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LETTER TO THE EDITOR

Exact evaluation of the collapse phase boundary for two-dimensional directed polymers

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Abstract. The phase boundary of the collapsed phase for a directed polymer on a square lattice in the presence of an attractive wall and monomer–monomer interactions is calculated exactly using transfer-matrix techniques. The position of the multicritical point is also identified.

Polymer adsorption on a substrate has received considerable attention both because of its intrinsic merit as an interesting problem in statistical mechanics [1] and because of its technological importance in the stabilization of colloidal dispersions used in paints, pharmaceuticals and foodstuffs [2]. While the adsorption of a self-avoiding walk is now well understood [3–7], models where monomer–monomer interactions compete with the surface attraction have only become the focus of attention recently [8–11].

In this letter we calculate the phase boundaries of a directed self-avoiding walk with nearest-neighbours attractive interactions in the presence of an adsorbing wall.

We consider a directed polymer on a strip of width N_y as shown in figure 1. The polymer is directed in that steps in the negative x direction are forbidden. Hence, the position of the polymer in column i, n_i, is unique. The attraction to the substrate is modelled by assigning an energy K to each column in which $n_i = 1$ or N_y. Nearest-neighbour interactions between monomers are introduced through an attractive energy J between bonds which occupy the same row in adjacent columns.

This model was solved for $J = 0$ by Privman *et al* [7]. The full parameter space was explored numerically using finite-size scaling by Veal *et al* [10]. They found the

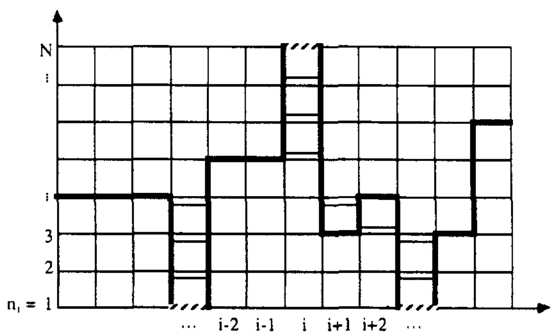

Figure 1. A directed polymer on a strip of width N. The polymer interacts with the surfaces of the strip (hatched lines). Monomer–monomer interactions are represented by double lines.

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three phases shown in figure 2 and gave values for the multicritical point conjectured to be exact. Subsequently Binder *et al* [11] have solved the problem exactly for $K=0$. In this letter we extend their work and calculate exactly the boundary of the collapsed phase. We identify the multicritical point and confirm the conjecture of Veal *et al* [10].

Our analysis commences by defining the grand partition function

$$Z=\sum_{\text{walks}} \omega^L \kappa^l \tau^n \tag{1}$$

where ω is the fugacity, $\kappa=\exp(-K/k_BT)$ and $\tau=\exp(-J/k_BT)$. L is the number of monomers in the walk, l the number of visits to the wall and n the number of monomer-monomer interactions.

Z may be rewritten as a sum of partition functions, Z_{L_x}, for polymers with L_x steps in the x direction

$$Z=\sum_{L_x} Z_{L_x}. \tag{2}$$

To evaluate Z we write Z_{L_x} in terms of a transfer matrix, T [12]. Due to the monomer-monomer interactions we need to use a transfer matrix of dimensionality N_y^2. The elements of the transfer matrix, labelled by $\alpha=(n_{i-1}, n_i)$, $\beta=(n_i, n_{i+1})$ are

$$T_{\alpha,\beta}=\omega^{L_{\alpha,\beta}}\kappa^{l_{\alpha,\beta}}\tau^{n_{\alpha,\beta}} \tag{3}$$

where

$$L_{\alpha,\beta}=1+\tfrac{1}{2}[|n_{i-1}-n_i|+|n_i-n_{i+1}|]$$
$$l_{\alpha,\beta}=\delta_{n_{i-1},1}+\delta_{n_{i-1},N_y}$$
$$n_{\alpha,\beta}=\tfrac{1}{2}\min(|n_{i-1}-n_i|, |n_i-n_{i+1}|)(1-\mathrm{sgn}((n_{i-1}-n_i)(n_i-n_{i+1}))).$$

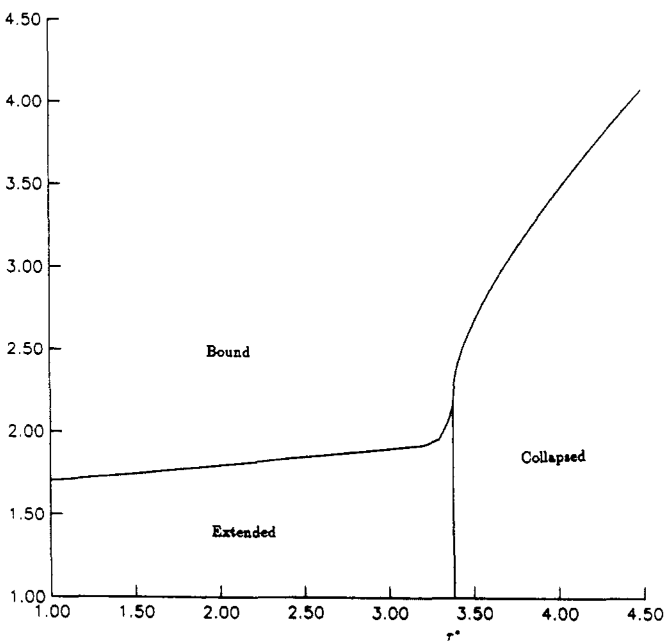

Figure 2. Phase diagram of the directed polymer showing the extended, collapsed and bound phases. The boundaries between the collapsed and bound, and the collapsed and extended phases are exact while the boundary between the extended and bound phases is shown schematically.

