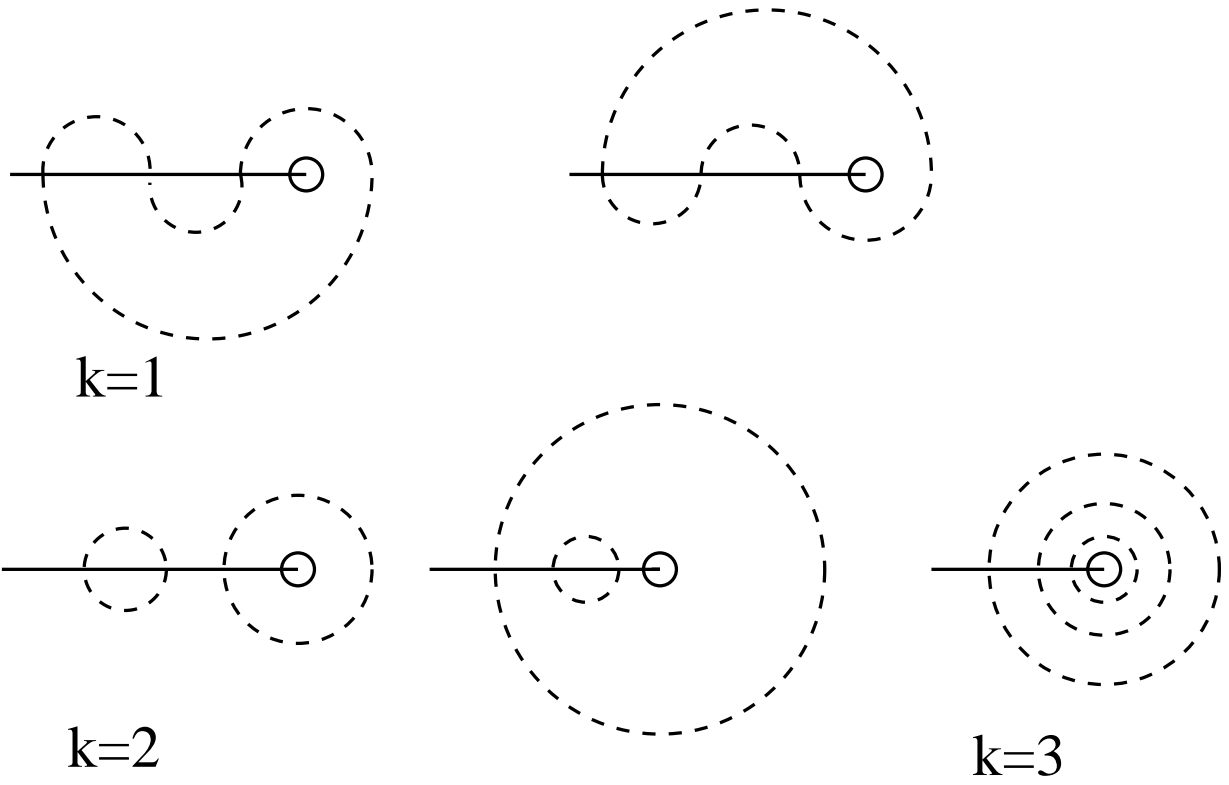
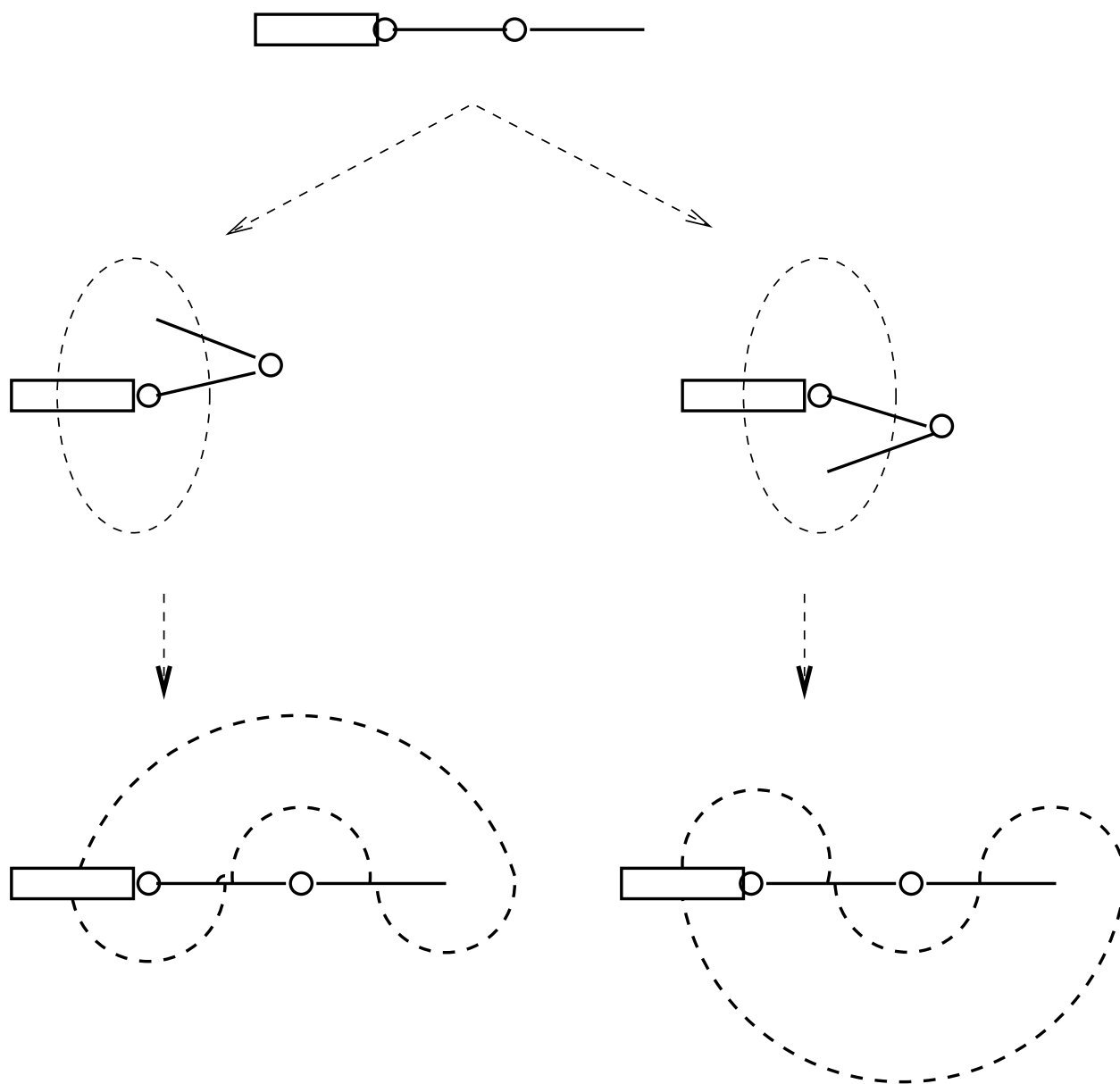


图 2: Meander with $n = 3$.

