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Entangled polymer rings in 2D and confinement

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Abstract. The statistical mechanics of polymer loops entangled in the two-dimensional array of randomly distributed obstacles of infinite length is discussed. The area of the loop projected onto the plane perpendicular to the obstacles is used as a collective variable in order to re-express a (mean-field) effective theory for the polymer conformation. It is shown explicitly that the loop undergoes a collapse transition to a randomly branched polymer with $R \propto lN^{1/4}$.

1. Introduction

The statistical mechanics of entangled polymers, i.e. polymer chains under topological constraints is a generally unsolved problem. The main difficulty is to specify distinct topological states of the polymer chain. Closed polymers, or polymer loops appear to be a much simpler system as they are either linked (with themselves or with one another) or unlinked. Linear chains, however, can always be disentangled. On a shorter time scale than the disentanglement time though, it seems justified to define topological states 'on the average', using the same formalism as for polymer loops.

Mathematically, the problem of specifying topological states of polymer loops is equivalent to the classification problem for knots and links [1]. Since the mid-eighties considerable progress has been made following Jones [2] as various new knot polynomials have been discovered (for a review on knots see [1]).

For an analytical theory of the polymer entanglement problem, the algebraic form of these invariants is not suitable (see section 5 for new perspectives). They are generally expressed in one, two or three variables which appear in the defining relations (known as skein relations). There is no immediate relation of these variables to the polymer conformation and consequently there is no reasonable way to couple the knot invariant to a statistical weight for a given polymer conformation. Algebraic knot theory seems to be applicable for the theory of entangled directed polymers [3], and certainly does so in computer simulations (e.g. [4–7]).

The degrees of freedom appearing in the statistical weight of a given polymer conformation are usually expressed in terms of segment positions $\boldsymbol{r}(s)$ which is a mapping $[0, N] \to R^d$ from the contour variable s to d-dimensional space [8]. For $d = 3$, one invariant showing an explicit dependance on these variables is the the so called Gauss invariant for two given closed loops C_α and C_β parametrized by $\boldsymbol{r}_\alpha(s)$, $\boldsymbol{r}_\beta(s)$

$$\Phi(C_\alpha, C_\beta) = \frac{1}{4\pi} \oint_{C_\alpha} \mathrm{d}s \oint_{C_\beta} \mathrm{d}s' \, \dot{\boldsymbol{r}}_\alpha(s) \wedge \dot{\boldsymbol{r}}_\beta(s') \cdot \frac{\boldsymbol{r}_\alpha(s) - \boldsymbol{r}_\beta(s')}{|\boldsymbol{r}_\alpha(s) - \boldsymbol{r}_\beta(s')|^3} \tag{1}$$

which is invariant with respect to continuous deformations of the loops, was first used by Edwards to discuss entangled polymer loops [9, 10]. It is also called the Gaussian linking

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number (sometimes also the winding number). As Edwards already noted, in $d = 3$ the Gauss invariant does not uniquely specify a given link. There is, in fact, an infinite series of higher order link invariants that appear quite naturally in a perturbative expansion of a field-theoretical representation of the generalized Jones polynomial [11, 12]. For special cases such as a random walk winding around an obstacle of infinite length, rigorous results can be obtained using the Gauss invariant, as it has been discussed in detail by Wiegel [13].

As even the Gauss invariant is difficult to handle mathematically for a rigorous treatment of the three-dimensional entanglement problem, many mean-field-type arguments have been used [8] for a rough characterization of the topological states. Tube models for entangled polymer melts are the most prominent approaches, which seem to lead to contradictory conclusions for open linear polymer chains and closed ring polymers. Therefore more detailed knowledge about the topological states of polymer systems is needed. In general, this seems to be a difficult task, and to overcome mathematical and conceptual difficulties simple and model-type situations must be studied, to learn about more complex ones. Only recently more detailed situations are under consideration by using the path integral approach and the Gaussian linking number constraint [14].

To give an example that shows the complexity of the structure of the theory we mention the following development: the 'easiest' topological arrangement of closed polymer rings is the non-concatenated melt of rings, since all winding numbers between different rings are zero. Scaling arguments for the typical size of a ring, $R \propto N^{\nu}$, have been put forward [15], giving an estimate of $\nu = \frac{2}{5}$. This result seems to be in rough agreement with computer simulation [16] (see also [17, 18]). The more detailled analytical many chain theory in [14] supported the scaling result, although the theory is more involved than simple scaling.

