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LETTER TO THE EDITOR

Unbinding of semiflexible directed polymers in 1 + 1 dimensions

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Abstract. The unbinding transition of a directed semiflexible polymer whose fluctuations are controlled by bending rigidity is studied in 1 + 1 dimensions. The chain is modelled by a restricted solid-on-solid model with a short-ranged substrate potential. All the statistical and thermodynamic properties are evaluated exactly. In particular, the phase diagram is determined and is compared with the case when fluctuations are controlled by surface tension.

In the present work we study the behaviour of a directed polymer chain in the vicinity of an attracting substrate. A directed chain can propagate only in the positive direction of a given axis, which we choose to be the x -axis and take it parallel to the substrate. Experimentally such chains result when the polymer is subject to a flow field [1]. In two dimensions, the transverse fluctuations perpendicular to the substrate are restricted to (say) the z -direction. In this (1 + 1)-dimensional geometry, the chain may be thought of as an interface dividing two separate phases (see figure 1). Indeed, due to the analogy with interfaces, the theoretical description of the fluctuations of these chains in terms of various solid-on-solid (sos) models[†] involves surface tension.

Using the sos model (with surface tension) it has recently been shown that at a well defined temperature the directed polymer unbinds from attracting line defects or one-dimensional substrates [3]. This adsorption-desorption transition is second order;

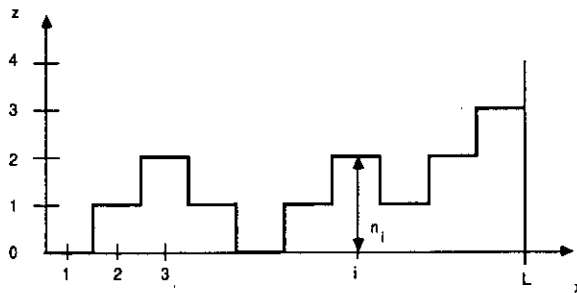


Figure 1. A typical configuration of a directed polymer in the restricted solid-on-solid model. Heavy lines of unit length denote individual monomers and for a given value of x there can be only a single monomer in the vertical direction. The chain is grafted at one end to the substrate.

[†] For a review of sos models see, for example, [2].

the relative number of monomers attached to the line defect vanishes linearly when the transition is approached from below. If attraction between monomers is included, instead of the second-order transition the chain may unbind via a first-order transition into a collapsed phase [4].

As a separate development, the fluctuations of membranes are also actively being studied [5]. These fluctuations are known to be driven by bending rigidity [6]. A 'membrane' in 1+1 dimensions is then equivalent to a semiflexible polymer. It is known that certain linear macromolecules, such as DNA, may have a large persistence length, in which case rigidity has to be incorporated into the study of their statistical behaviour. The unbinding of semiflexible polymers in 1+1 dimension has been studied within the SOS model using a number of approximate techniques, like Flory approximation, scaling arguments, numerical transfer matrix methods and Monte Carlo simulations [7-9].

In the present work we study the unbinding of semiflexible polymers for the case of short-ranged binding potentials. We use a restricted SOS (RSOS) model (see below), which allows the evaluation of the partition function of the chain exactly. The resulting phase diagram for the transition shows a number of distinct features when compared with the case when the fluctuations are driven by surface tension.

Consider the chain shown in figure 1. Let the chain be grafted with its left end to the line defect, which is put at $z=0$. The statistical weight of a given configuration of the polymer is expressed by a Boltzmann factor, $\exp(-E\{n_i\}/T)$, with the energy

$$E\{n_i\} = J \sum_{i=1}^{L-1} |(n_{i+1} - n_i) - (n_i - n_{i-1})| + K \sum_{i=1}^{L-1} |(n_{i+1} - n_i)| - u \sum_{i=0}^L \delta_{n_i,0}. \quad (1)$$

Here i measures the (integer) steps along the x -axis. Vertical bars denote absolute value. The integer-valued height variables, n_i , are measured along the z -direction and vary between zero and N_z . They describe the transverse fluctuations of the chain. The first term in (1), which is proportional to the discretized second derivative with respect to z , is the bending energy; J is the bending stiffness. The second term describes fluctuations due to surface tension. The third term, with $u > 0$, describes the wall attraction due to the substrate. We take the Boltzmann constant to be unity. When $J=0$, the model defined by (1) has been extensively used to study wetting phenomena in 1+1 dimensions [2]. Here we are interested in fluctuations due to bending rigidity, and, therefore put $K=0$.

