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1992 J. Phys. A: Math. Gen. 25 4659

(http://iopscience.iop.org/0305-4470/25/17/023)

J. Phys. A: Math. Gen. 25 (1992) 4659-4672. Printed in the UK

Algebraic invariants of knots and disordered Potts model

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Received 5 November 1991

Abstract. We propose the reformulation of the Kauffman bracket invariant of the knot in terms of statistical mechanics of the 2D disordered Potts model. This allows us to put the question of the determination of knot entropy (or of the probability of an arbitrary knot formation) in terms of the usual statistical mechanics. To demonstrate the possibilities of our approach we give constructive estimation for the trivial knot formation probability for a long strongly contracted closed random path confined in a thin slit. We use the mean-field approximation for the free energy of the Potts system at the point of the transition from the paramagnetic phase to the spin-glass one.

1. Introduction

Let us consider the knot as being a closed path embedded in 3D space. Objects of such type, having different physical nature, play an important role in many branches of physics. Previously, some topological problems were investigated in connection with quantum field and string theories, 2D gravitation, polymer and DNA physics [1-3].

There exist two classes of questions in the theory of such knot-like objects: to the first class we attribute problems of construction of topological invariants, definition of topological classes, etc; the second class deals with the problems of the determination of the entropy (or available volume in the phase space) for the path with fixed topological state.

The first class of problems is quite well understood at present due to the very elegant results concerning construction of new topological invariants, such as Jones [4], and HOMFLY polynomials [5] and Kauffman bracket invariants [6]. On the other hand, the second class of problems mentioned above has been less well investigated. Very few results are known in this field:

(i) The fact of asymptotical exponential decay of the probability of trivial knot formation with increase of path length has been established by rigorous theorem [7].

(ii) The probabilities of realization of various types of a knot, as well as some other related quantities, have been numerically calculated via computer simulation technique by Vologodskii *et al* [8, 9] and followers [11-14] for randomly closed paths of strongly restricted length generated by the Monte Carlo method. The probabilities, P_i, of formation of any arbitrary type of knot labelled here as, i, (the case $i=0$ corresponds to the trivial knot) were calculated as functions of the chain length (more precisely, of the effective number of segments, l, per chain): $P_i = P_i(L/l)$. The case of an infinitely thin chain was considered first in [8]. The influence of excluded volume effects, i.e. of the chain thickness, d (in the units of the effective segment length), was

0305-4470/92/174659+14$04.50

investigated in [10]. In recent work [14] the simulation procedure was extended up to chains of lengths of order $L/l = 2000$, and the exponential asymptote of the type

$$P_0(L/l, d/l) \sim \exp(-L/L_0(d/l)) \tag{1}$$

was obtained for trivial knot probability in the limit $L \to \infty$ in accordance with the rigorous mathematical theorem [7]. As to the characteristic length $L_0(d/l)$, it increases sharply with chain thickness. Combining the results of [8] and [14], we can write down the following phenomenological expression:

$$L_0(d/l) \approx L_0(0) \exp(27 d/l). \tag{2}$$

(This formula was derived working with A V Vologodskii). Thus, the probability of any non-trivial knot formation, $1 - P_0$, grows rapidly from the swollen coil regime ($d/l \sim 1$) to the Gaussian coil regime ($d/l \to 0$) [13, 14].† Moreover, this probability increases even more sharply in the course of polymer contraction, i.e. of the coil-to-globule transition [13].

(iii) Few simple models, such as random walk near the single obstacle and random walk in the lattice of obstacles, have been analytically investigated (see, for example [15] and references therein).

In the present paper we propose to apply recent achievements in the theory of topological invariants, namely the construction of Kauffman bracket polynomials [6], for the investigation of the problem of knot entropy.

We start with the usual construction of the topological invariant, based on the consideration of 2D projection of the knot. Let us recall that the topological state of the knot can be described completely by defining the passages of intersecting parts of the path on knot projection (if the knot is turned into the so-called general position, where, on the projection, only the pair intersections remain).

Our approach is based on the following idea. The above-mentioned projection can be considered as a disordered 2D lattice. The passages can be characterized as the two-state Ising spin variables. Fixation of the topological state of the knot corresponds to the quenching of these spins. Since the Kauffman invariant can be presented as some special kind of partition function, we can reformulate our problem of knot entropy determination in terms of the thermodynamic properties of the disordered 2D Potts model. Using this formulation, we give in the present paper the constructive estimation of the trivial knot formation probability for the simplest physical system, namely, for a long closed random path confined in a thin slit.