An important step forward to formulate the problem by field-theoretic methods was made by Brereton and Shah [19]. A test loop in the melt was considered that is entangled with many other chains. The resulting theory can be mapped to Euclidean electrodynamics in $3 = 2+1$ dimensions coupled to a $\mathrm{O}(n)\phi^4$ theory for the conformation of a self-avoiding walk (in the limit $n \to 0$ [20, 21]). It is the basis for work by Nechaev and Rostiashvili [22] in two dimensions.

As a matter of fact, for $d = 2$ the Gauss invariant becomes rigorous for 'simple', i.e. non-self-intersecting loops. It reads

$$G_i(C) = \frac{1}{2\pi} \oint_C \mathrm{d}s\, \dot{\boldsymbol{r}}(s) \cdot \nabla(\ln|\boldsymbol{r}(s) - \boldsymbol{r}_i|) \wedge \boldsymbol{\eta}. \tag{2}$$

Here the vector $\boldsymbol{r}(s)$ represents the segment positions of the polymer loop in the plane. In equation (1), the role of the polymers entangled with the loop is taken formally by obstacles at the positions $\boldsymbol{r}_i$. $\boldsymbol{\eta}$ is a unit vector perpendicular to plane [22]. $G_i(C)$ is also called the winding number of the loop. Equation (2) may also be expressed in terms of a Cauchy integral in the complex plane and is related to the oriented area of the loop in the plane [23]. For so-called 'complex' loops, i.e. loops with points of self-intersection, special care is needed as the invariant equation (2) might give zero although the loops are entangled (see Rostiashvili *et al* [24]).

The theoretical basis of this paper is the field theory by Brereton *et al* [19]. It was studied by Nechaev and Rostiashvili [22, 24] in order to discuss the behaviour of a polymer loop in an array of randomly distributed parallel line obstacles [22, 24] whose spatial distribution is quenched. A first-order transition for critical length N_{c} for the polymer loop was found when the quenched average over the winding number distribution was taken. It has been interpreted as a collapse transition (for $N > N_{\mathrm{c}}$) to an octopus conformation resembling a randomly branched polymer with no self-interaction with an end-to-end vector scaling of

the size $R \propto N^{1/4}$, where N is the total length of the ring [25–27].

In fact, in the work below it will be shown explicitly (within the approximation made in [22]) that the conjectured scaling behaviour is valid even for annealed disorder with respect to the spatial distribution of obstacles. This assumption is reasonable if the obstacles are supposed to represent other polymers entangled with a given loop, and was also made in the original theory by Brereton *et al* [19]. We will obtain the same free energy (in the mean-field approximation) as Nechaev *et al* [22]—yet in a physically more transparent form—and consequently, the same transition behaviour.

We will exploit the fact that the interaction due to the topological constraint is a so-called 'area law', i.e. it is proportional to the area enclosed by the loop. This is an exact result known in quantum field theory in the context of Wilson loops and the confinement problem for abelian gauge fields (see e.g. [28]). Therefore, the area of the loop is equal to first order to the effective potential found in [22] and is dependent on the conformational fields and topological quantities.

The paper is organized as follows. In section 2 we clarify that the effective interaction is proportional to the area being the order parameter of the problem. In section 3, we show on the level of polymer field theory how the area appears in the effective interaction and how it depends on the conformational fields (in the mean-field approximation). The critical behaviour of the order parameter as a function of topological parameters is discussed. A new upper bound for the range of stability for the mean-field solution (in the replica-symmetric case) is found. In section 4, the conjectured scaling like for randomly branched polymers is shown, and in section 5 a brief outlook on the complete, i.e. $d = 3$ entanglement problem is given.

2. The area as the order parameter

In the work of Nechaev and Rostiashvili [22] it is not evident at first sight that the first-order phase transition caused by topological disorder corresponds to a classical collapse transition, similarly to the case of a polymer immersed in a poor solvent [21]. We expect indeed structural differences between a collapsed chain in poor solvent and a 'collapsed ring' under topological constraints.

