Problems of probabilistic topology: the statistics of knots and non-commutative random walks

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<u>Abstract.</u> This paper reviews the state of affairs in a modern branch of mathematical physics called probabilistic topology. In particular we consider the following problems: (i) we estimate the probability of trivial knot formation on a lattice using the Kauffman algebraic invariants and show the connection of this problem with the thermodynamic properties of 2D disordered Potts model; (ii) we investigate the limiting behavior of random walks in multiconnected spaces and on non-commutative groups related to knot theory. We discuss the application of the abovementioned problems in the statistical physics of polymer chains. On the basis of non-commutative probability theory we derive some new results in the statistical physics of entangled polymer chains which unite rigorous mathematical facts with intuitive physical arguments.

1. Introduction

It would not be an exaggeration to say that contemporary physical science is becoming more and more mathematical.

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Received 8 July 1997, revised 10 November 1997 Uspekhi Fizicheskikh Nauk **168** (4) 369–405 (1998) Translated by S K Nechaev; edited by M S Aksent'eva This fact is too strongly manifested to be completely ignored. Hence I permit myself to bring forward two possible conjectures:

(a) On the one hand there are hardly any newly discovered physical problems which are beyond the well established methods of modern theoretical physics. This leads to the fact that nowadays real physical problems seem to be less numerous than the mathematical methods for their investigation.

(b) On the other hand mathematical physics is a fascinating field which absorbs new ideas from different branches of modern mathematics, translates them into the physical language and hence fills the abstract mathematical constructions with new fresh content. This ultimately leads to creating new concepts and stimulates the search for new deep conformities to natural laws in known physical phenomena.

The penetration of new mathematical ideas in physics sometime has a rather paradoxical character. It is not a secret that the difference in means (in languages) and goals of physicists and mathematicians leads to mutual misunderstanding, making the very subject of investigation obscure. What is true in general is certainly true in particular. To clarify the point, let us turn to the statistics of entangled uncrossable random walks — the well-known subject of the statistical physics of polymers. Actually, since the 1970s, after Conway's works, when the first algebraic topological invariants — Alexander polynomials — became very popular in mathematical literature, physicists working in statistical topology have acquired a much more powerful topological



Figure 1. Links between topologically – probabilistic problems. Solid boxes — problems, discussed in the paper; dashed boxes — problems not included in the consideration.

invariant than the simple Gauss linking number. The constructive utilization of algebraic invariants in the statistical physics of macromolecules has been developed in the classical works of A Vologodskii and M Frank-Kamenetskii [1]. However until recently in the overwhelming majority of works the authors have continued using the commutative Gauss invariant just making references to its imperfectness.

One of the reasons for such inertia consists in the fact that new mathematical ideas are often formulated as 'theorems of existence' and it takes much time to retranslate them into a physically acceptable form which may serve as a real computational tool.

We intend to use some recent advances in algebraic topology and the theory of random walks on non-commutative groups for reconsidering the old problem — evaluating the entropy of randomly generated knots and entangled random walks in a given homotopic state. Let us emphasize that this is a real physical paper, and when it is possible the rigorous statements are replaced by some physically justified conjectures. Generally speaking, the work is devoted to an analysis of probabilistic problems in topology and their applications in the statistical physics of polymer systems with topological constraints.

Let us formulate briefly the main results of our work.

1. The probability for a long random walk to form a knot randomly with a specific topological invariant is computed. This problem is considered using the Kauffman algebraic invariants and the connection with the thermodynamic properties of 2D Potts model with 'quenched' and 'annealed' disorder in interaction constants is discussed.

2. The limit behavior of random walks on the noncommutative groups related to the knot theory is investigated. Namely, the connection between the limit distribution for the Lyapunov exponent of products of non-commutative random matrices — generators of 'braid group' — and the asymptotic of powers ('knot complexity') of algebraic knot invariants is established. This relation is applied for calculating the knot entropy. In particular, it is shown that the 'knot complexity' corresponds to the well known topological invariant, 'primitive path', repeatedly used in the statistics of entangled polymer chains.

3. The random walks on multi-connected manifolds is investigated using conformal methods and the non-abelian topological invariants are constructed. It is shown that many non-trivial properties of the limit behavior of random walks with topological constraints can be explained in the context of random walks on hyperbolic groups.

4. The limit behavior of entangled random paths established above is used for investigation of the statistical properties of a so-called 'crumpled globule' (a trivial ring without self-intersections in a strongly contracted state).

The connection between all these problems is shown in Fig. 1.

2. Knot diagrams as disordered spin systems

2.1 Brief review of statistical problems in topology

The interdependence of such branches of modern theoretical and mathematical physics as the theory of integrable systems, algebraic topology and conformal field theory has proved to be a powerful catalyst for the development of a new direction in topology, namely, of analytical topological invariant construction by means of exactly solvable statistical models.

Today it is widely believed that the following three cornerstone findings have brought a fresh stream into topology:

— A deep relation has been found between the Temperley-Lieb algebra and the Hecke algebra representation of the braid group. This fact resulted in the remarkable geometrical analogy between the Yang-Baxter equations, appearing as a necessary condition of the transfer matrix commutativity in the theory of integrable systems on the one hand, and one of Reidemeister moves, used in the knot invariant construction on the other hand.

— It has been discovered that the partition function of the Wilson loop with the Chern–Simons action in the topological field theory coincides with the representation of the known non-abelian algebraic knot invariants written in terms of the time-ordered path integral.

— The need for new solutions of the Yang-Baxter equations has given a power impetus to the theory of quantum groups. Later on a related set of problems was separated into an independent branch of mathematical physics.

Of course the above mentioned findings do not exhaust the list of all brilliant achievements in that field during the last decade, but apparently these new accomplishments have used profound 'ideological' changes in the topological science: now we can hardly consider topology as an independent branch of pure mathematics where each small step forward takes so much effort that it seems incidental.

Thus in the middle of the 80s the 'quantum group' gin was released. It linked classical problems in topology, statistical physics and field theory by a common mathematical formalism. A new look at the old problems and the beauty of the formulated ideas made an impression on physicists and mathematicians. As a result, in the last few years the number of works devoted to the search of the new applications of the quantum group apparatus has grown exponentially going beyond the framework of original domains. As an example of the persistent penetration of the quantum group ideas in physics we can cite the works on anyon superconductivity [2], intensively discussing problems on 'quantum random walks' [3], the investigation of spectral properties of 'quantum deformations' of harmonic oscillators [4] and so on.

Time will show whether such 'quantum group expansion' is physically justified or merely does tribute to today's fashion. However it is clear that physics has acquired a new convenient language allowing the construction of new 'nonabelian objects' and to work with them.

Among the vast number of works devoted to different aspects of the theory of integrable systems, the topological applications connected to the construction of knot and link invariants and their representation in terms of partition functions of some known 2D-models deserve our special attention. There exist several reviews [5] and books [6] on this subject and our aim by no means consists in a reinterpretation or compilation of their contents. We attempt a consecutive account of recently solved *probabilistic* problems in topology as well as attract attention to some interesting, still unsolved, questions lying on the border of topology and probability theory. Of course we employ the knowledge acquired in algebraic topology utilizing the construction of new topological invariants made by V F R Jones [5] and L H Kauffman [7].

Besides the traditional fundamental topological issues concerning the construction of new topological invariants, investigation of homotopic classes and fibre bundles we mark a set of adjoint but much less studied problems. First of all, we mean the problem of so-called 'knot entropy' calculation. Most generally it can be formulated as follows. Take the lattice \mathbb{Z}^3 embedded in the space \mathbb{R}^3 . Let Ω_N be the ensemble of all possible closed non-self-intersecting *N*-step loops with one common fixed point on \mathbb{Z}^3 ; by ω we denote the particular trajectory configuration. The question is: what is the probability \mathcal{P}_N that the trajectory $\omega \in \Omega_N$ belongs to some specific homotopic class. Formally this quantity can be represented in the following way

$$\mathcal{P}_{N}\{\operatorname{Inv}\} = \frac{1}{\Omega_{N}} \sum_{\{\omega \in \Omega_{N}\}} \Delta[\operatorname{Inv}\{\omega\} - \operatorname{Inv}]$$

$$\equiv \frac{1}{\Omega_{N}} \sum_{\{\mathbf{r}_{1},...,\mathbf{r}_{N}\}} \Delta[\operatorname{Inv}\{\mathbf{r}_{1},...,\mathbf{r}_{N}\} - \operatorname{Inv}] (1 - \Delta[\mathbf{r}_{i} - \mathbf{r}_{j}]) \Delta[\mathbf{r}_{N}],$$

(2.1)

where $\text{Inv}\{\omega\}$ is the functional representation of the knot invariant corresponding to the trajectory with the bond coordinates $\{\mathbf{r}_1 \dots, \mathbf{r}_N\}$; Inv is the topological invariant characterizing a knot of specific homotopic type and $\Delta(x)$ is the Kronecker function: $\Delta(x = 0) = 1$ and $\Delta(x \neq 0) = 0$. The first Δ -function in Eqn (2.1) cuts the set of trajectories with the fixed topological invariant while the second and the third Δ -functions ensure the *N*-step trajectory to be non-self-intersecting and to form a closed loop respectively.

The distribution function \mathcal{P}_N {Inv} satisfies the normalization condition

$$\sum_{\substack{\text{all homotopic}\\ \text{classes}}} \mathcal{P}_N\{\text{Inv}\} = 1.$$
(2.2)

The entropy S_N {Inv} of the given homotopic state of the knot represented by an *N*-step closed loop on \mathbb{Z}^3 reads

$$S_N\{\operatorname{Inv}\} = \ln\left[\Omega_N \mathcal{P}_N\{\operatorname{Inv}\}\right]. \tag{2.3}$$

The problem concerning the determination of knot entropy has been discussed time and again by leading physicists. However the number of new analytic results in this field was insufficient till the beginning of the 80s: in about 90 percent of published materials authors used the Gauss linking number or some of its abelian modifications for classification of a topological state of knots and links while the disadvantages of this approach were explained in the remaining 10 percent. We do not include in this list the celebrated investigations of A V Vologodskiĭ et. al. [1] devoted to the first fruitful usage of the non-abelian Alexander algebraic invariants for computer simulations in statistical biophysics. We discuss physical applications of these topological problems at length in Section 5.

Despite the clarity of the geometrical image, the topological ideas are very hard to formalize because of the non-local character of topological constraints. Besides, the main difficulty in attempts to calculate analytically the knot entropy is due to the absence of a convenient analytic representation of the complete topological invariant. Thus, to succeed, at least partially, in computation of the knot entropy we simplify the general problem replacing it by the problem of calculating the distribution function for the knots with defined topological invariants. That problem differs from the original one because none of the known topological invariants (Gauss linking number, Alexander, Jones, HOM-FLY) are complete. The only exception are Vassiliev invariants [8], which are beyond the scope of the present book. Strictly speaking we are unable to estimate exactly the correctness of such a replacement of the homotopic class by the mentioned topological invariants. Thus under the definition of the topological state of the knot or entanglement we simply understand the determination of the corresponding topological invariant.

The problems where ω [see Eqn (2.1)] is the set of realizations of the random walk, i.e. the Markov chain are of special interest. In that case the probability of finding a closed *N*-step random walk in \mathbb{R}^3 in some prescribed topological state can be presented in the following way

$$\mathcal{P}_{N}\{\operatorname{Inv}\} = \int \dots \int \prod_{j=1}^{N} \mathrm{d}\mathbf{r}_{j} \prod_{j=1}^{N-1} g(\mathbf{r}_{j+1} - \mathbf{r}_{j}) \delta[\operatorname{Inv}\{\mathbf{r}_{1}, \dots, \mathbf{r}_{N}\} - \operatorname{Inv}] \delta[\mathbf{r}_{N}], \qquad (2.4)$$

where $g(\mathbf{r}_{j+1} - \mathbf{r}_j)$ is the probability of finding the j + 1th step of the trajectory in the point \mathbf{r}_{j+1} if *j*th step is in \mathbf{r}_j . In the limit $a \to 0$ and $N \to \infty$ (Na = L = const) in three-dimensional space we have the following expression for $g(\mathbf{r}_{j+1} - \mathbf{r}_j)$

$$g(\mathbf{r}_{j+1} - \mathbf{r}_j) = \left(\frac{3}{2\pi a^2}\right)^{3/2} \exp\left(-\frac{3(\mathbf{r}_{j+1} - \mathbf{r}_j)^2}{2a^2}\right)$$
$$\simeq \left(\frac{3}{2\pi a^2}\right)^{3/2} \exp\left\{\frac{3}{2a}\left(\frac{\mathrm{d}\mathbf{r}(s)}{\mathrm{d}s}\right)^2\right\}.$$
(2.5)

Introducing the 'time', s, along the trajectory we rewrite the distribution function $\mathcal{P}_N\{\text{Inv}\}$ [Eqn (2.4)] in the path integral form with the Wiener density measure

$$\mathcal{P}_{N}\{\operatorname{Inv}\} = \frac{1}{\mathcal{Z}} \int \dots \int \mathcal{D}\{\mathbf{r}\} \exp\left\{-\frac{3}{2a} \int_{0}^{L} \left(\frac{\mathrm{d}\mathbf{r}(s)}{\mathrm{d}s}\right)^{2} \mathrm{d}s\right\}$$
$$\times \delta[\operatorname{Inv}\{\mathbf{r}(s)\} - \operatorname{Inv}], \qquad (2.6)$$

and the normalization condition is as follows

$$\mathcal{Z} = \sum_{\substack{ ext{all different} \ ext{knot invariants}}} \mathcal{P}_N \{ ext{Inv} \}$$

The form of Eqn (2.6) up to the Wick turn and the constants coincides with the scattering amplitude α of a free quantum particle in a multi-connected phase space. Actually, for the amplitude α we have

$$\alpha \sim \sum_{\substack{\text{all paths from a given topological class}}} \exp\left\{\frac{\mathbf{i}}{h} \int \dot{\mathbf{r}}^2(s) \, \mathrm{d}s\right\}.$$
 (2.7)

If the phase trajectories can be mutually transformed by means of continuous deformations, then the summation in Eqn (2.7) should be extended to all available paths in the system, but if the phase space consists of different topological domains, then the summation in Eqn (2.7) refers to the paths from the exclusively defined class and the 'knot entropy' problem arises.

2.2 Abelian problems in the statistics of entangled random walks and the incompleteness of the Gauss invariant

As far back as 1967 S F Edwards had discovered the basis of the statistical theory of entanglements in physical systems. In [9] he proposed a way of exactly calculating the partition function of a self-intersecting random walk topologically interacting with an infinitely long uncrossible string (in 3D case) or obstacle (in 2D-case). That problem had been considered in mathematical literature even earlier — see paper [10] for instance — but S F Edwards was apparently the first to recognize the deep analogy between abelian topological problems in the statistical mechanics of Markov chains and quantum-mechanical problems (like Bohm– Aharonov) of particles in magnetic fields. The review of classical results is given in [12], whereas some modern advantages are discussed in [11].

The 2D version of the Edwards' model is formulated as follows. Take a plane with an excluded origin, producing the topological constraint for the random walk of length L with the initial and final points \mathbf{r}_0 and \mathbf{r}_L respectively. Let trajectory make n turns around the origin (Fig. 2). The question is in calculating the distribution function $\mathcal{P}_n(\mathbf{r}_0, \mathbf{r}_L, L)$.

In the said model the topological state of the path C is fully characterized by number of turns of the path around the origin. The corresponding abelian topological invariant is known as Gauss linking number and when represented in the



Figure 2. Random walk on the plane near the single obstacle.

contour integral form, reads

$$\operatorname{Inv}\{\mathbf{r}(s)\} \equiv G\{C\} = \int_{C} \frac{y \, \mathrm{d}x - x \, \mathrm{d}y}{x^2 + y^2}$$
$$= \int_{C} \mathbf{A}(\mathbf{r}) \, \mathrm{d}\mathbf{r} \equiv 2\pi n + \vartheta \,, \qquad (2.8)$$

where

$$\mathbf{A}(\mathbf{r}) = \xi \times \frac{\mathbf{r}}{r^2}, \quad \xi = (0, 0, 1)$$
 (2.9)

and ϑ is the angular distance between ends of the random walk.

Substituting Eqn (2.8) into Eqn (2.6) and using the Fourier transform of the δ -function, we arrive at

$$\mathcal{P}_{n}(\mathbf{r}_{0},\mathbf{r}_{L},L) = \frac{1}{\pi La} \exp\left(\frac{r_{0}^{2} + r_{L}^{2}}{La}\right) \int_{-\infty}^{\infty} I_{|\lambda|}\left(\frac{2r_{0}r_{L}}{La}\right) \\ \times \exp\left[i\lambda(2\pi n + \vartheta)\right] d\lambda, \qquad (2.10)$$

which reproduces the well known old result [9] (some very important generalizations one can find in [11]).

A physically significant quantity obtained on the basis of Eqm (2.10) is the entropic force

$$f_n(\rho) = -\frac{\partial}{\partial \rho} \ln \mathcal{P}_n(\rho, L) , \qquad (2.11)$$

which acts on the closed chain ($\mathbf{r}_0 = \mathbf{r}_L = \rho, \vartheta = 0$) when the distance between the obstacle and a certain point of the trajectory changes. Apparently the topological constraint leads to a strong attraction of the path to the obstacle for any $n \neq 0$ and to weak repulsion for n = 0.

Another exactly solvable 2D-problem closely related to that under discussion deals with the calculation of the partition function of a random walk with a given algebraic area. The problem concerns the determination of the distribution function $\mathcal{P}_S(\mathbf{r}_0, \mathbf{r}_L, L)$ for a random walk with the fixed ends and specific algebraic area S.

As a possible solution, D S Khandekar and F W Wiegel [13] again represented the distribution function in terms of the path integral Eqn (2.6) with the replacement

$$\delta \Big[\operatorname{Inv} \{ \mathbf{r}(s) \} - \operatorname{Inv} \Big] \to \delta \Big[S \{ \mathbf{r}(s) \} - S \Big], \qquad (2.12)$$

where the area is written in the Landau gauge:

$$S\{\mathbf{r}(s)\} = \frac{1}{2} \int_{C} y \, \mathrm{d}x - x \, \mathrm{d}y = \frac{1}{2} \int_{C} \widetilde{\mathbf{A}}(\mathbf{r}) \dot{\mathbf{r}} \, \mathrm{d}s, \quad \widetilde{\mathbf{A}} = \xi \times \mathbf{r}$$
(2.13)

[compare to Eqs (2.8), (2.9)].

The final expression for the distribution function reads ([12])

$$\mathcal{P}_{S}(\mathbf{r}_{0},\mathbf{r}_{L},L) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dg \exp(iqS) \mathcal{P}_{q}(\mathbf{r}_{0},\mathbf{r}_{L},L), \quad (2.14)$$

where

$$\mathcal{P}_q(\mathbf{r}_0, \mathbf{r}_L, L) = \frac{\lambda}{4\pi \sin(La\lambda/4)} \exp\left\{\frac{\lambda}{2}(x_0y_L - y_0x_L) - \frac{\lambda}{4} \times \left[(x_L - x_0)^2 + (y_L - y_0)^2\right] \cot\frac{La\lambda}{4}\right\} (2.15)$$

and $\lambda = -iq$.

For closed trajectories Eqs (12.14), (2.15) can be simplified essentially, giving

$$\mathcal{P}_{S}^{cl}(N) = 2La\cosh^{2}\left(\frac{2\pi S}{La}\right).$$
(2.16)

Different aspects of this problem have been extensively studied in [11].

There is no principal difference between the problems of random walk statistics in the presence of a single topological obstacle or with a fixed algebraic area — both of them have the 'abelian' nature. Nevertheless we would like to concentrate on the last problem because of its deep connection with the famous Harper–Hofstadter model dealing with the spectral properties of a 2D electron hopping on a discrete lattice in a constant magnetic field [14]. Actually, rewrite Eqn (2.4) with the substitution Eqn (2.12) in form of recursion relation in the number of steps, N:

$$\mathcal{P}_{q}(\mathbf{r}_{N+1}, N+1) = \int d\mathbf{r}_{N}g(\mathbf{r}_{N+1} - \mathbf{r}_{N})$$
$$\times \exp\left[\frac{\mathrm{i}q}{2}\xi(\mathbf{r}_{N} \times \mathbf{r}_{N+1})\right]\mathcal{P}_{q}(\mathbf{r}_{N}, N). \quad (2.17)$$

For the discrete random walk on \mathbb{Z}^2 we use the identity

$$\int \mathbf{d}\mathbf{r}_N g(\mathbf{r}_{N+1} - \mathbf{r}_N)(\ldots) \to \sum_{\{\mathbf{r}_N\}} w(\mathbf{r}_{N+1} - \mathbf{r}_N)(\ldots) ,\quad (2.18)$$

where $w(\mathbf{r}_{N+1} - \mathbf{r}_N)$ is the matrix of the local jumps on the square lattice; *w* is supposed to be symmetric:

$$w = \begin{cases} \frac{1}{4}, \text{ for } (x, y) \to (x, y \pm 1) \text{ and } (x, y) \to (x, \pm 1, y), \\ 0 \text{ otherwise.} \end{cases}$$
(2.19)

Finally, in the Landau gauge we get :

1 1

$$\frac{4}{\varepsilon}W(x, y, q, \varepsilon) = \exp\left(\frac{1}{2}iqx\right)W(x, y - 1, q)$$

$$+ \exp\left(-\frac{1}{2}iqx\right)W(x, y + 1, q)$$

$$+ \exp\left(\frac{1}{2}iqy\right)W(x - 1, y, q)$$

$$+ \exp\left(-\frac{1}{2}iqy\right)W(x + 1, y, q), \quad (2.20)$$

where $W(x, y, q, \varepsilon)$ is the generating function defined via the relation $W(x, y, q, \varepsilon) = \sum_{N=0}^{\infty} \varepsilon^N \mathcal{P}_S(\mathbf{r}_N, N)$ and q plays the

role of the magnetic flux through the contour bounded by the random walk on the lattice.

There is one point which is still out of our complete understanding. On the one hand the continuous version of the described problem has very clear abelian background due to the use of commutative 'invariants' like the algebraic area, Eqn (2.13). On the other hand it has been recently discovered [15] that the so-called Harper equation, i.e. Eqn (2.20), written in the gauge $S{\mathbf{r}} = \int_C y \, dx$, exhibits a hidden quantum group symmetry related to the so-called C^* algebra [16] which is strongly non-abelian. Usually in statistical physics we expect that the continuous limit (when lattice spacing tends to zero with corresponding rescaling of parameters of the model) of any discrete problem does not change the observed physical picture, at least qualitatively. But for the considered model the spectral properties of the problem are extremely sensitive to the actual physical scale of the system and depend strongly on the lattice geometry.

The generalization of the above stated problems concerns, for instance, the computation of the partition function for the random walk entangled with k > 1 obstacles on the plane located in the points $\{\mathbf{r}_1, \ldots, \mathbf{r}_k\}$. At first sight, the approach based on the usage of the Gauss linking number as a topological invariant might allow us to solve such a problem easily. Let us replace the vector potential $\mathbf{A}(\mathbf{r})$ in Eqn (2.8) by the following

$$\mathbf{A}(\mathbf{r}_1,\ldots,\mathbf{r}_k) = \xi \times \sum_{j=1}^k \frac{\mathbf{r} - \mathbf{r}_j}{|\mathbf{r} - \mathbf{r}_j|^2} \,. \tag{2.21}$$

The topological invariant in this case will be the algebraic sum of turns around obstacles, which seems to be a natural generalization of the Gauss linking number to the case of many-obstacle entanglements.

However, the following problem is bound to arise: for a system with two or more obstacles it is possible to imagine closed trajectories entangled with a few obstacles together but not entangled with every one. In Figure 3 the so-called 'Pochhammer contour' is shown. Its topological state with respect to the obstacles cannot be described using any abelian version of the Gauss-like invariants.