Our calculations are restricted in many ways. We will present and discuss them in the conclusions, but just now we would like to emphasize that our paper is aimed at the presentation of topological problems as a matter of ordinary calculations widely used in statistical mechanics. This is why we adopt here only the simplest approximations. Of course, all the steps of the calculation procedure can be improved, but this seems to be rather technical problem.

The paper is organized as follows. In section 2 we describe in brief the Kauffman construction of the Jones invariant and convert the Kauffman invariant of regular isotopy written in terms of our model, to the 2D Potts model (with some special number of spin states) in quenched disorder. In section 3 we apply replica-like conjectures for

† We would like to emphasize that real polymer chains under the so-called θ-conditions, perhaps, do not behave as the ideal one (with $d = 0$) from a topological point of view: the second virital coefficient of segment–segment interaction vanishes at the θ-point, but the topological constraints nevertheless remain.

calculating the fraction of topologically trivial lattice knots in the mean-field approximation using the usual replica-broken solution for Potts glass.

2. Kauffman bracket invariant as the partition function of the Potts model in quenched disorder

2.1. Formulation of the model

To define the model, let us consider the 2D regular square lattice. We suppose that it represents the projection of our knot to the plane. The crossings on the projection are the lattice vertices; N, is their total number. Let us turn the lattice to the standard position, where each lattice bond forms angles $\pm\pi/4$ with respect to the x-axis (see figure 1). Then we have two kinds of crossings of the path projection in the vertices of our 2D lattice:

(a) 

and

(b) 

Let us attribute the values of the spin-like variables, b_i, to each lattice vertex, i, (see below). Since the lattice as a whole is produced by one single path, i.e. this lattice corresponds to the knot (but not to the link), some special boundary conditions should be valid (see figure 1). In particular N can take odd values only.

Of course there are 2^N different realizations of the lattice. Now we would like to put the following *physical* question: what is the fraction $P_0(N)$ of *unknotted* paths on the lattice among all 2^N possible paths?

2.2. Kauffman representation of Jones invariants for knots and links

To analyse the topological state of the path corresponding to a given set of $\{b_i\}$ values we are going to use the Kauffman topological invariant. Let us start with a brief

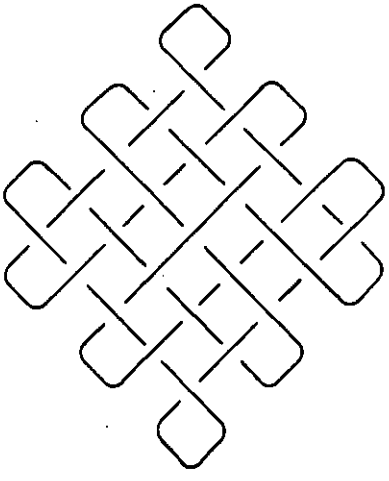

Figure 1. Lattice representation of 2D projection of the knot.

reproduction of the Kauffman construction of the topological invariant for knots and links [16, 17].

For the knot plane projection with defined passages the following Reidemeister theorem is valid [17]: different knots (or links) are topologically isomorphic to each other if and only if they can be transformed continuously into one another by means of a sequence of simple local Reidemeister moves of types 1, 2 and 3—see figure 2. Two knots are called *regular isotopic* if they are isomorphic with respect to the last two types of moves (2 and 3); meanwhile, if they are isomorphic with respect to all types of Reidemeister moves, they are called *ambient isotropic*. As can be seen from figure 2, a Reidemeister move of type 1 leads to cusp creation on the knot projection. Thus for a real physical path in a thin slit we can restrict our consideration to the case of knots of regular isotropy. At the same time it is noteworthy that all real 3D knots (links) are of ambient isotopy.

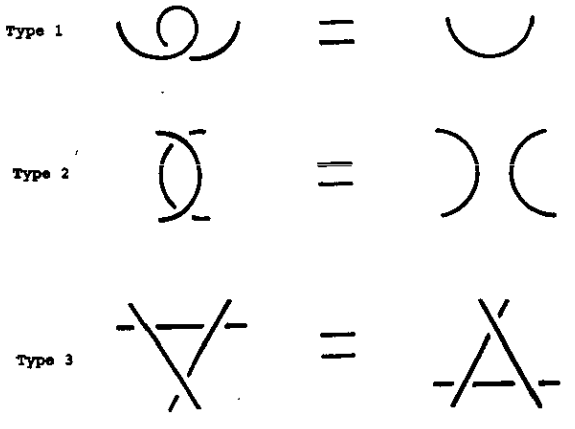

Figure 2. Reidemeister moves of types 1, 2 and 3.

