

An exactly soluble model of directed polymers with multiple phase transitions

G. Forgacs, Klaus G. Ziegler

Angaben zur Veröffentlichung / Publication details:

Forgacs, G., and Klaus G. Ziegler. 1995. "An exactly soluble model of directed polymers with multiple phase transitions." *Europhysics Letters (EPL)* 29 (9): 705–10.
<https://doi.org/10.1209/0295-5075/29/9/009>.

Nutzungsbedingungen / Terms of use:

licgercopyright

Dieses Dokument wird unter folgenden Bedingungen zur Verfügung gestellt: / This document is made available under these conditions:

Deutsches Urheberrecht

Weitere Informationen finden Sie unter: / For more information see:

<https://www.uni-augsburg.de/de/organisation/bibliothek/publizieren-zitieren-archivieren/publiz/>



An Exactly Soluble Model of Directed Polymers with Multiple Phase Transitions.

G. FORGACS(*) and K. ZIEGLER(**)

(*) *Department of Physics, Clarkson University - Potsdam, NY 13699-5820, USA*

(**) *Institut für Theorie der Kondensierten Materie, Universität, Physikhochhaus D-76128 Karlsruhe, Germany*

PACS. 64.70.Dv – Solid-liquid transitions.

PACS. 64.70.Rh – Commensurate-incommensurate transitions.

PACS. 64.60.Kw – Multicritical points.

Abstract. – Polymer chains with hard-core interaction on a two-dimensional lattice are modeled by directed random walks. Two models, one with intersecting walks (IW) and another with non-intersecting walks (NIW) are presented, solved and compared. The exact solution of the two models, based on a representation using Grassmann variables, leads, surprisingly, to the same analytic expression for the polymer density and identical phase diagrams. There are three different phases as a function of hopping probability and single site monomer occupancy, with a transition from the dense polymer system to a polymer liquid (A) and a transition from the liquid to an empty lattice (B). Within the liquid phase there exists a self-dual line with peculiar properties. The derivative of polymer density with respect to the single site monomer occupancy diverges at transitions A and B, but is smooth across and along the self-dual line. The density-density correlation function along the direction x , perpendicular to the axis of directedness has a power law decay $1/x^2$ in the entire liquid phase, in both models. The difference between the two models shows up only in the behavior of the correlation function along the self-dual line: it decays exponentially in the IW model and as $1/x^4$ in the NIW model.

A directed random walker makes steps along a given (z) axis only in one (forward) direction. Random fluctuations are present in the transverse directions [1]. Such walks are the subject of great interest since they may model diverse phenomena like polymers under flow [2], tracer diffusion [3], electrorheological fluids [4], commensurate-incommensurate phase transitions [5], vortex lines in high- T_c superconductors [6, 7], world lines of quantum particles [8], the behavior of interfaces in $1 + 1$ dimensions [9], some aspects of biomembranes [10], etc. They share a number of properties of dimers [9] and vortex models [11].

Directedness makes analytic calculations considerably easier, and a number of exact results exist both for a single walk and cases with many walks.

In the present work we concentrate on some generic properties of random walks. We introduce and solve exactly a model with non-intersecting walks. Using the same formalism, we also obtain the solution of a similar model, which allows for intersections. The comparison of the two models reveals some surprising effects. The interesting feature of our systems is

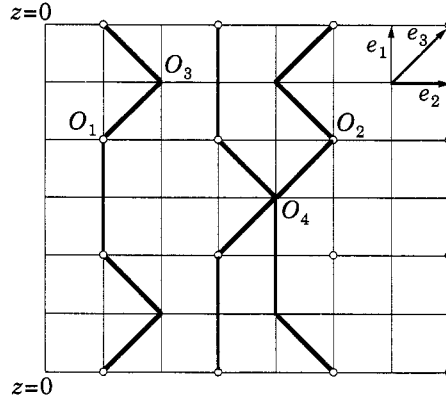


Fig. 1. – The schematic representation of the lattice where the model presented in this work is defined. The figure shows a typical configuration of some of the directed polymers. The use of periodic boundary conditions in the z -direction is indicated explicitly. For more details see text.

that along with second-order phase transitions, observed in previous investigations of similar models [12-14], they contain a self-dual line, with characteristics of yet another critical phenomenon.