To clarify the point we can apply this to the concept of the homotopy group [17]. Consider the topological space $\mathcal{R} = \mathbb{R}^2 - \{\mathbf{r}_1, \mathbf{r}_2\}$ where $\{\mathbf{r}_1, \mathbf{r}_2\}$ are the coordinates of the removed points (obstacles) and choose an arbitrary reference point $\mathbf{r}_0 \neq \mathbf{r}_j$, $j \in [1, 2]$. Consider the ensemble of all directed trajectories starting and finishing at the point \mathbf{r}_0 . Take the *basis loops* $\gamma_1(s)$ and $\gamma_2(s)$ (0 < s < L) representing the rightclock turns around the points \mathbf{r}_1 and \mathbf{r}_2 respectively. The same



Figure 3. Pochammer contour entangled with two obstacles together but not entangled with every one.

trajectories passed in the counter-clockwise direction are denoted by $\gamma_1^{-1}(s)$ and $\gamma_2^{-1}(s)$.

The *multiplication* of the paths is their composition: for instance, $\gamma_1\gamma_2 = \gamma_1 \circ \gamma_2$. The unit (trivial) path is the composition of an arbitrary loop with its inverse:

$$e = \gamma_i \gamma_i^{-1} = \gamma_i^{-1} \gamma_i, \quad i = \{1, 2\}.$$
 (2.22)

The loops $\gamma_i(s)$ and $\tilde{\gamma}_i(s)$ are called *equivalent* if one can be transformed into another by means of a monotonic change of variables $s = s(\tilde{s})$. The homotopic classes of directed trajectories form the group with respect to the paths multiplication; the unity is the homotopic class of the trivial paths. This group is known as the *homotopy group* $\pi_1(\mathcal{R}, \mathbf{r}_0)$.

Any closed path on \mathcal{R} can be represented by a 'word' consisting of set of letters $\{\gamma_1, \gamma_2, \gamma_1^{-1}, \gamma_2^{-1}\}$. Taking into account Eqn (2.22), we can reduce each word to the minimal irreducible representation. For example, the word $W = \gamma_1 \gamma_2^{-1} \gamma_1 \gamma_1 \gamma_1^{-1} \gamma_2^{-1} \gamma_2 \gamma_1^{-1} \gamma_2^{-1}$ can be transformed to the irreducible form: $W = \gamma_1 \gamma_2^{-1} \gamma_2^{-1}$. It is easy to understand that the word $W \equiv$ e represents only the unentangled contours. The entanglement in Fig. 3 corresponds to the irreducible word $W = \gamma_1^{-1} \gamma_2 \gamma_1 \gamma_2^{-1} \equiv 1$. The non-abelian character of the topological constraints is reflected in the fact that different entanglements do not commute: $\gamma_1\gamma_2 \neq \gamma_2\gamma_1$. At the same time, the total algebraic number of turns (Gauss linking number) for the path in Fig. 3 is equal to zero, i.e. it belongs to the trivial class of homology. Speaking more formally, the mentioned example is the direct consequence of a well known fact in topology: the classes of homology of knots (of entanglements) do not coincide in general with the corresponding homotopic classes. The first ones for the group π_1 can be distinguished by the Gauss invariant, while the problem of characterizing the homotopy class of a knot (entanglement) by an analytically defined invariant is one of the main problems in topology.

The principal difficulty connected with application of the Gauss invariant is due to its incompleteness. Hence, exploiting the abelian invariants for adequate classification of topologically different states in systems with multiple topological constraints is very problematic.

2.3 Non-abelian algebraic knot invariants

The most obvious topological questions concerning the knotting probability during the random closure of the random walk cannot be answered using the Gauss invariant due to its weakness.

A break through in that field was made in 1975–1976 when the algebraic polynomials were used for the topological state identification of closed random walks generated by the Monte-Carlo method [1]. It has been recognized that the Alexander polynomials, being much stronger invariants than the Gauss linking number, could serve as a convenient tool for the calculation of the thermodynamic properties of entangled random walks. That approach actually appeared to be very fruitful and the main part of our modern knowledge on knot and link statistics was obtained with the help of these works and their subsequent modifications.

In the present section we develop the analytic approach in the statistical theory of knots considering the basic problem — the probability of finding a randomly generated knot in a specific topological state. We would like to reiterate that our investigation would be impossible without utilizing the algebraic knot invariants discovered recently. Below we reproduce briefly the construction of Jones invariants following the Kauffman approach in the general outline.

2.3.1 Disordered Potts model and generalized dichromatic polynomials. The graph expansion for the Potts model with the disorder in the interaction constants can be defined by means of a slight modification of the well known construction of the ordinary Potts model [18, 19]. Let us recall the necessary definitions.

Take an arbitrary graph \mathcal{L} with N vertices. To each vertex of the given graph we attribute the 'spin' variable σ_i $(i \in [1, N])$ which can take q states labelled as $1, 2, \ldots, q$ on the simplex. Suppose that the interaction between spins belonging to the connected neighboring graph vertices only contributes to the energy. Define the energy of the spins' interaction as follows

$$E_{kl} = J_{kl} \delta(\sigma_k, \sigma_l)$$

=
$$\begin{cases} J_{kl}, \ \sigma_k = \sigma_l, \ (\sigma_k, \sigma_l) - \text{neighbors}, \\ 0 \text{ otherwise}, \end{cases}$$
(2.23)

where J_{kl} is the interaction constant which varies for different graph edges and the equality $\sigma_k = \sigma_l$ means that the neighboring spins take equal values on the simplex.

The partition function of the Potts model now reads

$$Z_{\text{potts}} = \sum_{\{\sigma\}} \exp\left\{\sum_{\{kl\}} \frac{J_{kl}}{T} \delta(\sigma_k, \sigma_l)\right\},$$
(2.24)

where T is the temperature.

Expression Eqn (2.24) gives for q = 2 the well-known representation of the Ising model with the disordered interactions extensively studied in the theory of spin glasses [20]. (Later on we would like to fill in this old story with a new 'topological' sense.)

To proceed with the graph expansion of the Potts model [19], rewrite the partition function (2.24) in the following way

$$Z_{\text{potts}} = \sum_{\{\sigma\}} \prod_{\{kl\}} \left[1 + v_{kl} \,\delta(\sigma_k, \sigma_l) \right], \quad v_{kl} = \exp\left(\frac{J_{kl}}{T}\right) - 1.$$
(2.25)

If the graph \mathcal{L} has N edges then the product Eqn (2.25) contains N multipliers. Each multiplier in that product consists of two terms: 1 and $v_{kl} \delta(\sigma_k, \sigma_l)$. Hence the partition function Eqn (2.25) is decomposed into the sum of 2^N terms.

Each term in the sum is in one-to-one correspondence with some part of the graph \mathcal{L} . To make this correspondence clearer, it should be considered that an arbitrary term in the sum represents the product of N multipliers described above in ones from each graph edge. We accept the following convention:

(a) If for some edge the multiplier is equal to 1, we remove the corresponding edge from the graph \mathcal{L} ;

(b) If the multiplier is equal to $v_{kl}\delta(\sigma_k,\sigma_l)$ we keep the edge in its place.

After repeating the same procedure with all graph edges, we find a unique representation for all terms in the sum, Eqn (2.25), by collecting the components (either connected or not) of the graph \mathcal{L} .

Take a typical graph G consisting of m edges and C connected components where the separated graph vertex is

$$Z_{\text{potts}} = \sum_{\{G\}} q^C \prod_{\{kl\}}^m v_{kl} \,, \tag{2.26}$$

where the product $\prod_{\{kl\}}^{m}$ runs over all edges in the fixed graph *G*.

It should be noted that the graph expansion Eqn (2.26) where $v_{kl} \equiv v$ for all $\{k, l\}$ coincides with the well known representation of the Potts system in terms of a *dichromatic polynomial* (see, for instance, [18, 19]).

Another comment concerns the number of spin states, q. As can be seen, in the derivation presented above we did not account for the fact that q has to take positive integer values only. From this point of view the representation Eqn (2.26) has an advantage with respect to the standard representation Eqn (2.24) and can be considered an analytic continuation of the Potts system to the non-integer and even complex values of q. We show in the subsequent sections how the defined model is connected to the algebraic knot invariants.

2.3.2 Reidemeister moves and the state model for construction of algebraic invariants. Let K be a knot (or link) embedded in 3D-space. First of all we project the knot (link) onto a plane and obtain a 2D-knot diagram in the so-called general position (denoted by K as well). This means that only pair crossings can be at the points of paths intersections. Then for each crossing we define the passages, i.e. parts of the trajectory on the projection going 'below' and 'above' in accordance with its natural positions in 3D-space.

For the knot plane projection with defined passages the following theorem is valid: (Reidemeister [22]):

Two knots embedded in \mathbb{R}^3 can be deformed continuously one into the other if and only if the diagram of one knot can be transformed into the diagram corresponding to another knot via the sequence of simple local moves of types I, II and III shown in Fig. 4.

Work [22] provides us with a proof of this theorem. Two knots are called *regular isotopic* if they are isotopic with respect to the two last Reidemeister moves (II and III); meanwhile, if they are isotopic with respect to all moves, they are called *ambient isotopic*. As can be seen from Fig. 4, the Reidemeister move of type I leads to the creation of a cusp



Figure 4. Reidemeister moves of types I, II and III.

on the projection. At the same time it should be noted that all real 3D-knots (links) are of ambient isotopy.

Now, after the Reidemeister theorem has been formulated, it is possible to describe the construction of the polynomial 'bracket' invariant in the way proposed by L H Kauffman [7, 23]. This invariant can be introduced as a certain partition function being the sum over the set of some formal ('ghost') degrees of freedom.

Let us consider a 2D-knot diagram with defined passages as a certain irregular lattice (graph). The crossings of path on the projection are the lattice vertices. Turn all these crossings to the standard positions where parts of the trajectories in each graph vertex are normal to each other and form angles of $\pm \pi/4$ with the x-axis. It can be proven that the result does not depend on such a standardization.

There are two types of vertices in our lattice — (a) and (b) which we label by the variable $b_i = \pm 1$ as it is shown below:

(a)
$$b_i = +1$$
, (b) $b_i = -1$.

The next step in the construction of the algebraic invariant is the introduction of two possible ways of *vertex splitting*. Namely, we attribute to each way of graph splitting the following statistical weights: A to horizontal splitting and Bto vertical for a vertex of type (a); B to horizontal splitting and A to vertical for a vertex of type (b). This can be schematically reproduced in the following picture:



the constants A and B to be defined later.

For the knot diagram with N vertices there are 2^N different microstates, each of them representing the set of splittings of all N vertices. The entire microstate, S, corresponds to the knot (link) disintegration to a system of disjoint and non-self-intersecting circles. The number of such circles for the given microstate S we denote as S. The following statement belongs to L Kauffman ([7]).

Consider the partition function

$$\langle K \rangle = \sum_{\{S\}} d^{\mathcal{S}-1} A^i B^j , \qquad (2.27)$$

where $\sum_{\{S\}}$ means summation over all possible 2^N graph splittings, *i* and j = N - i being the numbers of vertices with weights *A* and *B* for the given realization of all splittings in the microstate *S* respectively.

The polynomial in A, B and d represented by the partition function Eqn (2.27) is the topological invariant of knots of regular isotopy if and only if the following relations among the weights A, B and d are fulfilled:

$$AB = 1,$$

$$ABd + A^{2} + B^{2} = 0.$$
(2.28)

The sketch of the proof is as follows. Denote by $\langle ... \rangle$ the statistical weight of the knot or a part of it. The $\langle K \rangle$ -value equals the product of all weights of knot parts. Using the definition of vertex splittings, it is easy to test the following

identities valid for unoriented knot diagrams

$$\left\langle \begin{array}{c} \\ \end{array}\right\rangle = \left\langle \begin{array}{c} \\ \end{array}\right\rangle A + \left\langle \begin{array}{c} \\ \end{array}\right\rangle B, \\ \left\langle \begin{array}{c} \\ \end{array}\right\rangle = \left\langle \begin{array}{c} \\ \end{array}\right\rangle B + \left\langle \begin{array}{c} \\ \end{array}\right\rangle A, \end{array}$$
(2.29)

completed by the 'initial condition'

$$\langle K \cup O \rangle = d \langle K \rangle$$
, if K is not empty, (2.30)

where O denotes the separated trivial loop.

The *skein relations* Eqn (2.29) correspond to the above defined weights of horizontal and vertical splittings while relation Eqn (2.30) defines the statistical weights of the composition of an arbitrary knot and a single trivial ring. These diagrammatic rules are well defined only for fixed 'boundary condition' of the knot (i.e., for the fixed part of the knot outside the brackets). Suppose that by convention the polynomial of the trivial ring is equal to unity:

$$\langle O \rangle = 1 \,. \tag{2.31}$$

Now it can be shown that under an appropriate choice of relations between *A*, *B* and *d*, the partition function Eqn (2.27) represents the algebraic invariant of the knot. The proof is based on direct testing of the invariance of the $\langle K \rangle$ -value with respect to Reidemeister moves of types II and III. For instance, for a Reidemeister move of type II we have:

$$\left\langle \overbrace{\bigcirc}\right\rangle = \left\langle \overbrace{\bigcirc}\right\rangle ABd + \left\langle \overbrace{\bigcirc}\right\rangle B^{2} + \left\langle \overbrace{\bigcirc}\right\rangle A^{2} + \left\langle \overbrace{\bigcirc}\right\rangle AB = \left\langle \bigcirc\right\rangle (ABd + A^{2} + B^{2}) + \left\langle \bigcirc\right\rangle AB. (2.32)$$

Therefore, the invariance with respect to the Reidemeister move of type II can be obtained immediately if we set the statistical weights in the last line of Eqn (2.32) as written in Eqn (2.28). Actually, the topological equivalence of the two knot diagrams is restored with respect to the Reidemeister move of type II only if the right- and left-hand sides of Eqn (2.28) are identical. It can also be tested that the condition of obligatory invariance with respect to the Reidemeister move of type III does not violate the relations Eqn (2.28).

The relations Eqn (2.28) can be converted into the form

$$B = A^{-1}, \quad d = -A^2 - A^{-2},$$
 (2.33)

which means that the Kauffman invariant Eqn (2.27) is the Laurent polynomial in *A*-value only.

Finally, Kauffman showed that for oriented knots (links) the invariant of ambient isotopy (i.e., the invariant with respect to all Reidemeister moves) is defined via the relation:

$$f[K] = (-A)^{3T_W(K)} \langle K \rangle, \qquad (2.34)$$

here Tw(K) is the twisting of the knot (link), i.e. the sum of signs of all crossings defined by the convention:

(a)
$$+1$$
, (b) -1

(not to be confused with the definition of the variable b_i introduced above). Eqn (2.34) follows from the following chain of equalities

The state model and bracket polynomials introduced by L H Kauffman seem to be very special. They explore only the peculiar geometrical rules such as summation over the formal 'ghost' degrees of freedom — all possible knot (link) splittings with simple defined weights. But one of the main advantages of the described construction is connected with the fact that Kauffman polynomials in *A*-value coincide with Jones knot invariants in *t*-value (where $t = A^{1/4}$).

Jones polynomial knot invariants were first discovered by V F R Jones during his investigation of the topological properties of braids (see Section 3 for details). Jones' proposition concerns the establishment of a deep connection between the braid group relations and the Yang-Baxter equations ensuring the necessary condition of transfer matrix commutativity [6]. The Yang–Baxted equations play an exceptionally important role in the statistical physics of integrable systems (such as ice, Potts, O(n), 8-vertex, quantum Heisenberg models [19]).

2.4 Lattice knot diagrams as a disordered Potts model

An attempt to apply Kauffman invariants of regular isotopy to the investigation of the statistical properties of random walks with topological constraints in a thin slit was made recently [24]. Below we extend the ideas of the work [24] considering the topological state of the knot as a special kind of a *quenched disorder*.

Let us specify the model under consideration. Take a square lattice \mathcal{M} turned to an angle $\pi/4$ with respect to the *x*-axis and project a knot embedded in \mathbb{R}^3 onto \mathcal{M} supposing that each crossing point of the knot diagram coincides with one lattice vertex without fall (there are no empty lattice vertices) — see Fig. 5. Define the passages in all *N* vertices and choose such boundary conditions which ensure the lattice to form a single closed path; that is possible when \sqrt{N} (i.e. *N*) is an odd number. The *frozen pattern* of all passages $\{b_i\}$ on the lattice together with the boundary conditions fully determine the topology of some 3D knot.

Of course, the model under consideration is rather rough because we neglect the 'space' degrees of freedom due to trajectory fluctuations and keep the pure topological specificity of the system. Later on in Chapter 4 we discuss the applicability of such a model for real physical systems and produce arguments in support of its validity.

The basic question of interest is as follows: what is the probability $\mathcal{P}_N\{f[K]\}$ of finding a knot diagram on our lattice \mathcal{M} in a topological state characterized by some specific Kauffman invariant $f[K\{b_1,\ldots,b_N\}]$ among all 2^N microrealizations of the disorder $\{b_i\}$ in the lattice vertices. That probability distribution reads [compare to Eqn (2.1)]



Figure 5. Lattice knot with topological disorder realized in a quenched random pattern of passages.

$$\mathcal{P}_{N}\left\{f[K]\right\} = \frac{1}{2^{N}} \sum_{\{b_{i}\}} \Delta\left[f\left[K\{b_{1}, b_{2}, \dots, b_{N}\}\right] - f[K]\right], (2.35)$$

where $f[K\{b_1, \ldots, b_N\}]$ is the representation of the Kauffman invariant as a function of all passages $\{b_i\}$ on the lattice \mathcal{M} . These passages can be regarded as a sort of quenched 'external field' (see below).

Our main idea for dealing with $\mathcal{P}_N{f[K]}$ consists in two steps:

(a) first we convert the Kauffman topological invariant into the known and well-investigated Potts spin system with the disorder in interaction constants;

(b) then we apply the methods of the physics of disordered systems to the calculation of the thermodynamic properties of the Potts model. This enables us finally to extract the estimation for the requested distribution function.

Strictly speaking, we could have disregarded point (a), because it does not lead directly to the answer to our main problem. Nevertheless we follow the mentioned sequence of steps in pursuit of two goals: (1) we would like to prove that the topologically-probabilistic problem can be solved within the framework of the standard thermodynamic formalism; (2) we would like to employ the knowledge already accumulated in the physics of disordered Potts systems to avoid some unnecessary complications. Let us emphasize that the meanfield approximation and formal replacement of the model with short-range interactions by one with infinite long-range interactions serves as a common computational tool in the theory of disordered systems and spin glasses.

2.4.1 Algebraic invariants of regular isotopy. The general outline of topological invariant construction concerns the search for the functional, $f[K\{b_1, \ldots, b_N\}]$, which is independent of the knot shape i.e. is invariant with respect to all Reidemeister moves.

Recall that the Potts representation of the Kauffman polynomial invariant of regular isotopy for some given pattern of 'topological disorder', $\{b_i\}$, deals with simultaneous splittings in all lattice vertices representing the polygon decomposition of the lattice \mathcal{M} . Such lattice disintegration looks like a densely packed system of disjoint and non-self-intersecting circles. The collection of all polygons (circles) can

be interpreted as a system of so-called *Eulerian circuits* completely filling the square lattice. Eulerian circuits are in one-to-one correspondence with the graph expansion of some disordered Potts systems introduced in Section 2.3.1 (see details below and in [27]).

Rewrite the Kauffman invariant of regular isotopy, $\langle K \rangle$, in form of disordered Potts model defined in the previous section. Introduce the two-state 'ghost' spin variables, $s_i = \pm 1$ in each lattice vertex independent on the crossing in the same vertex

$$\bigcup_{i=1}^{n} s_i = +1; \quad \bigcup_{i=1}^{n} s_i = -1.$$

Irrespective of the orientation of the knot diagram shown in Fig. 5 (i.e. restricting with the case of regular isotopic knots), we have

$$\langle K\{b_i\}\rangle = \sum_{\{S\}} (A^2 + A^{-2})^{S-1} \exp\left(\ln A \sum_{i=1}^N b_i s_i\right).$$
 (2.36)

Written in such a form, the partition function $\langle K\{b_i\}\rangle$ represents the weighted sum of all possible *Eulerian circuits*[†] on the lattice \mathcal{M} . Let us show explicitly that the microstates of the Kauffman system are in one-to-one correspondence with the microstates of some disordered Potts model on a lattice. Apparently for the first time, a similar statement was expressed in paper [7]. To be careful, we would like to use the following definitions:

(i) Let us introduce the lattice \mathcal{L} dual to the lattice \mathcal{M} , or more precisely, one of two possible (odd and even) diagonal dual lattices, shown in Fig. 6. It can be easily noticed that the edges of lattice \mathcal{L} are in one-to-one correspondence with the vertices of lattice \mathcal{M} . Thus, the disorder on the dual lattice \mathcal{L} is determined on the *edges*. In turn, the edges of lattice \mathcal{L} can be divided into the subgroups of vertical and horizontal bonds. Each *kl*-bond of lattice \mathcal{L} carries the 'disorder variable' b_{kl} being a function of the variable b_i located in the correspond-



Figure 6. Disintegration of the knot diagram on the \mathcal{M} -lattice into an ensemble of non-self-intersecting loops (Eulerian circuits) and a graph representation of the Potts model on the dual \mathcal{L} -lattice.

† A Eulerian circuit is a trajectory on the graph which visits once and only once all the graph edges.

ing *i*-vertex of lattice \mathcal{M} . The simplest and most sitable choice of the function $b_{kl}(b_i)$ is as in Eqn (2.46) (or vice versa for another choice of dual lattice); *i* is the vertex of the lattice \mathcal{M} belonging to the *kl*-bond of the dual lattice \mathcal{L} .

(ii) For the given configuration of splittings on \mathcal{M} and chosen dual lattice \mathcal{L} let us accept the following convention: we mark the edge of the \mathcal{L} -lattice by the solid line if this edge is not intersected by some polygon on the \mathcal{M} -lattice and we leave the corresponding edge unmarked if it is intersected by any polygon — as it is shown in Fig. 6. Similarly, the sum $\sum s_i b_i$ in Eqn (2.36) can be rewritten in terms of marked and unmarked bonds on the \mathcal{L} -lattice

$$\sum_{i} s_{i}b_{i} = \sum_{\text{marked}} s_{i}b_{i} + \sum_{\text{unmarked}} s_{i}b_{i} = \sum_{\text{marked}} s_{i}b_{i} + \sum_{\text{marked}} s_{i}b_{i}$$

+
$$\sum_{\text{unmark}}^{\text{horizontal}} s_{i}b_{i} + \sum_{\text{unmarked}}^{\text{vertical}} s_{i}b_{i} = -\sum_{\text{marked}}^{\text{horizontal}} b_{kl} - \sum_{\text{marked}}^{\text{vertical}} b_{kl}$$

+
$$\sum_{\text{unmarked}}^{\text{horizontal}} b_{kl} + \sum_{\text{unmarked}}^{\text{vertical}} b_{kl} = \sum_{\text{all edges}} b_{kl} - 2\sum_{\text{marked}} b_{kl},$$

(2.37)

where we used the relation

$$\sum_{\text{unmarked}} b_{kl} + \sum_{\text{marked}} b_{kl} = \sum_{\text{all edges}} b_{kl} \, .$$

(iii) Let m_s be the number of marked edges and C_s be the number of connected components of the marked graph. Then the Euler relation reads:

$$\mathcal{S} = 2C_s + m_s - N + \chi. \tag{2.38}$$

Eqn (2.38) can be proved directly. The χ -value depends on the genus of the surface, which can be covered by the given lattice, (i.e. χ depends on the boundary conditions). In the thermodynamic limit $N \ge 1$ the χ -dependence should disappear (at least for flat surfaces), so the standard equality $S = 2C_s + m_s - N$ will be assumed below.