Writing Z in terms of T gives

$$Z \propto T^2(1-T)^{-1}. \tag{4}$$

Z develops a singularity when λ_0, the largest eigenvalue of T, is equal to unity. In this limit $\langle L\rangle \to \infty$. We defined a critical fugacity, $\omega_\infty(\kappa, \tau)$, by

$$\lambda_0[\omega_\infty] = 1. \tag{5}$$

It was found [10, 11] that the collapsed phase occupies the region in phase space where $\omega\tau > 1$. Here the largest eigenvalue of T depends exponentially upon N_y and the polymer has finite density as well as infinite length. The transition boundary is given by $\omega_\infty\tau = 1$.

Substituting the condition $\omega\tau = 1$ into the transfer matrix it can be rewritten in the form

$$T_{\alpha,\beta} = \omega^{L'_{\alpha,\beta}}\kappa^{l_{\alpha,\beta}} \tag{6}$$

where

$$L'_{\alpha,\beta} = L_{\alpha,\beta} - n_{\alpha,\beta} = 1 + \tfrac{1}{2}|n_{i-1} - n_{i+1}|$$

$$l_{\alpha,\beta} = \delta_{n_{i-1},1} + \delta_{n_{i-1},N_y}$$

L' does not depend on n_i. Therefore Z_{L_x} can be reduced to the product of partition functions for two sublattices made up of alternate columns of the full lattice. Another way of looking at this is that the full matrix may be written as the direct product† of two identical matrices (Owczarek, private communication),

$$T^2 = t \otimes t \tag{7}$$

where t is an N_y by N_y matrix with elements

$$t_{i,j} = \omega^{L_{i,j}}\kappa^{l_{i,j}} \tag{8}$$

where

$$L_{i,j} = 1 + \tfrac{1}{2}|i-j|$$

$$l_{i,j} = \delta_{i,1} + \delta_{i,N_y}.$$

It is clear from (7) that the largest eigenvalues of T and t are the same and hence λ_0 may be found from t [7].

The eigenvalue spectrum of t consists (in the limit $N_y \to \infty$) of a continuous set of eigenvalues corresponding to an unbound state and at most one bound state eigenvector and corresponding eigenvalue.

For the transition between the free and collapsed phases the largest eigenvalue corresponds to the top edge of the continuous spectrum,

$$\lambda_0^{\text{unbound}} = \frac{\omega(1+\omega^{1/2})}{(1-\omega^{1/2})}. \tag{9}$$

This is independent of κ. Setting $\lambda_0 = 1$ gives a value for ω_∞, and hence $\tau = 1/\omega_\infty$, on the phase boundary

$$\omega_\infty = \tfrac{1}{9}[(17+3\sqrt{33})^{1/3} + (17-3\sqrt{33})^{1/3} - 1]^2 = 0.295\,5977\ldots. \tag{10}$$

† This may be written in terms of components as $T_{(l-1)N_y+k,(j-1)N_y+i} = t_{i,j}t_{k,l}$.

For the boundary between the adsorbed and collapsed phases the largest eigenvalue corresponds to the bound state and is given by

$$\lambda_0^{\text{bound}} = \omega\kappa + \frac{\omega^2\kappa}{\kappa(1-\omega)-1}. \tag{11}$$

Putting $\lambda_0^{\text{bound}} = 1$ and $\omega_\infty\tau = 1$ gives the boundary between the bound and collapsed phases

$$\kappa = \frac{\tau+1}{2} + \frac{\sqrt{(\tau^2+1)^2 - 4\tau^3}}{2(\tau-1)}. \tag{12}$$

The multicritical point is then found from the simultaneous solution of $\lambda^{\text{bound}} = \lambda^{\text{unbound}} = 1$ and $\omega\tau = 1$

$$\kappa^* = (1-\omega_\infty^{*1/2})^{-1} = 2.191\,4878\ldots \tag{13}$$

$$\omega_\infty^* = 0.295\,5977\ldots \tag{14}$$

$$\tau^* = 3.382\,9757.\ldots \tag{15}$$

The expression for κ^* is in agreement with the conjecture of Binder *et al* [11].

Physically (6) corresponds to considering only the 'excess' bonds, those not involved in monomer-monomer interactions. The condition $\lambda_0 \to 1$ now corresponds to the number of excess bonds becoming infinite. This point corresponds to the transition from the collapsed phase to the extended phases.

In summary in this letter we give exact results for the boundary of the collapsed phase in a model of a directed polymer attracted to an adsorbing substrate with monomer-monomer interactions. The position of the multicritical point between the bound, extended and collapsed phases is also calculated exactly.

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After this work was completed we learnt that similar results have been obtained by F Igloi, Institute für Theoretische Physik, Universität zu Köln, Federal Republic of Germany.

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