The elements of the transfer matrix associated with (1) have to be labelled by a pair of height variables and can be written as

$$T_{(n_{i+1}, n_i), (n_i, n_{i-1})} = \omega^{|(n_{i+1} - n_i) - (n_i - n_{i-1})|} \kappa^{\delta_{n_i,0}} \quad (2)$$

where $\omega = e^{-J/T}$ and $\kappa = e^{u/T}$. In the existing studies of semiflexible polymers in terms of the restricted SOS (RSOS) model the restriction is imposed on the difference of the slope of the height variables. Using the discrete slope variables $v_i = (n_{i+1} - n_i)$, the exponent of ω in (2) becomes $|v_i - v_{i-1}|$. In the RSOS model this difference takes on values 0, 1. Since the difference of the n_i variables itself still can take on any value, the transfer matrix has dimensionality N_z^2 with all its elements different from zero. As a consequence, the largest eigenvalue and the corresponding eigenvector can be determined only by using approximate methods [7]. In the continuum version of the model the eigenvalue equation reduces to a partial differential equation [8], and one has to impose boundary conditions on both the n and v variables. In what follows, we impose restrictions on the difference of the n variables and allow $(n' - n)$ to take

on only the values 0 and ± 1 . This automatically restricts the difference of the slope variables $|v_i - v_{i-1}|$ to the values 0, 1, 2. With this modification many elements of the transfer matrix become zero by definition. The eigenvalue problem for T is still more complicated than in the case of wetting, but it can be shown by simple substitution that the following ansatz for an eigenvector solves all the eigenvalue equations:

$$\phi_{nn'} = \begin{cases} b_0 & \text{for } n = n' = 0 \\ b_1 e^{-\mu} & \text{for } n = 0, n' = 1 \\ a_{(n-n')} e^{-n'\mu} & \text{for } n \geq 1. \end{cases} \quad (3)$$

Since this expression, as a function of the index nn' does not have a node, it is a good candidate for the largest eigenvector of T . Inserting (3) into the eigenvalue equation, and fixing the normalization of ϕ by putting $a_0 = 1$, it follows that $b_1 = a_{-1}$. Denoting the eigenvalue corresponding to (3) by λ , one obtains the following system of equations for the unknowns $b_0, a_{-1}, a_1, \mu, \lambda$:

$$\kappa b_0 + \kappa \omega a_{-1} e^{-\mu} = \lambda b_0 \quad (4)$$

$$\kappa \omega b_0 + \kappa \omega^2 a_{-1} e^{-\mu} = \lambda a_1 \quad (5)$$

$$\omega a_1 e^{\mu} + \omega + \omega^2 a_{-1} e^{-\mu} = \lambda a_1 \quad (6)$$

$$\omega a_1 e^{\mu} + 1 + \omega a_{-1} e^{-\mu} = \lambda \quad (7)$$

$$\omega^2 a_1 e^{\mu} + \omega + a_{-1} e^{-\mu} = \lambda a_{-1}. \quad (8)$$

From the last three equations λ can be expressed as a function of ω and μ as

$$\lambda^3 - 3\lambda^2 + \lambda[1 - \omega^4 + 2(1 - \omega^2) \cosh \mu] - (\omega^2 - 1)^2 = 0. \quad (9)$$

Finally the parameter μ can be eliminated from (9), using equations (4) and (5). The unbinding transition takes place at $\mu = 0$, which is equivalent to a transition temperature $T_U = T(K, u)$. As can be seen from (9), for small deviations from the transition $\lambda(\mu) = \lambda(0) + \text{constant} \times \mu^2$. As a consequence, the free energy also contains a piece quadratic in μ , and, therefore, the specific heat has a jump at the transition, which is then second order. For $T > T_U$, the eigenstates of the transfer matrix are extended and the eigenvalues form a continuum in the limit $N_z \rightarrow \infty$. The largest eigenvalue in the unbound phase is at the edge of the continuum determined by $\lambda(0)$, which can be easily determined from (9)

$$\lambda(0) = 1 + \frac{1}{2}\omega[\omega + \sqrt{\omega^2 + 8}]. \quad (10)$$

Inserting this expression into (4) and (5) with $\mu = 0$ one obtains the phase boundary between the bound and unbound phases

$$\kappa = \frac{1 + \omega[\omega + \sqrt{\omega^2 + 8}]}{1 + \omega^2}. \quad (11)$$