By means of definitions (i)–(iii), we can easily convert Eqn (2.36) into the form: N

$$\langle K\{b_{kl}\} \rangle = (A^2 + A^{-2})^{-(N+1)} \prod_{\text{all edges}}^{m} [A^{b_{kl}}]$$

$$\times \sum_{\{G\}} (A^2 + A^{-2})^{2C_s} \prod_{\text{marked}}^{m_s} [A^{-2b_{kl}}(-A^2 - A^{-2})]$$

$$(2.39)$$

where we used Eqn (2.37) and the fact that N + 1 is even. Comparing Eqn (2.39) with Eqn (2.25) we immediately conclude that

$$\sum_{\{G\}} (A^2 + A^{-2})^{2C_s} \prod_{\text{marked}}^m \left[A^{-2b_{kl}} (-A^2 - A^{-2}) \right]$$
$$\equiv \sum_{\{\sigma\}} \prod_{\{kl\}} \left[1 + v_{kl} \delta(\sigma_k, \sigma_l) \right], \qquad (2.40)$$

which coincides with the partition function of the Potts system written in the form of a dichromatic polynomial. Therefore, we have

$$v_{kl} = A^{-2b_{kl}}(-A^2 - A^{-2}) = -1 - A^{-4b_{kl}},$$

$$q = (A^2 + A^{-2})^2.$$
(2.41)

Since the 'disorder' variables b_{kl} take the discrete values ± 1 only, we get the following expression for the interaction constant J_{kl}

$$\frac{J_{kl}}{T} = \ln\left[1 - (A^2 + A^{-2})A^{-2b_{kl}}\right] = \ln\left[-A^{-4b_{kl}}\right].$$

Combining Eqs (2.39)-(2.41) we obtain the following statement.

(a) Take an N-vertex knot diagram on the lattice \mathcal{M} with given boundary conditions and a fixed set of passages $\{b_i\}$.

(b) Take the dual lattice \mathcal{L} in one-to-one correspondence with \mathcal{M} where one vertex of \mathcal{M} belongs to one edge of \mathcal{L} .

The Kauffman topological invariant $\langle K(A) \rangle$ of regular isotopy for knot diagrams on \mathcal{M} admits representation in the form of a 2D Potts system on a dual lattice \mathcal{L} :

$$\langle K(A) \rangle = H(A, \{b_{kl}\}) Z_{\text{potts}}[q(A), \{J_{kl}(b_{kl}, A)\}], \quad (2.42)$$

where:

$$H(A, \{b_{kl}\}) = (A^2 + A^{-2})^{-(N+1)} \exp\left(\ln A \sum_{\{kl\}} b_{kl}\right)$$
(2.43)

is a trivial multiplier (H does not depend on Potts spins);

$$Z_{\text{potts}}[q(A), \left\{J_{kl}(b_{kl}, A)\right\}]$$
$$= \sum_{\{\sigma\}} \exp\left\{\sum_{\{kl\}} \frac{J_{kl}(b_{kl}, A)}{T} \delta(\sigma_k, \sigma_l)\right\}$$
(2.44)

is the Potts partition function with interaction constants, J_{kl} , and number of spin states, q, defined as follows

$$\frac{J_{kl}}{T} = \ln[-A^{-4b_{kl}}], \quad q = (A^2 + A^{-2})^2; \quad (2.45)$$

and the variables b_{kl} play the role of disorder on the edges of the lattice \mathcal{L} dual to the lattice \mathcal{M} . The connection between b_{kl} and b_i is defined by convention

$$b_{kl} = \begin{cases} -b_i, \text{ if edge } (kl) \text{ is vertical,} \\ b_i, \text{ if edge } (kl) \text{ is horizontal.} \end{cases}$$
(2.46)

Eqn (2.44) has the sense of a partition function of the 2D disordered Potts system with random nearest-neighbor interactions whose distribution remains arbitrary. The set of passages $\{b_{kl}\}$ uniquely determines the actual topological state of the woven carpet for the definite boundary conditions. Therefore the topological problem of the knot invariant determination is reduced to a normal statistical problem of calculation of the partition function of the Potts model with the disorder in the interaction constants. Of course, this correspondence is still rather formal because the polynomial variable A is absolutely arbitrary and can take even complex values, but for some regions of A that thermodynamic analogy makes sense and could be useful as we shall see below.

The specific feature of the Potts partition function which gives the representation of the Kauffman algebraic invariant is connected with the existence of a relation between the temperature T and the number of spin states q [see Eqn (2.44)] according to which T and q cannot be considered anymore as independent variables.

2.4.2 Algebraic invariants of ambient isotopy. The invariance of the algebraic topological invariant, f[K], with respect to all Reidemeister moves [see Eqn (2.34)] for our system shown in Fig. 5 is related to the oriented Eulerian circuits called *Hamiltonian walks*[†].

Let us suppose that the orientation of the knot diagram shown in Fig. 5 is chosen according to the natural orientation of the path representing a knot K in \mathbb{R}^3 . For the defined boundary conditions we get the so-called *Manhattan lattice* consisting of woven threads with alternating directions.

It follows from the definition of twisting Tw(K) (see Section 2.3.2) that Tw(K) changes sign if the direction of one arrow in the vertex is reversed. Reversing the direction of any arrows in the given vertex an even number of times we return the sign of twisting to the initial value.

We define groups of 'even' and 'odd' vertices on the lattice \mathcal{M} as follows. The vertex *i* is called *even* (*odd*) if it belongs to the horizontal (vertical) bond (*kl*) of the dual lattice \mathcal{L} . Now it is easy to prove that the twisting of the knot on the Manhattan lattice \mathcal{M} can be written in terms of the above defined variables b_{kl} . Finally the expression for the algebraic invariant of ambient isotopy f[K] on the lattice \mathcal{L} reads

$$f[K] = \exp\left(3\ln[-A]\sum_{\{kl\}} b_{kl}\right) \left\langle K(\{b_{kl}\}, A)\right\rangle, \qquad (2.47)$$

where $\langle K(\{b_{kl}\}, A) \rangle$ is defined by Eqn (2.42).

2.5 Notion about annealed and quenched realizations of topological disorder

The fixed topological structure of a trajectory of a given length fluctuating in space is a typical example of quenched disorder. Actually, the knot structure is formed during the random closure of the path and cannot be changed without path rupture. Because of the topological constraints the entire phase space of the ensemble of randomly generated closed loops is divided into separate domains resembling the multivalley structure of the spin glass phase space. Every domain corresponds to a sub-space of the path configuration with a fixed value of the topological invariant.

The methods of theoretical description of the systems with quenched disorder in interaction constants are rather well developed, especially in regard to the investigation of *spin glass models* [20]. Central to these methods is the concept of *self-averaging* which can be explained as follows. Take some additive function F (the free energy, for instance) of some disordered spin system. The function F is the self-averaging quantity if the observed value, F_{obs} , of any macroscopic sample of the system coincides with the value F_{av} averaged over the ensemble of disorder realizations:

$$F_{\rm obs} = \langle F \rangle_{\rm av}$$
.

The central technical problem is in the calculation of the free energy $F = -T \ln Z$ averaged over the randomly distributed quenched pattern in the interaction constants. In this section we show that this famous thermodynamic problem of spin glass physics is closely related to the knot entropy computation.

Another problem arises when averaging the partition function Z (but not the free energy) over the disorder. Such

a problem is much simpler from the computational point of view and corresponds to the case of *annealed* disorder. Physically such a model corresponds to the situation when the topology of the closed loop can be changed. It means that the topological invariant, i.e. the Potts partition function, has to be averaged over all possible realizations of the pattern disorder in the ensemble of open (i.e. unclosed) loops on the lattice. It has been shown in [26] that the calculation of the mean values of topological invariants allows the extraction of rather rough but non-trivial information about the knot statistics.

2.5.1 Entropy of knots. Replica methods. Our main goal is the computation of the probability distribution $\mathcal{P}_N\{f[K]\}$ [see Eqn (2.35)]. Although we are unable to evaluate this function exactly, the representation of $\mathcal{P}_N\{f[K]\}$ in terms of the disordered Potts system enables us to give an upper estimate for the fraction of randomly generated paths belonging to some definite topological class (in particular, to the trivial one). We use the following chain of inequalities restricting ourselves to the case of regular isotopic knots for simplicity ([24]):



The first inequality is due to the fact that the Kauffman invariant of regular isotopic knots is not a complete topological invariant, whereas the last probability in the chain can be written as follows

$$\mathcal{P}_{N}\left\{K(A^{*})\right\} = \sum_{\{b_{kl}\}} \Theta\left\{b_{kl}\right\} \Delta\left[\left\langle K\{b_{kl}, A^{*}\}\right\rangle - \left\langle K(A^{*})\right\rangle\right], \quad (2.49)$$

where \sum means summation over all possible configurations of the 'crossing field' $\{b_{kl}\}$, the Δ -function cuts out all states of the field $\{b_{kl}\}$ with specific value of Kauffman invariant $\langle K\{b_{kl}, A^*\} \rangle \equiv \langle K(A^*) \rangle$ and $\Theta\{b_{kl}\}$ is the probability of realization of a given crossings configuration.

In principle the distribution $\Theta\{b_i\}$ depends on the statistics of the path in the underlying 3D space and is determined physically by the process of knot formation. Here we restrict ourselves to the following simple suppositions:

(i) We regard the crossings $\{b_i\}$ in different vertices of the \mathcal{M} -lattice as completely uncorrelated variables (or, in other words, we assume that the variables $\{b_{kl}\}$ defined on the edges of the \mathcal{L} -lattice are statistically independent):

$$\Theta\{b_i\} = \prod_{i=1}^{N} P(b_i);$$
 (2.50)

(ii) We suppose variable b_i (or b_{kl}) to take values ± 1 with equal probabilities, i.e.:

$$P(b_i) = \frac{1}{2}\delta(b_i - 1) + \frac{1}{2}\delta(b_i + 1).$$
(2.51)

[†] A Hamiltonian walk is a closed path which visits once and only once all vertices of the given *oriented* graph.

The probability of trivial knot formation can be estimated now as follows

$$\mathcal{P}_{N}^{(0)}(A^{*}) \leq \sum_{\{b_{kl}\}} \Theta\{b_{kl}\} \Delta \Big[\ln \big\langle K\{b_{kl}, A^{*}\} \big\rangle \Big]$$
$$\simeq \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}y \int \dots \int \prod_{kl} P(b_{kl}) \,\mathrm{d}b_{kl} \big\langle K^{\mathrm{i}y}\{b_{kl}, A^{*}\} \big\rangle$$
(2.52)

where $\langle K(A^*) \rangle \equiv 1$ for trivial knots.

Thus our problem is reduced to the calculation of noninteger complex moments of the partition function, i.e., values of the type $\langle K^{iy}\{b_{kl}, A^*\}\rangle$. An analogous problem of evaluation of non-integer moments is well known in spinglass theory. Indeed, the averaging of the free energy of the system, \overline{F} , over a quenched random field is widely performed via the so-called *replica-trick* [28]. The idea of the method is as follows. Consider the identity $Z^n \equiv \exp(n \ln Z)$ and expand the right-hand side up to the first order in *n*. We get $Z^n = 1 + n \ln Z + O(n^2)$. Now we can write

$$F = -\ln Z = -\lim_{n \to 0} \frac{Z^n - 1}{n} \,.$$

We proceed with the calculation of the complex moments of the partition function $\langle K\{b_{kl}\}\rangle$. In other words we would like to find the averaged value $\overline{\langle K^n \rangle}$ for integer values of *n*. Then we put n = iy and compute the remaining integral in Eqn (2.52) over *y*-values. Of course, this procedure needs to be verified and it would be most desirable to compare our predictions with the data obtained in numerical simulations. However let us stress that our approach is no more curious than the replica one, and it would be extremely desirable to test the results obtained by means of computer simulations.

The outline of our calculations is as follows. We begin by rewriting the averaged Kauffman invariant using the standard representation of the replicated Potts partition function and extract the corresponding free energy $\overline{F(A)}$ in the frameworks of the infinite-range mean-field theory in two dimensions. Minimizing $\overline{F(A)}$ with respect to A we find the equilibrium value A^* . Then we compute the desired probability of trivial knot formation $\mathcal{P}_N^{(0)}(A^*)$ evaluating the remaining Gaussian integrals.

Averaging the *n*th power of the Kauffman invariant over independent values of the 'crossing field' $b_{kl} = \pm 1$ we get

$$\overline{\langle K^{n}(A) \rangle} = \int \dots \int \prod_{kl} P(b_{kl}) \, \mathrm{d}b_{kl} K^{2n} \{ b_{kl} \}$$
$$= \left[2 \cosh(2\beta) \right]^{-2n(N+1)} \sum_{\{\sigma\}} \prod_{kl} \exp\left\{ \mathrm{i}\pi \sum_{kl} \delta(\sigma_{k}^{\alpha}, \sigma_{l}^{\alpha}) + \ln \cosh\left[\beta \sum_{\alpha=1}^{n} \left(4\delta(\sigma_{k}^{\alpha}, \sigma_{l}^{\alpha}) - 1 \right) \right] \right\}, \qquad (2.53)$$

where $\beta = \ln A$. Let us break for a moment the connection between the number of spin states, q, and the interaction constant and suppose $|\beta| \leq 1$. Later on we shall verify the selfconsistency of this approximation. Now the exponent in the last expression can be expanded as a power series in β . Keeping the terms of order β^2 only, we rewrite Eqn (2.53) in the standard form of the *n*-replica Potts partition function

$$\overline{\langle K^{n}(A) \rangle} = \left[2 \cosh(2\beta) \right]^{-2n(N+1)} \exp\left[N\left(\frac{1}{2}\beta^{2}n^{2}\right) \right]$$
$$\times \sum_{\{\sigma_{1},...,\sigma_{n}\}} \exp\left\{ \frac{J^{2}}{2} \sum_{kl}^{N} \sum_{\alpha\neq\beta}^{n} \sigma_{ka}^{\alpha} \sigma_{kb}^{\beta} \sigma_{la}^{\alpha} \sigma_{lb}^{\beta} \right.$$
$$\left. + \left(\frac{J^{2}}{2}(q-2) + \bar{J}_{0} \right) \sum_{kl}^{N} \sum_{\alpha=1}^{n} \sigma_{ka}^{\alpha} \sigma_{lb}^{\beta} \right\}, (2.54)$$

where spin indexes a, b change over the interval [0, q-1], $\beta^2 \ll 1$ and

$$J^{2} = 16\beta^{2},$$

$$\bar{J}_{0} = i\pi - 4\beta^{2}n,$$

$$q = 4 + 16\beta^{2} > 4.$$
(2.55)

According to the results of Cwilich and Kirkpatrick [29] and later works (see, for instance, [30]), spin-glass ordering takes place and the usual ferromagnetic phase makes no essential contribution to the free energy under the condition

$$\frac{\bar{J}_0}{J} < \frac{q-4}{2}$$
 (2.56)

Substituting Eqn (2.55) into Eqn (2.56) it can be seen that Re [l.h.s.] < Re [r.h.s] in Eqn (2.56) for all β . Thus, we expect that the spin-glass ordering (in the infinite-range model) corresponds to the solutions

$$egin{aligned} &m_a^lpha = \left\langle q\delta(\sigma_k^lpha, a) - 1
ight
angle = 0\,, \ &Q_{ab}^{lphaeta} = \left\langle q\delta(\sigma_k^lpha, a) - 1
ight
angle \left\langle q\delta(\sigma_k^eta, b) - 1
ight
angle
eq 0\,, \end{aligned}$$

where m_a^{α} and $Q_{ab}^{\alpha\beta}$ are the ferromagnetic and spin-glass order parameters respectively. If it is so, we can keep the term in the exponent [Eqn (2.54)] corresponding to inter-replica interactions only.

We now follow the standard scheme of analysis of Potts spin glasses partition function exhaustively described in [29– 31]; the main steps of this analysis are briefly shown below. Performing the Hubbard–Stratonovich transformation to the scalar fields $Q_{iab}^{\alpha\beta}$ and implying a homogeneous isotropic solution of the form $Q_{iab}^{\alpha\beta} = Q_i^{\alpha\beta} \delta_{ab}$, we can write down the value $\overline{\langle K^n \rangle}$ Eqn (2.54) as follows [29]:

$$\overline{\langle K^n \rangle} = \exp\left\{ N \left[\ln \frac{\pi}{J^2} n(n-1)(q-1)^2 - \ln \left(2 \cosh \frac{J}{2} \right) + \frac{J^2 n^2}{32} \right] \right\}$$
$$\times \sum_{\{\sigma\}} \int \prod_i dQ_i^{\alpha\beta} \exp\left\{ - \int H\{Q_i^{\alpha\beta}\} d^2x \right\}, (2.57)$$

where

$$H\{Q^{\alpha\beta}\} = (q-1) \left[\frac{1}{4} \left(\frac{2}{J^2} - 1 \right) \sum_{\alpha \neq \beta} (Q^{\alpha\beta})^2 - \frac{1}{6} \sum_{\alpha \neq \beta \neq \gamma} Q^{\alpha\beta} Q^{\beta\gamma} Q^{\gamma\alpha} - \frac{q-2}{12} \sum_{\alpha \neq \beta} (Q^{\alpha\beta})^3 - \frac{q-2}{4} \sum_{\alpha \neq \beta \neq \gamma} (Q^{\alpha\beta})^2 Q^{\beta\gamma} Q^{\gamma\alpha} - \frac{1}{8} \sum_{\alpha \neq \beta \neq \gamma \neq \delta} Q^{\alpha\beta} Q^{\beta\gamma} Q^{\gamma\delta} Q^{\delta\alpha} - \frac{q^2 - 6q + 6}{48} \sum_{\alpha\beta} (Q^{\alpha\beta})^4 \right].$$
(2.58)

In [29, 31] it was shown that the mean-field replica symmetric solution of the mean-field Potts spin glass is unstable for $q \ge 2$ and the right ansatz of Eqs (2.57)–(2.58) corresponds to the first level of the Parisi replica breaking scheme for spin glasses. Hence, we have

$$Q^{\alpha\beta} = \begin{cases} Q, & \text{if } \alpha \text{ and } \beta \text{ belong to the} \\ & \text{same group of } m \text{ replicas}, \\ 0 & \text{otherwise.} \end{cases}$$
(2.59)

Analysis shows that for q > 4 (our case) the transition to the glassy state corresponds to m = 1 which implies the accessory condition $F_{pm} = F_{sg}$, where F_{pm} and F_{sg} are the free energies of paramagnetic and spin-glass phases respectively. The transition occurs at the point

$$1 - \frac{2}{J^2} = \frac{(q-4)^2}{3(q^2 - 18q + 42)} \,. \tag{2.60}$$

Substituting Eqn (2.55) into Eqn (2.60) we find the selfconsistent value of reverse temperature of a spin-glass transition, β_{tr} :

$$\beta_{\rm tr} \approx 0.35 \,. \tag{2.61}$$

This numerical value is consistent with the condition $\beta_{tr}^2 \ll 1$ implied above in the course of expansion of Eqn (2.54).

According to the results of the work [29] the *n*-replica free energy near the transition point has the following form

$$F \simeq \frac{1}{64} Nn(q-1)^2 Q_{\rm tr} \left(\frac{1}{\beta^2} - \frac{1}{\beta_{\rm tr}^2}\right)^2, \qquad (2.62)$$

with

$$Q_{\rm tr} = \frac{2(4-q)}{q^2 - 18q + 42} > 0 \tag{2.63}$$

the resulting expression of the spin-glass order parameter.

From Eqn (2.62) we conclude that the free energy \overline{F} reaches its minimum as a function of $A = \exp(\beta)$ just at the point $A^* = \exp(\beta_{tr})$. Using Eqs (2.62) and (2.63) we rewrite the expression for the averaged *n*-replica Kauffman invariant $\overline{\langle K^n \rangle}$ in the vicinity of β_{tr} as follows (compare to [29]):

$$\overline{\langle K^{2n} \rangle} \simeq \exp\left\{ Nn^2 \left[(3 + 16\beta^2)^2 \ln \frac{\pi}{16\beta^2} + \frac{\beta^2}{2} \right] - Nn \left[(3 + 16\beta^2)^2 \ln \frac{\pi}{16\beta^2} + \ln 2 + \frac{\beta^2}{2} - \frac{(3 + 16\beta^2)^2 (\beta^{-2} - \beta_{\rm kp}^{-2})^2 \beta_{\rm kp}^2}{(4 + 16\beta_{\rm tr}^2)^2 - 18(4 + 16\beta_{\rm tr}^2) + 42} \right] \right\}.$$
 (2.64)

Substituting Eqn (2.64) into Eqn (2.52) and bearing in mind that n = iy, we can easily evaluate the remaining Gaussian integral over *y*-values and obtain the result for $\mathcal{P}_N^{(0)}(A)$. As was mentioned above, to get the simplest estimate for the probability of trivial knot formation, we use the last inequality in the chain of equations (2.48) corresponding to the choice $A = A^* \equiv \exp(\beta_{\rm tr})$:

$$\mathcal{P}_N^{(0)}(A^*) \simeq \exp(-cN), \quad c \approx 1.$$
(2.65)

This dependence is not surprising from the point of view of statistical mechanics because the value $\eta = \mathcal{P}_N^{(0)}(A^*)$ is proportional to the free energy of the Potts system. But from the topological point of view the value η has the sense of the typical 'complexity' of the knot (see also Section 3). The fact that η grows linearly with N means that the maximum of the distribution function $P(\eta, N)$ is in the region of very 'complex' knots, i.e. knots far from trivial. This circumstance directly follows from the non-commutative nature of topological interactions.

3. Random walks on locally non-commutative groups

Recent years have been marked by the emergence of more and more problems related to the consideration of physical processes on non-commutative groups. In trying to classify such problems, we distinguish between the following categories in which the non-commutative origin of phenomena appear with perfect clarity:

1. Problems connected with the spectral properties of the Harper–Hofstadter equation [14] dealing with the electron dynamics on the lattice in a constant magnetic field. We mean primarily the consideration of groups of magnetic translations and properties of quantum planes [15, 32].

2. Problems of classical and quantum chaos on hyperbolic manifolds: spectral properties of dynamical systems and the derivation of trace formulae [33-35] as well as the construction of probability measures for random walks on modular groups [36].

3. Problems giving rise to the application of quantum group theory in physics: deformations of classical abelian objects such as harmonic oscillators [4] and standard random walks [3].

4. Problems of knot theory and statistical topology: the construction of non-abelian topological invariants [5, 23], the consideration of probabilistic behavior of the words on the simplest non-commutative groups related to topology (such as braid groups) [37], and statistical properties of 'anyonic' systems [38].

5. Classical problems of random matrix and random operator theory and localization phenomena: the determination of Lyapunov exponents for products of random non-commutative matrices [39-41], the study of the spectral properties and the calculation of the density of states of large random matrices [21, 42].

Certainly, such a division of problems into these categories is very speculative and reflects to a marked degree the author's personal point of view. However, we believe that the enumerated items reflect, at least partially, the currently growing interest in theoretical physics of the ideas of noncommutative analysis. Let us stress that we do not touch upon the pure mathematical aspects of non-commutative analysis in this paper and the problems discussed in the present work mainly concern points 4 and 5 of the list above.

In the present section we continue analyzing the statistical problems in knot theory, but our attention is paid to some more delicate matters related to investigation of correlations in knotted random paths caused by topological constraints. The methods elaborated in Section 2 allow us to discuss these questions but we find it more reasonable to take a look at the problems of knot entropy estimation in terms of conventional random matrix theory. We believe that many non-trivial properties of the knot entropy problem can be clearly explained in the context of the limit behavior of random walks over the elements of some non-commutative (hyperbolic) groups [46].

Another reason which forces us to consider the limit distributions (and conditional limit distributions) of Markov chains on *locally non-commutative discrete groups* is due to the fact that this class of problems could be regarded as the first step in a consistent harmonic analysis on multiconnected manifolds (like Teichmüller space); see also Section 4.

3.1 Brownian bridges on simple non-commutative groups and knot statistics

As said above, problems dealing with the investigation of the limit distributions of random walks on non-commutative groups are not a new in probability theory and statistical physics.

However in the context of a 'topologically-probabilistic' consideration, problems dealing with distributions of noncommutative random walks are practically out of discussion, except for very few special cases [41, 43, 49]. Particularly, in these works it has been shown that the statistics of random walks with a fixed topological state with respect to the regular array of obstacles on the plane can be obtained from the limit distribution of the so-called 'Brownian bridges' (see the definition below) on the universal covering — the graph with the topology of a Cayley tree. The analytic construction of a non-abelian topological invariant for the trajectories on the double punctured plane and statistics of a simple non-trivial random braid B_3 was briefly discussed in [44].