$$M_3^1 = 2, \quad M_3^2 = 2, \quad M_3^3 = 1$$

2.2 Compact Folding of Polymer



☒ 3: Meander and Compact Folding of Polymer

2.3 Folding Pathway of Polymer

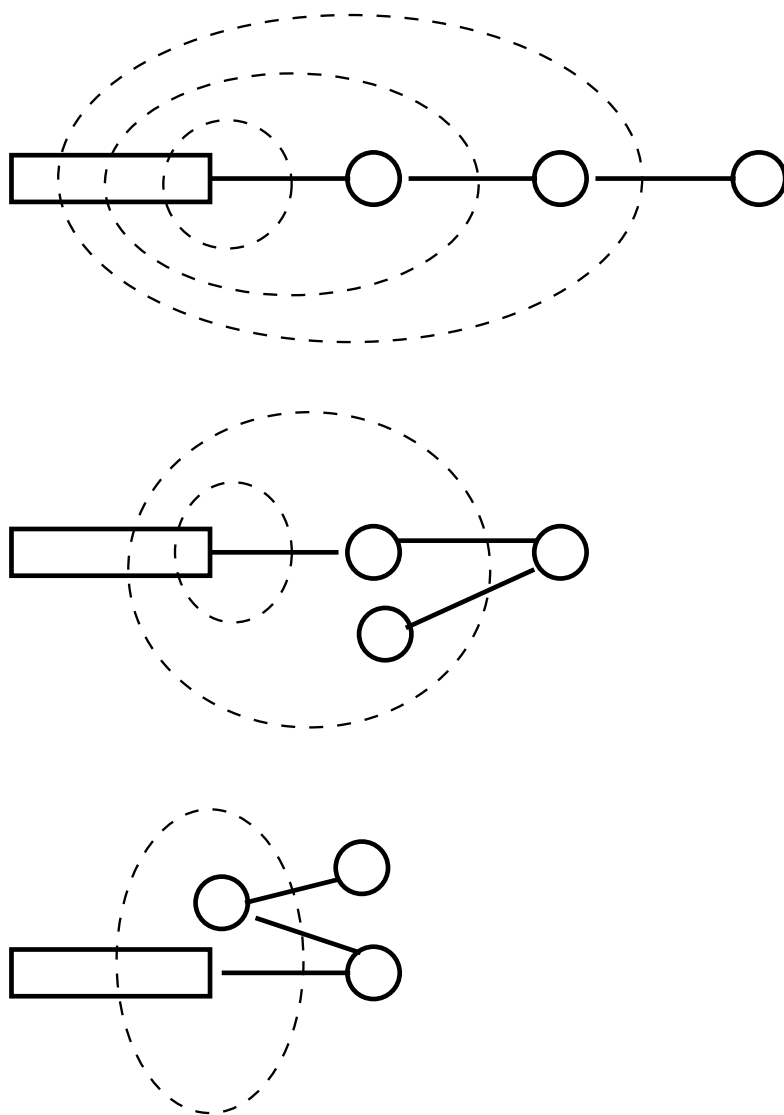


图 4: Folding Pathway and Meander

2.4 Meander Number: Numerical Data

表 1: The numbers M_n^k of inequivalent (semi)-meanders of order n with k connected components for $1 \leq n \leq 12$, obtained by exact enumeration on the computer.

| k \ n | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|-------|---|---|---|---|----|----|-----|-----|------|
| 1 | 1 | 1 | 2 | 4 | 10 | 24 | 66 | 174 | 504 |
| 2 | 0 | 1 | 2 | 6 | 16 | 48 | 140 | 428 | 1308 |
| 3 | 0 | 0 | 1 | 3 | 11 | 37 | 126 | 430 | 1454 |
| 4 | 0 | 0 | 0 | 1 | 4 | 17 | 66 | 254 | 956 |
| 5 | 0 | 0 | 0 | 0 | 1 | 5 | 24 | 104 | 438 |
| 6 | 0 | 0 | 0 | 0 | 0 | 1 | 6 | 32 | 152 |
| 7 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 7 | 41 |
| 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 8 |
| 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |

Enumerated Up to $n \leq 29$.

2.5 Properties of M_n^k

$$\begin{aligned}M_n^n &= 1 \\M_n^{n-1} &= n - 1 \\ \sum_{k=1}^n M_n^k &= C_n\end{aligned}\tag{4}$$

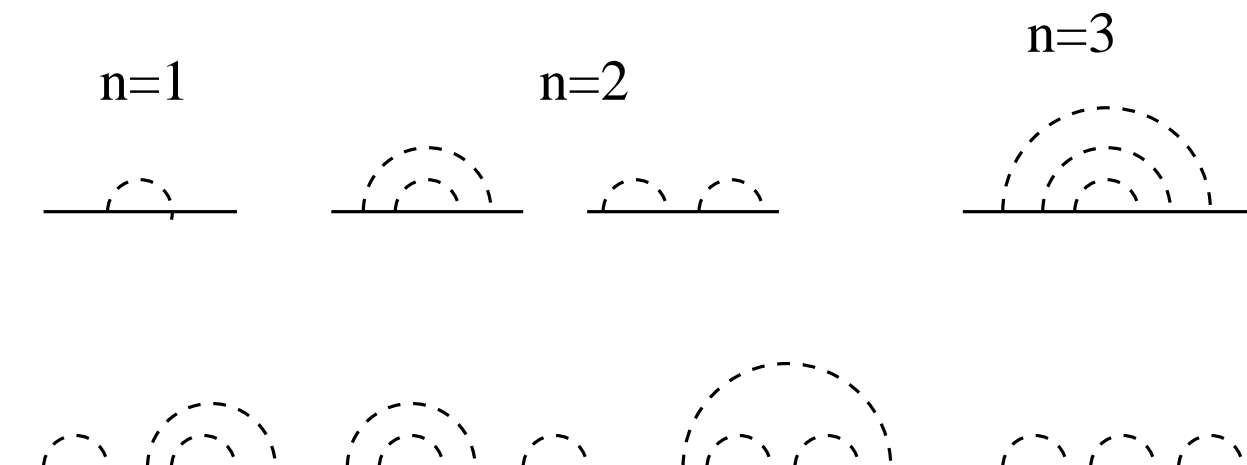
C_n : Catalan Number

$$C_n \equiv \frac{1}{2n+1} {}^{2n+1}C_n = \frac{(2n)!}{n!(n+1)!} \simeq \frac{1}{\sqrt{\pi}} \frac{4^n}{n^{\frac{1}{2}}}\tag{5}$$

$$C_1 = 1 \quad C_2 = 2, \quad C_3 = 5, \quad C_4 = 14\tag{6}$$

2.6 Arch and Catalan Number

$C_n =$ Number of Arch Configuration with $2n$ bridges (7)

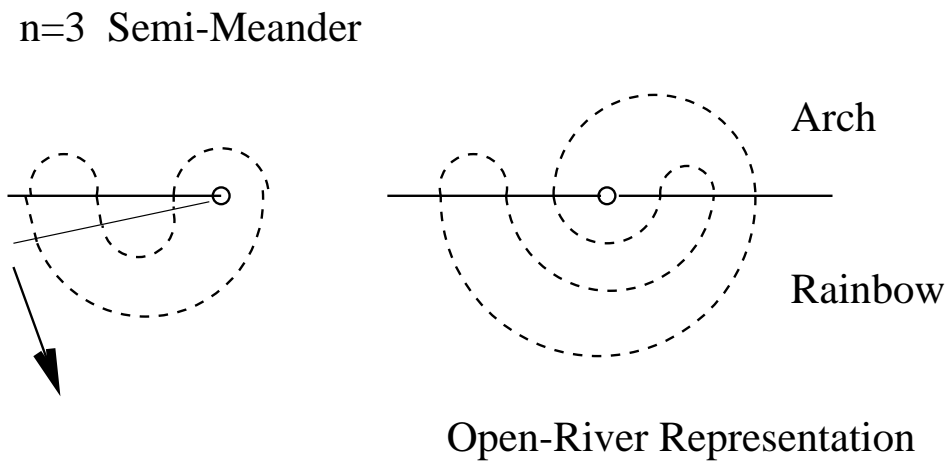


$$C_1=1 \quad C_2=2 \quad C_3=5$$

☒ 5: Arch and Catalan Number

2.7 Open-River Representation

$$\text{Meander} = \text{Arch} + \text{Rainbow} \quad (8)$$



⊠ 6: Arch + Rainbow = Meander

$$\sum_{k=1}^n M_n^k = C_n \quad (9)$$

2.8 Catalan Number C_n

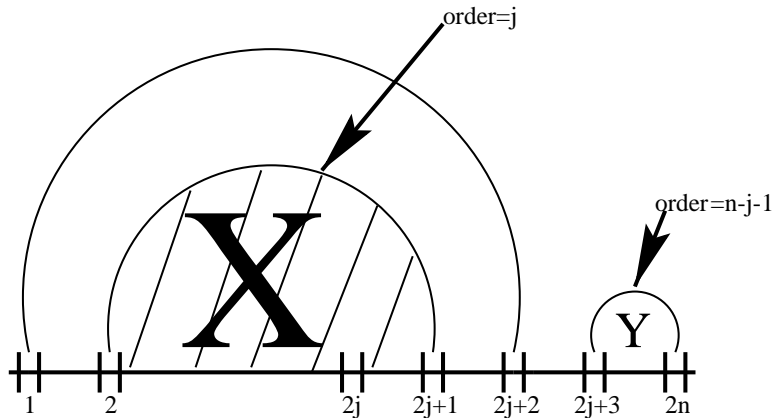


图 7:

$$C_n = \sum_{j=0}^{n-1} C_j \times C_{n-j-1} \quad \text{with} \quad C_0 = 1 \quad (10)$$

Generating function $C(x)$:

$$C(x) = \sum_{n=0}^{\infty} C_n x^n = 1 + C_1 x + C_2 x^2 + \dots \quad (11)$$

$C(x)$ satisfy the following algebraic relation.