The Kauffman invariant is introduced as a certain partition function, which is the sum over the set of some ghost degrees of freedom. These ghost variables correspond to two possible ways of vertex splitting:

vertical 

and

horizontal 

To each state of spin, i.e. to each way of splitting, the following statistical weights should be attributed:

- A to vertical splitting and B to horizontal if the vertex is of kind (a) and, in contrast,
- B to vertical splitting and A to horizontal for the vertex of kind (b).

For the system of N vertices there exist 2^N different microstates, each of them represents the set of splittings of all N vertices. Each microstate, S, corresponds to lattice disintegration to the system of disjoint and non-self-intersecting circles. The number of circles for microstate S let us call $|S|$.

Then the original Kauffman polynomial can be written down as follows [17]:

$$K = \sum_{\{S\}} d^{|S|-1} A^i B^j \tag{3}$$

where $\Sigma_{\{S\}}$ means summation over all possible microstates of the knot (or link) for an unchanged topological state of lattice realization, i and $j = N - i$ are the numbers of vertices with weights A and B respectively in the given realization of microstate S.

The partition function of the system described above represents the Laurent polynomial in A, B and d values. This function, for some special choice of relations among weights A, B and d, is the topological invariant of knots of regular isotopy. The proof, based on direct checking of invariance of K with respect to Reidemeister moves of types 2 and 3, shows [17] that A, B and d values obey the following relations:

$$B = A^{-1} \qquad d = -A^2 - A^{-2} \tag{4}$$

and it means that the Kauffman invariant (3) can be represented as a Laurent polynomial in A. The case $K = 1$ corresponds to paths topologically isomorphic to a trivial ring.

The state model and bracket polynomials introduced by Kauffman seem to be very special because they explore only very special geometrical rules such as summation over formal ghost degrees of freedom (splittings). Nevertheless, Kauffman showed also that bracket polynomials are deeply connected with Jones polynomials [4]. The substitution $A = t^{-1/4}$ converts the f $[A]$-Kauffman polymial of knots *of ambient isotopy* (which is invariant under all three Reidemeister moves) in A to the original Jones $V(t)$-polynomial in t [6, 17].

To emphasize the broad region of applicability of the system described above, we would note the following fact. Recently, in [18, 19] during investigation of 3D quantum field theory with Chern-Simons action, a deep connection was established between expectation values of Wilson lines with non-trivial topology and the partition function (3) determining the polynomial invariant of the knot or link.

2.3. Invariant for regular isotopic knots on square lattice and graph expansion for 2D Potts model

First of all let us rewrite (3) with conditions (4) in more readable form. To do that we define the spin variables, b_i, characterizing the natural disorder of the lattice, in the following way:

$$b_i = \begin{cases} +1 & \text{crossing of kind } (a) \\ -1 & \text{crossing of kind } (b) \end{cases}$$

meanwhile, for splittings we introduce 'ghost' spin variables, s_i, as follows:

$$s_i = \begin{cases} +1 & \text{vertical splitting} \\ -1 & \text{horizontal splitting.} \end{cases}$$

The A variable in equations (3) and (4) is arbitrary and can be considered as a complex one, therefore it would be better to write it in the following way:

$$A = \mathrm{i}\exp(\beta) \qquad -A^2 - A^{-2} = 2\cosh(2\beta). \tag{5}$$

In terms of b_i and s_i spins and β variable, the Kauffman invariant of regular isotopy reads

$$K\{b_i\} = \sum_{\{S\}} [2\cosh(2\beta)]^{|S|-1} \exp\left[(\mathrm{i}\pi/2 + \beta) \sum_i b_i s_i \right] \tag{6}$$

where the summation in the exponent runs over all N vertices and $\Sigma_{\{s\}}$ means the summation over possible states of all spins s_i.

We will show that the value $K\{b_i\}$ can be represented as the partition function of the Potts model on the square lattice with q-state spins, (q being given by $q = (A^2 + A^{-2})^2 = 4\cosh^2(2\beta)$) and with disordered interaction of nearest neighbours adsorbed by b_i variables.

To explain the Potts representation of the Kauffman invariant (6), let us recall first of all that an arbitrary configuration of simultaneous splittings represents the so-called polygon decomposition of the lattice, which looks like a densely packed system of disjoint and non-self-intersecting circles. Each concrete polygon decomposition is determined completely by the polygons' backbone—see figure 3. In turn, the configuration of backbones completely filling the lattice can be interpreted as the graph expansion for the high-temperature phase of the Potts system [20]. It is noteworthy that just this system was considered [21] in the context of the physics of 2D densely packed polymers with volume interactions, because it resembles the system of Euler walks completely filling the square lattice.