Below we calculate the conditional limit distributions of the Brownian bridges on the braid group B_3 and derive the limit distribution of powers of Alexander polynomial of knots generated by random B_3 -braids. We also discuss the limit distribution of random walks on locally free groups and express some conjectures about the statistics of random walks on the group B_n . A more extended discussion of the results concerning the statistics of Markov chains on braid and locally free groups can be found in [52-54].

3.1.1 Basic definitions and statistical model. The braid group B_n of *n* strings has n - 1 generators $\{\sigma_1, \sigma_2, \ldots, \sigma_{n-1}\}$ with the following relations:

1.

$$\sigma_{i}\sigma_{n+1}\sigma_{i} = \sigma_{n+1}\sigma_{i}\sigma_{n+1} \quad (1 \le n < n-1),$$

$$\sigma_{i}\sigma_{j} = \sigma_{j}\sigma_{i} \quad (|i-j| \ge 2),$$

$$\sigma_{i}\sigma_{i}^{-1} = \sigma_{i}^{-1}\sigma_{i} = e. \quad (3.1)$$

Any arbitrary word written in terms of 'letters' — generators from the set $\{\sigma_1, \ldots, \sigma_{n-1}, \sigma_1^{-1}, \ldots, \sigma_{n-1}^{-1}\}$ — gives a particular *braid*. The geometrical interpretation of braid generators is shown below:



The *length* of the braid is the total number of letters used, while the *minimal irreducible length* hereafter referred to as the 'primitive word' is the shortest non-contractible length of a

particular braid which remains after applying all possible group relations Eqn (3.1). Diagrammatically the braid can be represented as a set of crossed strings going from the top to the bottom appeared after subsequent gluing the braid generators.

The closed braid appears after gluing the 'upper' and the 'lower' free ends of the braid on the cylinder.

Any braid corresponds to some knot or link. So, it is feasible principal possibility to use the braid group representation for the construction of topological invariants of knots and links. However the correspondence between braids and knots is not mutually single valued and each knot or link can be represented by an infinite series of different braids. This fact should be taken into account in the course of knot invariant construction.

Take a knot diagram K in a general position on the plane. Let f[K] be the topological invariant of the knot K. One of the ways to construct the knot invariant using the braid group representation is as follows.

1. Represent the knot by some braid $b \in B_n$. Take the function f

$$f: B_n \to C$$

Require f to take the same value for all braids b representing the given knot K. That condition is established in the well-known Markov–Birman theorem (see, for instance, [55]):

The function $f_K{b}$ defined on the braid $b \in B_n$ is the topological invariant of a knot or link if and only if it satisfies the following 'Markov condition'

$$f_{K}\{b' \ b''\} = f_{K}\{b'' \ b'\},$$

$$f_{K}\{b' \ \sigma_{n}\} = f_{K}\{\sigma_{n} \ b'\} = f_{K}\{b'\}, \qquad b', b'' \in B_{n}, \qquad (3.2)$$

where b' and b'' are two subsequent sub-words in the braid (see Fig. 7).

2. Now the invariant $f_K{b}$ can be constructed using the linear functional φ{b} defined on the braid group and called *a Markov trace*. It has the following properties

$$\begin{aligned} \varphi\{b' b''\} &= \varphi\{b'' b'\},\\ \varphi\{b' \sigma_n\} &= \tau \varphi\{b'\},\\ \varphi\{b' \sigma_n^{-1}\} &= \bar{\tau} \varphi\{b'\}, \end{aligned}$$
(3.3)



Figure 7. Geometric representation of Eqn (3.2).

where

$$\tau = \varphi\{\sigma_i\}, \quad \bar{\tau} = \varphi\{\sigma_i^{-1}\}, \quad i \in [1, n-1].$$
 (3.4)

The invariant $f_K{b}$ of the knot K is connected with the linear functional φ{b} defined on the braid b as follows

$$f_{K}\{b\} = (\tau\bar{\tau})^{-(n-1)/2} \left(\frac{\bar{\tau}}{\tau}\right)^{[\#(+)-\#(-)]/2} \varphi\{b\}, \qquad (3.5)$$

where #(+) and #(-) are the numbers of 'positive' and 'negative' crossings in the given braid correspondingly.

The Alexander algebraic polynomials are the first wellknown invariants of such a type. At the beginning of the 1980s Jones discovered the new knot invariants. He used the braid representation 'passed through' the Hecke algebra relations, where the Hecke algebra, $H_n(t)$, for B_n satisfies both braid group relations Eqn (3.1) and an additional "reduction" relation (see the works [55, 56])

$$\sigma_i^2 = (1-t)\sigma_i + t. \tag{3.6}$$

Now the trace $\varphi\{b\} = \varphi(t)\{b\}$ can be said to take the value in the ring of polynomials of one complex variable *t*. Consider the functional $\varphi(t)$ over the braid $\{b' \sigma_i b''\}$. Eqn (3.6) allows us to get the recursion (skein) relations for $\varphi(t)$ and for the invariant $f_K(t)$ (see for details [58]):

$$\varphi(t)\{b'\sigma_i b''\} = (1-t)\varphi(t)\{b'b''\} + t\varphi(t)\{b'\sigma_i^{-1}b''\}, \quad (3.7)$$

and

$$f_{K}^{+}(t) - t\left(\frac{\bar{\tau}}{\tau}\right)f_{K}^{-}(t) = (1-t)\left(\frac{\bar{\tau}}{\tau}\right)^{1/2}f_{K}^{0}(t), \qquad (3.8)$$

where $f_K^+ \equiv f\{b' \sigma_i b''\}$, $f_K^- \equiv f\{b' \sigma_i^{-1} b''\}$, $f_K^0 \equiv f\{b' b''\}$ and the fraction $\bar{\tau}/\tau$ depends on the representation used.

3. The tensor representations of the braid generators can be written as follows

$$\sigma_{i}(u) = \lim_{u \to \infty} \sum_{klmn} R_{ln}^{km}(u) I^{(1)} \otimes$$
$$\dots I^{(i-1)} \otimes E_{nk}^{i} \otimes E_{ml}^{i+1} \otimes I^{(i+1)} \otimes \dots I^{(n)}, \qquad (3.9)$$

where $I^{(i)}$ is the identity matrix acting in the position *i*; E_{nk} is a matrix with $(E_{nk})_{pq} = \delta_{np}\delta_{kq}$ and R_{ln}^{km} is the matrix satisfying the Yang–Baxter equation

$$\sum_{abc} R_{cr}^{bq}(v) R_{kc}^{ap}(u+v) R_{jb}^{ia}(u) = \sum_{abc} R_{bq}^{ap}(u) R_{cr}^{ia}(u+v) R_{ka}^{jb}(v) \,.$$
(3.10)

In that scheme both known polynomial invariants (Jones and Alexander) ought to be considered. In particular, it has been discovered in [57, 58] that the solutions of Eqn (3.10) associated with the groups $SU_q(2)$ and GL(1,1) are linked to Jones and Alexander invariants correspondingly. To be more specific:

(a) $\bar{\tau}/\tau = t^2$ for Jones invariants, $f_K(t) \equiv V(t)$. The corresponding skein relations are

$$t^{-1}V^{+}(t) - tV^{-}(t) = (t^{-1/2} - t^{1/2})V^{0}(t); \qquad (3.11)$$

(b) $\bar{\tau}/\tau = t^{-1}$ for Alexander invariants, $f_K(t) \equiv \nabla(t)$. The corresponding skein relations† are

$$\nabla^{+}(t) - \nabla^{-}(t) = (t^{-1/2} - t^{1/2})\nabla^{0}(t).$$
(3.12)

To complete this brief review of the construction of polynomial invariants from the representation of the braid groups it should be mentioned that the Alexander invariants also allow another useful description [59]. Write the generators of the braid group in the so-called Magnus representation

$$\sigma_{j} \equiv \hat{\sigma}_{j} = \begin{pmatrix} 1 & 0 & \cdots & & \\ 0 & \ddots & & & \\ \vdots & & A & & \vdots \\ & & & \ddots & 0 \\ & & & \ddots & 0 & 1 \end{pmatrix} \leftarrow j \text{th row},$$

$$A = \begin{pmatrix} 1 & 0 & 0 \\ t & -t & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$
(3.13)

Now the Alexander polynomial of the knot represented by the closed braid $W\{K\} = \prod_{j=1}^{N} \sigma_{\alpha_j}$ of length *N* can be written as follows

$$(1 + t + t^{2} + \ldots + t^{n-1})\nabla(t)\{K\} = \det\left[\prod_{j=1}^{N} \hat{\sigma}_{\alpha_{j}} - \mathbf{e}\right],$$
(3.14)

where the index *j* runs 'along the braid', i.e. labels the number of generators used, while the index $\alpha = \{1, ..., n-1, n, ..., 2n-2\}$ marks the set of braid generators (letters) ordered as follows $\{\sigma_1, ..., \sigma_{n-1}, \sigma_1^{-1}, ..., \sigma_{n-1}^{-1}\}$. In our further investigations we repeatedly address this representation.

We are interested in the limit behavior of the knot or link invariants when the length of the corresponding braid tends to infinity, i.e. when the braid 'grows'. In this case we can rigorously define some topological characteristics, simpler than the algebraic invariant, which we call the *knot complexity*.

Call the knot complexity, η , the power of some algebraic invariant, $f_K(t)$ (Alexander, Jones, HOMFLY) (see also [26])

$$\eta = \lim_{|t| \to \infty} \frac{\ln f_K(t)}{\ln t} \,. \tag{3.15}$$

Remark. By definition, the 'knot complexity' takes one and the same value for rather broad class of topologically different knots corresponding to algebraic invariants of one and the same power, being from this point of view weaker topological characteristics than a complete algebraic polynomial. Let us summarize the advantages of knot complexity.

(i) One and the same value of η characterizes a narrow class of 'topologically similar' knots which is, however, much broader than the class represented by the polynomial invariant $f_K(t)$. This enables us to introduce smoothed measures and distribution functions for η .

[†] Let us stress that the standard skein relations for Alexander polynomials can be obtained from Eqn (3.12) replacing $T^{1/2}$ by $-t^{1/2}$.

(ii) The knot complexity η correctly describes (at least from the physical point of view) the limit cases: $\eta = 0$ corresponds to 'weakly entangled' trajectories whereas $\eta \sim N$ matches the system of 'strongly entangled' paths.

(iii) The knot complexity keeps all the non-abelian properties of the polynomial invariants.

(iv) The polynomial invariant can give exhaustive information about the knot topology. However when dealing with the statistics of randomly generated knots, we frequently look for rougher characteristics of 'topologically different' knots. A similar problem arises in statistical mechanics when passing from the microcanonical ensemble to the Gibbs one: we lose some information about the details of a particular realization of the system but acquire smoothness of the measure and are able to apply standard thermodynamic methods to the system in question.

The main purpose of the present section is the estimation of the limit probability distribution of η for the knots obtained by randomly generated closed B_n -braids of the length N. It should be emphasized that we essentially simplify the general problem 'of knot entropy'. Namely, we introduce an additional requirement that the knot should be represented by a braid from the group B_n without fail.

We begin the investigation of the probability properties of algebraic knot invariants by analyzing the statistics of random loops ('Brownian bridges') on simple non-commutative groups. Most generally the problem can be formulated as follows. Take a discrete group \mathcal{G}_n with a fixed finite number of generators $\{g_1, \ldots, g_{n-1}\}$. Let v be the uniform distribution on the set $\{g_1, \ldots, g_{n-1}, g_1^{-1}, \ldots, g_{n-1}^{-1}\}$. For convenience we suppose $h_j = g_i$ for j = i and $h_j = g_i^{-1}$ for j = i + n - 1; $v(h_j) = 1/(2n-2)$ for any j. We construct the (right-hand) side random walk (the random word) on \mathcal{G}_n with a transition measure v, i.e. the Markov chain $\{\xi_n\}$, $\xi_0 = e \in \mathcal{G}_n$ and $\operatorname{Prob}(\xi_j = u|\xi_{j-1} = v) = v(v^{-1}u) = 1/(2n-2)$. This means that with probability 1/(2n-2) we add the element h_{x_N} to the given word $h_{N-1} = h_{\alpha_1}h_{\alpha_2} \dots h_{\alpha_{N-1}}$ from the right-hand side[†].

The random word W formed by N letters taken independently with a uniform probability distribution v = 1/(2n-2)from the set $\{g_1, \ldots, g_{n-1}, g_{n-1}^{-1}\}$ is called the Brownian bridge (BB) of length N on the group \mathcal{G}_n if the shortest (primitive) word of W is identical to unity.

Two questions require most of our attention:

(1) What is the probability distribution P(N) of the Brownian bridge on the group \mathcal{G}_n ?

(2) What is the conditional probability distribution P(k, m|N) of the fact that the sub-word W' consisting of the first *m* letters of the *N*-letter word *W* has the primitive path *k* under the condition that the whole word *W* is the Brownian bridge on the group \mathcal{G}_n ? (Hereafter P(k, m|N) is referred to as the conditional distribution for BB.)

It has been shown in paper [41] that for the free group the corresponding problem can be mapped on the investigation of random walks on a simply connected tree. Below we briefly show some results concerning the limit behavior of the conditional probability distribution of **BB** on the Cayley tree. In the case of braids the more complicated group structure does not allow us to apply the same simple geometrical image directly. Nevertheless the problem of the limit distribution for random walks on B_n can be reduced to the consideration of the random walk on some graph $C(\Gamma)$. In

[†] We can construct the left-hand side Markov chain analogously.

case of the group B_3 we are able to construct this graph, whereas for the group B_n ($n \ge 4$) we give upper estimate for the limit distribution of the random walks considering the statistics of Markov chains on so-called local groups.

3.1.2 Random process on *PSL*(2, \mathbb{Z}), *B*₃ and the limit distribution of powers of the Alexander invariant. We begin with computing the distribution function for the conditional random process on the simplest non-trivial braid group *B*₃. The group *B*₃ can be represented by 2×2 matrices. To be specific, the braid generators σ_1 and σ_2 in the Magnus representation [59] look as follows:

$$\sigma_1 = \begin{pmatrix} -t & 1\\ 0 & 1 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 1 & 0\\ t & -t \end{pmatrix}, \quad (3.16)$$

where t is 'the spectral parameter'. It is well known that for t = -1 the matrices σ_1 and σ_2 generate the group $PSL(2,\mathbb{Z})$ in such a way that the whole group B_3 is its central extension with the center

$$(\sigma_1 \sigma_2 \sigma_1)^{4\lambda} = (\sigma_2 \sigma_1 \sigma_2)^{4\lambda} = (\sigma_1 \sigma_2)^{6\lambda}$$
$$= (\sigma_2 \sigma_1)^{6\lambda} = \begin{pmatrix} t^{6\lambda} & 0\\ 0 & t^{6\lambda} \end{pmatrix}.$$
(3.17)

We first restrict ourselves to the examination of the group $PSL(2,\mathbb{Z})$, for which we define $\tilde{\sigma}_1 = \sigma_1$ and $\tilde{\sigma}_2 = \sigma_2$ (at t = -1). The canonical representation of $PSL(2,\mathbb{Z})$ is given by the unimodular matrices S, T:

$$S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad T = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}.$$
 (3.18)

The braiding relation $\tilde{\sigma}_1 \tilde{\sigma}_2 \tilde{\sigma}_1 = \tilde{\sigma}_2 \tilde{\sigma}_1 \tilde{\sigma}_2$ in the $\{S, T\}$ -representation takes the form

$$S^2 T S^{-2} T^{-1} = 1. (3.19)$$

In addition we have

$$S^4 = (ST)^3 = 1. (3.20)$$

This representation is well known and signifies the fact that in terms of $\{S, T\}$ -generators the group $PSL(2, \mathbb{Z})$ is a free product $Z^2 \otimes Z^3$ of two cyclic groups of 2nd and 3rd orders correspondingly.

The connection of $\{S, T\}$ and $\{\tilde{\sigma}_1, \tilde{\sigma}_2\}$ is as follows

$$\tilde{\sigma}_1 = T \qquad (T = \tilde{\sigma}_1),$$

$$\tilde{\sigma}_2 = T^{-1}ST^{-1} \qquad (S = \tilde{\sigma}_1\tilde{\sigma}_2\tilde{\sigma}_1). \qquad (3.21)$$

The modular group $PSL(2, \mathbb{Z})$ is a discrete subgroup of the group $PSL(2, \mathbb{R})$. The fundamental domain of $PSL(2, \mathbb{Z})$ has the form of a circular triangle ABC with angles $\{0, \pi/3, \pi/3\}$ situated in the upper half-plane Im $\zeta > 0$ of the complex plane $\zeta = \zeta + i\eta$ (see Fig. 8 for details). According to the definition of the fundamental domain, at least one element of each orbit of $PSL(2,\mathbb{Z})$ lies inside the ABCdomain and two elements lie on the same orbit if and only if they belong to the boundary of the ABC-domain. The group $PSL(2,\mathbb{Z})$ is completely defined by its basic substitutions under the action of generators S and T:

$$S: \quad \zeta \to -\frac{1}{\zeta} ,$$

$$T: \quad \zeta \to \zeta + 1 .$$
(3.22)



Figure 8. Riemann surface for the modular group. The graph $C(\Gamma)$ representing the topological structure of $PSL(2, \mathbb{Z})$ is shown by the dashed line.

Let us choose an arbitrary element ζ_0 from the fundamental domain and construct a corresponding orbit. In other words, we raise a graph, $C(\Gamma)$, which connects the neighboring images of the initial element ζ_0 obtained under successive action of the generators from the set $\{S, T, S^{-1}, T^{-1}\}$ to the element ζ_0 . The corresponding graph is shown in the Fig. 8 by the broken line and its topological structure is clearly reproduced in Fig. 9. It can be seen that although the graph $C(\Gamma)$ does not correspond to the free group and has local cycles, its 'backbone', $C(\gamma)$, has a Cayley tree structure but with a reduced number of branches compared to the free group $C(\Gamma_2)$.



Figure 9. Graph $C(\Gamma)$ and its backbone graph $C(\gamma)$ (see the explanations in the text).

Turn to the problem of limit distribution of a random walk on the graph $C(\Gamma)$. The walk is determined as follows:

1. Take an initial point ('root') of the random walk on the graph $C(\Gamma)$. Consider the discrete random jumps over the neighboring vertices of the graph with the transition probabilities induced by the uniform distribution v on the set of generators $\{\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_1^{-1}, \tilde{\sigma}_2^{-1}\}$. These probabilities are [see Eqn (3.21)]

$$\operatorname{Prob}(\xi_n = T\zeta_0 \mid \xi_{n-1} = \zeta_0) = \frac{1}{4},$$

$$\operatorname{Prob}(\xi_n = (T^{-1}ST^{-1})\zeta_0 \mid \xi_{n-1} = \zeta_0) = \frac{1}{4},$$

$$\operatorname{Prob}(\xi_n = T^{-1}\zeta_0 \mid \xi_{n-1} = \zeta_0) = \frac{1}{4},$$

$$\operatorname{Prob}(\xi_n = (TS^{-1}T)\zeta_0 \mid \xi_{n-1} = \zeta_0) = \frac{1}{4}.$$
 (3.23)

The following facts should be taken into account: the elements $S\zeta_0$ and $S^{-1}\zeta_0$ represent one and the same point, i.e. coincide [as follows from Eqn (3.22)]; the process is Markovian in terms of the alphabet $\{\tilde{\sigma}_1, \ldots, \tilde{\sigma}_2^{-1}\}$ only; the total transition probability is conserved.

2. Define the shortest distance, k, along the graph between the root and terminal points of the random walk. According to its construction, this distance coincides with the length $|W_{\{S,T\}}|$ of the minimal irreducible word $W_{\{S,T\}}$ written in the alphabet $\{S, T, S^{-1}, T^{-1}\}$. The link of the distance, k, with the length $|W_{\{\tilde{\sigma}_1, \tilde{\sigma}_2\}}|$ of the minimal irreducible word $W_{\{\tilde{\sigma}_1, \tilde{\sigma}_2\}}$ written in terms of the alphabet $\{\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_1^{-1}, \tilde{\sigma}_2^{-1}\}$ is as follows: (a) $|W_{\{\tilde{\sigma}_1, \tilde{\sigma}_2\}}| = 0$ if and only if k = 0; (b) for $k \ge 1$ the length $|W_{\{\tilde{\sigma}_1, \tilde{\sigma}_2\}}|$ is asymptotic to: $|W_{\{\tilde{\sigma}_1, \tilde{\sigma}_2\}}| = k + o(k)$.

We define the 'coordinates' of the graph vertices in the following way (see Fig. 9):

(a) We apply the arrows to the bonds of the graph Γ corresponding to *T*-generators. A step with (against) the arrow means the application of $T(T^{-1})$.

(b) We characterize each elementary cell of the graph Γ by its distance, μ , along the graph backbone γ from the root cell.

(c) We introduce the variable $\alpha = \{1, 2\}$ which numerates the vertices in each cell. We assume that the walker stays in the cell *M* located at a distance μ along the backbone from the origin if and only if it visits one of two in-going vertices of *M*. Such labelling gives a unique coding of the whole graph $C(\Gamma)$.

Define the probability $U_{\alpha}(\mu, N)$ that the *N*-step random walk along the graph $C(\Gamma)$ starting from the root point ends in an α -vertex of the cell at the distance of μ steps along the backbone. It should be emphasized that $U_{\alpha}(\mu, N)$ is the probability of staying in *any* of $\mathcal{N}_{\gamma}(\mu) = 3 \times 2^{\mu-1}$ cells situated at the distance μ along the backbone.

It is possible to write the closed system of recursion relations for the functions $U_{\alpha}(\mu, N)$. However, here we attend to rougher characteristics of the random walk. Namely, we calculate the 'integral' probability distribution of the fact that the trajectory of the random walk starting from an arbitrary vertex of the root cell O ends in an arbitrary vertex point of the cell M situated at a distance μ along the graph backbone. This probability, $U(\mu, N)$, reads

$$U(\mu, N) = \frac{1}{2} \sum_{\alpha = \{1, 2\}} U_{\alpha}(\mu, N) .$$

The relation between the distances k, along the graph Γ , and μ along its backbone γ is such: $k = \mu + o(\mu)$ for $\mu \ge 1$, what ultimately follows from the constructions of the graphs $C(\Gamma)$ and $C(\gamma)$.

Suppose the walker stays in the vertex α of the cell *M* located at a distance $\mu > 1$ from the origin along the graph backbone $C(\gamma)$. The change in μ after making one arbitrary step from the set $\{\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_1^{-1}, \tilde{\sigma}_2^{-1}\}$ is summarized in the following table:

α :	= 1	lpha=2				
$\begin{split} \tilde{\sigma}_1 &= T \\ \tilde{\sigma}_2 &= T^{-1}ST - 1 \\ \tilde{\sigma}_1^{-1} &= T^{-1} \\ \tilde{\sigma}_2^{-1} &= TS^{-1}T \end{split}$	$\begin{split} \mu &\to \mu + 1 \\ \mu &\to \mu \\ \mu &\to \mu - 1 \\ \mu &\to \mu + 1 \end{split}$	$egin{array}{lll} & ilde{\sigma}_1 = T \ & ilde{\sigma}_2 = T^{-1}ST^{-1} \ & ilde{\sigma}_1^{-1} = T^{-1} \ & ilde{\sigma}_2^{-1} = TS^{-1}T \end{array}$	$\begin{array}{l} \mu \rightarrow \mu - 1 \\ \mu \rightarrow \mu + 1 \\ \mu \rightarrow \mu + 1 \\ \mu \rightarrow \mu \end{array}$			

It is clear that for any value of α , two steps increase the length of the backbone, μ , one step decreases it and one step leaves μ unchanged.

Let us introduce the effective probabilities: p_1 — to jump to some specific cell among 3 neighboring ones of the graph $C(\Gamma)$ and p_2 — to stay in the given cell. Because of the symmetry of the graph, the conservation law has to be written as $3p_1 + p_2 = 1$. By definition we have: $p_1 = v = 1/4$. Thus we can write the following set of recursion relations for the integral probability $U(\mu, N)$

$$U(\mu, N+1) = \frac{1}{4}U(\mu+1, N) + \frac{1}{4}U(\mu, N) + \frac{1}{2}U(\mu-1, N)$$
$$(\mu \ge 2),$$
$$U(\mu, N+1) = \frac{1}{4}U(\mu+1, N) + \frac{1}{2}U(\mu, N) \quad (\mu = 1),$$
$$U(\mu, N = 0) = \delta_{\mu, 1}.$$
(3.24)

The solution of Eqn (3.24) gives the limit distribution for the random walk on the group $PSL(2, \mathbb{Z})$.

