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Winding-angle distribution for two-dimensional polymers at the θ-point [1]

Thomas Prellberg *, Barbara Drossel

Department of Theoretical Physics, University of Manchester, Manchester M13 9PL, UK

Abstract

We calculate winding-angles distributions of polymer models at the θ-point in two dimensions by means of Coulomb gas techniques. Our results suggest that breaking the symmetry of the model by distinguishing between parallel and antiparallel interactions changes the universality class.

The study of polymers is one of the most fascinating fields of current research, because of its relevance not only for material sciences, but also for the understanding of proteins. Depending on the chemical and physical environment, a polymer in a dilute solution can be either swollen or collapsed, or at the θ-point, which is the boundary point between the two. Such polymers can be modeled by interacting self-avoiding random walks (SAWs) with an interaction energy ε between (non-consecutive) bonds that are on the same plaquette of the underlying lattice. As the temperature is decreased, the SAW undergoes the above-mentioned transition at a the θ-temperature, provided that $\varepsilon < 0$. The relation between the polymer length N (monomer number) and its radius of gyration R is characterized by the exponent ν, which assumes the values $\frac{3}{4}$, $\frac{4}{7}$, and $\frac{1}{2}$ above, at, and below the θ-temperature in two dimensions.

For θ-point polymers, there are various competing exactly solvable models which share the same length-scale exponent $\nu = \frac{4}{7}$, but differ with respect to other exponents. One such model is given by loops on the honeycomb lattice with annealed vacancies [1], whereas another model is given by kinetically grown loops on the Manhattan lattice [2,3], which can be mapped to percolation cluster perimeters for bond percolation on the square lattice at the percolation threshold. These two models differ in, e.g., the partition function exponent γ which takes on the values $\frac{8}{7}$ for the model on the honeycomb lattice and $\frac{6}{7}$ on the Manhattan lattice. This opens up intriguing questions regarding the universality of the collapse transition. In this paper, we investigate this question from the point

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* Corresponding author. E-mail: prel@a13.ph.man.ac.uk.

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of view of winding-angle distributions and propose a solution by relating the difference in scaling to the occurrence of parallel interactions. In particular, we claim that breaking the symmetry between parallel and antiparallel interactions changes the universality class of the collapse. In a two-dimensional phase diagram parametrized by parallel and antiparallel interaction energies, one therefore obtains a line of percolation-type collapse points ending in the usual θ-point on the symmetry line.

A polymer in two dimensions is modeled by a SAW on a two-dimensional regular lattice. The steps of the walk, which coincide with lattice bonds, can be viewed as monomers. Each site of the lattice can only be visited once. This condition models the excluded volume effect of the polymer. Short-range interactions between monomers are taken into account by assigning an energy ε to each pair of (non-consecutive) nearest-neighbor sites. The weight for each interaction is given by $\omega = \exp(-\varepsilon/k_B T)$, where T is the temperature and k_B is the Boltzmann constant. The partition function for a polymer of N steps is then $Z_N = \sum_m g_N^{(m)} \omega^m$, where m is the number of interactions, and $g_N^{(m)}$ is the number of configurations (starting at a given point) with this interaction number.

In the swollen regime, the partition function is known to scale as $Z_N \approx A\mu^N N^{\gamma-1}$, with $\gamma = \frac{43}{32}$ [4]. At the θ-point $\omega \equiv \omega_\theta$, the value of γ (denoted γ_t) is known to be $\gamma_t = \frac{8}{7}$ [1]. It is also known that $\gamma_t = \frac{6}{7}$ for a self-avoiding walk that is part of a percolation cluster hull and therefore has no parallel interactions [2,3]. Since $\nu = \frac{4}{7}$ [5] for both of these models, they are both at the collapse transition. Like the exponent γ, the winding-angle distribution is closely related to the frequency of parallel interactions. For this reason one might expect that the change of γ is linked to a similar behavior of the winding-angle distribution. Our results for the winding-angle distribution below confirm indeed such a link. For self-avoiding walks, the winding-angle distribution is generally described by a Gaussian $p(\theta) \propto \exp(-\theta^2/2C \ln N)$, with a variance $C \ln N$ [6,7]. Such Gaussian distributions with a variance proportional to $\ln N$ occur generically for radially scale-invariant polymers, given that the winding center is visited only a finite number of times [8]. The value of C is 2 in the swollen phase and $\frac{24}{7}$ at the θ-point of a polymer with no orientation dependence in the interaction [7]. These results follow from an analytical calculation on an hexagonal lattice. The calculation for the swollen phase is nicely confirmed by an exact enumeration on a square lattice, where we obtain $C = 2.0005(6)$ for polymers up to length $N = 26$, using differential approximant analysis [9].