We first discuss the NIW model depicted in fig. 1. Chains are pinned with one of their ends at $z = 0$. In order to avoid crossing of walks in the vertical direction only steps of length $2a$ are allowed, where a is the lattice spacing. Each such chain can be parametrized with two indices, r and j . Here r are lattice sites denoted by open circles in fig. 1. The index j takes values 0 or 1. $j = 0$ if a site is an r -site, and, as a consequence, can be reached from another r -site making two steps along the elementary vectors e_1 (site O_1 in fig. 1) or e_3 (site O_2 in fig. 1). $j = 1$ for a site which can be reached from an r -site by making a single step in the direction of the vector e_3 (site O_3 in fig. 1) or from a $j = 1$ site directly below (site O_4 in fig. 1). Chains start at $z = 0$, at r -sites (also needed to avoid crossing). This is model A of ref. [14] which was used to describe phase transitions in biomembranes. In the present article we investigate correlations in this model (as well as in the IW model) to provide a deeper understanding of the statistics than what can be obtained from the thermodynamic properties studied in ref. [14].

We impose periodic boundary conditions both in the x and z directions. We assume a hard-core potential between walks: chains repel each other with infinite energy upon contact. Therefore, the contribution of the configuration in fig. 1 to the partition function is zero because of point O_4 . We assign unit weight to a step in the vertical direction (with length $2a$ along the vector e_1), and a weight w to a step along the diagonals of the elementary square. The weight (fugacity) of an empty site is denoted by μ . Introducing a pair of Grassmann variables [15] $\{\Psi_{r,j}, \bar{\Psi}_{r,j}\}$ for each lattice site, the configurations of our system can be generated from the partition function

$$Z = \int \exp \left[\sum_{r, r'} \sum_{j=0,1} \Psi_{r,j} G_{r,r';j,j'}^{-1} \bar{\Psi}_{r',j'} \right] \mathcal{D}\Psi \mathcal{D}\bar{\Psi} = \det G^{-1}. \quad (1)$$

Here $\mathcal{D}\Psi \mathcal{D}\bar{\Psi}$ denotes the Berezin integration [15] over all Grassmannians, and, the lattice

Green's function is given by its Fourier components

$$\tilde{G}_k^{-1} = \begin{pmatrix} \exp[ik_1] - \mu & w \exp[ik_1](1 + \exp[ik_2]) \\ w(1 + \exp[-ik_2]) & \exp[ik_1] - \mu \end{pmatrix}. \quad (2)$$

The 2×2 -matrix structure reflects the dependence on the index $j = 0, 1$; k_1 and k_2 are the components of the two-dimensional momentum vector along the x - and z -directions, respectively. On a lattice with N sites expression (2) leads to a free energy

$$\frac{1}{N} \log Z = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} \log \left(\mu^2 - 4w^2 \exp[ik_1] \cos^2 \frac{k_2}{2} - 2\mu \exp[ik_1] + \exp[2ik_1] \right). \quad (3)$$

In what follows we first outline the calculation of the density n_r of lines at site r and of the density-density correlation function. The probability that a line goes through the site (r, j) is given by

$$n_r = \langle 1 - \mu \bar{\Psi}_{r,0} \Psi_{r,0} \rangle = n, \quad (4)$$

where the last equation follows from translational invariance. The average value in (4) is to be calculated using the partition function given by (1) and (3). It is easy to see that n can be expressed in terms of the Green's function as

$$n = 1 + \mu G_{r,r;00}. \quad (5)$$

The calculation of the Green's function is tedious but straightforward. Starting from the Fourier components of the Green's function in (2), the diagonal matrix elements of G read

$$G_{r,r;00} = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{\mu - \exp[ik_1]}{(\mu - \exp[ik_1])^2 - 2w^2 \exp[ik_1](1 + \cos k_2)} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi}. \quad (6)$$

By evaluating the double integral in (6), we finally arrive at

$$n = 1 - \frac{1}{2\pi} \cos^{-1} \left[1 - \frac{(1 + \mu)^2}{2(\mu + w^2)} \right] \mp \frac{1}{2\pi} \cos^{-1} \left[1 - \frac{(1 - \mu)^2}{2w^2} \right]. \quad (7)$$

Here \mp corresponds, respectively, to cases $\mu > 1$ and $\mu < 1$.