The probability distribution U(k, N) of the fact that the randomly generated N-letter word $W_{\{\tilde{\sigma}_1, \tilde{\sigma}_2\}}$ with the uniform distribution v = 1/4 over the generators $\{\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_1^{-1}, \tilde{\sigma}_2^{-1}\}$ can be contracted to the minimal irreducible word of length k, has the following limit behavior

$$U(k,N) \simeq \frac{h}{\sqrt{\pi}(4-h)} \left(\frac{h}{4(h-2)}\right)^{N} \\ \times \begin{cases} \frac{1}{N^{3/2}}, & k = 0, \\ \frac{k}{N^{3/2}} 2^{k/2} \exp\left(-\frac{k^{2}h}{4N}\right), & 1 \ll k \end{cases}$$
(3.25)

where $h = 2 + \sqrt{2}/2$.

Corollary. The probability distribution U(k, m|N) of the fact that in a randomly generated N-letter trivial word in the alphabet $\{\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_1^{-1}, \tilde{\sigma}_2^{-1}\}$ the sub-word of the first *m* letters has a minimal irreducible length k reads

$$U(k,m|N) = \frac{h}{\sqrt{\pi}(4-h)} \frac{k^2}{\left[m(N-m)\right]^{3/2}} \\ \times \exp\left\{\frac{k^2h}{4}\left(\frac{1}{m} + \frac{1}{N-m}\right)\right\}.$$
 (3.26)

Actually, the conditional probability distribution $U(\mu, m|N)$ that the random walk on the backbone graph, $C(\gamma)$, starting in the origin, after the first m (m/N = const) steps visits some graph vertex situated at a distance μ and after N steps returns to the origin, is determined as follows

$$U(\mu, m|N) = \frac{U(\mu, m)U(\mu, N - m)}{U(\mu = 0, N)\mathcal{N}_{\gamma}(\mu)}, \qquad (3.27)$$

where $\mathcal{N}_{\gamma} = 3 \times 2^{\mu-1}$ and $U(\mu, N)$ is given by (3.25).

The problem considered above helps us in calculating the conditional distribution function for the powers of Alexander polynomial invariants of knots produced by randomly generated closed braids from the group B_3 .

The closure of an arbitrary braid $b \in B_3$ of the total length N gives the knot (link) K. Split the braid b into two parts b'and b" with corresponding lengths m and N - m and make the 'phantom closure' of the sub-braids b' and b'' as shown in Fig. 10. The phantomly closed sub-braids b' and b'' correspond to the set of phantomly closed parts ('sub-knots') of the knot (link) K. The next question is what is the conditional probability of finding these sub-knots in the state characterized by the complexity η when the knot (link) K as a whole is characterized by the complexity $\eta = 0$ (i.e. the topological state of K 'is close to trivial')?



Figure 10. Construction of a Brownian bridge for knots represented by B₃braids.

We introduce normalized generators of the group B_3

$$||\sigma_j^{\pm 1}|| = (\det \sigma_j^{\pm 1})^{-1} \sigma_j^{\pm 1}.$$

to neglect the insignificant commutative factor dealing with the norm of matrices σ_1 and σ_2 . Now we can rewrite the power of Alexander invariant [Eqn (3.14)] in the form

$$\eta = |\#(+) - \#(-)| + \overline{\eta}, \qquad (3.28)$$

where #(+) and #(-) are the numbers of generators σ_{α_i} or σ_{α}^{-1} in a given braid and $\overline{\eta}$ is the power of the normalized matrix product $\prod_{j=1}^{N} ||\sigma_{\alpha_j}||$. The condition of the Brownian bridge implies $\eta = 0$ (i.e. #(+) - #(-) = 0 and $\overline{\eta} = 0$). Write

$$|\sigma_1|| = T(t), \qquad ||\sigma_2|| = T^{-1}(t)S(t)T^{-1}(t), \qquad (3.29)$$

where T(t) and S(t) are the generators of the 't-deformed' group $PSL_t(2, \mathbb{Z})$

$$T(t) = \begin{pmatrix} \sqrt{-t} & 0\\ 0 & \frac{1}{\sqrt{-t}} \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{-t}}\\ 0 & 1 \end{pmatrix},$$
$$S(t) = \begin{pmatrix} \frac{1}{\sqrt{-t}} & 0\\ 0 & \sqrt{-t} \end{pmatrix} \begin{pmatrix} 0 & 1\\ -1 & 0 \end{pmatrix}.$$
(3.30)

The group $PSL_t(2, \mathbb{Z})$ preserves the relations of the group $PSL(2,\mathbb{Z})$ unchanged, i.e., $[T(t)S(t)]^3 = S^4(t) =$ $T(t)S^{2}(t)T^{-1}(t)S^{-2}(t) = 1$ [compare to Eqn (3.19)]. Hence, if we construct the graph $C(\Gamma_t)$ for the group $PSL_t(2,\mathbb{Z})$ connecting the neighboring images of an arbitrary element from the fundamental domain, we ultimately come to the conclusion that the graphs $C(\Gamma_t)$ and $C(\Gamma)$ (see Fig. 9) are topologically equivalent. This is the direct consequence of the fact that group B_3 is the central extension of $PSL(2,\mathbb{Z})$. It should be emphasized that the metric properties of the graphs $C(\Gamma_t)$ and $C(\Gamma)$ differ because of different embeddings of groups $PSL_t(2, \mathbb{Z})$ and $PSL(2, \mathbb{Z})$ into the complex plane.

Thus, the matrix product $\prod_{j=1}^{N} ||\sigma_{\alpha_j}||$ for the uniform distribution of braid generators is in one-to-one correspondence with the *N*-step random walk along the graph $C(\Gamma)$. Its power coincides with the respective geodesic length along the backbone graph $C(\gamma)$. Thus we conclude that limit distribution of random walks on the group B_3 in terms of normalized generators (3.29) is given by Eqn (3.25) where *k* should be regarded as the power of the product $\prod_{\alpha=1}^{N} ||\sigma_{\alpha_j}||$. Hence we come to the following statement.

Take a set of knots obtained by closure of B_3 -braids of length N with a uniform distribution over the generators. The conditional probability distribution $U(\bar{\eta}, m|N)$ for the normalized complexity $\bar{\eta}$ of the Alexander polynomial invariant [see (3.28)] has Gaussian behavior and is given by Eqn (3.26) where $k = \bar{\eta}$.

3.2 Random walks on locally free groups

We aim at getting the asymptote of the conditional limit distributions of BB on the braid group B_n . For the case n > 3 it presents a problem which is yet unsolved. However we can estimate the limit probability distributions of BB on B_n considering the limit distributions of random walks on the so-called 'local groups' [44, 48, 52–54].

The group $\mathcal{LF}_{n+1}(d)$ we call locally free if the generators, $\{f_1, \ldots, f_n\}$ obey the following commutation relations:

(a) Each pair (f_j, f_k) generates a free subgroup of the group \mathcal{F}_n if |j - k| < d;

(b) $f_j f_k = f_k f_j$ for $|j - k| \ge d$.

(Below we restrict ourselves to the case d = 2 where $\mathcal{LF}_{n+1}(2) \equiv \mathcal{LF}_{n+1}$).

The limit probability distribution for an N-step random walk $(N \ge 1)$ on the group \mathcal{F}_{n+1} to have the minimal irreducible length μ is

$$\mathcal{P}(\mu, N) \simeq \frac{\text{const}}{N^{3/2}} \exp\left(-\frac{N}{6}\right) \mu \sinh\mu \exp\left(-\frac{3\mu^2}{2N}\right) \ (n=3)$$
$$\mathcal{P}(\mu, N) \simeq \frac{1}{2\sqrt{14\pi N}} \exp\left\{-\frac{8}{7N}\left(\mu - \frac{3}{4}N\right)^2\right\} \ (n \ge 1) \ . \tag{3.31}$$

We propose two independent approaches valid in two different cases: (1) for n = 3 and (2) for $n \ge 1$.

(1) The following geometrical image seems useful. Establish a one-to-one correspondence between a random walk in some *n*-dimensional Hilbert space $\mathcal{LH}^n(x_1, \ldots, x_n)$ and a random walk on the group \mathcal{LF}_{n+1} , written in terms of generators $\{f_1, \ldots, f_n^{-1}\}$. To be more specific, suppose that when a generator, say, f_j , (or f_j^{-1}) is added to the given word in \mathcal{LF}_n , the walker makes one unit step towards (away from for f_j^{-1}) the axis $[0, x_j]$ in the space $\mathcal{LH}^n(x_1, \ldots, x_n)$.

Now the relations (a), (b) of the definition of the locally free group could be reformulated in terms of metric properties of the space \mathcal{LF}_n . Actually, relation (b) indicates that successive steps along the axes $[0, x_j]$ and $[0, x_k]$ ($|j - k| \ge 2$) commute, hence the section (x_j, x_k) of the space \mathcal{LH}_n is flat and has the Euclidean metric $dx_j^2 + dx_k^2$. The situation with the random trajectories in the sections $(x_j, x_{j\pm 1})$ of the Hilbert space \mathcal{LH}_n appears to be completely different. Here the steps of the walk obey the free group relations (a) and the walk itself is mapped onto the walk on the Cayley tree. It is well known that Cayley tree can be uniformly embedded (without gaps and self-intersections) into a 3-pseudosphere which gives a representation of the non-Euclidean plane with constant negative curvature. Thus, sections (x_j, x_{j+1}) have the metric of the Lobachevskiĭ plane which can be written in the form $(dx_i^2 + dx_{i\pm 1}^2)/x_i^2$.

For the group \mathcal{LF}_4 these arguments result in the following metric of an appropriate space $\mathcal{LH}^{(3)}$

$$ds^{2} = \frac{dx_{1}^{2} + dx_{2}^{2} + dx_{3}^{2}}{x_{2}^{2}}.$$
(3.32)

Actually, the space section (x_1, x_3) is flat whereas the space sections (x_1, x_2) and (x_2, x_3) have the Lobachevskiĭ plane metric. The non-Euclidean (hyperbolic) distance between two points M' and M'' in the space \mathcal{H}^3 is defined as follows

$$\cosh \mu(M'M'') = 1 + \frac{1}{x_2(M')x_2(M'')} \\ \times \sum_{i=1}^{3} \left[x_i(M') - x_i(M'') \right]^2, \quad (3.33)$$

where $\{x_1, x_2, x_3\}$ are the Euclidean coordinates in the 3D-halfspace $x_2 > 0$ and μ is regarded as a geodesic on a 4-pseudosphere (Lobachevskiĭ space).

Some well known results concerning the limit behavior of random walks in spaces of constant negative curvature are reviewed in the next section where solutions of the diffusion equations in the Lobachevskiĭ plane and space are given by Eqn (3.49) and Eqn (3.51) correspondingly. Thus we can conclude that the distribution function for a random walk in Lobachevskiĭ space $\mathcal{P}_s(\mu, N)$ defined by Eqs (3.51)–(3.54) also gives the probability for the *N*-letter random word (written in terms of uniformly distributed generators on \mathcal{F}_4) to have the primitive word of length μ [see Eqn (3.31)].

(2) For the group \mathcal{LF}_{n+1} $(n \ge 1)$ we extract the limit behavior of the distribution function exactly evaluating the volume of the maximal non-commutative subgroup of \mathcal{LF}_{n+1} .

Let $V_n(\mu)$ be the number of all non-equivalent primitive words of length μ on the group \mathcal{LF}_{n+1} . When $\mu \ge 1$, $V_n(\mu)$ has the following asymptote:

$$V_n(\mu) = \text{const} \left[1 + 2\left(3 - \frac{4\pi^2}{n^2}\right) \right]^{\mu} \simeq 7^{\mu} \quad (n \ge 1) \,. \quad (3.34)$$

To get Eqn (3.34) we write each primitive word W_p of length μ in the group \mathcal{LF}_{n+1} in the so-called *normal order* (all f_{α_i} are different) similar to the so-called 'symbolic dynamics' used in the consideration of chaotic systems

$$W_p = (f_{\alpha_1})^{m_1} (f_{\alpha_2})^{m_2} \dots (f_{\alpha_s})^{m_s}, \qquad (3.35)$$

where $\sum_{i=1}^{s} |m_i| = \mu$ $(m_i \neq 0 \forall i; 1 \leq s \leq \mu)$ and the sequence of generators f_{α_i} in Eqn (3.35) for all f_{α_i} satisfies the following local rules:

(i) If $f_{\alpha_i} = f_1$, then $f_{\alpha_{i+1}} \in \{f_2, f_3, \dots, f_{n-1}\}$;

(ii) If $f_{\alpha_i} = f_k$ (1 < k \leq n - 1), then $f_{\alpha_{i+1}} \in \{f_{k-1}, f_{k+1}, \dots, f_{n-1}\}$;

(iii) If $f_{\alpha_i} = f_n$, then $f_{\alpha_{i+1}} = f_{n-1}$.

These local rules prescribe the enumeration of all distinct primitive words. If the sequence of generators in the primitive word W_p does not satisfy the rules (i) – (iii), we commute the generators in the word W_p until the normal order is restored. Hence, the normal order representation provides us with a unique coding of all non-equivalent primitive words in the group \mathcal{LF}_{n+1} .

The calculation of the number of distinct primitive words, $V_n(\mu)$, of the given length μ is rather straightforward:

$$V_n(\mu) = \sum_{s=1}^{\mu} R(s) \sum_{\{m_1,\dots,m_s\}}^{\prime} \Delta \left[\sum_{i=1}^{s} |m_i| - \mu \right], \qquad (3.36)$$

where R(s) is the number of all distinct sequences of *s* generators taken from the set $\{f_1, \ldots, f_n\}$ and satisfying the local rules (i) – (iii) while the second sum gives the number of all possible representations of the primitive path of length μ *for the fixed sequence of generators* ('prime' means that the sum runs over all $m_i \neq 0$ for $1 \leq i \leq s$; Δ is the Kronecker Δ -function).

It should be mentioned that the local rules (i) – (iii) define the generalized Markov chain with the states given by the $n \times n$ coincidence matrix \hat{T}_n where the rows and columns correspond to the generators f_1, \ldots, f_n :

		f_1	f_2	f_3	f_4		f_{n-1}	f_n	
$\widehat{T}_n(d) =$	$ \begin{array}{c} f_1\\ f_2\\ f_3\\ f_4\\ \vdots\\ f_{n-1}\\ f_n \end{array} $	0 1 0 : 0 0 0	1 0 1 0 : 0 0	1 1 0 1 : 0 0	$ \begin{array}{c} 1 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{array} $	···· ··· ···	1 1 1 : 0 1	$ \begin{array}{c} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \\ 0 \end{array} $	(3.37)

The number of all distinct normally ordered *sequences of words* of length *s* with allowed commutation relations is given by the following partition function

$$R_n(s,d) = \mathbf{v}_{\rm in} \left[\widehat{T}_n(d) \right]^s \mathbf{v}_{\rm out} \,, \tag{3.38}$$

where

$$\mathbf{v}_{\text{in}} = \left(\begin{array}{cc} n\\ 1\\ \cdots \end{array}\right), \quad \mathbf{v}_{\text{out}} = \begin{pmatrix} 1\\ \vdots\\ 1 \end{pmatrix} \right\}_{n}. \quad (3.39)$$

Supposing that the main contribution in Eqn (3.36) results from $s \ge 1$ we take for $R_n(s)$ the following asymptotic expression

$$R_n(s)\Big|_{s \ge 1} = (\lambda_n^{\max})^s, \quad \lambda_n^{\max} = 3 - \frac{4\pi^2}{n^2} + O\left(\frac{1}{n^3}\right), (3.40)$$

where λ_n^{\max} is the highest eigenvalue of the matrix \hat{T}_n $(n \ge 1)$.

The remaining sum in Eqn (3.36) is independent of R(s), so its calculation is trivial:

$$\sum_{\{m_1,\dots,m_s\}}^{\prime} \Delta \left[\sum_{i=1}^s |m_i| - \mu \right] = 2^s \frac{(\mu - 1)!}{(s - 1)!(\mu - s)!} \,. \tag{3.41}$$

Collecting all terms in Eqn (3.36) and evaluating the sum over *s* we arrive at Eqn (3.34). The value $V_n(\mu, d)$ grows exponentially fast with μ and the 'speed' of this growth is clearly represented by the fraction

$$z_{\rm eff} - 1 = \frac{V_n(\mu+1)}{V_n(\mu)} \bigg|_{\mu \gg 1} \simeq 7 - \frac{8\pi^2}{n^2} , \qquad (3.42)$$

where z_{eff} is the coordinational number of the effective tree associated with the locally free group.

Thus, a random walk on the group \mathcal{LF}_{n+1} can be viewed as follows. Take the *free* group Γ_n with generators $\{\tilde{f}_1, \ldots, \tilde{f}_n\}$ where all \tilde{f}_i $(1 \le i \le n)$ do not commute. The group Γ_n has a structure of a 2*n*-branching Cayley tree, $C(\Gamma_n)$, where the number of distinct words of length μ is equal to $\tilde{V}_n(\mu)$,

$$\widetilde{V}_n(\mu) = 2n(2n-1)^{\mu-1}.$$
(3.43)

The graph $C(\mathcal{LF}_{n+1})$ corresponding to the group \mathcal{LF}_{n+1} can be constructed from the graph $C(\Gamma_n)$ in accordance with the following recursion procedure: (a) Take the root vertex of the graph $C(\Gamma_n)$ and consider all vertices at the distance $\mu = 2$. Identify those vertices which correspond to the equivalent words in group \mathcal{LF}_{n+1} ; (b) Repeat this procedure taking all vertices at the distance $\mu = (1, 2, ...)$ and 'gluing' them at the distance $\mu + 2$ according to the definition of the locally free group. By means of the described procedure we raise a graph which on average has $z_{\text{eff}} - 1$ distinct branches leading to the 'next coordinational sphere'. Thus this graph coincides (on average) with a z_{eff} -branching Cayley tree.

Although the local structure of the graph $C(\mathcal{LF}_{n+1})$ is very complex, Eqn (3.42) enables us to find the asymptote of the random walk on the graph $C(\mathcal{LF}_{n+1})$. Once having z_{eff} , we can write down the master equation for the probability $\mathcal{P}(\mu, N)$ to find the walker at the distance μ from the origin after N random steps on the graph $C(\mathcal{LF}_{n+1})$:

$$\mathcal{P}(\mu, N+1) = \left(1 - \frac{1}{z_{\text{eff}}}\right) P(\mu - 1, N) + \frac{1}{z_{\text{eff}}} P(\mu + 1, N)$$
$$(\mu \ge 2). \tag{3.44}$$

The recursion relation (3.44) coincides with the equation describing a random walk on the half-line with the drift from the origin. Taking into account this analogy we can complete Eqn (3.44) by the boundary conditions [52]. However the exact form of the boundary conditions does not influence the asymptotic solution of Eqn (3.44) in the vicinity of the maximum of the distribution function:

$$\begin{split} \mathcal{P}(\mu,N) \simeq & \frac{1}{2\sqrt{2\pi(z_{\rm eff}-1)N}} \\ & \times \exp\left\{-\frac{z_{\rm eff}^2}{8(z_{\rm eff}-1)N}\left(\mu-\frac{z_{\rm eff}-2}{z_{\rm eff}}N\right)^2\right\}. \end{split}$$

Thus we obtain the desired distribution function [Eqn (3.31)] for the primitive word length for a random walk on the group \mathcal{LF}_{n+1} .

Eqn (3.31) gives the estimate from below for the limit distribution of the primitive words on the group B_n for $n \ge 1$.

We find further investigation of the random walks on the groups $\mathcal{LF}_{n+1}(d)$ for different values of *d* very perspective. It should give insight for consideration of random walk statistics on 'partially commutative groups'. Moreover, the set of problems considered there has a deep relation with the spectral theory of random matrices.

3.3 Brownian bridges on the Lobachevskii plane and products of non-commutative random matrices

The problem of word enumeration on a locally non-commutative group has an evident connection with the statistics of Markov chains on graphs having a Cayley tree-like structure and, hence, with random walk statistics on surfaces of a constant negative curvature. (We stressed once that the Cayley tree-like graphs are isometrically embedded in surfaces of a constant negative curvature).

Recall that the distribution function, $P(\mathbf{r}, t)$, for a free random walk in *D*-dimensional Euclidean space obeys the standard heat equation:

$$\frac{\partial}{\partial t}P(\mathbf{r},t) = \mathcal{D}\Delta P(\mathbf{r},t)$$

with the diffusion coefficient D = 1/(2D) and appropriate initial and normalization conditions

$$P(\mathbf{r}, t = 0) = \delta(\mathbf{r}), \qquad \int P(\mathbf{r}, t) \,\mathrm{d}\mathbf{r} = 1.$$

Correspondingly, the diffusion equation for the scalar density $P(\mathbf{q}, t)$ of the free random walk on a Riemann manifold reads (see [62] for instance)

$$\frac{\partial}{\partial t}P(\mathbf{q},t) = \mathcal{D}\frac{1}{\sqrt{g}} \frac{\partial}{\partial q_i} \left(\sqrt{g} \left(g^{-1}\right)_{ik} \frac{\partial}{\partial q_k}\right) P(\mathbf{q},t), \quad (3.45)$$

where

$$P(\mathbf{q}, t = 0) = \delta(\mathbf{q}), \qquad \int \sqrt{g} P(\mathbf{q}, t) \,\mathrm{d}\mathbf{q} = 1 \tag{3.46}$$

and g_{ik} is the metric tensor of the manifold; $g = \det g_{ik}$.

Eqn (3.45) has been subjected to thorough analysis for manifolds of constant negative curvature. Below we reproduce the corresponding solutions for the best known cases: for 2*D*- and 3*D*-Lobachevskiĭ spaces (often referred to as 3- and 4-pseudospheres) labelling them by indices '*p*' and '*s*' for the 2*D*- and 3*D*-cases correspondingly.

For the Lobachevskiĭ plane one has

$$||g_{ik}|| = \left| \begin{vmatrix} 1 & 0 \\ 0 & \sinh^2 \mu \end{vmatrix} \right|, \qquad (3.47)$$

where μ stands for the geodesic length on a 3-pseudosphere. The corresponding diffusion equation now reads

$$\frac{\partial}{\partial t} P_{\pi}(\mu, \varphi, t) = \mathcal{D}\left(\frac{\partial^2}{\partial \mu^2} + \coth \mu \frac{\partial}{\partial \mu} + \frac{1}{\sinh^2 \mu} \frac{\partial^2}{\partial \varphi^2}\right) \times P_{p}(\mu, \varphi, t) .$$
(3.48)

The solution of Eqn (3.48) is believed to have the following form

$$P_{\rm p}(\mu, t) = \frac{\exp(-t\mathcal{D}/4)}{4\pi\sqrt{2\pi(t\mathcal{D})^3}} \int_{\mu}^{\infty} \frac{\xi \exp\left[-\xi^2/(4t\mathcal{D})\right]}{\sqrt{\cosh\xi - \cosh\mu}} d\xi$$
$$\simeq \frac{\exp(-t\mathcal{D}/4)}{4\pi t\mathcal{D}} \left(\frac{\mu}{\sinh\mu}\right)^{1/2} \exp\left(-\frac{\mu^2}{4t\mathcal{D}}\right). (3.49)$$

For the Lobachevskii space the corresponding metric tensor is

$$||g_{ik}|| = \left\| \begin{array}{ccc} 1 & 0 & 0 \\ 0 & \sinh^2 \mu & 0 \\ 0 & 0 & \sinh^2 \mu \sin^2 \theta \end{array} \right\|.$$
(3.50)

Substituting Eqn (3.45) for Eqn (3.50) we have

$$P_{\rm s}(\mu,t) = \frac{\exp(-t\mathcal{D})}{8\pi\sqrt{\pi(t\mathcal{D})^3}} \frac{\mu}{\sinh\mu} \exp\left(-\frac{\mu^2}{4t\mathcal{D}}\right). \tag{3.51}$$

For the first time this spherically symmetric solution of the heat equation [Eqn (3.45)] in the Lobachevskii space was received in [63].