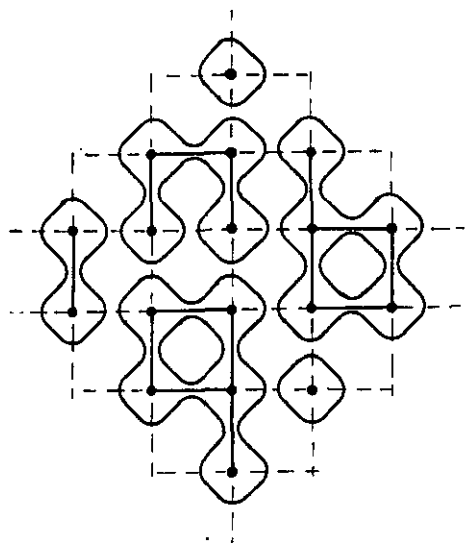

Figure 3. Splitting of the knot projection on the lattice and graph representation of microstate of 2D Potts model.

After these empirical conjectures, we are going to show, that the systematization of the microstates for the Kauffman system is the same as for the Potts model on a disordered lattice (this idea was expressed for the first time in a slightly different way in [22]; see also [23]). To be more careful, we would like to use the following definitions:

(i) Let us introduce the dual lattice, more precisely, one of the two (odd and even) possible diagonal dual lattices, as is shown in figure 3. Using the dual lattice, the disorder should be determined on the lattice *edges* (instead of the *vertices* as on the original lattice). The following definition is most suitable:

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

(or vice versa for another choice of dual lattice), i is the vertex of the original lattice, which belongs to the (kl) bond of the dual lattice.

(ii) For the given splitting let us mark the centres of elementary cells in each polygon by dots and the edges of the dual lattice connecting these centres by solid lines (see figure 3). Since the edges of the dual lattice are in one-to-one correspondence with the vertices of the original lattice, the sum $\Sigma\, s_i b_i$ in (6) can be transformed as follows:

$$\begin{aligned}\sum_i s_i b_i &= \sum_{\text{mark}} s_i b_i + \sum_{\text{nonmark}} s_i b_i \\ &= \sum_{\text{mark}}^{\text{horiz}} s_i b_i + \sum_{\text{mark}}^{\text{vert}} s_i b_i + \sum_{\text{nonmark}}^{\text{horiz}} s_i b_i + \sum_{\text{nonmark}}^{\text{vert}} s_i b_i \\ &= -\sum_{\text{mark}}^{\text{horiz}} b_{kl} - \sum_{\text{mark}}^{\text{vert}} b_{kl} + \sum_{\text{nonmark}}^{\text{horiz}} b_{kl} + \sum_{\text{nonmark}}^{\text{vert}} b_{kl} \\ &= \sum_{\text{nonmark}} b_{kl} - \sum_{\text{mark}} b_{kl}. \end{aligned} \tag{7}$$

(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

$$|S| = 2C_s + m_s - N + \chi \tag{8}$$

where χ is the so-called Euler index. Equation (8) can be easily proved in the direct way. The χ value depends on the topological class of the surface which can be covered by the given lattice, i.e. on the boundary conditions, and in the thermodynamic limit $N \gg 1$ it should be neglected, so that below we will suppose the usual equality $|S| = 2C_s + m_s - N$.

Using the conventions (i)-(iii), we can convert (6) to the form

$$\begin{aligned} K\{b_{kl}\} = \exp\left[-(\beta - \mathrm{i}\pi/2)\sum_{kl} b_{kl}\right](2\cosh(2\beta))^{-(N+1)} \\ \times \sum_{\{G\}} (2\cosh(2\beta))^{2C_s} \prod_{\text{mark}} [2\cosh(2\beta)\exp((2\beta - \mathrm{i}\pi)b_{kl})] \end{aligned} \tag{9}$$

where $\Sigma_{\{G\}}$ implies the summation over all possible configurations of marked graphs on the dual lattice.

The expression (9) is one possible representation of the so-called dichromatic polynomial [20, 24], closely connected to the high-temperature expansion of the partition function of the Potts model. Let us introduce q-state Potts spins, σ_k, in the vertices, k, of the dual lattice and define spin interactions with the usual rules:

$$\delta(\sigma_k, \sigma_l) = \begin{cases} 1 & \text{if } \sigma_k = \sigma_l,\ k \text{ and } l \text{ are nearest neighbours} \\ 0 & \text{otherwise.} \end{cases}$$

Taking into account that on the square lattice the total number of edges is even, it is easy to derive the final expression for the Kauffman invariant of regular isotopy, K, in terms of the Potts model on a disordered dual lattice:

$$K\{b_{kl}\} = (2\cosh(2\beta))^{-(N+1)} \sum_{\{\sigma\}} \exp\left\{\sum_{kl} \beta b_{kl}(4\delta(\sigma_k, \sigma_l) - 1) + \mathrm{i}\pi \sum_{kl} \delta(\sigma_k, \sigma_l)\right\} \tag{10}$$

Equation (10) has the sense of the partition function of the 2D Potts model with random nearest-neighbour interactions, proportional to $b_{kl} = \pm 1$ with some probability distribution. At the same time the set of passages $\{b_{kl}\}$ completely determines the actual topological state of the weaved carpet for the definite boundary conditions. Therefore the topological problem of the determination of the knot invariant is reduced to the usual statistical problem of calculating the well-defined partition function in quenched disorder. From this point of view, we can attribute to the variable β in (10) the sense of reverse temperature.