The result given in (7) corresponds to the phase diagram shown in fig. 2. $\mu = 1 \pm 2w$ (A and B, respectively, in fig. 2) are lines of phase transitions from a dense system of directed polymers ($n = 1$) to a polymer liquid ($0 < n < 1$) and finally to a system without directed polymers. Approaching the phase transition lines from the regions II and III along directions parallel to the w -axis, one finds $\partial n / \partial \mu \sim 1/\sqrt{\varepsilon}$, where $\varepsilon = 1 - (1 - \mu)/2w$ and $\varepsilon = 1 - (\mu - 1)/2w$, respectively for the two cases. There is another critical phenomenon at $\mu = 1$ (broken line in fig. 2). Across this line the above partial derivative of the density varies smoothly. This critical behavior can be understood from the density-density correlation function C_{x_2} , which measure the correlation perpendicular to the polymer direction. C_{x_2} is given in terms of the Green's function

$$G_{r,r+xe_2} \equiv G_x = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{(\mu - \exp[ik_1]) \exp[ik_2 x]}{(\mu - \exp[ik_1])^2 - 2w^2 \exp[ik_1](1 + \cos k_2)} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} \quad (8)$$

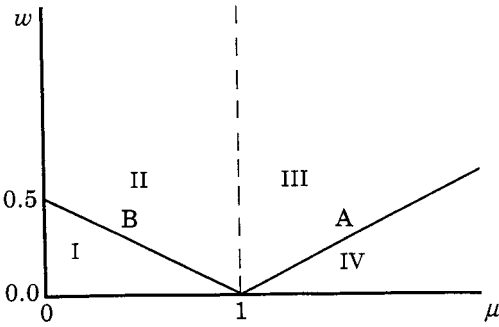


Fig. 2.

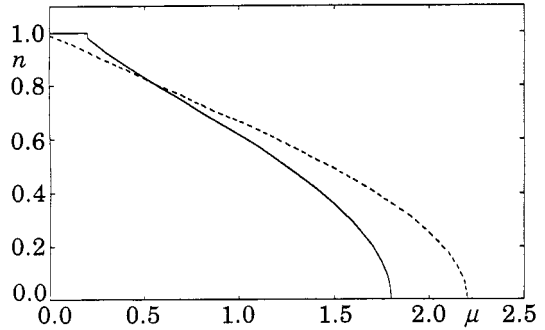


Fig. 3.

Fig. 2. – The phase diagram of the model. In regions I and IV, $n = 1$ and $n = 0$, respectively.

Fig.3. – The behavior of the density of polymer lines along lines $w = 0.4$ (full line) and $w = 0.6$ (dashed line) in fig. 2.

as

$$C_x = \mu^2 G_x G_{-x}. \quad (9)$$

Performing the k_1 integration in (8), one arrives at

$$G_x = \frac{1}{2} \int_{-k^*}^{k^*} \frac{2\mu(1-\mu) + \alpha}{\sqrt{\alpha^2 + 4\mu\alpha}} \exp[ik_2 x] \frac{dk_2}{2\pi}, \quad (10)$$

with $k^* = \cos^{-1}[(1-\mu)^2/2w^2 - 1]$ and $\alpha = 2w^2(1 + \cos k_2)$. k^* takes the values π and 0 along the line $\mu = 1$ and the transition lines $\mu = 1 \pm 2w$, respectively. The calculation of the integral in (10) is an exercise in complex contour integration, and in the large- x limit can be performed analytically for any value of k^* , with the result

$$G_x \sim \begin{cases} \frac{(-1)^x}{x^2} & \text{for } k^* = \pi, \\ \cos\left(\frac{k^*}{2}\right) \frac{\cos(k^* x)}{x} & \text{for } k^* \neq \pi. \end{cases} \quad (11)$$

Finally, the density-density correlation function decays as $1/x^4$ along the line $\mu = 1$ and as $1/x^2$ elsewhere in the liquid phase.

The special property of the line $\mu = 1$ is also elucidated by noting that the expressions for the density of polymer lines, given in (7) are invariant under a «duality transformation» $\mu \rightarrow 1/\mu$ and $w \rightarrow w/\mu$. This duality at $\mu = 1$ reflects the equivalence of directed polymer lines and lines of empty sites on the lattice. $\mu = 1$ is a self-dual line along which polymers and empty sites compete with the same weight. This competition leads to a faster decay of the density-density correlation function.

In regions I and IV in fig. 2, n has the values 1 and 0, respectively. Figure 3 shows the behavior of n along the lines $w = 0.4$ and $w = 0.6$.