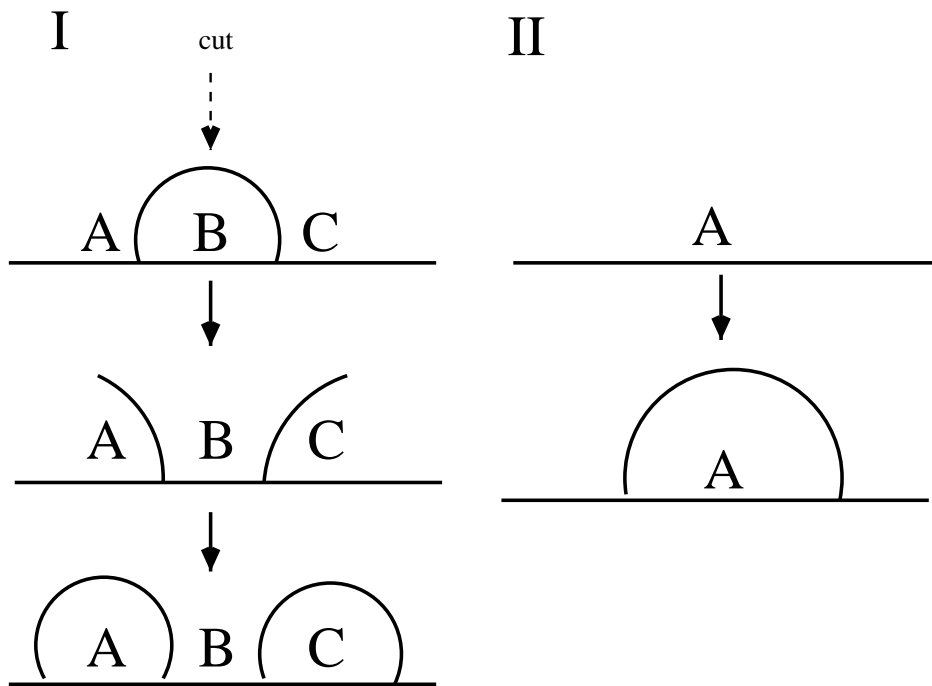
$$xC(x)^2 = C(x) - 1 \quad (12)$$

$$C(x) = \frac{1 - \sqrt{(1 - 4x)}}{2x} \quad (13)$$

2.9 How to Analyze

- Enumeration upto $n \leq 29$
Ph.Di Francesco, O.Golinelli and E.Guitter
- Transfer-Matrix
Ph. Di Francesco, O.Golinelli and E.Guitter
- Monte-Carlo Method (Population Sampling Method)
 $k = 1$ O.Golinelli, $k \geq 2$ S.Mori
- Mean-Field Method
- Temperley-Lieb Algebra
Ph.Di Francesco, O.Golinelli and E.Guitter
- Matrix Model
S.Land and A.Zvonkin, Ph.Di Francesco and E.Guitter

2.10 Numerical Methods



☒ 8: Construction of Arch : Process I and II

- Process I : Cut Exterior Arch and Pull its Ends all the way around the others and reconnect them below.

$$k \rightarrow k, n \rightarrow n + 1$$

- Process II : Draw a Circle around the Meander.

$$k \rightarrow k + 1, n \rightarrow n + 1$$

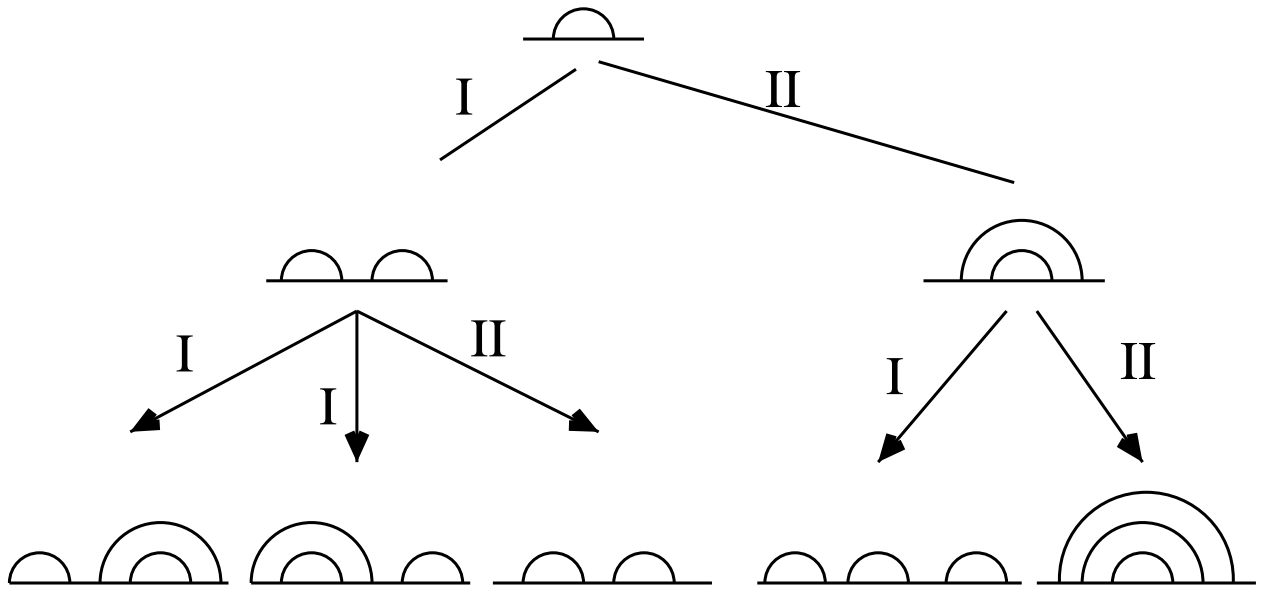


图 9: Arch $n \leq 3$

2.11 Asymptotic Behavior

From Enumeration, Monte-Carlo Method

O.Golinelli

$$M_n^k \sim \frac{R_k^n}{n^{\gamma_k}} \text{ with } R_1 \simeq 3.5018(3) \text{ and } \gamma_1 = 2.056(10) \quad (14)$$

S.Mori

表 2: γ_k

| | | | | | |
|------------|-------|-------|-------|-------|-------|
| k | 1 | 2 | 3 | 4 | 5 |
| γ_k | 2.0 | 1.4 | 0.45 | -0.57 | -1.53 |
| k | 6 | 7 | 8 | 9 | 10 |
| γ_k | -2.53 | -3.53 | -4.53 | -5.53 | -6.6 |

表 3: R_k

| | | | | | |
|-----------------|--------|-------|-------|-------|-------|
| k | 1 | 2 | 3 | 4 | 5 |
| $\log(R_k/3.5)$ | 0.0 | 0.005 | 0.003 | 0.001 | 0.001 |
| k | 6 | 7 | 8 | 9 | 10 |
| $\log(R_k/3.5)$ | 0.0001 | 0.001 | 0.001 | 0.001 | 0.001 |

From Enumeration, Transfer Matrix, Matrix Model

Meander-Polynomial $m_n(q)$:

$$m_n(q) \equiv \sum_{k=1}^n M_n^k q^k \quad (15)$$

$$\begin{aligned} m_1(q) &= q & m_2(q) &= q + q^2 \\ m_3(q) &= 2q + 2q^2 + q^3 \end{aligned} \quad (16)$$