3. Replica broken mean-field solution for the fraction of unknotted paths

Now, using the Potts representation of the Kauffman invariant of regular isotropy (10), we would like to obtain the estimate of the simplest characteristic of the polymer chain knotting, namely the probability of trivial knot formation. Since the knot topology is described by the configuration of the field $\{b_{kl}\}$, our problem can be formulated in the following way: There exist a number of configurations of the $\{b_{kl}\}$ field corresponding to trivial knot topology. What is the fraction of these configurations among all possible ones?

We can present only the upper estimation of this probability using the following chain of inequalities:

$$\begin{pmatrix}\text{probability of}\\ \text{trivial knot}\\ \text{formation}\end{pmatrix} \leqslant \begin{pmatrix}\text{probability of}\\ \text{realization of knot}\\ \text{with } K(\beta)=1 \text{ for } \textit{all } \beta\end{pmatrix} \leqslant \begin{pmatrix}\text{probability of}\\ \text{realization of knot with}\\ K(\beta)=1 \text{ for } \textit{arbitrary } \beta\end{pmatrix} \leqslant \begin{pmatrix}\text{maximal probability}\\ \text{over all } \beta \text{ for}\\ \text{knot with } K(\beta)=1\end{pmatrix}. \tag{11}$$

The first inequality is due to the fact that the Kauffman invariant of regular isotopy, $K\{b_{kl}\}$, is not proved to be a full topological invariant. (In particular we do not know any examples of non-trivial knots with $K(\beta) \equiv 1$.) The last probability in this chain can be evaluated in the usual way:

$$Z_0(\beta) = \sum_{kl} \mathcal{P}\{b_{kl}\}\delta(K\{b_{kl}, \beta\} - 1)$$

$$= 2\int D\{b_{kl}\}\mathcal{P}\{b_{kl}\}\delta(\ln K^2\{b_{kl}, \beta\}) \tag{12}$$

where Σ_{kl} or $\int D\{b_{kl}\}$ means summation over all possible configurations of the 'crossings field' $\{b_{kl}\}$, δ function cuts out all states of the field $\{b_{kl}\}$ with $K(\beta) \equiv 1$ and $\mathcal{P}\{b_{kl}\}$ is the probability of realization of the given $\mathcal{P}\{b_{kl}\}$ configuration. The freedom of choice of the concrete value of β we shall use later in accordance with the last inequality in the chain.

The probability distribution $\mathcal{P}\{b_{kl}\}$ is determined physically by the process of knot formation. In the present paper we will restrict ourselves to the simplest suppositions, namely:

(1) we will regard different crossings to be stastically independent of each other, i.e., $\mathcal{P}\{b_{kl}\}=\Pi_{kl}P(b_{kl})$; we assume this approximation to be valid for a contracted (globular) polymer;

(2) we suppose each crossing to have two possible positions with the same probability equal to $\frac{1}{2}$, i.e.

$$P(b_{kl})=\tfrac{1}{2}(\delta(b_{kl}-1)+\delta(b_{kl}+1)). \tag{13}$$

We assume this distribution to be valid for a polymer confined in a thin slit.

Using the usual integral representation for the scalar δ function, and changing the order of integral evaluations, we can rewrite equation (12) in the following form:

$$Z_0(\beta)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}y\int\ldots\int\prod_{kl}P(b_{kl})\,\mathrm{d}b_{kl}K^{2\mathrm{i}y}\{b_{kl},\beta\}. \tag{14}$$

Thus our problem is reduced to the calculation of the non-integer complex moments of the partition function, i.e. the values of the type $\langle K^{2\mathrm{i}y}\{b_{kl},\beta\}\rangle$. An analogous problem of evaluation of non-integer moments is well known in spin-glass theory. Indeed, for the averaging of the free energy of the system, F, over a quenched random field, the replica trick is widely applied:

$$\langle F\rangle=-\lim_{n\to 0}\frac{\langle Z^n\rangle-1}{n}$$

where the moments of the partition function are usually averaged for positive integer values of n, and in the final expression analytical continuation to the case $n=0$ is performed.