In our opinion one fact must be given attention. The distribution functions $P_p(\mu, t)$ and $P_s(\mu, t)$ give the probabilities of finding a random walk starting at the point $\mu = 0$ after time t in some *specific* point located at the distance μ in the corresponding non-Euclidean space. The probability of finding the terminal point of a random walk after time t somewhere at a distance μ is

$$\mathcal{P}_{\mathbf{p},\mathbf{s}}(\mu,t) = P_{\mathbf{p},\mathbf{s}}(\mu,t)\mathcal{N}_{\mathbf{p},\mathbf{s}}(\mu), \qquad (3.52)$$

where

$$\mathcal{N}_{\mathrm{p}}(\mu) = \sinh \mu \tag{3.53}$$

is the perimeter of circle of radius μ on the Lobachevskiĭ plane and

$$\mathcal{N}_{\rm s}(\mu) = \sinh^2 \mu \tag{3.54}$$

is the area of a sphere of radius μ in the Lobachevskiĭ space.

The difference between $P_{p,s}$ and $\mathcal{P}_{p,s}$ is insignificant in euclidean geometry, whereas in non-Euclidean space it becomes dramatic because of the consequences of the behavior of Brownian bridges in spaces of constant negative curvature.

Using the definition of the Brownian bridge, let us calculate the probabilities of finding an *N*-step random walk (starting at $\mu = 0$) after first *t* steps at the distance μ in the Lobachevskiĭ plane (space) under the condition that it returns to the origin on the last step. These probabilities are $(N \rightarrow \infty)$

$$\mathcal{P}_{p}(\mu, t|0, N) = \frac{P_{p}(\mu, t)\mathcal{P}_{p}(\mu, N-t)}{P_{p}(0, t)} \simeq \frac{N}{4\pi\mathcal{D}t(N-t)}\mu\exp\left\{-\frac{\mu^{2}}{4\mathcal{D}}\left(\frac{1}{t}+\frac{1}{N-t}\right)\right\},\$$

$$\mathcal{P}_{s}(\mu, t|0, N) = \frac{P_{s}(\mu, t)\mathcal{P}_{s}(\mu, N-t)}{P_{s}(0, t)} \simeq \frac{N^{3/2}}{8\pi t^{3/2}(N-t)^{3/2}}\mu^{2}\exp\left\{-\frac{\mu^{2}}{4\mathcal{D}}\left(\frac{1}{t}+\frac{1}{N-t}\right)\right\}.$$
 (3.55)

Hence we come to the standard Gaussian distribution function with zero mean.

Equations (3.55) describing the random walk on the Riemann surface of constant negative curvature have direct application to the conditional distributions of Lyapunov exponents for products of some non-commutative matrices. Let us consider the first of Eqn (3.55). Changing the variables $\mu = \ln(1 + |z|)/(1 - |z|)$; $\varphi = \arg z$ where z = x + iy, $\overline{z} = x - iy$ we map the 3-pseudosphere (μ, φ) onto the unit disk |z| < 1 known as the Poincare representation of the Lobachevskiĭ plane. The corresponding conformal metric reads $dl^2 = (4 dz d\overline{z})/(1 - |z|^2)^2$. Using the conformal transform z = (1 + iw)/(1 - iw) we recover the so-called Klein representation of the Lobachevskiĭ plane, where $dl^2 = -(4 dw d\overline{w})/(w - \overline{w})^2$ and the model is defined in Imw > 0 (w = u + iv; $\overline{w} = u - iv$).

The following relations can be verified using conformal representations of the Lobachevskiĭ plane metric (see, for instance, [17]). The fractional group of motions of the Lobachevskiĭ plane is isomorphic to:

(i) the group $SU(1,1)/\pm 1 \equiv PSU(1,1)$ in the Poincare model;

(ii) the group $SL(2, \mathbb{R})/\pm 1 \equiv PSL(2, \mathbb{R})$ in the Klein model.

Moreover, it is known (see, for example, [34]) that the Lobachevskii plane H can be identified with the group $\mathcal{H} = SL(2, \mathbb{R})/SO(2)$. This relation enables us to resolve (at least qualitatively) the following problem. Take the Brownian bridge on the group $\mathcal{H} = SL(2, \mathbb{R})/SO(2)$, i.e. demand the products of *N* independent random matrices $\widehat{\mathcal{M}}_k \in \mathcal{H} \ (0 \leq k \leq N)$ to be identical to the unit matrix. Consider the limit distribution of the Lyapunov exponent, δ , for the first *m* matrices in those products. To have a direct mapping of this problem onto the random walk in the Lobachevskii plane, write the corresponding stochastic recursion equation for some vector $\mathbf{W}_k = \begin{pmatrix} u_k \\ v_k \end{pmatrix}$

$$\mathbf{W}_{k+1} = \widehat{\mathcal{M}}_k \mathbf{W}_k, \quad \mathbf{W}_1 = \begin{pmatrix} 1\\1 \end{pmatrix}, \qquad (3.56)$$

where $\mathcal{M}_k \in \mathcal{H}$ for all $k \in [1, N]$. The BB-condition means that

$$\mathbf{W}_N = \mathbf{W}_1 \quad \text{for } N \ge 1 \,. \tag{3.57}$$

Let us consider the simplest case

$$\widehat{\mathcal{M}}_k = 1 + \widehat{M}_k, \quad \operatorname{norm}\left[\widehat{M}_k\right] \ll 1.$$
 (3.58)

In this case the discrete dynamic equation (3.56) can be replaced by the differential one. Its stationary measure is determined by the corresponding Fokker–Plank equation (3.45). The Lyapunov exponent, $\hat{\delta}$ of the product of random matrices $\widehat{\mathcal{M}}$ coincides with the length of geodesics in the Klein representation of the Lobachevskiĭ plane. Hence, under the conditions (3.57), (3.58) we have for $\hat{\delta}$ the usual Gaussian distribution coinciding with the first of Eqn (3.55). Without the BB-condition (i.e. for 'open walks') we reproduce the standard Fürstenberg behavior [39].

Although this consideration seems rather crude (for details see Appendix A), it clearly shows the origin of the main result:

The 'Brownian bridge' condition for random walks in a space of constant negative curvature makes the space 'effectively flat' turning the corresponding limit probability distribution for random walks to the ordinary central limit distribution.

The question whether this result is valid for the case of the random walk in non-Euclidean spaces of non-constant negative curvature still remains.

Finally we would like to introduce some conjectures which naturally generalize our consideration.

The complexity η of any known algebraic invariants (Alexander, Jones, HOMFLY) for the knot represented by the B_n -braid of length N with the uniform distribution over generators has the following limit behavior:

$$P(\eta, N) \sim \frac{\text{const}}{N^{3/2}} \eta \exp\left(-\alpha(n)N + \beta(n)\eta - \frac{\eta^2}{\delta(n)N}\right),$$

(3.59)

where $\alpha(n)$, $\beta(n)$, $\delta(n)$ are numerical constants depending on *n* only.

The knot complexity η in an ensemble of Brownian bridges from the group B_n shown in Fig. 10 has a Gaussian distribution, where

$$\langle \eta \rangle = 0, \quad \langle \eta^2 \rangle = \frac{1}{2} \delta(n) N.$$
 (3.60)

These conjectures are yet to be proven. The main idea is to employ the relation between the knot complexity η , the length of the shortest non-contractible word and the length of geodesics on some hyperbolic manifold.

4. Conformal methods in the statistics of random walks with topological constraints

The last few years have been marked by considerable progress in understanding the relationship between Chern–Simons topological field theory, the construction of the algebraic knot and link invariants and conformal field theory (see, for review, [64]).

Although the general concepts have been well elaborated in the field-theoretic context, their application in related areas of mathematics and physics, such as, for instance, probability theory and statistical physics of chain-like objects is highly limited.

The present section is mainly concerned with the conformal methods in statistical analysis which allow us to correlate the problems discussed in Sections 1 and 2 and the limit distributions of random walks on multiconnected Riemann surfaces. To be more specific, we show on the level of differential equations how simple geometrical methods can be applied to the construction of non-commutative topological invariants. The latter might serve as non-abelian generalizations of the Gauss linking numbers for random walks on multi-punctured Riemann surfaces. We also study the connection between the topological properties of random walks on the double punctured plane and behavior of fourpoint correlation functions in the conformal theory with central charge c = -2. The approach developed is applied to the investigation of the statistics of 2D-random walks with multiple topological constraints. For instance, the methods presented here allow us to extract non-trivial critical exponents for the contractible (i.e., unentangled) random walks in the regular lattices of obstacles. Some of our findings support the conjectures of Sections 2 and 3 and have direct application in the statistics of strongly entangled polymer chains (see Section 5).

4.1 Construction of non-abelian connections for Γ_2 and $PSL(2,\mathbb{Z})$ from conformal methods

We analyzed random walk of length L with a effective elementary step a $(a \equiv 1)$ on the complex plane z = x + iywith two points removed. Suppose the coordinates of these points are A $(z_1 = (0,0))$ and B $(z_2 = (c,0))$ $(c \equiv 1)$. Such a choice does not indicate a loss of generality because by means of simultaneous rescaling of the effective step, a, of the random walk and of the distance, c, between the removed points we can always obtain any arbitrary values of a and c.

Consider the closed paths on z and attribute the generators g_1 , g_2 of some group G to the turns around the points A and B if we move along the path in the clockwise direction (we apply g_1^{-1} , g_2^{-1} for counter-clockwise motion) — see Fig. 11.



Figure 11. (a) — the double punctured complex plane *z* with two basis loops C_1 and C_2 enclosing points M_1 and M_2 ; (b) — the universal covering ζ with fundamental domain corresponding to the free group Γ_2 . The contours P_1 and P_2 are the images of the loops C_1 and C_2 .

The question is: what is the probability $P(\mu, L)$ for a random walk of length *L* on the plane *z* to form a closed loop with the shortest non-contractible word written in terms of the generators $\{g_1, g_2, g_1^{-1}, g_2^{-1}\}$ of having length μ (see also Section 2).

Let the distribution function $P(\mu, L)$ be formally written as a path integral with a Wiener measure

$$P(\mu, L) = \frac{1}{Z} \int \dots \int \mathcal{D}\{z\} \exp\left\{-\frac{1}{a^2} \int_0^L \left(\frac{dz(s)}{ds}\right)^2 ds\right\} \\ \times \delta \left[W\{g_1, g_2, g_1^{-1}, g_2^{-1} | z\} - \mu\right],$$
(4.1)

where $\mathcal{Z} = \int P(\mu, L)d\mu$ and $W\{\ldots | z\}$ is the length of the shortest word on *G* as a functional of the path on the complex plane.

Conformal methods enable us the construct the connection and the topological invariant W for the given group as well as to rewrite Eqn (4.1) in a closed analytic form which is solvable at least in the limit $L \to \infty$.

Let $\zeta(z)$ be the conformal mapping of the double punctured plane z = x + iy on the universal covering $\zeta = \xi + i\lambda$. The Riemann surface ζ is constructed in the following way. Make three cuts on the complex plane z between the points *A* and *B*, between *B* and (∞) and between (∞) and *A* along the line Im z = 0. These cuts separate the upper (Im z > 0) and lower (Im z < 0) half-planes of *z*. Now perform a conformal transform of the half-plane Im z > 0 to the fundamental domain of the group $G\{g_1, g_2\}$ — the curvilinear triangle lying in the half-plane Im $\zeta > 0$ of the plane ζ . Each fundamental domain represents the Riemann sheet corresponding to the fibre bundle above *z*. The whole covering space ζ is the unification of all such Riemann sheets.

The coordinates of the initial and final points of any trajectory on the universal covering ζ determine (see [66]): (a) the coordinates of corresponding points on z; (b) the homotopy class of any path on z. In particular, the contours on ζ are closed if and only if $W\{g_1,g_2|z\} \equiv 1$, i.e. they belong to the trivial homotopy class.

The coordinates of the ends of the trajectory on the universal covering ζ can be used as the topological invariant for the path on the double punctured plane *z* with respect to the action of the group *G*.

Thus, we characterize the topological invariant, Inv(C), of some closed directed path *C* starting and ending at an arbitrary point $z_0 \neq \{z_1, z_2, \infty\}$ on the plane *z* by the coordinates of the initial, $\zeta_{\text{in}}(z_0)$, and final, $\zeta_{\text{fin}}(z_0)$, points of the corresponding contour *P* in the covering space ζ . The contour *P* connects the images of the point z_0 on the different Riemann sheets. Write $\text{Inv}_{(z)}(C)$ as a full derivative along the contour *C*:

$$\operatorname{Inv}_{(z)}(C) \stackrel{\text{def}}{=} \zeta_{\text{in}} - \zeta_{\text{fin}} = \oint_C \frac{\mathrm{d}\zeta(z)}{\mathrm{d}z} \,\mathrm{d}z \,. \tag{4.2}$$

The physical interpretation of the derivative $d\zeta(z)/dz$ is very straightforward. Actually, the invariant, Inv(C), can be associated with the flux through the contour C on the plane (x, y):

$$Inv(C) \equiv Inv_{(x,y)}(C) = \oint_C \nabla \zeta(x, y) \mathbf{n} \, \mathrm{d}\mathbf{r}$$
$$= \oint_C \mathbf{v} \times \nabla \zeta(x, y) \mathbf{v}(s) \, \mathrm{d}s \,, \tag{4.3}$$

where: **n** is the unit vector normal to the curve *C*, $d\mathbf{r} = \mathbf{e}_x dx + \mathbf{e}_y dy$ on the plane (x, y); $\mathbf{v}(s) = d\mathbf{r}/ds$ denotes the 'velocity' along the trajectory; and ds stands for the differential path length. The simple transformations used in Eqn (4.3) are: (a) $\mathbf{n}d\mathbf{r} = \mathbf{e}_x dy - \mathbf{e}_y dx = d\mathbf{r} \times v$; (b) $\nabla \zeta(x, y)(d\mathbf{r} \times v) = (v \times \nabla \zeta(x, y)) d\mathbf{r}$, where v = (0, 0, 1) is the unit vector normal to the plane (x, y).

The vector product

$$\mathbf{A}(x,y) = \mathbf{v} \times \nabla \zeta(x,y) \tag{4.4}$$

can be considered a non-abelian generalization of the vector potential of a solenoidal 'magnetic field' normal to the plane (x, y) and crossing it at the points (x_1, y_1) and (x_2, y_2) . Thus, **A** defines the *flat connection* of the double punctured plane *z* with respect to the action of the group *G*.

It is easy to show how the basic formulae (4.2) and (4.3) transform in the case of the commutative group $G_{\text{comm}}\{g_1, g_2\}$ which distinguishes only the classes of homology of the contour *C* with respect to the removed points on the plane. The corresponding conformal transform is performed by the function $\zeta(z) = \ln(z - z_1) + \ln(z - z_2)$. This immediately gives the abelian connection and the Gauss linking number

as a topological invariant:

$$\mathbf{A}(\mathbf{r}) = \mathbf{v} \times \sum_{j=\{1,2\}} \frac{\mathbf{r} - \mathbf{r}_j}{|\mathbf{r} - \mathbf{r}_j|^2},$$

$$\operatorname{Inv}(C) = \oint_C \mathbf{A}(\mathbf{r}) \, \mathrm{d}\mathbf{r} = 2\pi (n_1 + n_2)$$

where n_1 and n_2 are the winding numbers of the path *C* around the points M_1 and M_2 of the plane (x, y).

Substituting Eqn (4.3) written in Euclidean coordinates (x, y) for Eqn (4.1) and using the Fourier transform for the δ -function, we can rewrite equation (4.1) as follows

$$P(\mu, L) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-\mathrm{i}q\mu) P(q, L) \,\mathrm{d}q \,, \tag{4.5}$$

where

$$P(q,L) = \frac{1}{\mathcal{Z}} \int \dots \int \mathcal{D}\{\mathbf{r}\} \exp\left\{-\frac{1}{a^2} \int_0^L \left[\left(\frac{d\mathbf{r}(s)}{ds}\right)^2 - iq\mathbf{A}(\mathbf{r})\frac{d\mathbf{r}(s)}{ds}\right] ds\right\}.$$
 (4.6)

The function P(q, L) coincides with the Green function $P(\mathbf{r}_0, \mathbf{r} = \mathbf{r}_0, q, L)$ of the non-stationary Schrödinger-like equation for free particle motion in a 'magnetic field' with vector potential (4.4):

$$\frac{\partial}{\partial L} P(\mathbf{r}_0, \mathbf{r}, q, L) - \left(\frac{1}{2a}\nabla - \mathrm{i}q\mathbf{A}(\mathbf{r})\right)^2 P(\mathbf{r}_0, \mathbf{r}, q, L)$$
$$= \delta(L)\delta(\mathbf{r} - \mathbf{r}_0), \qquad (4.7)$$

where q plays the role of a 'charge' and the magnetic field is considered transversal, i.e. rot $\mathbf{A}(\mathbf{r}) = 0$.

We describe now the constructive way of getting the desired conformal transform. The single-valued inverse function $z(\zeta) \equiv \zeta^{-1}(z)$ is defined in the fundamental domain of ζ — the triangle *ABC*. The multivalued function $\phi(\zeta)$ is determined as follows:

— the function $\phi(\zeta)$ coincides with $z(\zeta)$ in the basic fundamental domain;

— in all other domains of the covering space ζ the function $\phi(\zeta)$ is analytically continued through the boundaries of these domains by means of fractional transformations consistent with the action of the group *G*.

Consider two basic contours P_1 and P_2 on ζ being the conformal images of the contours C_1 and C_2 (Fig. 11b). The function $\phi(z)$ ($z \neq \{z_1, z_2, \infty\}$) obeys the following transformations:

$$\phi[z \xrightarrow{C_1} z] \to \tilde{\phi}_1(z) = \frac{a_1 \phi(z) + b_1}{c_1 \phi(z) + d_1},$$

$$\phi[z \xrightarrow{C_2} z] \to \tilde{\phi}_2(z) = \frac{a_2 \phi(z) + b_2}{c_2 \phi(z) + d_2},$$
(4.8)

where

$$\begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix} = g_1, \quad \begin{pmatrix} a_2 & b_2 \\ c_2 & d_2 \end{pmatrix} = g_2$$
 (4.9)

are the matrices of basic substitutions of the group $G\{g_1, g_2\}$.

We assume $\zeta(z)$ to be a ratio of two fundamental solutions, $u_1(z)$, and, $u_2(z)$, of some second order differential equation with peculiar points $\{z_1 = (0,0), z_2 = (0,1, z_3 = (\infty)\}$. As follows from the analytic theory of differential equations [68], the solutions $u_1(z)$ and $u_2(z)$ undergo linear transformations when the variable z moves along the contours C_1 and C_2 :

$$C_1: \begin{pmatrix} \tilde{u}_1(z)\\ \tilde{u}_2(z) \end{pmatrix} = g_1 \begin{pmatrix} u_1(z)\\ u_2(z) \end{pmatrix}, \quad C_2: \begin{pmatrix} \tilde{u}_1(z)\\ \tilde{u}_2(z) \end{pmatrix} = g_2 \begin{pmatrix} u_1(z)\\ u_2(z) \end{pmatrix}.$$
(4.10)

The problem of restoring the form of the differential equation knowing the monodromy matrices g_1 and g_2 of the group G known as Riemann-Hilbert problem has a long history [68]. In our particular case we restrict ourselves to the well investigated groups Γ_2 (the free group) and $PSL(2,\mathbb{Z})$ (the modular group). Thus, we have the following second-order differential equations:

$$z(z-1)\frac{d^2}{dz^2}u^{(f)}(z) + (2z-1)\frac{d}{dz}u^{(f)}(z) + \frac{1}{4}u^{(f)}(z) = 0$$
(4.11)

for the free group and

$$z(z-1)\frac{\mathrm{d}^2}{\mathrm{d}z^2} u^{(m)}(z) + \left(\frac{5}{3}z-1\right)\frac{\mathrm{d}}{\mathrm{d}z} u^{(m)}(z) + \frac{1}{12} u^{(m)}(z) = 0$$
(4.12)

for the modular group.

The function which performs the conformal mapping of the upper half-plane Im z > 0 on the fundamental domain (the curvilinear triangle *ABC*) of the universal covering ζ now reads

$$\zeta(z) = \frac{u_1^{(f,m)}(z)}{u_2^{(f,m)}(z)}, \qquad (4.13)$$

where $u_{1,2}^{(f)}(z)$ and $u_{1,2}^{(m)}(z)$ are the basic solutions of (4.11) and (4.12) for Γ_2 and $PSL(2, \mathbb{Z})$ respectively.

As an example we give an explicit form of the complex potential A(z) for the free group Γ_2 . Substituting Eqn (4.2) for Eqn (4.13), we get

$$A(z) = \frac{\mathrm{d}\zeta(z)}{\mathrm{d}z} = \frac{1}{2(z-1)} \left(\frac{F_1(z)F_4(z)}{F_2^2(z)} - \frac{F_3(z)}{F_2(z)} \right), \quad (4.14)$$

where

$$\begin{split} F_1(z) &= \int_1^{1/\sqrt{z}} \frac{\mathrm{d}\varkappa}{\sqrt{(1-\varkappa^2)(1-z\varkappa^2)}} \,, \\ F_2(z) &= \int_0^1 \frac{\mathrm{d}\varkappa}{\sqrt{(1-\varkappa^2)(1-z\varkappa^2)}} \,, \\ F_3(z) &= \int_1^{1/\sqrt{z}} \sqrt{\frac{1-\varkappa^2}{1-z\varkappa^2}} \mathrm{d}\varkappa \,, \quad F_4(z) = \int_0^1 \sqrt{\frac{1-\varkappa^2}{1-z\varkappa^2}} \mathrm{d}\varkappa \,. \end{split}$$

The asymptote of (4.14) is as follows

$$\frac{\mathrm{d}\zeta(z)}{\mathrm{d}z} \sim \begin{cases} z^{-1}, & z \to 0, \\ (z-1)^{-1}, & z \to 1 \end{cases}$$

(compare to the abelian case).

4.2 Random walk on a double punctured plane and conformal field theory

The geometrical construction described in the previous section is evidently related to the conformal field theory. In the most direct way this relation could be understood as follows. The ordinary differential equations Eqn (4.11) and Eqn (4.12) can be associated with equations on the four-point correlation function of some (still not defined) conformal field theory. The question remains whether it is always possible to adjust the central charge c of the corresponding Virosoro algebra and the conformal dimension Δ of the critical theory to the coefficients in equations like (4.11), (4.12). The question is positive and we show this for the example of a random walk on a double punctured plane with the monodromy of the free group.

We restrict ourselves to the 'critical' case of infinitely long trajectories, i.e. we suppose $L \to \infty$. In field-theoretic language that means the consideration of the massless free field theory on z. Actually, the partition function of the selfintersecting random walk on z written in the field representation is generated by the scalar Hamiltonian $H = (\nabla \phi)^2/2 + m\phi^2$ where the mass m acts as the 'chemical potential' conjugated to the length of the path $(m \sim 1/L)$. Thus, for $L \to \infty$ we have $m_c = 0$ which corresponds to the critical point in conformal theory [65].