$$m_n(q) \sim \frac{R(q)^n}{n^{\gamma(q)}} \quad (17)$$

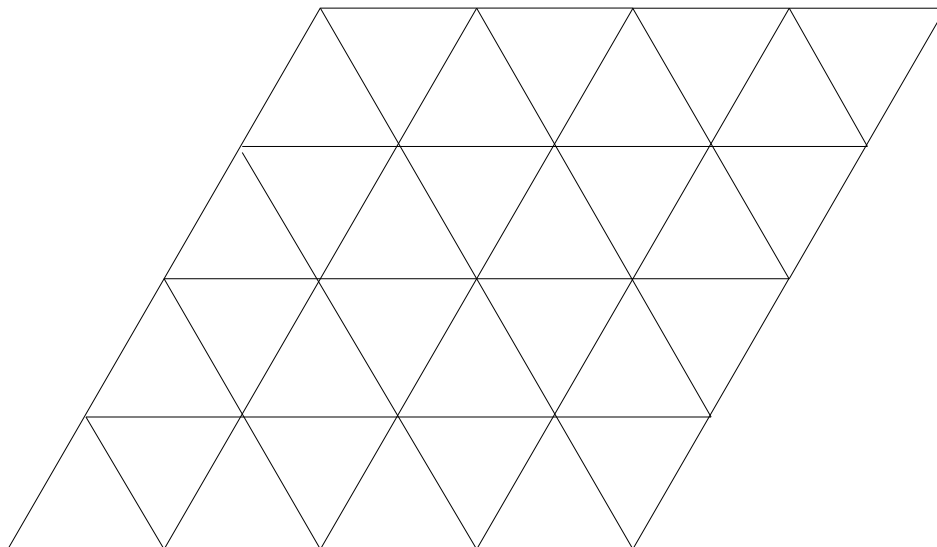
with $R(1) = 4$ and $\gamma(1) = \frac{3}{2}$

$$\text{as } m_n(1) = C_n \simeq \frac{4^n}{n^{\frac{3}{2}}}$$

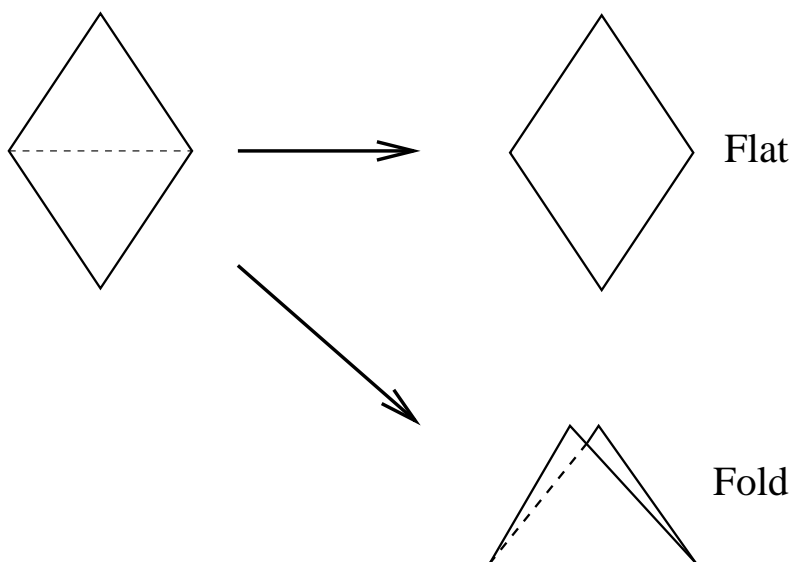
$$\begin{aligned} \text{with } R(\infty) &= q \text{ and } \gamma(\infty) = 0 \\ \text{as } m_n(q) &\simeq q^n \text{ for } q \rightarrow \infty \end{aligned} \quad (18)$$

3 Folding of the Regular Triangular Lattice

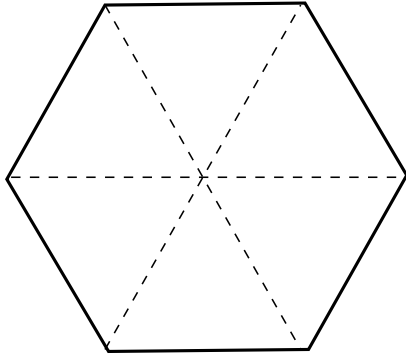
Regular Triangular Lattice



Embedded in 2-dimensional Space \rightarrow Fold or Flat



Folding of Elementary Hexagon:



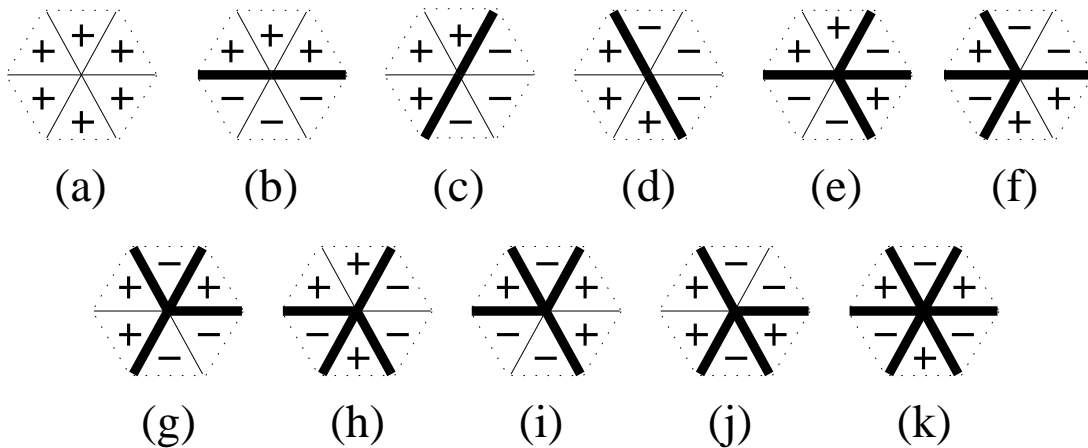
6 Bonds ----> 64 States ?

Only 11 Physical States

11 local fold environments for elementary Hexagon

Face Up ----- > $S = +1$

Face Down ----- > $S = -1$



Model System:

Geometric Constraints :

$$\sigma_v \equiv \sum_{i \text{ around } v} S_i = 0 \pmod{3} \quad (19)$$

Constrained Z_2 Spin System : 11 vertex model

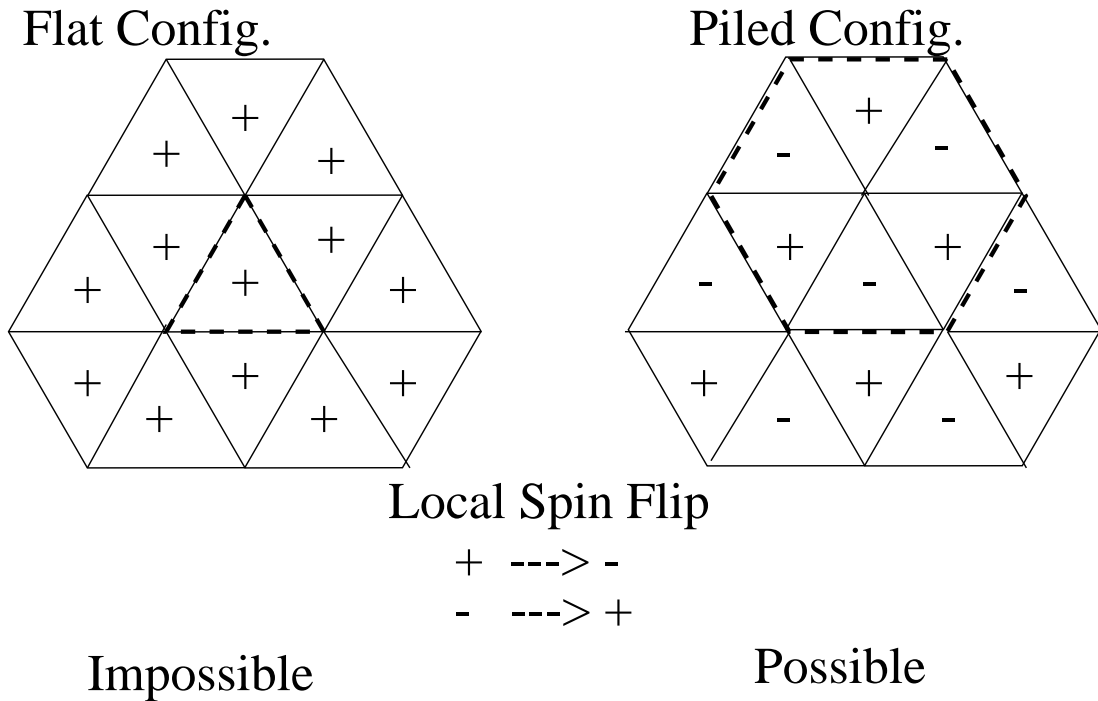
Hamiltonian:

$$\mathcal{H}_{Ising} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i \quad (20)$$

and

$$K = \beta J = J/k_B T \text{ and } h = \beta H \quad (21)$$

Structure of Phase Space: (Ph. Di Francesco and E.Guitter)



Local Spin Excitation :