We are going to act in a similar way for calculation of the non-integer complex moments of the partition function $K\{b_{kl}\}$. In other words we would like to calculate the averaged value $\langle K^{2n}\rangle$ for integer values of n. Then we put $n=\mathrm{i}y$ and calculate the remaining integral in (14) over y. Of course, this procedure in principle needs to be verified. Although our approach is no more curious than the replica approach, it would be extremely desirable to check the results of our calculations by means of computer simulations. Thus, the calculation of the value $\langle K^{2\mathrm{i}y}\rangle$, we replace with the calculation of the value $\langle K^{2n}\rangle$, where n is an integer and positive. Averaging over independent $b_{kl}=\pm 1$, we obtain

$$\begin{aligned}\langle K^{2n}\rangle&=\int\ldots\int\prod_{kl}P(b_{kl})\,\mathrm{d}b_{kl}K^{2n}\{b_{kl}\}\\&=[2\cosh(2\beta)]^{-2n(N+1)}\\&\quad\times\sum_{\{\sigma\}}\prod_{kl}\exp\left\{\ln\cosh\left[\beta\sum_{\alpha=1}^{2n}(4\delta(\sigma_k^\alpha,\sigma_l^\alpha)-1)\right]\right\}\end{aligned} \tag{15}$$

where we have used the identity $\exp\{\mathrm{i}\pi\sum_{\alpha=1}^{2n}\delta(\sigma_k^\alpha,\sigma_l^\alpha)\}=\exp(2\mathrm{i}\pi m)\equiv 1$ $(m=\{0,\pm 1,\pm 2,\ldots\})$.

Now let us suppose formally the values of the number of spin states, q, and the reverse temperature, β, to be independent variables, i.e. for a moment let us break the connection $q=4\cosh^2(2\beta)$, and suppose q to be an integer and β to be small ($\beta^2\ll 1, \beta>0$); N is odd. Then the exponent in the last expression can be expanded as a

power series in β. Keeping only the terms of order β^2, we can rewrite (15), i.e. the averaged $2n$ replica partition function of Potts model, in the following standard form:

$$\langle K^{2n}\rangle = [2\cosh(2\beta)]^{-2n(N+1)} \exp[N(2\beta^2 n^2 + q - 1)]$$
$$\times \sum_{\{\sigma_1 \ldots \sigma_{2n}\}} \exp\left\{\frac{J^2}{2}\sum_{kl}^{N}\sum_{\alpha\neq\beta}^{2n} \sigma_{ka}^{\alpha}\sigma_{kb}^{\beta}\sigma_{la}^{\alpha}\sigma_{lb}^{\beta}\right.$$
$$\left.+\left(\frac{J^2}{2}(q-2)+J_0\right)\sum_{kl}^{N}\sum_{\alpha=1}^{2n}\sigma_{ka}^{\alpha}\sigma_{lb}^{\beta}\right\} \tag{16}$$

where spin indexes a, b change in the interval $[0, q-1]$ and the connection between q and β variables can be restored, since q takes non-integer values. Thus

$$J^2 = 16\beta^2$$
$$J_0 = -8\beta^2 n \tag{17}$$
$$q = 4 + 16\beta^2 > 4.$$

According to the results of [25], the spin-glass ordering takes place and the usual ferromagnetic phase makes no essential contribution to the free energy under the condition

$$\frac{J_0}{J} + \frac{q-2}{2} < 1. \tag{18}$$

Substituting (17) into (18) it is easy to see that for all β and n the last inequality is valid. Thus, we need keep only the first term in the exponent, corresponding to interaction of the replicas.

Now we can follow the standard scheme of analysis of the replica partition function for the spin-glass-like system. For the Potts model this is exhaustively described in [25], and briefly presented in the appendix. For $q > 4$ (see equations (17)) there is the stable spin-glass solution and the transition point can be found from the condition $F_{\text{paramagnetic}} = F_{\text{spin glass}}$ which gives the following relation between J and q at the transition point:

$$1 - \frac{2}{J^2} = \frac{(q-4)^2}{3(q^2 - 18q + 42)}. \tag{19}$$

Substituting (17) into (19) and restoring the initial connection between J and q, we find the self-consistent value of reverse temperature of spin-glass transition, β_{tr}:

$$\beta_{\text{tr}} = 0.35. \tag{20}$$

This numerical value is consistent with the condition $\beta_{\text{tr}}^2 \ll 1$ implied above in the course of expansion of (16).