In order to understand better the nature of the phase transition, it is desirable to introduce an order parameter that fits to the problem, which is in our case the area of the 2D projection of a *simple* loop. Following Cardy [29] we use the covariant expression

$$A = \int \mathrm{d}^2\boldsymbol{x} \int \mathrm{d}^2\boldsymbol{x}' \, \langle A_\mu(\boldsymbol{x}) A_\nu(\boldsymbol{x}') \rangle J_\mu(\boldsymbol{x}) J_\nu(\boldsymbol{x}') \tag{3}$$

where $\boldsymbol{x} = (x, y)$ is a vector in two-dimensional Euclidean space. Variables J_μ are the polymer current densities or tangent vector densities $J_\mu(\boldsymbol{x}) = \int_0^N \mathrm{d}s \, \dot{r}_\mu(s) \delta(\boldsymbol{x} - \boldsymbol{r}(s))$ where N is the chemical length of the chain. The gauge fields A_μ are of the $U(1)$ type and their correlator is gauge dependent. Using the gauge $A_1 = 0$ it reads as $\langle A_\mu(\boldsymbol{x}) A_\nu(\boldsymbol{x}') \rangle = -\frac{1}{2} \delta_{\mu 0} \delta_{\nu 0} |y - y'| \delta(x - x')$, and it becomes obvious that the right-hand side of (3) is indeed an area.

When using expression (3) for the definition of the area some care is needed. The above equation is valid only for non-self-intersecting loops which will be the scope of the present treatment. In the case of self-intersections, negative area contributions may cancel positive ones giving a total zero area (see above the discussion following (2)).

We next recall the incorporation of constraint (2) in the partition sum for the loop [22].

For a fixed number of obstacles c enclosed by the loop the partition function is given by

$$Z(c) = \int \mathcal{D}\boldsymbol{r}(s)\delta(\boldsymbol{r}(N)-\boldsymbol{r}(0))\delta\left(c - \oint_C \mathrm{d}s\,\dot{\boldsymbol{r}}(s)\cdot\boldsymbol{A}\right) \times \exp\left(-\frac{1}{l^2}\oint \mathrm{d}s\,\dot{\boldsymbol{r}}^2(s) - \frac{a^2}{2}\oint \mathrm{d}s \oint \mathrm{d}s'\,\delta(\boldsymbol{r}(s)-\boldsymbol{r}(s'))\right) \tag{4}$$

where l is the Kuhn segment length, and a^2 is the 2D excluded volume. From equation (2) we see that the gauge field $\boldsymbol{A}$ is given by $\sum_{i=1}^{N}\nabla(\ln|\boldsymbol{r}(s)-\boldsymbol{r}_i|)\wedge\boldsymbol{\eta}$ so that the delta function fixes the winding number in terms of the 2D Gauss invariant. It satisfies $\nabla\cdot\boldsymbol{A}=0$ and $\nabla\wedge\boldsymbol{A}=\boldsymbol{\eta}(\varphi(\boldsymbol{r})-\varphi_0)$ where $\varphi(\boldsymbol{r})=\sum_i\delta(\boldsymbol{r}-\boldsymbol{r}_i)$ and φ_0 is the mean density of obstacles in the xy-plane.

In contrast to [22] we suppose that first, the spatial distribution of obstacles is annealed whereas second, the distribution of winding numbers c, i.e. obstacles enclosed by the loop is quenched. The first assumption is reasonable if the obstacles are to represent other polymers (of infinite length) entangled with the loop, which is an important feature of a model that projects the original three-dimensional entanglement problem to two dimensions.

The second assumption is clear from the fact that once a given winding number c is fixed for the loop, it should remain fixed in the process of averaging over both the conformations of the loop and the positions of obstacles. As a consequence, we take the *annealed* average over the spatial distribution of obstacles to be the Gaussian

$$P(\varphi(\boldsymbol{r})) \sim \exp\left(-\frac{1}{2\varphi_0}\int \mathrm{d}^2\boldsymbol{x}\,(\varphi(\boldsymbol{r})-\varphi_0)^2\right) \sim \exp\left(-\frac{1}{2\varphi_0}\int \mathrm{d}^2\boldsymbol{x}\,(\nabla\wedge\boldsymbol{A})^2\right). \tag{5}$$

The *quenched* distribution of the number of obstacles c is assumed to be a Gaussian with mean c_0 and dispersion Δ_c,

$$P(c) \sim \exp\left(-\frac{(c-c_0)^2}{2\Delta_c}\right) \tag{6}$$

and is used to average the free energy.