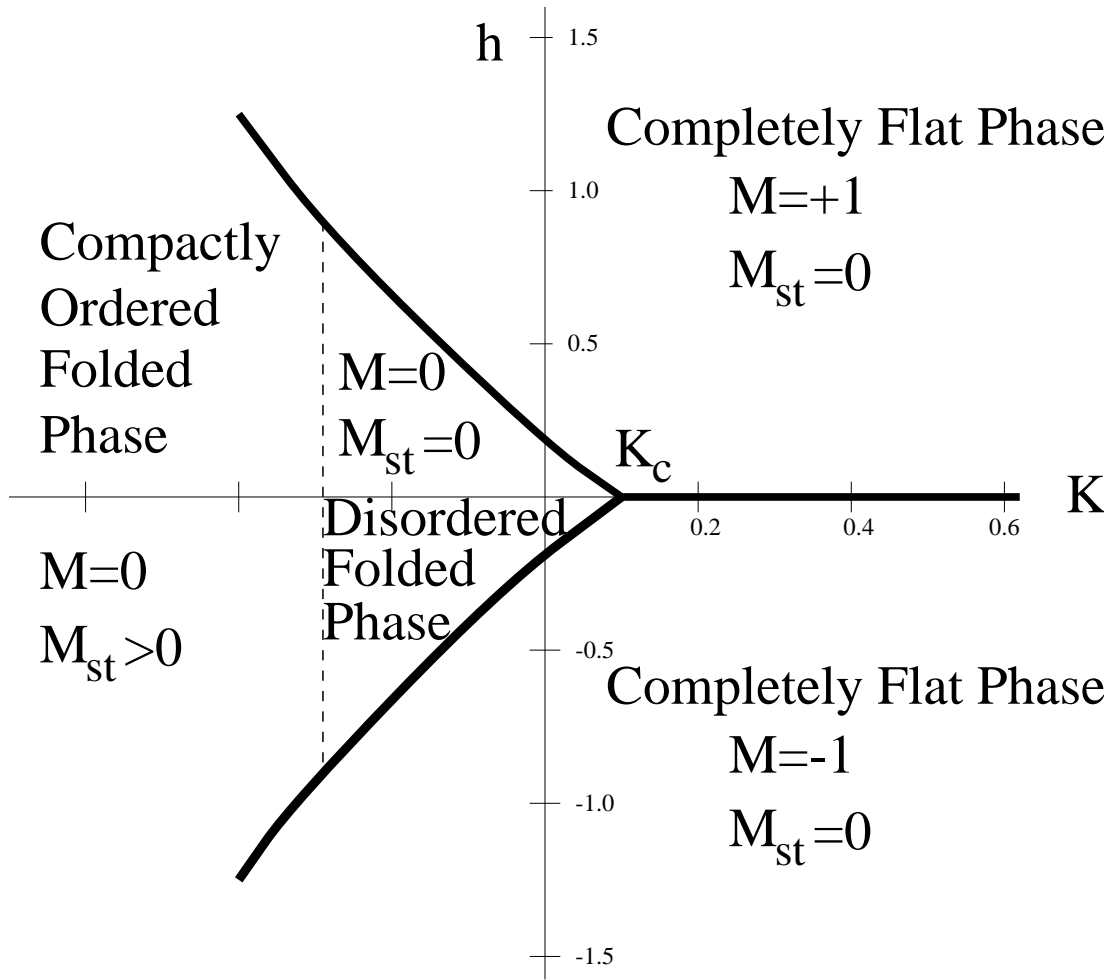
- (1) Impossible for Flat Configuration
- (2) Possible for Piled Configuration: Reversing All Spins in an Hexagon

Entropy or Number of States N_S for N Triangles:

$$N_S \sim q^N > 2^{\frac{1}{6} \times N} \quad (22)$$

$$q = \frac{\sqrt{3}}{2\pi} \Gamma(1/3)^{\frac{3}{2}} = 1.208717 \dots \quad (23)$$

Phase Diagram in the (K, h) -plane:(Ph. Di Francesco, E.Guitter and S.Mori etc)



$$M = \frac{1}{N} \left\langle \left(\sum_{\triangle} S_i + \sum_{\nabla} S_i \right) \right\rangle \quad (24)$$

$$M_{st} = \frac{1}{N} \left\langle \left(\sum_{\triangle} S_i - \sum_{\nabla} S_i \right) \right\rangle \quad (25)$$

Three-Coloring Formulation:

The Folding Problem is equivalent to 3-coloring Problem of the Bonds

Three Colors R (0), G (1), B (2), ordered cyclically (modulo 3).

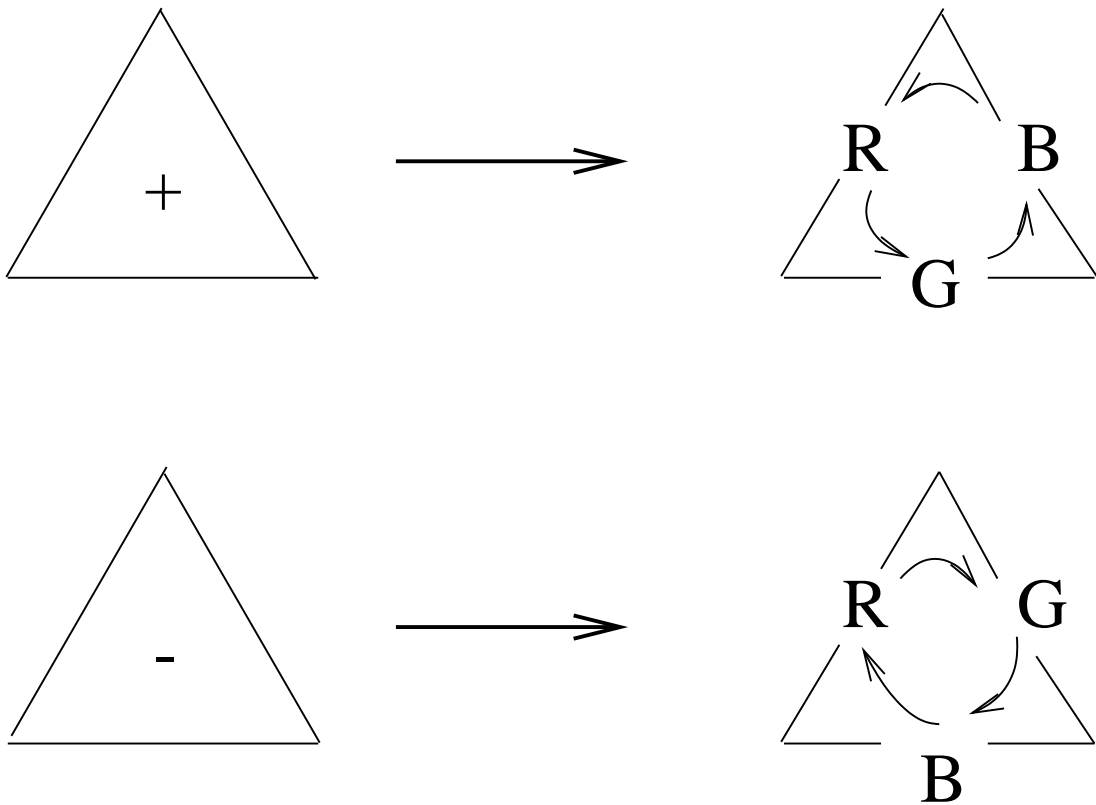
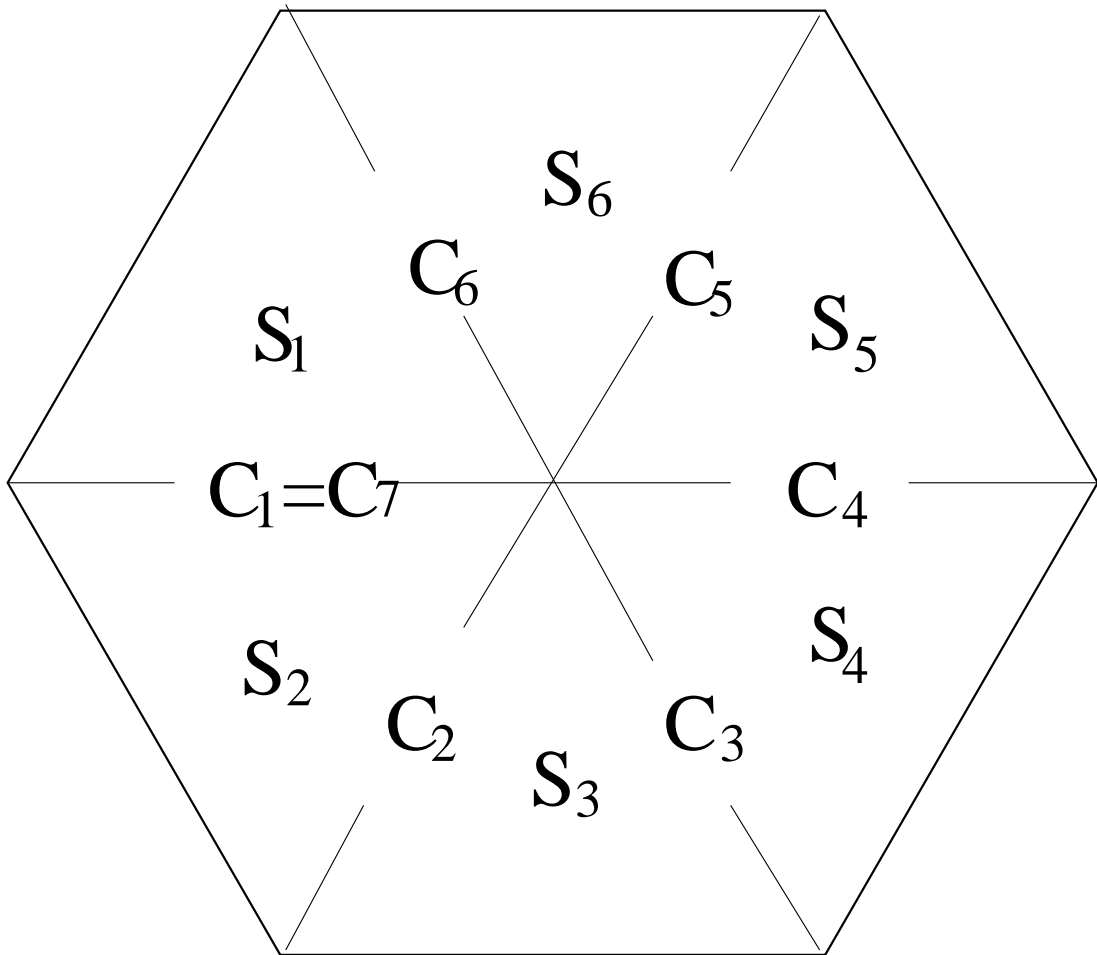