According to the results of [25], near the transition point the $2n$ replica free energy has the following form

$$F \simeq \frac{1}{32} Nn(q-1)^2 Q_{\text{tr}} \left(\frac{1}{\beta^2} - \frac{1}{\beta_{\text{tr}}^2}\right)^2 \tag{21}$$

where

$$Q_{\text{tr}} = \frac{2(4-q)}{q^2 - 18q + 42} > 0. \tag{22}$$

Using these equations, we can rewrite the expression for the averaged $2n$ replica Kauffman invariant $\langle K^{2n}\rangle$ in the vicinity of β_{tr} (see appendix—equation (28)) as follows:

$$\langle K^{2n}\rangle \simeq \exp\left\{ Nn^2\left[4(3+16\beta^2)^2 \ln\frac{\pi}{16\beta^2}+2\beta^2\right]\right.$$
$$-Nn\left[2(3+16\beta^2)^2\ln\frac{\pi}{16\beta^2}+2\ln 2+\beta^2\right.$$
$$\left.\left.-\frac{(3+16\beta^2)^2(\beta^{-2}-\beta_{tr}^{-2})^2\beta_{tr}^2}{(4+16\beta_{tr}^2)^2-18(4+16\beta_{tr}^2)+42}\right]+N(3+16\beta^2)\right\}. \tag{23}$$

Substituting (23) into (14) and remembering, that $n=\mathrm{i}y$, we can easily evaluate the remaining Gaussian integral over y and obtain the result for $Z_0(\beta)$. As was mentioned above, to get the simplest estimation for the probability of trivial knot formation, we use the last inequality in the chain of equations (11) which corresponds to $\beta \simeq \beta_{tr}$:

$$Z_0(\beta_{tr}) \simeq \exp(0.31N). \tag{24}$$

4. Discussion

The result of the calculations described in the previous section can be formulated as the following upper estimate for the probability of trivial knot formation:

$$P_0 \leqslant Z_0(\beta_{tr})/2^N = \exp(-N/N_0) \tag{25}$$

where the 'characteristic length' $N_0 \simeq 2.6$.

It is noteworthy that very close estimation can be obtained in the following simple way. Let us present our unknotted closed trajectory as the double folded one, i.e. in the form of a system of hairpins. Let us place now some of them along one of the lattice directions and then let us sew this system with the other hairpins along the orthogonal direction. It is clear that there are $2^{N/2} \simeq \exp(N/2.9)$ possible ways of such a sewing. The corresponding estimation for probability is of the order $2^{N/2}/2^N \simeq \exp(-N/2.9)$.

Let us recall that N is the number of crossings on the 2D knot projection. This value depends not only on the chain length L/l but also on the degree of compactness of the chain embedded in real 3D space. One can give a simple estimation of N as a function of the chain length L/l using the standard concept of swelling ratio, α, adopted in polymer physics† ($\alpha^2 = \langle R^2\rangle / Ll$, where $\langle R^2\rangle$ and Ll are the mean square end-to-end distances for swollen or collapsed real chain and ideal Gaussian chain, respectively). Actually, in our notation N is the number of lattice vertices, i.e. the number of self-crossings on the chain trace on the 2D projection. For the Gaussian chain of length L its projection is also Gaussian and $N(L) \sim (L/l)\ln(L/l)$. In the most interesting case of polymer chain compression (for example in some cavity, external field or in poor solvent; such a compressed regime is the case for most biopolymers) the term

† Under any equilibrium conditions the value of α is determined by the chain length, L, temperature, solvent quality, etc. As is well known, $\alpha \sim 1$ for the Gaussian coil, i.e. for θ-solvent, $\alpha \sim L^{1/10}$ for the swollen coil, i.e. for good solvent and $\alpha \sim L^{-1/6}$ for the globular chain, i.e. for poor solvent.

$N_{\text{independent}} \sim Ld/R^2$ should be added to $N(L)$ due to the intersections between the uncorrelated parts of the polymer chain, R^2 being the mean square gyration radius of the chain 3D fold. On the other hand, in the swollen coil regime $N(L)$ should be far smaller than that for the Gaussian regime. It can be estimated roughly as $N(L) \sim (Ll/r^2)^y (L/l) \ln(L/l)$, where $y < 1$ is some critical exponent; its calculation is beyond our consideration here. Thus as a reasonable interpolation we use the following formula:

$$N(L, R) = (\alpha^{-2})^y (L/l) \ln(L/l) + \alpha^{-2}. \tag{26}$$

Substituting this result into (25) we obtain the following estimation for the dependency of P_0 probability on the swelling ratio:

$$P_0 \leqslant \exp(\text{const}(L/l)\alpha^{-2})(L/l)^{(L/l)\alpha^{-2y}}. \tag{27}$$

Equation (27) implies that the probability of chain knotting grows dramatically with the decrease of chain size from a swollen coil to a Gaussian coil and from a Gaussian coil to a globular chain. This concept is in a good qualitative agreement with the empirical equation (1) and with the data of computer simulations [13].