The winding number constraint in the partition sum is expressed by a Fourier transform introducing the variable g, a chemical potential conjugate to c:

$$\delta\left(c - \oint_C \mathrm{d}s\,\dot{\boldsymbol{r}}(s)\cdot\boldsymbol{A}\right) = \int \frac{\mathrm{d}g}{2\pi}\,\mathrm{e}^{\mathrm{i}gc - \mathrm{i}g\oint_C \mathrm{d}s\,\dot{\boldsymbol{r}}(s)\cdot\boldsymbol{A}}. \tag{7}$$

The distribution of winding numbers $P(c)$ may then be transformed into a distribution $P(g)$ for the chemical potential [22]. For later purposes it is crucial to note that the g^2 averaged over $P(g)$ is

$$[g^2]_g = \frac{1}{\Delta_c}\left(1-\frac{c_0^2}{\Delta_c}\right). \tag{8}$$

The partition function is now expressed in terms of g. After averaging over the the spatial distribution of obstacles, it reads

$$\langle Z(g)\rangle_{\boldsymbol{A}} = \mathcal{N}\int \mathcal{D}\boldsymbol{A}\,\delta(\nabla\cdot\boldsymbol{A})\int \mathcal{D}\boldsymbol{r}(s)\,\delta(\boldsymbol{r}(N)-\boldsymbol{r}(0)) \times \exp\left(-\frac{1}{2\varphi_0}\int \mathrm{d}^2\boldsymbol{x}\,(\nabla\wedge\boldsymbol{A})^2 - \mathrm{i}g\oint_C \mathrm{d}s\,\dot{\boldsymbol{r}}(s)\cdot\boldsymbol{A} - \frac{1}{l^2}\oint \mathrm{d}s\,\dot{\boldsymbol{r}}^2(s) - \frac{a^2}{2}\oint \mathrm{d}s\oint \mathrm{d}s'\,\delta(\boldsymbol{r}(s)-\boldsymbol{r}(s'))\right) \tag{9}$$

where $\mathcal{N}$ is a normalization factor for the average over the gauge fields.

Carrying out the integral over the gauge fields $\boldsymbol{A}$, one obtains

$$\langle Z(g)\rangle_{\boldsymbol{A}} = \int \mathcal{D}\boldsymbol{r}(s)\delta(\boldsymbol{r}(N)-\boldsymbol{r}(0)) \times \exp\left(-\frac{\varphi_0 g^2}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{x}'\,\langle A_\mu(\boldsymbol{x})A_\nu(\boldsymbol{x}')\rangle J_\mu(\boldsymbol{x})J_\nu(\boldsymbol{x}') -\frac{1}{l^2}\oint \mathrm{d}s\,\dot{\boldsymbol{r}}^2(s)-\frac{a^2}{2}\oint \mathrm{d}s\oint \mathrm{d}s'\,\delta(\boldsymbol{r}(s)-\boldsymbol{r}(s'))\right). \tag{10}$$

The resulting term in the exponential is proportional to the area of the loop. In fact, the interaction reads as

$$\beta H_{\mathrm{int}} = \frac{\varphi_0 g^2}{2}A. \tag{11}$$

If we replace g^2 by its mean value (8) we obtain

$$\beta H_{\mathrm{int}} = \frac{\varphi_0}{2\Delta_{\mathrm{c}}}\left(1-\frac{c_0^2}{\Delta_{\mathrm{c}}}\right)A. \tag{12}$$

The approximation considered in [22] is limited to range of values for φ_0 and Δ_{c} which require the factor in front of A to be always positive (as to further restrictions on the set of values for these parameters where a mean-field solution is valid, see the end of section 3). Consequently, in order to minimize its energy the loop tends to collapse, decreasing its area.

3. The area as a collective variable and polymer field theory

We now introduce the area explicitly as collective variable in the partition sum using $1=\int \mathrm{d}A\,\delta(A-\hat{A})$ where $\hat{A}$ is given by (3). After transforming the delta function and some standard manipulations we then have

$$\langle Z(g)\rangle_{\boldsymbol{A}} = \mathcal{N}\int \mathrm{d}A\int \mathrm{d}\alpha\int \mathcal{D}\boldsymbol{r}(s)\delta(\boldsymbol{r}(N)-\boldsymbol{r}(0)) \times \exp\left(\mathrm{i}\alpha A-\left(\mathrm{i}\alpha+\frac{\varphi_0 g^2}{2}\right)\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{x}'\,\langle A_\mu(\boldsymbol{x})A_\nu(\boldsymbol{x}')\rangle J_\mu(\boldsymbol{x})J_\nu(\boldsymbol{x}') -\frac{1}{l^2}\oint \mathrm{d}s\,\dot{\boldsymbol{r}}^2(s)-\frac{a^2}{2}\oint \mathrm{d}s\oint \mathrm{d}s'\,\delta(\boldsymbol{r}(s)-\boldsymbol{r}(s'))\right). \tag{13}$$