图 10: Color Assignments for Bonds



☒ 11: Coloring is Consistent if $c_7 = c_1$

$$C_{i+1} = C_i + S_i \pmod{3}$$

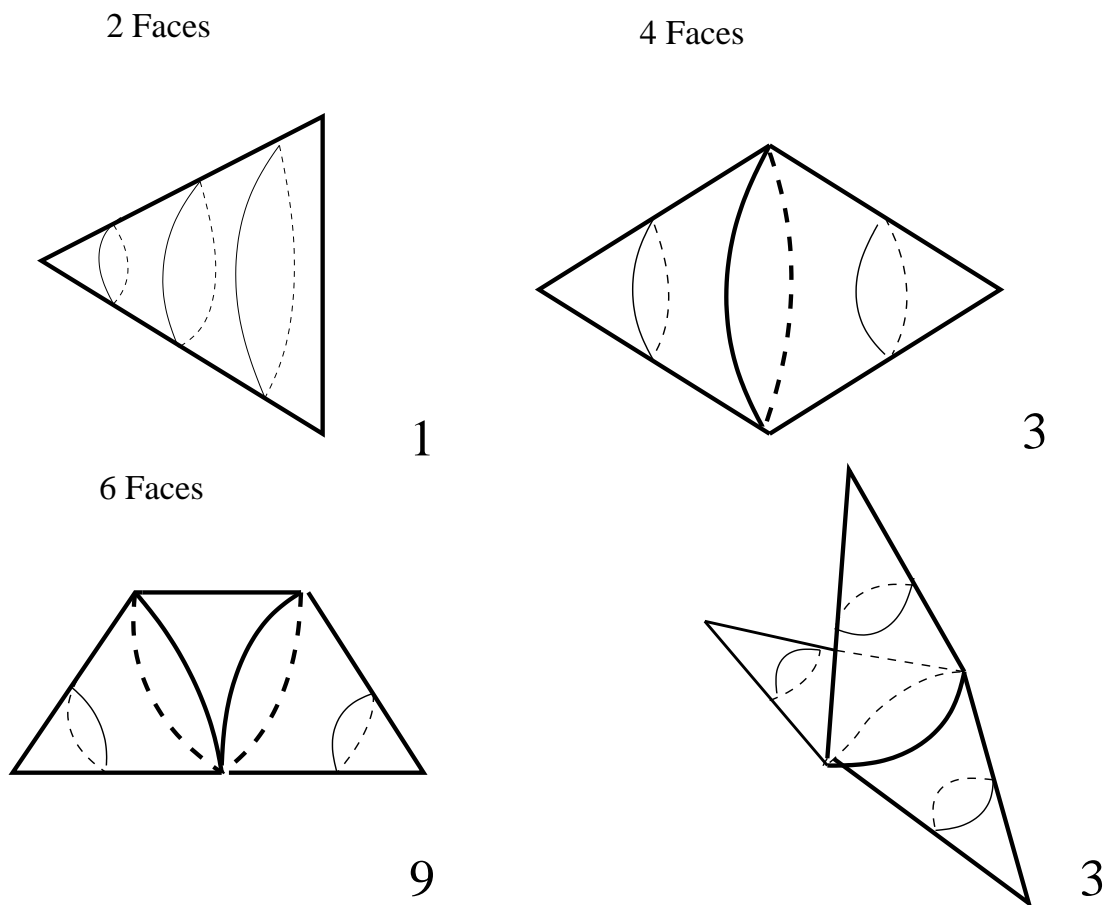
After One Turn,

$$C_7 = C_1 + \sum_{i=1}^6 S_i = 0 \pmod{3}$$

4 Folding of the Foldable Randomly Triangulated Surface

Fluid Membrane = Randomly Triangulated Surface + Foldability

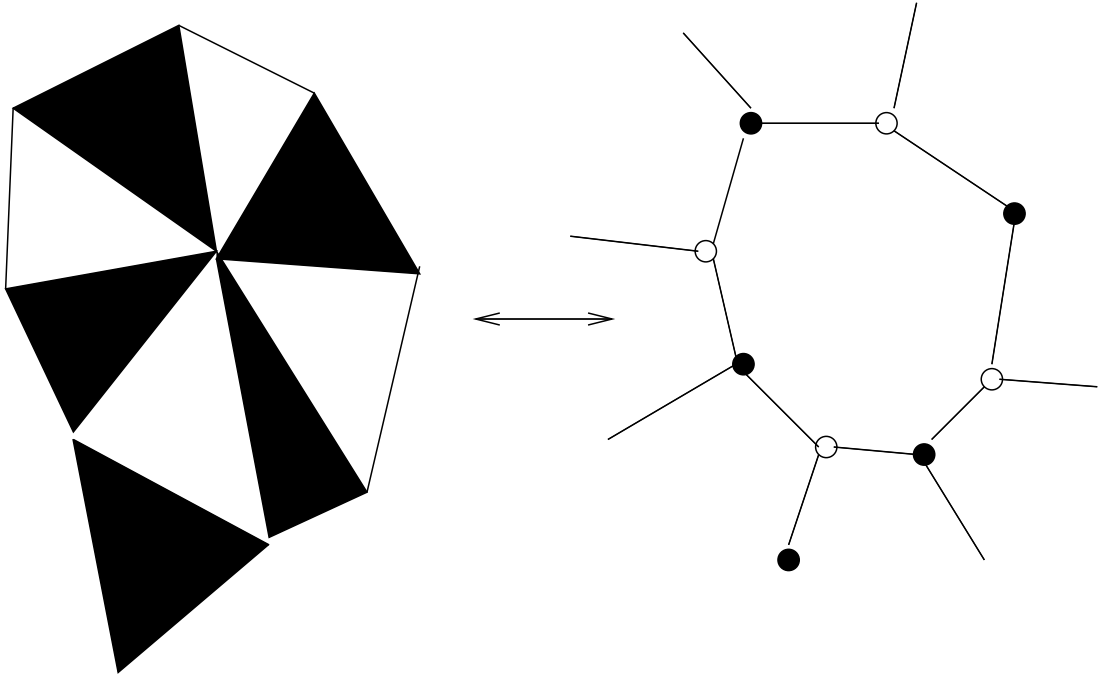
Foldable Triangulated Surface = Eulerian Triangulated Surface (Planar Surface Case)