As was mentioned in the introduction, our calculations are oversimplified in the following ways:

(1) The incompleteness of the Kauffman invariant makes impossible the estimation of accuracy of the results of our approach. We would like to emphasize only that in spite of the incompleteness of algebraic invariants they are much stronger than a Gaussian one and, moreover, Jones, HOMFLY and Kauffman invariants are even more powerful than Alexander ones.

(2) The knot 2D projection was supposed to be the regular lattice; we believe that our approach can be generalized for the more realistic case of a disordered lattice using the results of the theory of the Potts model on such a lattice presented in [26].

(3) We have used the simplified version of the Kauffman invariant, namely the invariant of regular isotopy; the more realistic ambient isotopy needs consideration of the directed path [17] and can be reduced to the Potts model by analogy with the problem of Hamiltonian walks on a Manhattan lattice [21].

(4) We have neglected the Euler index χ in (8), supposing the thermodynamic limit. Investigations of boundary effects and the role of topology of the underlying lattice seem to be of interest.

(5) The supposition of independence of different crossings on the knot projection seems to be acceptable for the contracted globular polymer chain. The symmetry of the two types of crossing for each lattice vertex takes place for the chain confined in a thin slit, but it is easy to omit this requirement for the general case.

(6) The procedure of analytic continuation of the averaged $2n$ replica Kauffman invariant to complex values of n needs to be verified.

(7) We have estimated the probability that the Kauffman invariant, K, is equal to 1 at one value of β only, namely at $\beta = \beta_{\text{tr}}$; for a trivial knot, K, should be equal to unity at all values of β simultaneously.

(8) We have used the self-consistent field approximation for $Z(\beta_{\text{tr}})$. This question should be analysed from the point of view of how this approximation perturbs the estimation, equation (24).

We hope that it will be possible to improve our calculations, but let us stress once more that our main aim in the present paper was to convert the determination of knot entropy (or probability) into the problem of normal statistical mechanics.

Acknowledgments

We are grateful to N Reshetikhin for introduction to the problem and A Vologodskii for useful discussions. SN would like to thank J L Lebowitz for the invitation to stay at Rutgers University and for the stimulating atmosphere during this visit.

Appendix

Performing the Hubbard-Stratonovich transformation to the scalar fields $Q_{iab}^{\alpha\beta}$ and implying the homogeneous isotropic solution of the form $Q_{iab}^{\alpha\beta} = Q_i^{\alpha\beta}\delta_{ab}$, we can write the value $\langle K^{2n}\rangle$ (equation (16)) as follows:

$$\langle K^{2n}\rangle = \exp\left\{N\left[q-1+\ln\left(\frac{\pi}{J^2}\right)2n(2n-1)(q-1)^2-\ln\left(2\cosh\left(\frac{J}{2}\right)\right)+n^2\frac{J^2}{8}\right]\right\}$$
$$\times\sum_{\{\sigma\}}\int\prod \mathrm{d}Q_i^{\alpha\beta}\exp\left\{-\int H\{Q_i^{\alpha\beta}\}\,\mathrm{d}^2x\right\} \tag{28}$$

where

$$H\{Q^{\alpha\beta}\} = (q-1)\left[\frac{1}{4}\left(\frac{2}{J^2}-1\right)\sum_{\alpha\neq\beta}(Q^{\alpha\beta})^2-\frac{1}{6}\sum_{\alpha\neq\beta\neq\gamma}Q^{\alpha\beta}Q^{\beta\gamma}Q^{\gamma\alpha}\right.$$
$$-\frac{q-2}{12}\sum_{\alpha\neq\beta}(Q^{\alpha\beta})^2-\frac{q-2}{4}\sum_{\alpha\neq\beta\neq\gamma}(Q^{\alpha\beta})^2Q^{\beta\gamma}Q^{\gamma\alpha}$$
$$\left.-\frac{1}{8}\sum_{\alpha\neq\beta\neq\gamma\neq\delta}Q^{\alpha\beta}Q^{\beta\gamma}Q^{\gamma\delta}Q^{\delta\alpha}-\frac{q^2-6q+6}{48}\sum_{\alpha\beta}(Q^{\alpha\beta})^4\right]. \tag{29}$$

In [25] it was shown that the mean-field replica-symmetry-broken ansatz of equations (28) and (29) correspond to the first level of Parisi scheme for Ising spin glass and can be presented in the form

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

Substituting this ansatz into (16) the mean-field solution (equation (23)) can easily be found.

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