Let us define $\mathrm{i}\tilde{\alpha}=\mathrm{i}\alpha+\varphi_0 g^2/2$ for a moment, and express α in terms of $\tilde{\alpha}$, and make the change $\alpha\to\tilde{\alpha}$ in the integration variable. This procedure looks strange at first glance, because the new integration variable $\tilde{\alpha}$ now becomes complex. Below we show that this is not a serious problem for the purpose of this paper. After these manipulations we obtain

$$\langle Z(g)\rangle_{\boldsymbol{A}} = \mathcal{N}\int \mathrm{d}A\int \mathrm{d}\tilde{\alpha}\int \mathcal{D}\boldsymbol{r}(s)\delta(\boldsymbol{r}(N)-\boldsymbol{r}(0)) \times \exp\left(-\frac{\varphi_0 g^2}{2}A+\mathrm{i}\tilde{\alpha}A-\mathrm{i}\tilde{\alpha}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{x}'\,\langle A_\mu(\boldsymbol{x})A_\nu(\boldsymbol{x}')\rangle J_\mu(\boldsymbol{x})J_\nu(\boldsymbol{x}') -\frac{1}{l^2}\oint \mathrm{d}s\,\dot{\boldsymbol{r}}^2(s)-\frac{a^2}{2}\oint \mathrm{d}s\oint \mathrm{d}s'\,\delta(\boldsymbol{r}(s)-\boldsymbol{r}(s'))\right). \tag{14}$$

In the next step, the term depending on the gauge field correlator is expressed in terms of a Gaussian integration:

$$\langle Z(g)\rangle_{\boldsymbol{A}} = \mathcal{N}\int \mathcal{D}\boldsymbol{A}\delta(\nabla\cdot\boldsymbol{A})\int \mathrm{d}A\int \mathrm{d}\tilde{\alpha}\int \mathcal{D}\boldsymbol{r}(s)\delta(\boldsymbol{r}(N)-\boldsymbol{r}(0))$$
$$\times\exp\Bigg(-\frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\,(\nabla\wedge\boldsymbol{A})^2 - \mathrm{i}e\int \mathrm{d}^2\boldsymbol{x}\,A_\mu(\boldsymbol{x})J_\mu(\boldsymbol{x}) - \frac{\varphi_0 g^2}{2}A + \mathrm{i}\tilde{\alpha}A$$
$$-\frac{1}{l^2}\oint \mathrm{d}s\,\dot{\boldsymbol{r}}^2(s) - \frac{a^2}{2}\oint \mathrm{d}s\oint \mathrm{d}s'\,\delta(\boldsymbol{r}(s)-\boldsymbol{r}(s'))\Bigg) \tag{15}$$

where e is a shorthand notation for $\sqrt{2\mathrm{i}\tilde{\alpha}}$ and is the 'coupling constant' of the analoguous Wilson loop problem, well known in quantum field theory [28]. We note again that e is complex, but it will turn out below that this is not a problem. The partition sum has now a structure similar to the original formulation considered in [22] and is suitable for a field-theoretic treatment. Note that the interaction $\frac{1}{2}\varphi_0 g^2 A$ has been completely separated from the conformational average and the average over the distribution of obstacles. The area is related to the conformation directly only via the coupling constant e or $\tilde{\alpha}$, respectively. In fact, the problem will be first examined for a given realization of these variables. In the last step, the parameter $\tilde{\alpha}$ will be eliminated to give back the dependance of the area on the conformation of the loop.

To proceed further, we consider only consider the functional intregation over the positions $\boldsymbol{r}(s)$, i.e. the partition function

$$Z(e;[\boldsymbol{A}]) = \mathcal{N}\int \mathcal{D}\boldsymbol{r}(s)\delta(\boldsymbol{r}(N)-\boldsymbol{r}(0))\exp\Bigg(-\frac{1}{l^2}\oint \mathrm{d}s\,\dot{\boldsymbol{r}}^2(s)$$
$$-\frac{a^2}{2}\oint \mathrm{d}s\oint \mathrm{d}s'\,\delta(\boldsymbol{r}(s)-\boldsymbol{r}(s')) - \mathrm{i}e\int \mathrm{d}^2\boldsymbol{x}A_\mu(\boldsymbol{x})J_\mu(\boldsymbol{x})\Bigg).$$