We now derive a different value $C = \frac{6}{7}$ for a self-avoiding walk that is part of a percolation cluster hull and, therefore, has no parallel interactions. In order to find its winding-angle distribution, we use a procedure similar to the one in Refs. [5,7], which is conveniently performed on an hexagonal lattice. We start with the $O(n)$-loop model [4] with the partition function

$$Z_{O(n)} = \int \prod_k d^N S_k \prod_{\langle i,j \rangle} (1 + \beta \boldsymbol{S}_i \cdot \boldsymbol{S}_j) = \sum_{\mathcal{G}} \beta^l n^P \,. \tag{1}$$

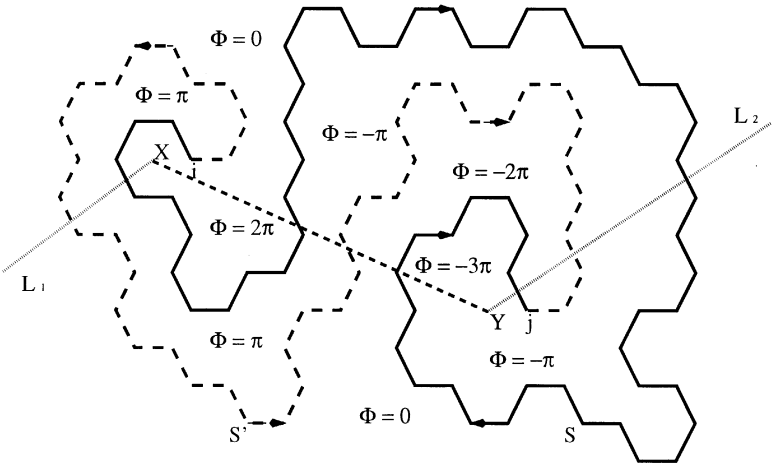

Fig. 1. Illustration of the calculation of the winding-angle distribution.

Here i,j,k are lattice sites, $\langle i,j\rangle$ nearest neighbors, and $\boldsymbol{S}$ an n-vector: $|\boldsymbol{S}|^2 = n$. The second sum is performed over all graphs $\mathscr{G}$ of P non-intersecting polygons of total length l. For $n \in [-2,2]$, the loop model has a critical point $\beta_c = [2+(2-n)^{1/2}]^{-1/2}$. For $n = 1$ and $\beta = 1$, each loop has the same weight. These loops can be interpreted as percolation cluster hulls for site percolation on the dual triangular lattice at the percolation threshold. We are interested in the winding-angle distribution of a segment of a loop. Fig. 1 illustrates the following calculation. We look at the function

$$G_{O(n)}(\boldsymbol{X}-\boldsymbol{Y},e_1,e_2) = \sum_{\mathscr{G}_1} W_{O(N)}(\mathscr{G}_1) e^{ie_1\pi(n_1+n_1')+ie_2\pi(n_2+n_2')} . \tag{2}$$

$\mathscr{G}_1$ are like the graphs $\mathscr{G}$ above, but with both points i and j lying on the same loop. Both parts S and S' of the loop are given the same orientation from i to j. $n_1(n_1')$ and $n_2(n_2')$ count the number of intersections of the oriented paths $S(S')$ with L_1 and L_2, respectively, crossing in different directions having a different sign. Without the phase factor, $G_{O(n)}$ is a four-spin correlation function, with two spins at i and two spins at j. To calculate Eq. (2), we transform it into a solid-on-solid (SOS) model. Height variables ϕ are defined on the centers of the hexagons, such that two adjacent heights are equal or different by $\pm\pi$. The polygons, once arbitrarily oriented, become domain walls with a step of $+\pi$ on the left of any oriented line. Along the straight line connecting $\boldsymbol{X}$ to $\boldsymbol{Y}$, the height changes by 2π. In the SOS language, this corresponds to a dislocation line with a vortex at $\boldsymbol{X}$ and an antivortex at $\boldsymbol{Y}$ [5]. At the vertices of the honeycomb lattice, the SOS walls turn by $\pm\pi/3$. The SOS weight W_{SOS} is calculated as the product along the walls of local factors $\beta\exp(iu)$ ($\beta\exp(-iu)$) at each left (right) turning vertex. Summing over the two independent orientations of each polygon (except, of course, the special polygon connecting i and j) gives a phase

factor $2\cos 6u$ for each polygon. The SOS weight of a graph $\mathscr{G}_1$ is then