We introduce the conformal operator, $\varphi(z)$, on the complex plane z. The dimension, Δ , of this operator is defined from the conformal correlator

$$\left\langle \varphi(z)\varphi(z')\right\rangle \sim \frac{1}{\left|z-z'\right|^{2\Delta}}$$
 (4.15)

Let us suppose $\varphi(z)$ to be a primary field, then the four-point correlation function $\langle \varphi(z_1)\varphi(z_2)\varphi(z_3)\varphi(z_4)\rangle$ satisfies the equation following from the conformal Ward identity [65, 69, 70]. In form of ordinary Riemann differential equation, Eqn (4.15) on the conformal correlator $\psi(z|z_1, z_2, z_3) =$ $\langle \varphi(z)\varphi(z_1)\varphi(z_2)\varphi(z_3)\rangle$ with the fixed points $\{z_1 = (0, 0), z_2 = (1, 0), z_3 = \infty\}$ reads [65, 69]

$$\begin{cases} \frac{3}{2(2\Delta+1)} \frac{d^2}{dz^2} + \frac{1}{z} \frac{d}{dz} + \frac{1}{z-1} \frac{d}{dz} - \frac{\Delta}{z^2} \\ - \frac{\Delta}{(z-1)^2} + \frac{2\Delta}{z(z-1)} \end{cases} \psi(z|z_1, z_2, z_3) = 0.$$

Performing the substitution $\psi(z|z_1, z_2, z_3) = [z(z-1)]^{-2\Delta} \times u(z)$ we get the equation

$$z(z-1)u''(z) - \frac{2}{3}(1-4\Delta)(1-2z)u'(z) - \frac{2}{3}(2\Delta - 8\Delta^2)u(z) = 0, \qquad (4.16)$$

which coincides with Eqn (4.11) for one single value of Δ

$$\Delta = -\frac{1}{8} \,. \tag{4.17}$$

The conformal properties of the stress-energy tensor, T(z), are defined by the coefficients, L_n , in its Laurent expansion T(z): $T(z) = \sum_{n=-\infty}^{\infty} L_n/z^{n+2}$ These coefficients form the Virosoro algebra [65]

$$[L_n, L_m] = (n-m)L_{n+m} + \frac{1}{12}c(n^3 - n)\delta_{n+m,0},$$

where the parameter, c, is the central charge of the theory. Using the relation $c = 2\Delta(5 - 8\Delta)/(2\Delta + 1)$ established in [69] and Eqn (4.17) we obtain

$$c = -2. (4.18)$$

We find the following fact, mentioned by B. Duplantier, very intriguing. As he pointed out, the value $\Delta = -1/8$ [Eqn (4.17)] coincides with the surface exponent (i.e. with the conformal dimension of the two point correlator near the surface) for the dense phase of the O(n = 0) lattice model (or, which is the same, for the Potts model with q = 0) describing the statistics of the so-called 'Manhattan random walks' (also known as 'dense polymers' — see paper [27]). Recall that the Potts model has been already mentioned in Section 2 in connection with the construction of algebraic knot invariants. It is hard to believe that such a coincidence is chance and we hope that the relation between these problems will be elucidated in the near future.

The conformal invariance of the random walk [66, 67] together with the geometrical interpretation of the monodromy properties of the four-point conformal correlator established above enable us to express the following assertion:

The critical conformal field theory characterized by the values c = -2 and $\Delta = -1/8$ gives the field representation for an infinitely long random walk on a double punctured complex plane.

With respect to the four-point correlation function, we could ask what happens with the gauge connection $A_j(z)$ if the argument z_j of the primary field $\varphi(z_j)$ moves along the closed contour *C* around three punctures on the plane. From the general theory it is known that $A_j(z)$ can be written as

$$A_{j}(z) = \frac{2}{k} \sum_{i \neq j} \frac{R_{i}R_{j}}{z - z_{i}}, \qquad (4.19)$$

where k is the level of the corresponding representation of the Kac-Moody algebra and R_i , R_j are the generators of representation of the primary fields $\varphi(z_i)$, $\varphi(z_j)$ in the given group [71]. The holonomy operator $\chi(C)$ associated with $A_j(z)$ reads

$$\chi(C) = P \exp\left(-\oint_C A_j(z) \,\mathrm{d}z\right). \tag{4.20}$$

It would be interesting to compare Eqn (4.14) (with one puncture at infinity) to Eqn (4.19). Besides we could also expect that Eqn (4.2) would allow us to rewrite the holonomy operator (4.20) as follows

$$\chi(C) = \exp(\zeta_{\rm in} - \zeta_{\rm fin})\,.$$

At this point we finish the brief discussion of the fieldtheoretical aspects of the geometrical approach presented above.

4.3 Statistics of random walks with topological constraints in a two-dimensional lattice of obstacles

The conformal methods can be applied to the problem of calculating the distribution function for random walks in regular lattices of topological obstacles on the complex plane w = u + iv. Let the elementary cell of the lattice be an equal-sided triangle with side length *c*.

Introduce the distribution function $P(w_0, w, L|\text{hom})$ defining the probability of the fact that the trajectory of a

random walk starting at the point w_0 comes after 'time' *L* to the point *w* and *all paths going from* w_0 to *w* belong to the same homotopy class with respect to the lattice of obstacles. Formally we can write the diffusion equation

$$\frac{a}{4}\Delta_{w}P(w,L|\text{hom}) = \frac{\partial}{\partial L}P(w,L|\text{hom})$$
(4.21)

with initial and normalization conditions:

$$P(w, L = 0|\text{hom}) = \delta(z_0),$$

$$\sum_{\{\text{hom}\}} P(w_0, w, L|\text{hom}) = \frac{1}{\pi aL} \exp\left(-\frac{|w - w_0|^2}{aL}\right).$$

The conformal methods can be used to find the asymptotic solution of Eqn (4.21) when $L \ge a$. Due to the conformal invariance of the Brownian motion, the new random process in the covering space will again be random but in the metricdependent 'new time'. In particular, we are interested in the probability of finding the closed path of length L to be unentangled in the lattice of obstacles.

The construction of the conformal transformation $\zeta(w)$ (explicitly described in [66]) can be performed in two steps—see Fig. 11:

1. First, by means of auxiliary reflection w(z) we transfer the elementary cell of the *w*-plane to the upper half-plane of the Im (z) > 0 of the double punctured plane *z*. The function w(z) is determined by the Christoffel–Schwarts integral

$$w(z) = \frac{c}{B(1/3, 1/3)} \int_0^z \frac{\mathrm{d}\tilde{z}}{\tilde{z}^{2/3} (1 - \tilde{z})^{2/3}} \,. \tag{4.22}$$

where $B(\frac{1}{3}, \frac{1}{3})$ is the Beta-function. The correspondence of the branching points is as follows:

$$A(w = 0) \to \tilde{A}(z = 0), \quad B(w = c) \to \tilde{B}(z = 1),$$

$$C\left(w = c \exp\left(-i\frac{\pi}{3}\right)\right) \to \tilde{C}(z = \infty).$$

2. The construction of the universal covering ζ for the double punctured complex plane *z* is realized by means of automorphic functions. If the covering space is free of obstacles, the corresponding conformal transform should be as follows

$$-\frac{1}{\left(z'(\zeta)\right)^2}\left\{z(\zeta)\right\} = \frac{z^2 - z + 1}{2z^2(z - 1)^2},$$
(4.23)

where $\{z(\zeta)\}$ is the so-called Schwartz's derivative

$$\left\{z(\zeta)\right\} = \frac{z'''(\zeta)}{z'(\zeta)} - \frac{3}{2} \left(\frac{z''(\zeta)}{z'(\zeta)}\right)^2, \qquad z'(\zeta) = \frac{\mathrm{d}z}{\mathrm{d}\zeta}$$

It is well known in the analytic theory of differential equations [68] that the solution of Eqn (4.23) can be represented as ratio of two fundamental solutions of some second order differential equation with two branching points, namely, of Eqn (4.11). The final answer reads

$$z(\zeta) \equiv k^2(\zeta) = \frac{\theta_2^4(0, \exp(i\pi\zeta))}{\theta_3^4(0, \exp(i\pi\zeta))}, \qquad (4.24)$$

where $\theta_2(0,\zeta)$ and $\theta_3(0,\zeta)$ are the elliptic Jacobi Thetafunctions. We recall their definitions

$$\theta_2(\chi, \exp(i\pi\zeta)) = 2\exp\left(i\frac{\pi}{4}\zeta\right)$$
$$\times \sum_{n=0}^{\infty} \exp\left[i\pi\zeta n(n+1)\right]\cos(2n+1)\chi,$$
$$\theta_3(\chi, \exp(i\pi\zeta)) = 1 + 2\sum_{n=0}^{\infty}\exp(i\pi\zeta n^2)\cos 2n\chi. \quad (4.25)$$

The branching points \widetilde{A} , \widetilde{B} , \widetilde{C} have images in the vertex points of a zero-angled triangle lying in the upper half-plane of the plane ζ . We have from Eqn (4.24):

$$\widetilde{A}(z=0) \to \overline{A}(\zeta=\infty), \quad \widetilde{B}(z=1) \to \overline{B}(\zeta=0),$$

 $\widetilde{C}(z=\infty) \to \overline{C}(\zeta=-1).$

The half-plane Im $(\zeta) > 0$ functions as a covering space for the plane *w* with a regular array of topological obstacles. It does not contain any branching point and consists of an infinite set of Riemann sheets, each having the form of a zeroangled triangle. These Riemann sheets correspond to the fibre bundle of *w*.

The conformal approach gives us a well defined nonabelian topological invariant for the problem — the difference between the initial and final points of the trajectory in the covering space (see Srction 4.1). Thus, the diffusion equation for the distribution function $P(\zeta, L)$ in the covering space ζ with given initial point ζ_0 yields

$$\frac{a}{4}\frac{\partial^2}{\partial\zeta\partial\overline{\zeta}}P(\zeta,\zeta_0,L) = \left|w'(\zeta)\right|^2\frac{\partial}{\partial L}P(\zeta,\zeta_0,L),\qquad(4.26)$$

where we took into account that under the conformal transform the Laplace operator is transformed in the following way

$$\Delta_{w} = \left| \frac{\mathrm{d}\zeta}{\mathrm{d}w} \right|^{2} \Delta_{\zeta} , \qquad \left| \frac{\mathrm{d}\zeta}{\mathrm{d}w} \right|^{2} = \frac{1}{\left| w'(\zeta) \right|^{2}} .$$

In particular, the value $P(\zeta = \zeta_0, \zeta_0, L)$ gives the probability of the path of length L being unentangled (i.e. being contractible to a point) in the lattice of obstacles.

The expression for the Jacobian $|w'(\zeta)|^2$ can be found using the properties of Jacobi Theta-functions [72]. Write $w'(\zeta) = w'(z) z'(\zeta)$, where

$$\begin{split} w'(z) &= \frac{c}{B(1/3, 1/3)} \frac{\theta_3^{16/3}}{\theta_2^{8/3}} \,, \quad z'(\zeta) = \mathrm{i}\pi \frac{\theta_2^4 \,\, \theta_0^4}{\theta_3^4} \,, \\ \mathrm{i} \, \frac{\pi}{4} \theta_0^4 &= \frac{\mathrm{d}}{\mathrm{d}\zeta} \ln\left(\frac{\theta_2}{\theta_3}\right) \end{split}$$

(we omit the arguments for compactness).

The identity

$$\theta_1'(0, \exp(i\pi\zeta)) \equiv \left. \frac{\mathrm{d}\theta_1(\chi, \exp(i\pi\zeta))}{\mathrm{d}\chi} \right|_{\chi=0}$$

$$= \pi \theta_0 (\chi, \exp(i\pi\zeta)) \theta_2 (\chi, \exp(i\pi\zeta)) \theta_3 (\chi, \exp(i\pi\zeta))$$

enables us to get the final expression

$$|w'(\zeta)|^{2} = c^{2}h^{2}|\theta'_{1}(0, \exp(i\pi\zeta))|^{8/3},$$

$$h = \frac{1}{\pi^{1/3}B(1/3, 1/3)} \simeq 0.129,$$
 (4.27)

where

$$\theta_1(\chi, \exp(i\pi\zeta)) = 2 \exp\left(i\frac{\pi}{4}\zeta\right)$$
$$\times \sum_{n=0}^{\infty} (-1)^n \exp\left[i\pi n(n+1)\zeta\right] \sin(2n+1)\chi. \quad (4.28)$$

Return to Eqn (4.26) and perform the conformal transform of the upper half-plane Im $\zeta > 0$ to the interior of the unit circle on the complex plane τ in order to use the symmetry properties of the system. It is convenient to choose the following mapping of the vertices of the fundamental triangle \overline{ABC}

$$\begin{split} \bar{A}(\zeta = \infty) &\to A'(\bar{\zeta} = 1) \,, \\ \bar{B}(\zeta = 0) &\to B'\left(\tilde{\zeta} = \exp\left(-\mathrm{i}\frac{2\pi}{3}\right)\right) \,, \\ \bar{C}(\zeta = -1) &\to C'\left(\tilde{\zeta} = \exp\left(\mathrm{i}\frac{2\pi}{3}\right)\right) \,. \end{split}$$

The corresponding transform reads

$$\zeta(\tau) = \exp\left(-i\frac{\pi}{3}\right)\frac{\tau - \exp(i2\pi/3)}{\tau - 1} - 1, \qquad (4.29)$$

and the Jacobian $|w'(\tau)|^2$ takes the form

$$|w'(\tau)|^{2} = \frac{3c^{2}h^{2}}{|1-\tau|^{4}} \left| \theta_{1}' \Big(0, \exp\left(i\pi\zeta(\tau)\right) \Big)^{8/3} \right|.$$
(4.30)

In Figure 12 we plot the function $g(r, \psi) = (1/c^2)|w'(\tau)|^2$ where $\tau = r \exp(i\psi)$.



Figure 12. Relief of the function $g(r, \psi)$ — see explanations in the text.

The gain of such a representation becomes clear if we average the function $g(r, \psi)$ with respect to ψ . The numerical calculations give us:

$$\lim_{r \to 1} \left\langle g(r, \psi) \right\rangle_{\psi} \equiv \lim_{r \to 1} \frac{1}{2\pi} \int_{0}^{2\pi} g(r, \psi) \, \mathrm{d}\psi = \frac{\bar{\omega}}{\left(1 - r^{2}\right)^{2}} \,,$$
(4.31)

where $\bar{\omega} \simeq 0.0309$ (see the Fig. 13).



Figure 13. Plot of product $2\pi \langle g(r,\psi) \rangle_{\psi} \times (1-r^2)^2$ as a function of *r*.

Thus it is clear that for r rather close to 1 the diffusion is governed by the Laplacian on the surface of constant negative curvature (the Lobachevskiĭ plane). The representation of the Lobachevskiĭ plane in the unit circle and in the upper halfplane (i.e. Poincare and Klein models) was discussed in Section 3.4. Finally the diffusion equation (4.26) takes the following form:

$$\frac{\partial}{\partial N} P(r, \psi, N) = \mathcal{D}(1 - r^2)^2 \Delta_{r, \psi} P(r, \psi, N) , \qquad (4.32)$$

where $\mathcal{D} = a^2/4\bar{\omega}c^2$ is the 'diffusion coefficient' in the Lobachevskiĭ plane and N = L/a is the dimensionless chain length (i.e. effective number of steps).

Changing the variables $(r, \psi) \rightarrow (\mu, \psi)$, where $\mu = \ln(1+r)/(1-r)$, we get the unrestricted random walk on the 3-pseudosphere [see Eqn (3.49)]. Correspondingly the distribution function $P(\mu, N)$ reads

$$P(\mu, N) = \frac{\exp(-N\mathcal{D}/4)}{4\pi\sqrt{2\pi(N\mathcal{D})^3}} \int_{\mu}^{\infty} \frac{\xi \exp(-\xi^2/(4N\mathcal{D}))}{\sqrt{\cosh\xi - \cosh\mu}} \, \mathrm{d}\xi \,. \ (4.33)$$

The physical meaning of the geodesic length on the 3pseudosphere, μ , is straightforward: μ is the length of the socalled 'primitive path' in the lattice of obstacles, i.e. the length of the shortest path remaining after all topologically allowed contractions of the random trajectory in the lattice of obstacles. Hence, μ can be considered a non-abelian topological invariant, much more powerful than the Gauss linking number. This invariant is not complete except one point $\mu = 0$ where it precisely classifies the trajectories belonging to the trivial homotopic class. Let us note that the length η is proportional to the length of the primitive (irreducible) word written in terms of generators of the free group Γ_2 .

5. Physical applications. Polymer language in the statistics of entangled chain-like objects

Topological constraints essentially modify the physical properties of statistical systems consisting of chain-like objects of a completely different nature. It should be said that topological problems are widely investigated in connection with quantum field and string theories, 2D-gravitation, the statistics of vortices in superconductors and world lines of anyons, the quantum Hall effect, thermodynamic properties of entangled polymers etc. Modern methods of theoretical physics allow us to describe rather comprehensively the effects of non-abelian statistics on physical behavior for each particular referred system; however, in our opinion, the following general questions remain obscure:

How do the changes in the topological state of the system of entangled chain-like objects affect their physical properties?

How can the knowledge accrued in statistical topology be applied to the construction of the Ginzburg–Landau-type theory of fluctuating entangled chain-like objects?

In order to have a representative and physically clear image for the system of fluctuating chains with the full range of non-abelian topological properties it appears quite natural to formulate general topological problems in terms of the polymer physics. It allows us: to use a geometrically clear image of polymer with topological constraints as a model corresponding to the path integral formalism in the field theory, and to advance in the investigation of specific physical properties of biological and synthetical polymer systems where the topological constraints play a significant role.

For physicists, polymer objects are attractive for many reasons. First of all, the joining of monomer units in chains essentially reduces all equilibrium and dynamic properties of the system under consideration. Moreover, due to that joining the behavior of polymers is determined by spacetime scales larger than for low-molecular-weight substances. The chain-like structure of macromolecules causes the following peculiarities (see, for instance, [73]): so-called 'linear memory' (i.e. the fixed position of each monomer unit along the chain); low translational entropy (i.e. the restrictions on independent motion of monomer units due to the presence of bonds); large space fluctuations (i.e. just a single macromolecule can be regarded as a statistical system with many degrees of freedom).

It should be emphasized that the above mentioned 'linear memory' leads to the fact that different parts of polymer molecules fluctuating in space can not go through one another without chain rupture. For a system of nonphantom closed chains this means that only those chain conformations which can be transformed continuously into one another are available, which inevitably gives rise to the problem of knot entropy determination (see Section 2 for details).

5.1 Polymer chain in a 3D-array of obstacles

The 3D-model, 'polymer chain in an array of obstacles' (PCAO), can be defined as follows [43, 49, 66]. Suppose a polymer chain of length L = Na is placed between the edges of a simple cubic lattice with spacing c, where N and a are the number of monomer units in the chain and the length of the unit correspondingly. We assume that the chain cannot cross ('pass through') any edges of the lattice.

The PCAO-model can be considered as the basis for a mean-field-like self-consistent approach to the major problem of entropy calculation of ensembles of strongly entangled fluctuating chains. Namely, choose a test chain, specify its topological state and assume that the lattice of obstacles models the effect of entanglements with the surrounding chains ('background'). Neglecting the fluctuations of the background and the topological constraints which the test chain produces for itself, we lose information about the correlations between the test chain and the background. However even in the simplest case we arrive at some non-trivial results concerning the statistics of the test chain caused by topological interactions with the background. This means that for the investigation of properties of real polymer systems with topological constraints it is not enough to be able to calculate the statistical characteristics of chains in lattices of obstacles, but it is also necessary to be able to adjust any specific physical system to the unique lattice of obstacles, which is a much more complicated task.

So, let us take a closed polymer chain without volume interactions (i.e. a chain with self-intersections) in the trivial topological state with respect to the 3D lattice of obstacles. This means that the chain trajectory can be continuously contracted to a point. It is clear that because of the obstacles, the macromolecule will adopt a more compact conformation than the standard random walk without any topological constraints.

It is convenient to begin with the lattice realization of the problem. In this case the polymer chain can be represented as a closed *N*-step random walk on a cubic lattice with the length of the elementary step *a* being equal to the spacing of the array of obstacles, *c*. The general case $a \neq c$ will be considered later.

A random walk on a 3D-cubic lattice in the presence of a regular array of topological constraints produced by uncrossible strings on the dual lattice is equivalent to a free random walk on the graph — the Cayley tree with branching number z = 6.

The average space dimension $R(N) \equiv \sqrt{R^2(N)}$ of the closed unentangled *N*-step random walk is [43]:

$$R \sim a N^{1/4} \,. \tag{5.1}$$

The outline of the derivation of result (5.1) is as follows. First of all note that the Cayley tree with z branches (called latter as z-tree with z = 2D branches) plays the role of a universal covering and is just a visualization of the free group Γ_{∞} with an infinite number of generators. At the same time $\Gamma_{\infty}/\mathbb{Z}^{D} = \Gamma_{z/2}$, where $\Gamma_{z/2}$ is the free group with z generators. Writing down the recursion relations for the probability P(k, N) for an N-step random walk on the z-tree [compare to (3.24)-(3.44)], we can easily find the conditional limiting distribution for function the distribution for the function $P(k,m|N) = P(k,m)P(k,N-m)/z(z-1)^{k-1}$. Recall that P(k, m|N) gives the conditional probability distribution of the fact that two sub-chains C_1 and C_2 of lengths m and N - m have a common primitive path k under the condition that the composite chain $C_1 C_2$ of length N is closed and unentangled in regard to the obstacles:

$$P(k,m|N) \simeq \left(\frac{N}{2m(N-m)}\right)^{3/2} k^2 \exp\left(-\frac{k^2 N}{2m(N-m)}\right).$$
(5.2)

This equation enables us to get the following expressions for the mean length of the primitive path, $\langle k(m) \rangle$ of a *closed unentangled* N-link chain divided into two parts of lengths m and N - m correspondingly:

$$\left\langle k(m)\right\rangle = \sum_{k=0}^{N} k P(k, m|N) \simeq \frac{2}{\sqrt{\pi}} \sqrt{\frac{2m(N-m)}{N}} \quad (N \gg 1) \,.$$
(5.3)

The primitive path itself can be considered a random walk in a 3D space with the restriction that any step of the primitive

path should not be strictly opposite to the previous one. Therefore the mean-square distance in the space $\langle (\mathbf{r}_0 - \mathbf{r}_m)^2 \rangle$ between the ends of the primitive path of k(m) steps is

$$\langle (\mathbf{r}_0 - \mathbf{r}_m)^2 \rangle = \frac{z}{z-2} k a^2,$$
 (5.4)

where \mathbf{r}_m is the radius-vector of the link number *m* and the boundary conditions are: $\mathbf{r}_N = \mathbf{r}_0 = 0$. The mean-square gyration radius, $\langle R_g^2 \rangle$ of an *N*-step closed unentangled random walk in the regular lattice of obstacles reads

$$\langle R_g^2 \rangle = \frac{1}{2N^2} \sum_{n \neq m} \left\langle (\mathbf{r}_n - \mathbf{r}_m)^2 \right\rangle = \frac{1}{2N} \sum_{m=1}^N \left\langle (\mathbf{r}_0 - \mathbf{r}_m)^2 \right\rangle$$
$$= \frac{z}{z-2} \frac{\sqrt{2\pi}}{8} a^2 \sqrt{N}. \quad (5.5)$$

This result should be compared to the mean-square gyration radius of the closed chain without any topological constraints, $\langle R_{g,0}^2 \rangle = a^2 N/12$

The relation $R \sim N^{1/4}$ is reminiscent of the well-known expression for the dimension of a randomly branched ideal macromolecule. The gyration radius of an ideal 'lattice animal' containing N links is proportional to $N^{1/4}$. This means that both systems belong to the same universality class.

Now we turn to the mean-field calculation of the critical exponent v of a non-self-intersecting random walk in a regular lattice of obstacles [75]. Within the framework of Flory-type mean-field theory the non-equilibrium free energy, F(R), of the polymer chain of size R with volume interactions can be written as follows

$$F(R) = F_{\text{int}}(R) + F_{\text{el}}(R), \qquad (5.6)$$

where $F_{int}(R)$ is the energy of the chain self-interactions and $F_{el}(R)$ is the 'elastic', (i.e. pure entropic) contribution to the total free energy of the system. Minimizing F(R) with respect to *R* for fixed chain length, L = Na, we get the desired relation $R \sim N^{\nu}$.

Write the interacting part of the chain free energy written in the virial expansion

$$F_{\rm B3}(R) = V(B\rho^2 + C\rho^3), \qquad (5.7)$$

where $V \sim R^D$ is the volume occupied by the chain in *d*dimensional space; $\rho = N/V$ is the chain density; $B = b(T - \theta)/\theta$ and C = const > 0 are the two- and threebody interaction constants respectively. In the case B > 0 the third virial coefficient contribution to Eqn (5.7) can be neglected [73].