The partition function (16) describes the statistics of the loop for given external 'magnetic' field $\boldsymbol{A}$. It is formally the same partition function as $Z(g)$ in (9), and can be treated in terms of the n vector ϕ^4 theory in the limit $n\to 0$ [20] according to [19, 22]. To obtain the field theory, the following standard steps have to be carried out. First, the two-dimensional excluded volume interaction is expressed in terms of a Gaussian average over a pseudopotential [8]. Then, one has to consider the Green's function of the loop for a given realization of the gauge field $\boldsymbol{A}$ and the pseudopotential for the excluded volume. The Green's function is expressed in terms of a Gaussian field theory. The averages over the pseudopotential and the gauge field lead to consider an n-fold replicated field theory (see [22] for technical details). When the average over the pseudopotential is carried out, one finally obtains

$$Z_n(e;[\boldsymbol{A}]) = \prod_{i=1}^{n}\Bigg(\int \mathcal{D}\phi_i\int \mathcal{D}\phi_i^*\Bigg)\exp\Bigg(-\int \mathrm{d}^3\boldsymbol{R}\,\mathcal{H}[\boldsymbol{A},\phi_i,\phi_i^*]\Bigg) \tag{16}$$

with

$$\mathcal{H}[\boldsymbol{A},\phi_i,\phi_i^*] = \sum_{i=1}^{n}\phi_i\left(m^2 - \frac{l^2}{4}(\nabla_\perp - \mathrm{i}e\boldsymbol{A})^2 - \frac{l^2}{2}\nabla_\parallel^2\right)\phi_i^* + \frac{La^2}{4}\sum_{i,j=1}^{n}\phi_i\phi_i^*\phi_j\phi_j^*. \tag{17}$$

The fields ϕ_i are replica fields for polymer loops. The model has been embedded into three-dimensional space, so the excluded volume term is the embedded two-dimensional one with L being the mean size of the polymer in the z direction.

Now, the average over the obstacle distribution is taken as follows:

$$\langle Z_n(e;[\boldsymbol{A}])\rangle_{\boldsymbol{A}} = \mathcal{N}\int \mathcal{D}\boldsymbol{A}\delta(\nabla\cdot\boldsymbol{A})Z_n(e;[\boldsymbol{A}])\exp\left(-\tfrac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\,(\nabla\wedge\boldsymbol{A})^2\right). \tag{18}$$

The gauge fields are integrated out following [22]. To simplify the algebra, the Landau gauge is used. One obtains an effective action with the one-loop correction being given by

$$\mathcal{H}_{1\text{-loop}} = \int \frac{\mathrm{d}^2\boldsymbol{k}}{(2\pi)^2}\log\left(k^2 + Q\sum_i \phi_i\phi_i^*\right) \tag{19}$$

with $Q = \frac{1}{2}l^2e^2 = \mathrm{i}\tilde{\alpha}l^2$. As Q is complex, a complex logarithm in (19) has to be considered. It is easily shown that by restricting the analysis to one Riemannian sheet, the integral can be evaluated straightforwardly under the assumption that the ϕ_i are constant in space. This assumption is consistent with the result that the topologically restricted chain forms a dense object with very small density fluctuations. This corresponds indeed to the assumption of $\phi_i \approx$ constant.

In [22] the replica-symmetric case is studied because only in this case the effective potential approximation can be used. (For the details of solving integral (19) and the renormalization procedure we refer the reader to [22]).

In this case, we now approximate $\sum_i \phi_i\phi_i^* = n\phi\phi^*$. After renormalization according to [22] one obtains

$$\langle Z_n(e = e(\tilde{\alpha});[\boldsymbol{A}])\rangle_{\boldsymbol{A}} = \exp\left(-\int \mathrm{d}^3\boldsymbol{R}\,\mathcal{L}_{\text{eff}}\right) \tag{20}$$

with an effective Lagrangian

$$\mathcal{L}_{\text{eff}} = in\tilde{\alpha}\left(-\frac{l^2}{4\pi}|\phi|^2\ln(\frac{|\phi|^2}{M^2}) + \frac{l^2}{2\pi}|\phi|^2\right) + n(m^2 - La^2M^2)|\phi|^2 + n\frac{La^2}{4}|\phi|^4 \tag{21}$$

where M is an arbitrary subtraction point appearing due to the renormalization procedure. Because the fields ϕ are now constant in space, the integration in (21) gives simply a constant volume factor V. From equation (20) one obtains the contribution to the free energy as a function of $\tilde{\alpha}$ which is conjugate to the area. Devided by the system volume, it is given using the standard formula:

$$\begin{aligned} f(\tilde{\alpha}) = \frac{\mathcal{F}(\tilde{\alpha})}{V} &= \frac{1}{V}\frac{\partial}{\partial n}\langle Z_n(e = e(\tilde{\alpha});[\boldsymbol{A}])\rangle_{\boldsymbol{A}}|_{n=0} \\ &= \mathrm{i}\tilde{\alpha}\left(-\frac{l^2}{4\pi}|\phi|^2\ln\left(\frac{|\phi|^2}{M^2}\right) + \frac{l^2}{2\pi}|\phi|^2\right) + (m^2 - La^2M^2)|\phi|^2 + \frac{La^2}{4}|\phi|^4. \end{aligned} \tag{22}$$

The next step is to transform back from $\tilde{\alpha}$ to the area A. This is done by a Legendre transfrom (or by a Fourier transform of the partition function). Finally one has to add the area term $\frac{1}{2}\varphi_0 g^2 A$ to the free energy which yields the partition function averaged over the distribution of obstacles:

$$\langle Z(g)\rangle_{\boldsymbol{A}} = \int \mathrm{d}A\,\delta\left(A + \frac{l^2}{4\pi}V|\phi|^2\ln\left(\frac{|\phi|^2}{M^2}\right) - \frac{l^2}{2\pi}V|\phi|^2\right)\mathrm{e}^{-Vf(A,g)} \tag{23}$$

with the free energy density

$$f(A,g) = \frac{\varphi_0 g^2}{2V}A + (m^2 - La^2M^2)|\phi|^2 + \frac{La^2}{4}|\phi|^4. \tag{24}$$

The set of equations (23) and (24) is the fundamental result of this paper. The free energy density $f(A,g)$ is indeed the area law plus the renormalized action for the self-avoiding

walk loop. Integrating over the area gives back the result of [22] for the free energy density in terms of conformational fields and g only. Averaging the free energy density in (24) over the distribution of winding numbers using (8) one finally obtains

$$f(A) = [f(A,g)]_g = \frac{\varphi_0}{2V\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right)A + (m^2 - La^2M^2)|\phi|^2 + \frac{La^2}{4}|\phi|^4. \tag{25}$$

As a consequence of (25), the essential result we have obtained here is the dependance of the area on the fields ϕ in the mean-field approximation expressed in the delta function of (23).

$$A = -\frac{l^2}{4\pi}V|\phi|^2 \ln\left(\frac{|\phi|^2}{M^2}\right) + \frac{l^2}{2\pi}V|\phi|^2. \tag{26}$$

Introducing the segment density $\rho = |\phi|^2$ and choosing $M^2 = L^{-3}$ we then obtain

$$A = V\frac{l^2}{2\pi}(\rho - \tfrac{1}{2}\rho\ln(\rho L^3)). \tag{27}$$

Let us now investigate the behaviour of the area when the collapse transition occurs. It has been studied in detail in [22], so we just mention the results. In fact, the collapse transition takes place at the critical length N_c which is given by (see [22], but with the factor $1/32\pi$ replaced by $1/8\pi$):

$$\frac{1}{N_c} = \frac{l^2}{8\pi}\frac{\varphi_0}{\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right)\ln\left[\left(\frac{L}{a}\right)^2\frac{l^2}{4\pi}\frac{\varphi_0}{\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right)\right]. \tag{28}$$

As $1/N_c$ is always positive, the condition

$$\left(\frac{L}{a}\right)^2\frac{l^2}{4\pi}\frac{\varphi_0}{\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right) > 1 \tag{29}$$

follows for the stability of the mean-field solution. At $N = N_c$ the segment density is

$$\rho_c = \frac{1}{La^2}\frac{l^2}{4\pi}\frac{\varphi_0}{\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right). \tag{30}$$

Thus the critical area is

$$A_c = \frac{V}{2La^2}\left(\frac{l^2}{2\pi}\right)^2\frac{\varphi_0}{\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right)\left(1 - \frac{1}{2}\ln\left[\left(\frac{L}{a}\right)^2\frac{l^2}{4\pi}\frac{\varphi_0}{\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right)\right]\right). \tag{31}$$