☒ 12: Eulerian Triangulated Sphere

4.1 Matrix Model

Planar Eulerian Triangulated Surface = Dual Graph of Bipartite Tri-valent Planar Graphs



⊗ 13: Eulerian Triangulated Surface and its Dual

Generating Function in Matrix Model :

$$Z_N(t) = \int dA dB e^{-N \text{Tr}(V(A,B))}$$
$$V(A, B) = AB - \frac{\sqrt{t}}{3}(A^3 + B^3) \quad (26)$$

A,B: Hermitian Matrices of size $N \times N$

The Generating Function for Rooted Objects is

$$E(t) = kt \frac{d}{dt} F_0(t)$$

$$F_0(t) = \lim_{N \rightarrow \infty} \frac{1}{N^2} \log Z_N(t) \quad (27)$$

Results by W.Tutte “A Census of Planar Maps ” (1963)

$$E(t) = \frac{1}{32t^2} ((1 - 8t)^{\frac{3}{2}} - 1 + 12t + 24t^2) = \sum_{n=1} e_n t^n \quad (28)$$

and

$$e_n = \frac{3 \cdot 2^{n-1}}{(n+1)(n+2)} 2^n C_n = \frac{3}{n+2} \times 2^{n-1} C_n \quad (29)$$

$$e_1 = 1, \quad e_2 = 3, \quad e_3 = 12 \quad (30)$$

4.2 Toy Models

Toy Model for Polymer Membrane:

- Folding of Triangular Lattice
- Constrained Z_2 Spin System on the Dual of Triangular Lattice
- 3-Coloring Problem of Triangular Lattice

Toy Model for Fluid Membrane:

- Folding of Eulerian Randomly Triangulated Surface
- Constrained Z_2 Spin System on its Dual Random Diagram
- 3-Coloring Problem of the Random Diagram

How to Formulate.

- Matrix Model ?
Difficult and not yet solved
- Decorated Tree
also difficult and under progress

4.3 Combinatorial Solution by Decorated Tree

One-to-One Correspondence between Eulerian Triangulation and Well-Balanced Tree

by M.Bousquet-Mélow and G.Schaeffer (2000),
J.Bouttier, P.Di Francesco and E.Guitter (2002/cond-
mat/0206452)

Steps:

- Rooted Binary Tree with n White vertices, $n - 1$ edges and $n + 2$ white leaves (including the root)

$$C_n = \frac{1}{n + 2} 2^n C_n \quad (31)$$

- Decorated by $n - 1$ Black vertices and Black Buds to each edge

$$2^{n-1} C_n$$

- Match Buds to the closest Leaves in counter clockwise direction (Planar)

$n - 1$ Buds and Leaves Pair and 3 unmatched White leaves

- Well-balanced if the Root remains unmatched

$$\frac{3}{n + 2} 2^{n-1} C_n = e_n$$

From Decorated Tree to Rooted Bipartite Trivalent Planar Graph

- Fusing Bud-Leaf Pair into Edge
- Three unmatched leaves are connected to Additional Black Vertex
- Marked edge is that pointing from this vertex to the root leaf

Rooted Binary Tree

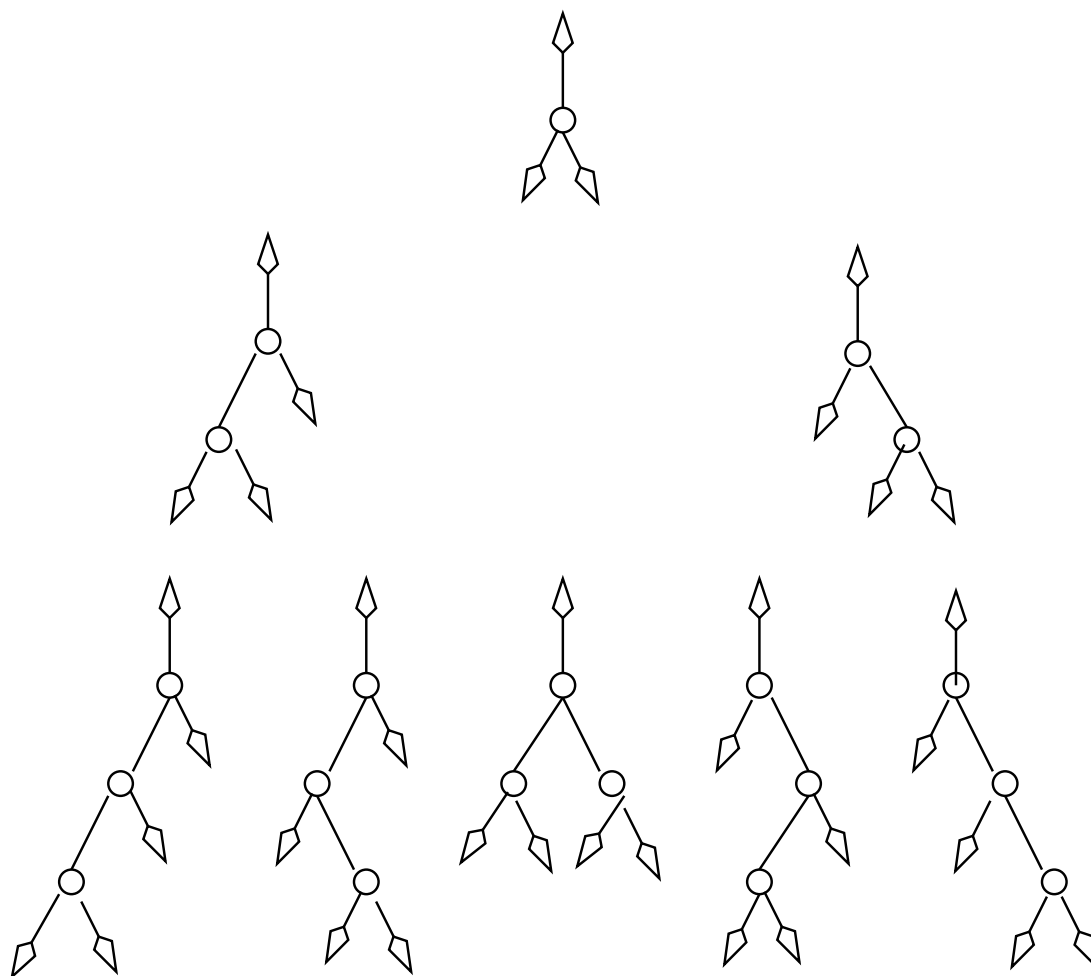


图 14: Binary Tree

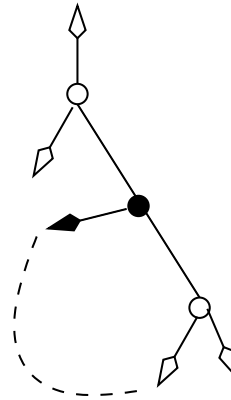
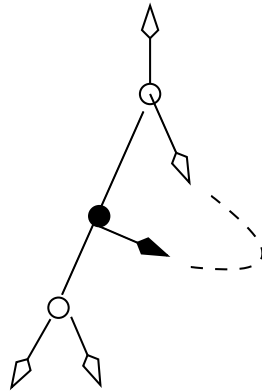
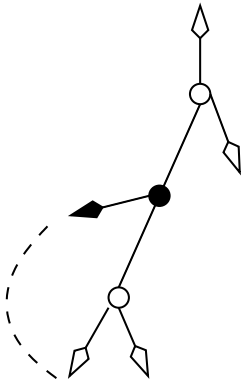
Recursion Relation:

$$C_n = \sum_{i=0}^{n-1} C_i \times C_{n-1-i}$$

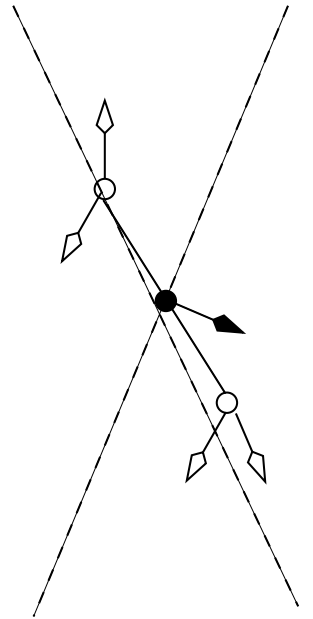
Decoration



$$c_2=2$$

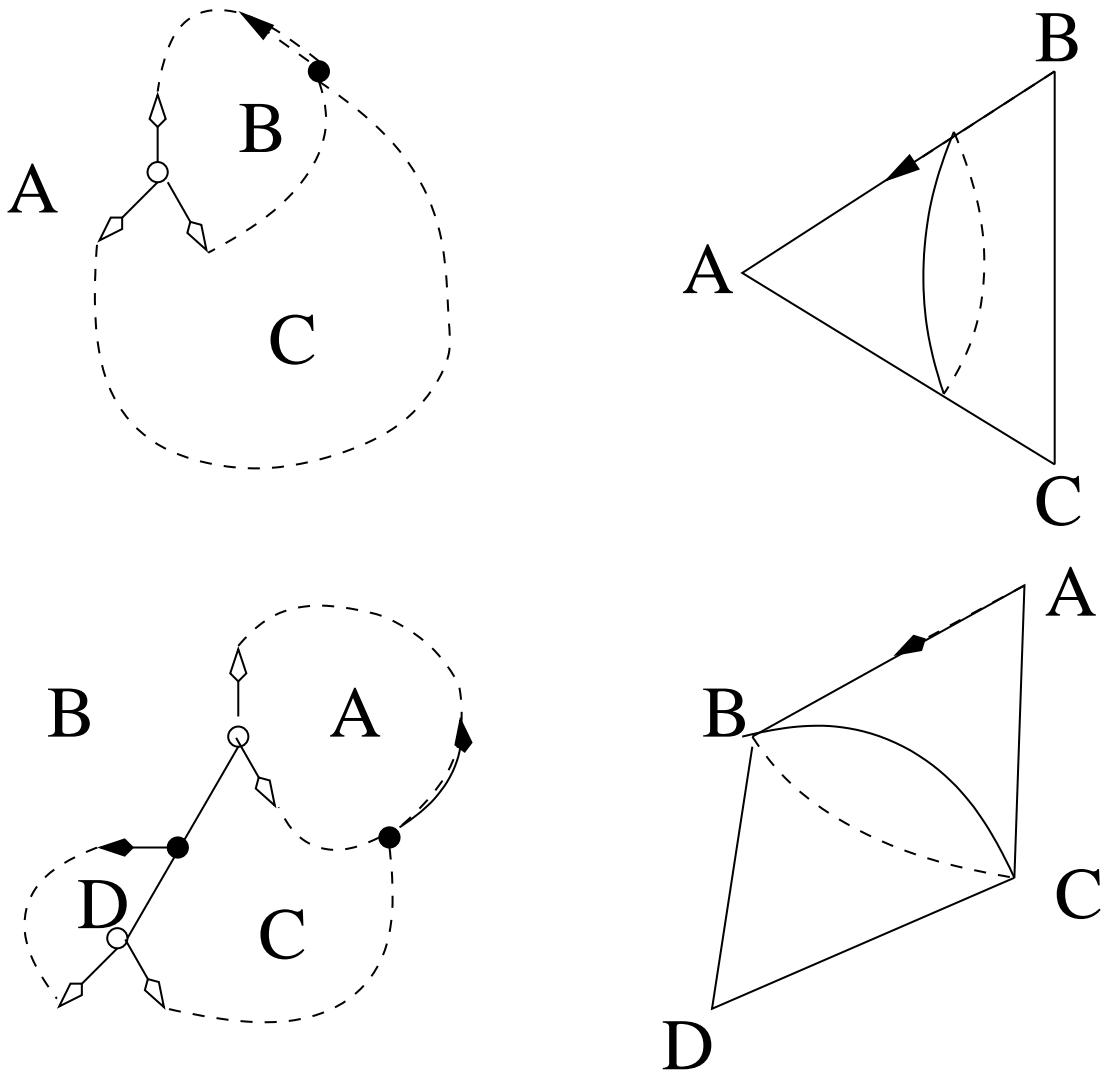


$$e_2=3$$



☒ 15: Decorated Binary Tree

Decorated Tree to Trivalent Graph



☒ 16: Decorated Binary Tree to Trivalent Tree and Triangulated Surface

Decorated Tree to Trivalent Graph

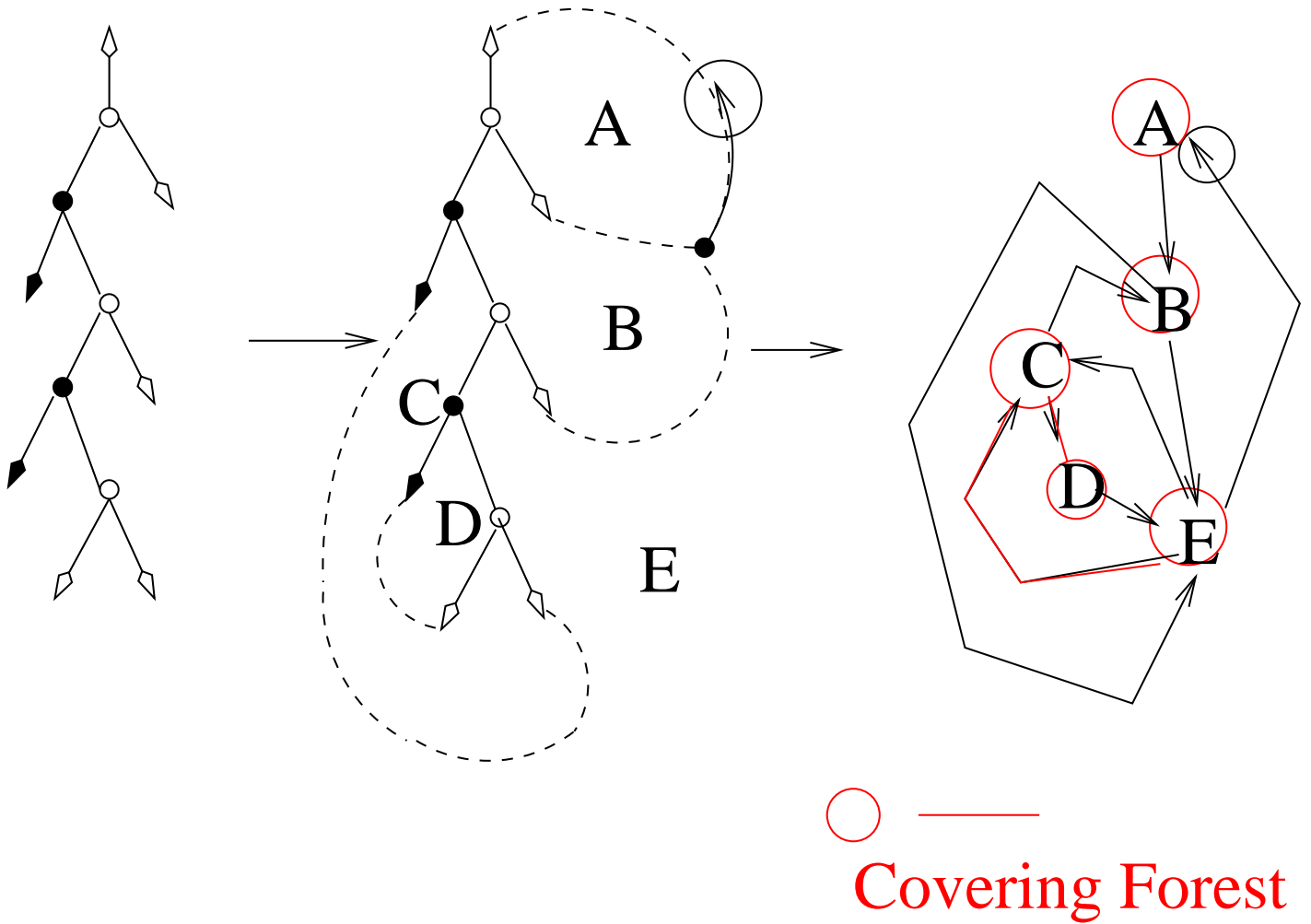


図 17: Decorated Binary Tree to Trivalent Tree and Triangulated Surface and Covering Forest

Under Construction(秋の物理学会の高分子分科のほうで)

5 Future Problem

- How to Describe Folding Path of Polymer
Not “Census “, but “Number of Folding Path”
“Physical” Move from Meander to Meander
- Physical Properties of Randomly Triangulated Surface
 - (1) Entropy
 - (2) Bending Energy and Phase Diagram
 - (3) How to Implement on Computer