$$W_{\mathrm{SOS}}(\mathscr{G}_1) = \beta^l n^P e^{iu(n_+ - n_-) + iu(n'_+ - n'_-) + 6iu(P_+ - P_-)} .$$

n_+ and n_- (n'_+ and n'_-) are the total number of local left and right turns of path S (S'). P_+ and P_- are the total number of right and left polygons surrounding i and j. In the asymptotic limit, we have $n_+ - n_- = 6(n_1 + n_2)$ and $n'_+ - n'_- = 6(n'_1 + n'_2)$. Let us define the SOS correlator

$$G_{\mathrm{SOS}}(\boldsymbol{X} - \boldsymbol{Y}, e'_1, e'_2) = \sum_{\mathscr{G}_1} W_{\mathrm{SOS}}(\mathscr{G}_1) e^{ie'_1\phi(\boldsymbol{X}) + ie'_2\phi(\boldsymbol{Y})} .$$

Equating this correlator with Eq. (2) above gives $n = 2\cos 6u$ and $e'_1 = e_1 + e_0$, $e'_2 = e_2 + e_0$, $e_1 + e_2 = 0$. The new constant e_0 is $e_0 = -6u/\pi$. Now, at $\beta = 1$, the SOS model renormalizes onto the low-temperature phase of the Coulomb-gas model for $g = \frac{2}{3}$ (if $n = 1$) [4], and

$$G_{\mathrm{SOS}}(e'_1, e'_2) = |\boldsymbol{X} - \boldsymbol{Y}|^{e'_1 e'_2/g + g m_1 m_2} . \tag{3}$$

The magnetic charges m_1 and m_2 are $m_1 = -m_1 = \frac{1}{2}$ [5], due to the vortex pair. The winding angle is finally extracted from

$$\left\langle e^{ie\pi(n_1 - n_2 + n'_1 - n'_2)} \right\rangle_{O(N)} = e^{-e^2 g^{-1} \ln|\boldsymbol{X} - \boldsymbol{Y}|} .$$

Fourier transformation yields immediately a Gaussian distribution for $n_1 - n_2 + n'_1 - n'_2$. Each of the two paths S and S' has the same number of intersections with L and L', and therefore $n_1 = n'_1$ and $n_2 = n'_2$. (In certain situations, n_1 and n'_1 differ by one, but this effect can be neglected in the thermodynamic limit, where the number of intersections becomes very large.) In terms of the angle $\hat{\theta} = \pi(n_1 - n_2 + n'_1 - n'_2)$ the resulting distribution reads

$$P(\hat{\theta}) = (16\pi g^{-1} \ln|\boldsymbol{X} - \boldsymbol{Y}|)^{-1/2} e^{-g\hat{\theta}^2/16 \ln|\boldsymbol{X} - \boldsymbol{Y}|} .$$

Since both paths make exactly the same contribution to $\hat{\theta}$, the winding angle of one path is given by $\hat{\theta}/2$. For large distances $|\boldsymbol{X} - \boldsymbol{Y}|$, the windings around $\boldsymbol{X}$ and $\boldsymbol{Y}$ are independent from each other and have the same probability distribution. Replacing $|\boldsymbol{X} - \boldsymbol{Y}|$ by N^ν (N being the length of the polymer), we arrive at the winding-angle distribution of path S around point $\boldsymbol{X}$,

$$P(\theta) = (4\pi\nu g^{-1} \ln N)^{-1/2} e^{-g\theta^2/2\nu \ln N} . \tag{4}$$

Inserting $g = \frac{2}{3}$ and $\nu = \frac{4}{7}$, we find $C = \frac{6}{7}$.[2] Numerical simulations with kinetic growth walks confirm nicely this result [10].

[2] This calculation can easily be generalized to "watermelon configurations", where the points i and j are connected by L paths. The constant C characterizing the winding angle distribution for one of these paths is then $C_L = 4\nu/L^2 g$.

We therefore see that the absence of parallel interactions changes the universality class of collapse. This effect is particular to two dimensions, since in higher dimensions a parallel interaction can locally be transformed into an antiparallel interaction, without changing the conformation of the polymer at a large scale. The implications for the general phase diagram for polymers with orientation-dependent interactions are discussed in Ref. [10]. In particular, it emerges that the symmetry breaking effect between parallel and antiparallel interactions observed here carries over into the collapsed phase. There, the symmetry line of equally strong parallel and antiparallel interactions becomes a phase boundary between the ordinary collapsed phase and a spiral collapsed phase.

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