The 'elastic' part of the free energy $F_{el}(R)$ of an unentangled closed chain of size R and length Na in the lattice of obstacles can be estimated as follows

$$F_{\rm el}(R) \approx \text{const} + \ln P(R, N)$$

= const + ln $\int dk P(k, N) P(R, k)$, (5.8)

where the distribution function P(k, m, N) is the same as in Eqn (5.2) and P(R, k) gives the probability of the primitive path of length k having a space distance between the ends equal to R:

$$P(R,k) = \left(\frac{D}{2\pi ack}\right)^{D/2} \exp\left(-\frac{DR^2}{2ack}\right).$$
 (5.9)

Substituting Eqn (5.8) for Eqs (5.2) and (5.9) we get the following estimate

$$F_{\rm el}(R) = -\left(\frac{R^4}{a^2 c^2 N}\right)^{1/3} + o(R^{4/3}).$$
(5.10)

Equations (5.7) and (5.10) allow us to rewrite Eqn (5.6) in the form

$$F(R) \simeq B \frac{N^2}{R^D} - \left(\frac{R^4}{a^2 c^2 N}\right)^{1/3}.$$
 (5.11)

Minimization of Eqn (5.11) with respect to R for fixed N yields

$$R \sim B^{3/(4+3D)}(ac)^{2/(4+3D)}N^{\nu}, \quad \nu = \frac{7}{4+3D}.$$
 (5.12)

The upper critical dimension for this system is $D_{\rm cr} = 8$. For D = 3 Eqn (5.12) gives $R \sim N^{7/13}$

It is interesting to compare Eqn (5.12) to the critical exponent v_{an} of the lattice animal with excluded volume in *D*-dimensional space, $v_{an} = 3/(4 + D)$, which gives $v_{an} = 3/7$ for D = 3. The difference in exponents signifies that the unentangled ring with volume interactions and the non-self-intersecting 'lattice animal' belong to *different universality classes* (despite that in the absence of volume interactions they belong to the same class).

5.2 Collapsed phase of unknotted polymer

In this section we show which predictions about the fractal structure of the strongly collapsed phase of an unknotted ring polymer can be made using the concept of a 'polymer chain in an array of obstacles'.

5.2.1 'Crumpled globule' concept in the statistics of strongly collapsed unknotted polymer loops. Take a closed non-selfintersecting polymer chain of length N in the trivial topological state[†]. After a temperature decrease the formation of the collapsed globular structure becomes thermodynamically favorable [78]. Supposing that the globular state can be described in the virial expansion we introduce as usual three-body interaction twoand constants: $B = b(T - \theta)/\theta < 0$ and C = const > 0. But in addition to the standard volume interactions we would like to take into account the non-local topological constraints which obviously have a repulsive character. In this connection we express our main assertion [79].

The condition for forming a trivial knot in a closed polymer significantl changes all the thermodynamic properties of a macromolecule and leads to specific non-trivial fractal properties for a line representing the chain trajectory in a globule.

We call such structure a *crumpled* (*fractal*) globule. We prove this statement consistently describing the given crumpled structure and showing its stability.

It is well-known that in a poor solvent there exists some critical chain length, g^* , depending on the temperature and energy of volume interactions, so that chains which have lengths greater than g^* collapse. Taking a long enough chain, we define these g^* -link parts as new block monomer units (crumples of minimal scale).

[†] The fact that the closed chain cannot intersect itself causes two types of interactions: (a) volume interactions which vanish for an infinitely thin chain and (b) topological constraints which remain even for a chain of zero thickness.

Consider now a part of a chain with several block monomers, i.e. crumples of the smallest scale. This new part should again collapse in itself, i.e. should form a crumple of the next scale if other chain parts do not interfere with it. The chain of such new sub-blocks (crumples of new scale) collapses again and so on till the chain as a whole (see Fig. 14) forms the largest final crumple. Thus the procedure is completed when all initial links are united into one crumple of the largest scale. It should be noted that the line representing the chain trajectory obtained through the procedure described above resembles the 3*D*-analogue of the well known self-similar *Peano curve*.



Figure 14. (a) – (c) Subsequent stages of collapse; (d) Self-similar structure of crumpled globule segregated on all scales.

A specific feature of the crumpled globule is the fact that different chain parts are not entangled with each other, they completely fill the allowed volume of space and are 'collapsed in themselves' starting from the characteristic scale g^* . It may seem that due to space fluctuations of the chain parts all that crumples could penetrate each other with the loops, destroying the self-similar scale-invariant structure described above. However it can be shown on the basis of the PCAO-model that if the chain length in a crumple of an arbitrary scale exceeds N_e then the crumples coming in contact do not mix with each other and remain segregated in space. Recall that N_e is the characteristic distance between neighboring entanglements along the chain expressed in number of segments and, as a rule, the values of N_e lie in the range 30-300 [73].

Since the topological state of the chain part in each crumple is fixed and coincides with the state of the whole chain (which is trivial) this chain part can be regarded as an unknotted ring. Other chain parts (other crumples) function as an effective lattice of obstacles surrounding the 'test' ring — see Fig. 15. Using the results of Section 5.1 [see Eqn (5.5)] we conclude that any *M*-link ring subchain without volume interactions not entangled with any of obstacles has size



Figure 15. (a) Part of the closed unknotted chain surrounded by other parts of the same chain; (b) Unentangled ring in lattice of obstacles. The obstacles replace the effect of topological constraints produced by other part of the same chain.

 $R^{(0)}(M) \sim aM^{1/4}$. If $R^{(0)}$ is the size of an equilibrium chain part in the lattice of obstacles, the entropy loss for a ring chain, S, as a function of its size, R, reaches a maximum for $R \simeq R^{(0)}$ [see Eqn (5.10)] and the chain swelling for values of R exceeding $R^{(0)}(M)$ is entropically unfavorable. At the same time in the presence of excluded volume the following obvious inequality must be fulfilled $R(M) \ge aM^{1/3}$, which follows from the fact that density of the chain in the globular phase $\rho \sim R^3/N$ is constant. In connection with the obvious relation $R(M) > R^{(0)}(M)$ we conclude that the swelling of chains in crumples due to their mutual inter-penetration with the loops does not result in an entropy gain and, therefore, does not occur in a system with finite density. It means that the size of the crumple on each scale is of the order of its size in the dense packing state and the crumples are mutually segregated in space. These questions are discussed in detail in the work [79].

The system of densely packed globulized crumples corresponds to a chain with the fractal dimension $D_f = 3$ ($D_f = 3$ is realized from the minimal scale, g^* , up to the whole globule size). The value g^* is of order

$$g^* = N_{\rm e}(\rho a^3)^{-2}$$
, (5.13)

where ρ is the globule density. This estimate was obtained in [79] using the following arguments: $g = (\rho a^3)^{-2}$ is the mean length of the chain part between two neighboring (along the chain) contacts with other parts; consequently N_{eg} is the mean length of the chain part between topological contacts (entanglements).

Of course, for phantom chains, the Gaussian blobs of size g are strongly overlapped by others because pair contacts between monomers are screened (because of so-called θ -conditions [78]). However for non-phantom chains these pair contacts are topologically essential because chain crossings are prohibited for any value and sign of the virial coefficient.

The entropy loss connected with crumpled state formation can be estimated as follows:

$$S \simeq -\frac{N}{g^*} \,. \tag{5.14}$$

Using Eqn (5.14) the corresponding crumpled globule density, ρ , can be obtained in the mean-field approximation via the minimization of its free energy. The density of the crumpled state is less than that of the usual equilibrium state which is connected with additional topological repulsive-type interactions between crumples:

$$\rho_{\rm crump} = \frac{\rho_{\rm eq}}{1 + {\rm const}(a^6/CN_{\rm e})} < \rho_{\rm eq} \,, \tag{5.15}$$

where $\rho_{\rm eq}$ is the density of the Lifshits globule.

The direct experimental verification of the proposed selfsimilar fractal structure of the unknotted ring polymer in the collapsed phase meets some technical difficulties. One of the ways to justify the 'crumpled globule' (CG) concept comes from its indirect manifestations in dynamic and static properties of different polymer systems. The following works should be mentioned in this context:

1. The two-stage dynamics of collapse of the macromolecule after abrupt changing of the solvent quality, found in recent light scattering experiments by B Chu and Q Ying (Stony Brook) [80].

2. The notion about the crumpled structure of the collapsed ring polymer allowed the explanation [84] of the experiments on compatibility enhancement in mixtures of ring and linear chains [85], as well as the construction of a quantitative theory of collapse for *N*-isopropilacrylamide gel in poor water [83].

3. Paper [82] where the authors claim observation of a crumpled globule in numerical simulations.

5.2.2 Knot formation probability. We can also utilize the CG-concept to estimate the trivial knot formation probability for the dense phase of the polymer chain. Let us repeat that the main part of our modern knowledge about knot and link statistics has been obtained with the help of numerical simulations based on the exploitation of algebraic knot invariants (Alexander, as a rule). Among the most important results we should mention the following:

— The probability of chain self-knotting, p(N), is determined as a function of chain length N under random chain closure [1, 86]. In the work [87] (see also the recent paper [88]) the simulation procedure was extended up to chains of order $N \simeq 2000$, where the exponential asymptote of type

$$P_0 \sim \exp\left(-\frac{N}{N_0(T)}\right).$$

was found for the trivial knot formation probability for chains in good and θ -solvents. A statistical study of random knotting probability using the Vassiliev invariants was undertaken in a recent work [88]. — The knot formation probability *p* is investigated as a function of the swelling ratio α ($\alpha < 1$) where $\alpha = (\langle R_g^2 \rangle / \langle R_{g,0}^2 \rangle)^{1/2}$, $\langle R_g^2 \rangle$ is the mean-square gyration radius of the closed chain and $\langle R_{g,0}^2 \rangle = Na^2/12$ is the same for an unperturbed ($\alpha = 1$) chain (see Fig. 16 [1]). It has been shown that this probability decreases sharply when a coil contracts from the swollen state with $\alpha > 1$ to the Gaussian state with $\alpha = 1$ [8971;] and especially when it collapses to the globular state [1, 86].



Figure 16. Dependence of non-trivial knot formation probability, *p* on swelling parameter, α , in globular state. *Points* — data from Ref. [1]; *dashed line*—approximation in weak compression regime [Eqn (5.21)]; *solid line* — approximation based on the concept of crumpled globule [Eqn (5.23)].

— It has been established that in the region $\alpha > 1$ the topological constraints are screened almost completely by volume interactions [89].

— It has been shown that two unentangled chains (of the same length) even without volume interactions in the coil state repel each other as impenetrable spheres with radii of order $(\langle R_{e,0}^2 \rangle)^{1/2}$ [1, 90].

Return to Fig. 16, where the knot formation probability p is plotted as a function of the swelling ratio, α , in the globular region ($\alpha < 1$). It can be seen that in the compression region, especially for $\alpha < 0.6$, data for numerical experiments are absent. It is difficult to discriminate between different knots in the strongly compressed regime because it is necessary to calculate the Alexander polynomial for each generated closed contour. It takes of order $O(l^3)$ operations (l is the number of self-interactions in the projection). This value becomes larger as the system becomes denser.

Let us present the theoretical estimates of the non-trivial knot formation probability $p(\alpha)$ in the dense globular state ($\alpha < 0.6$) based on the CG-concept. The trivial knot formation probability under random linear chain closure, can be defined by the relation:

$$q(\alpha) = \frac{Z(\alpha)}{Z_0(\alpha)}, \quad q(\alpha) = 1 - p(\alpha), \quad (5.16)$$

where $Z(\alpha)$ is the partition function of an unknotted closed chain with volume interactions for a fixed value of swelling parameter, α , and $Z_0(\alpha)$ is that of the 'shadow' chain without topological constraints but with the same volume interactions. Both partition functions can be estimated within the framework of the mean field theory. To do so, let us write down the classic Flory-type representation for the free energy of the chain with given α (in the equations below we take the temperature $T \equiv 1$):

$$F(\alpha) = -\ln Z(\alpha) = F_{\rm int}(\alpha) + F_{\rm el}(\alpha), \qquad (5.17)$$

where

$$F_{\rm el}(\alpha) = -S(\alpha) \,. \tag{5.18}$$

Here the contributions $F_{int}(\alpha)$ from the volume interactions to the free energies of unknotted and shadow chains of the same density (i.e. of the same α) are equivalent. Therefore, the only difference concerns the elastic part of the free energy, F_{el} , or, in other words, the conformational entropy. Thus, equation (5.16) can be written in the form:

$$q(\alpha) = \exp(-F(\alpha) - F_0(\alpha)) = \exp(S(\alpha) - S_0(\alpha)).$$
 (5.19)

According to Fixmann's calculations [91] the entropy of a phantom chain $S_0(\alpha)$ ($S_0(\alpha) = \ln Z_0(\alpha)$) in the region $\alpha < 1$ can be written in the following form:

$$S_0(\alpha) \simeq -\alpha^{-2} \,. \tag{5.20}$$

In the weak compression region $0.6 < \alpha \le 1$ the probability of non-trivial knotting, $p(\alpha)$, can be estimated from the expression for the phantom ring entropy Eqn (5.20). The best fit of numerical data [1] gives us

$$p(\alpha) = 1 - A_1 \exp(-B_1 \alpha^{-2})$$
 (0.6 < $\alpha \le 1$), (5.21)

where A_1 and B_1 are numerical constants.

The non-trivial part of our problem is reduced to the estimation of the entropy of strongly contracted closed unknotted ring ($\alpha \ll 1$). Using Eqs (5.13) and (5.14) and the definition of α we find

$$S(\alpha) \simeq -\frac{1}{N_{\rm e}} \alpha^{-6} \,. \tag{5.22}$$

In the region of interest ($\alpha < 0.6$) the α^{-2} -term can be neglected in comparison with α^{-6} . Therefore, the final probability estimate has the form:

$$p(\alpha) = 1 - A_2 \exp\left(-\frac{1}{N_e}\alpha^{-6}\right) \quad (\alpha < 0.6), \qquad (5.23)$$

where A_2 and N_e are numerical constants (their values are given below).

The probabilities of the non-trivial knot formation, $p(\alpha)$, in weak and strong compression regions are shown in Fig. 16 by the dotted and solid lines respectively. The values of the constants are: $A_1 = 1.2$, $B_1 = 0.25$, $A_2 = 0.925$, $N_e = 34$; they are chosen by comparing Eqs (5.21) and (5.23) with the numerical data of Ref. [1].

5.2.3 Quasi-knot concept in the collapsed phase of unknotted polymers. Speculations about the crumpled structure of strongly contracted closed polymer chains in the trivial topological state could be partially confirmed by the results of Sections 1 and 2. The crucial question is: *why do the crumples remain segregated in a weakly knotted topological state on all scales in course of chain fluctuations*? To clarify the point we begin by defining the topological state of a crumple, i.e. the unclosed part of the chain. Of course, a mathemati-

cally strict definition of a knot can be formulated for closed (or infinite) contours exclusively. However everyday experience tells us that even an unclosed rope can be knotted. Thus, it seems attractive to construct a non-rigorous notion of a *quasi-knot* for the description of long linear chains with free ends.

Such ideas were first expressed in 1973 by I M Lifshits and A Yu Grosberg [92] for the globular state of a chain. The main conjecture was rather simple: in the globular state the distance between the ends of the chain is of order $R \sim aN^{1/3}$, being much smaller than the chain contour length $L \sim Na$. Therefore, the topological state of a closed loop, consisting of the chain backbone and the straight end-to-end segment, might roughly characterize the topological state of the chain on the whole. The composite loop should be regarded as a quasi-knot of the linear chain.

The topological state of a quasi-knot can be characterized by the knot complexity, η , introduced in Section 3 [see Eqn (3.15)]. It should be noted that the quasi-knot concept failed for Gaussian chains where the large space fluctuations of the end-to-end distance lead to indefiniteness of the quasitopological state.

Our model of a crumpled globule can now be reformulated in terms of quasi-knots. Consider the ensemble of all closed loops of length L generated with the right measure in the globular phase. Let us extract from this ensemble the loops with $\eta(L) = 0$ and find the mean quasi-knot complexity, $\langle \eta(l) \rangle$, of an arbitrary subpart of length l (l/L = h = const; 0 < h < 1) of the given loop. In the globular state the probability $\pi(\mathbf{r})$ of finding the end of the chain of length L at some point **r** inside the globule of volume R^3 is of order $\pi(\mathbf{r}) \sim 1/R^3$ being independent on \mathbf{r} (this relation is valid when $La \gg R^2$). So, for the globular phase we could roughly suppose that the loops in the ensemble are generated with a uniform distribution. Thus our system satisfies the 'Brownian bridge' condition and according to the conjecture of Section 3, Eqn (3.60), we can apply the following scale-invariant estimate for the averaged quasiknot complexity $\sqrt{\langle \eta^2(l) \rangle}$

$$\sqrt{\langle \eta^2(l) \rangle} \sim l^{1/2} = h^{1/2} L^{1/2} .$$
 (5.24)

This value should be compared to the averaged complexity $\sqrt{\langle \eta^2(l) \rangle}$ of the part of the same length *l* in the equilibrium globule created by an open chain of length *L*, i.e. without the Brownian bridge condition

$$\sqrt{\langle \eta^2(l) \rangle} \sim l = hL \,. \tag{5.25}$$

Comparing Eqs (5.24) and (5.25) we conclude that any part of an unknotted chain in the globular state is far less knotted than the same part of an open chain in the equilibrium globule, which supports our mean-field consideration presented above. Let us stress that our statement is thermodynamically reliable and is independent of the kinetics of crumpled globule formation.

6. Some 'tight' problems of probability theory and statistical physics

Usually, in the conclusion it is accepted to overview the main results and imperceptibly prepare the reader to an idea of how important the work itself is... We would like not to go by the usual way and to make a formal conclusion, because the summary of received results together with a brief exposition of ideas and methods were indicated in the introduction and some incompleteness of the account could only stimulate the fantasy of the reader.

On the contrary, we will try to pay attention to some hidden difficulties, which we persistently met on our way, as well as to formulate possible, yet unsolved problems, logically following from our consideration. Thus, we shall schematically designate borders of the given research and shall allow the reader to decide whether a given subject deserves further attention or not.

6.1 Remarks and comments on Section 2

1. The derivation of Eqs (2.57)-(2.58) assumed the passage from a model with short-range interactions to the meanfield-theory, in which all spins are supposed to interact with each others. From the topological point of view such an approximation is unphysical and requires additional verification. We believe that the considered model could be investigated with the help of conformal theories and the renormalisation group technique in the case of 'weak disorder', i.e. when a strong asymmetry exists in the choice of vertex crossings on a lattice.

2. As was shown above, the utilization of the Jones topological invariant necessarily results in the study of the thermodynamic properties of a Potts model. In the work [57] it was mentioned, that Alexander polynomials are naturally connected to a partition function of a free fermion model and, hence, to an Ising model. Probably, the use of a similar functional representation of Alexander polynomials in the framework of our disordered model would result in simpler equations, concerned with the statistical properties of Ising spin glasses.

3. All results received in this work are stuck to a model, which is effectively two-dimensional, since we are interested in the statistical properties of a planar projection of a knot in which all space degrees of freedom are thrown away and only the topological disorder is kept. Thus, physically, the model corresponds to the situation of a globular polymer chain located in a narrow two-dimensional slit. In connection with that the following question is of significant interest: how do the space fluctuations of a trajectory in a three-dimensional space modify our consideration and, in particular, answer (2.65)?

6.2 Remarks and comments on Sections 3 and 4

1. The investigation of topological properties of trajectories on multiconnected manifolds (on planes with sets of removed points) from the point of view of the conformal field theory assumes a construction of topological invariants on the basis of monodromy properties of correlation functions of appropriate conformal theories. In connection with that there is a question concerning the possibility of construction of a conformal theory with the monodromies of the locally-free group considered in this work.

2. Without any doubt the question about the relation between topological invariants design and the spectral properties of dynamic systems on hyperbolic manifolds is of extreme importance. The nature of the connection mentioned consists in the prospective dependence between knot invariants (in the simplest case, Alexander polynomials), recorded in terms of a trace of products of elements of some hyperbolic group [see expression (3.14)] and trace formulae for some dynamic system on the same group. 3. Comparing the distribution function of primitive paths μ (4.33) with the distribution function of a knot complexity of η (3.15), we can conclude that both these invariants have the same physical sense: a random walk in a covering space, constructed for lattice of obstacles, is equivalent from the topological point of view to a random walk on a Cayley tree. Thus, the knot complexity is proportional to the length of the primitive (irreducible) word, written in terms of group generators, i.e. is proportional to a geodesic length on some surface of constant negative curvature. We believe that the detailed study of this interrelation will appear rather useful for the utilization of algebraic invariants in problems concerning the statistics of ensembles of fluctuating molecules with a fixed topological state for each separate polymer chain.

3. The questions considered in Section 3 admit an interpretation in the spirit of spin glass theories, discussed at length in Section 2. Let us assume, that there is a closed trajectory of length L, which we randomly drop on a plane with a regular set of removed points. Let one point of the trajectory be fixed. The following question appears: what is the probability of finding a random trajectory in a given topological state with respect to the set of removed points? The topological state of a trajectory is a typical example of quenched disorder. According to the general concept, in order to find an appropriate distribution function (statistical sum), it is necessary to average the moments of the topological invariant over a Gaussian distribution (i.e. with the measure of trajectories on a plane). The same assumptions permit us to assume that the function $g(r, \psi)$ (Jacobian of conformal transformation) — see Fig. 12 has a sense of an ultrametric 'potential', in which the random walk takes place and where each valley corresponds to some given topological state of the path. The closer r is to 1, the higher are the barriers between neighboring valleys. Thus, all reasonably long $(La \gg c^2)$ random trajectories in such a potential will become 'localized' in some strongly entangled state, in the sense that the probability of spontaneous disentanglement of a trajectory of length La is of the order of $\exp[-\text{const} \cdot (La/c^2)]$. Probably this analogy could be useful in a normal theory of spin glasses because of the presence of a explicit expression for the ultrametric Parisi phase space [20] in terms of doubleperiodic analytic functions.

6.3 Remarks and comments on Section 5

1. We would like to express a conjecture (see also [93]) concerning the possibility of reformulation of some topological problems for strongly collapsed chains (see Section 5.4) in terms of integration over the set of trajectories with fixed fractal dimension but without any topological constraints.

We have argued that in an ensemble of strongly contracted unknotted chains (paths) most of them have fractal dimension $D_f = 3$;

We believe that almost all paths in the ensemble of lines with fractal dimension $D_f = 3$ are topologically isomorphic to a fairly simple (i.e. close to trivial) knot.

Let us recall that the problem of the calculation of the partition function for closed polymer chain with topological constraints can be written as an integral over the set Ω of closed paths with a fixed value of the topological invariant (see Section 2):

$$Z = \int_{\Omega} D_w \{r\} e^{-H} = \int \dots \int D_w \{r\} e^{-H} \delta[I - I_0], \qquad (5.26)$$

where $D_w\{r\}$ means integration with the usual Wiener measure and $\delta[I - I_0]$ cuts the paths with a fixed value of the topological invariant (I_0 corresponding to trivial knots).

If our conjecture is true, then the integration over Ω in Eqn (5.26) for the chains in the globular phase (i.e. when $La \ge R^2$) can be replaced by an integration over all paths without any topological constraints, but with a special new measure, $D_f\{r\}$:

$$Z = \int \dots \int D_f \{r\} \mathrm{e}^{-H} \,. \tag{5.27}$$

The usual Wiener measure $D_w\{r\}$ is concentrated on trajectories with fractal dimension $D_f = 2$. Instead of that, the measure $D_f\{r\}$ with fractal dimension $D_f = 3$ for the description of statistics of unknotted rings should be used.

2. We believe that the distribution of knot complexity found for some model systems can serve as a starting point in construction of a mean-field Ginsburg–Landau — type theory of fluctuating polymer chains with a fixed topology. From a physical point of view it seems to be important to emphasise the mean-field theory which takes into account the influence of topological restrictions on phase transitions in bunches of entangled directed polymers.

3. Let us note that despite a number of experimental works, indirectly testifying for the existence of a fractal globule (see section 5 and references), the direct observation of this structure in real experiments involves to significant technical difficulties and has not so far been carried out. We believe that the organization of an experiment to determine the microstructure of an entangled ring molecule in a globular phase could introduce final clarity to the question of crumpled globule existence.

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