A_c essentially depends on the topological parameters c_0, the mean winding number, Δ_c, the dispersion of the winding number distribution, and φ_0 the mean density of obstacles in the plane. As A_c should remain non-negative we obtain a new upper bound in addition to the inequality (29):

$$\mathrm{e}^2 \geqslant \left(\frac{L}{a}\right)^2\frac{l^2}{4\pi}\frac{\varphi_0}{\Delta_c}\left(1 - \frac{c_0^2}{\Delta_c}\right) > 1 \tag{32}$$

where $\mathrm{e} = 2.714\ldots$ is Euler's constant (e is not to be confused with the coupling constant e defined earlier). Equation (32) indicates that at a certain value of the mean density of obstacles φ_0 the mean-field solution will break down. However, the specific value obtained for the upper bound is a result of the mean-field expression for the critical area A_c, equation (31), and should not be taken as a quantitative, but a qualitative result. Nechaev *et al* have stressed that the mean-field approximation is valid in the vicinity of the boundary curve defined by the lower bound inequality (29) [22] (see figure 1). The present approach using the area of the loop as the order parameter and giving the new upper bound gives strong support of this result that the mean-field solution is restricted to a small neigbourhood above the boundary curve.

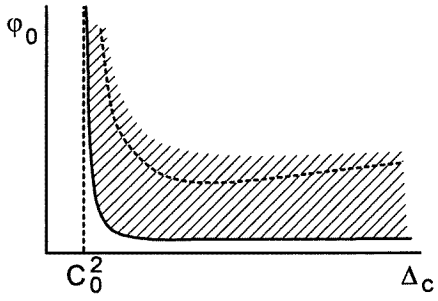

Figure 1. The phase diagram of the collapse transition. The shaded area bounded by the full curve corresponds to the collapsed state of the loop as obtained in [22]. The new upper bound in (32) gives rise to the new boundary curve (broken).

4. Final result and discussion

It has been argued in [22] that the collapsed phase can be identified with a randomly branched polymer. Here we give explicit support of this idea. Consider (27) and substitute $\rho = N/V$ in the mean-field approximation where $N \geqslant N_c$, i.e. above the critical length. We obtain

$$A = \frac{l^2}{2\pi} N\left(1 - \tfrac{1}{2}\ln(N) + \cdots\right). \tag{33}$$

Taking the terms in parentheses as the first powers of an exponential, one finds:

$$A = \frac{l^2}{2\pi} N(N^{-1/2}) = \frac{l^2}{2\pi} N^{1/2}. \tag{34}$$

Exploiting the result of Cardy [29] for SAWs in $d = 2$ that $\langle A\rangle \sim \langle R^2\rangle$, one obtains for $R = (\langle R^2\rangle)^{1/2}$:

$$R \sim l N^{1/4}. \tag{35}$$

This is the scaling behaviour for randomly branched polymers without excluded volume interaction. It is therefore very likely that the collapsed phase of the loop corresponds to a randomly branched polymer.

Note that the result of (34) corresponds to the free part of the free energy $\mathcal{F}$ in (24), i.e. without excluded volume. This is valid as a first approximation because the area A is not directly coupled to the density $\rho = |\phi|^2$ at the level of the free energy, and the excluded volume is not renormalized by the topological interactions in the mean-field approximation. Moreover, a Landau expansion in terms of segment density ρ and tangent vector density variables j_μ indicates that the ρ and j_μ decouple at first order because $k_\mu j_\mu(\boldsymbol{k}) = 0$, while interactions occur only at higher order [14].

As a consequence, the two-dimensional excluded volume must still be taken into account. That yields the well known $d = 2$ branched polymer scaling [26, 27] for the area or the mean sqare end-to-end vector respectively, i.e. $R^2 \sim l N^{5/4}$.

5. Outlook to the three-dimensional problem

Finally, let us point out some possible future perspectives for the $d = 3$ entanglement problem by coming to the mathematical difficulty of finding a correct knot invariant. While the known knot invariants in their algebraic form seem to be only of limited use in the polymer context, the work of Witten [11] showing an equivalence of the Jones polynomial (actually a more general one) and (in general non-abelian) Chern–Simons field theory has brought the knot problem closer to physics again. Witten showed that the expectation

value of Wilson lines averaged over a Chern–Simons action functional integral gives a knot invariant for framed links. This invariant can also be reproduced perturbatively giving the sqare of the Gauss invariant as a first approximation and higher order knot invariants [30, 31, 12].

In addition it has been shown recently that the invariants appearing in Chern–Simons perturbation theory are intimately related to so-called Vassiliev invariants (see e.g. [32] and the literature quoted therein).

These results may open new ways of solving the polymer entanglement problem by a 'topological perturbation theory'. It might give a range of validity for using the Gauss invariant for ensemble of random walk chains or rings.

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