If the restrictions imposed on the model as defined above (only steps of length $2a$ are allowed in the vertical direction, chains must start at $z = 0$, at r -sites) are relaxed, the model describes a system of intersecting random walks. The analogous calculations for the partition

function (\tilde{Z}), density of lines (\tilde{n}) and the correlation function (\tilde{C}_x) are even simpler in this case (one deals with a simple Bravais lattice as opposed to a lattice with basis in the case of non-intersecting walks). We only quote the results

$$\frac{1}{N} \log \tilde{Z} = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_1}{2\pi} \frac{dk_2}{2\pi} \log (\mu - 2w \exp [ik_1] \cos k_2 - \exp [2ik_1]). \quad (12)$$

Although the above expression for the free energy clearly differs from (1), surprisingly, for the density one obtains $\tilde{n} \equiv n$, where the expression for n is given in (7). This in turn implies that the phase diagram for the IW model is the same as the one obtained for the NIW model. Finally, the correlation function \tilde{C}_x can be calculated similarly to C_x in (9). However, instead of G_x in (10) we now have for $\mu = 1$

$$\tilde{G}_x = \frac{1}{2} \int_{-\pi}^{\pi} \frac{\alpha}{\sqrt{\alpha^2 + 4}} \exp [ik_2 x] \frac{dk_2}{2\pi} \quad (13)$$

with $\alpha = 2w \cos k_2$. Considering $\mu = 1$ and, for simplicity, $w = 1$ and comparing G_x and \tilde{G}_x , we notice that the arguments of the square root in the denominators are quite different. As a function of $z = \exp [ik_2]$ the square root of \tilde{G}_x is analytic in a vicinity of the unit circle. Therefore, the path of integration can be contracted to a smaller circle with $|z| < 1$. Consequently, \tilde{G}_x decays exponentially on the $\mu = 1$ line. Everywhere else in the liquid phase [13] it decays as $1/x$.

In conclusion, the analysis of the simple models of non-intersecting and intersecting directed polymer chains presented in this work (and studied earlier in ref. [13,14] leads, surprisingly, to identical thermodynamic properties. The phase diagram is unusually rich with multiple transition lines and phases. There are second-order phase transitions, with diverging second derivatives of the free energy. The region of the phase diagram between these transitions, the liquid phase (A and B in fig. 2) is critical in the sense that in it the density-density correlation function decays everywhere according to a power law. An additional feature of the phase diagram is a self-dual line in the liquid phase, which manifests itself also in the change of the decay of correlations. This change of correlations does not seem to affect the behavior of the thermodynamic quantities; they vary smoothly across the self-dual line. The difference between the two models, in our study shows up only in the behavior of the correlation function along this line.

* * *

One of us (GF) acknowledges useful discussions with S. Bhattacharjee.

REFERENCES

- [1] PRIVMAN V. and SVRAKIC N. M., *Directed Models of Polymers, Interfaces and Clusters: Scaling and Finite Size Properties, Lecture Notes Phys.*, **338** (Springer, Berlin) 1989.
- [2] LEE J. J. and FULLER G. G., *J. Coll. Int. Sci.*, **103** (1984) 568.
- [3] HARRIS T.E., *J. Appl. Prob.*, **2** (1965) 323; ALEXANDER S. and PINCUS P., *Phys. Rev. B*, **18** (1978) 2011.
- [4] HALSEY T. C. and TOOR W., *Phys. Rev. Lett.*, **65** (1990) 2820.
- [5] FISHER M. E., *J. Stat. Phys.*, **34** (1984) 667.

- [6] NELSON D. R., *Phys. Rev. Lett.*, **60** (1988) 1973; Nelson D. R. and SEUNG H. S., *Phys.Rev. B*, **39** (1989) 9153.
- [7] ZIEGLER K., *Europhys. Lett.*, **9** (1989) 277; *J. Stat. Phys.*, **64** (1991) 277; *Z. Phys. B*, **84** (1991) 163.
- [8] SCHULMAN L. S., *Techniques and Applications of Path Integrals* (John Wiley & Sons, New York, N.Y.) 1981.
- [9] FORGACS G., LIPOWSKY R. and NIEUWENHUIZEN TH. M., in *Phase Transitions and Critical Phenomena*, edited by C. DOMB and J. L. LEBOWITZ, Vol. 14 (Academic Press, London) 1991.
- [10] NAGLE J., YOKOI C. S. O. and BHATTACHARJEE S. M., in *Phase Transitions and Critical Phenomena*, edited by C. DOMB and J. LEBOWITZ, Vol. 13 (Academic Press, London) 1989.
- [11] BHATTACHARJEE S.M., *Europhys. Lett.*, **15** (1991) 815.
- [12] BHATTACHARJEE S. M. and NAGLE J. F., *Phys. Rev. A*, **31** (1985) 3199.
- [13] KORNILOV E. I. and LITVIN A. A., *Z. Phys B*, **84** (1991) 3.
- [14] NAGLE J. F., *J. Chem. Phys.*, **63** (1975) 1255.
- [15] BEREZIN F. A., *Method of Second Quantization* (Academic Press, London) 1966.