The phase diagram is shown in figure 2 together with the one obtained when the unbinding is controlled by the surface tension term in (1) (i.e. $J = 0$). Figure 2 shows the phase diagram for both positive and negative values of J and K that is for $\omega > 1$ and $\omega < 1$. (When $J = 0$ in (1), $\omega = e^{-K/T}$.) In the semiflexible region ($J > 0, K > 0, \omega < 1$) there is not a big difference between the two cases; actually for $\omega = 1$ the two curves attain the same value. For $\omega > 1$, which can be called the plastic region, fluctuations driven by the first and second derivative of the curve $z(x)$ lead to completely different results. It is easy to understand this difference between the two cases. Figure

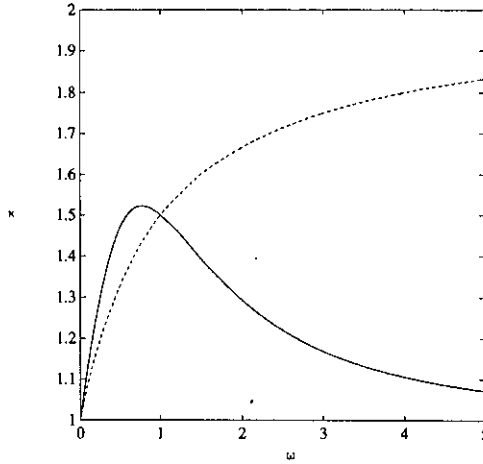


Figure 2. Phase diagram of the unbinding transition. Solid line: $J \neq 0, K = 0$ in equation (1), corresponding to unbinding controlled by bending rigidity. Dashed line: $J = 0, K \neq 0$ in equation (1), corresponding to unbinding controlled by surface tension.

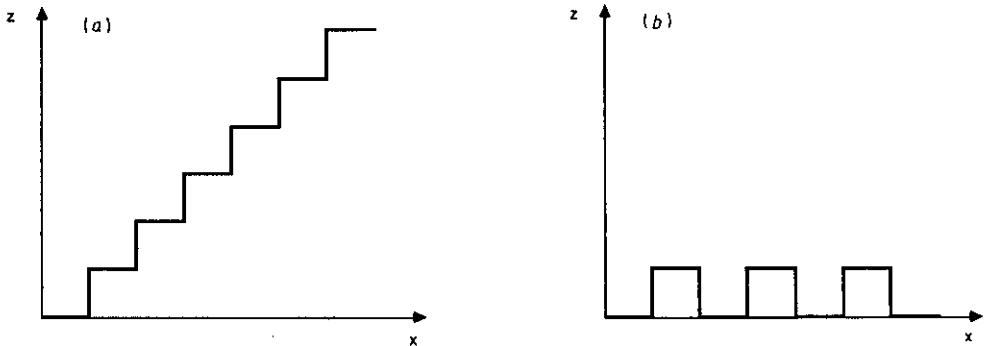


Figure 3. Typical configuration of the chain in the plastic phase. (a) $J = 0, K \neq 0$ in equation (1), (b) $J \neq 0, K = 0$ in equation (1).

3 shows configurations of the polymer within the RSOS model in the limit of infinite ω . In the case $J = 0, K \neq 0$, shown in figure 3(a) the chain benefits from getting further and further away from the substrate. (Note that the chain is always grafted with one of its ends to the substrate.) In this situation one needs an infinitely strong potential u or κ to bind the chain. In the case $J \neq 0, K = 0$ (figure 3(b)) there is a macroscopic number of monomers attached to the substrate even if $u = 0$, so the chain is bound even at $\kappa = 1$.

Once the largest eigenvalues and the corresponding eigenvectors are determined, all the relevant quantities of the system can be calculated. Approaching the unbinding transition from below, the mean position of the chain from the substrate, $l \equiv \langle n \rangle$ diverges linearly as $l \sim 1/\mu$. This defines the critical exponent $\psi = 1$ [2]. The mean fluctuation amplitude, or roughness, or perpendicular correlation length, which is defined by

$$\xi_{\perp} = [\langle (n - \langle n \rangle)^2 \rangle]^{1/2} \quad (12)$$

also diverges linearly with μ , giving $\nu_{\perp} = 1$ for the appropriate critical exponent. Another important length scale is the longitudinal (or parallel) correlation length, ξ_{\parallel} , whose

definition is

$$\langle [n_i - \langle n_i \rangle][n_j - \langle n_j \rangle] \rangle \sim \exp[-|i - j|/\xi_{\parallel}]. \quad (13)$$

Calculating the correlation function on the left-hand side of (13) in the bound phase close to the transition, one finds that ξ_{\parallel} diverges quadratically with μ , giving $\nu_{\parallel} = 2$ for the appropriate critical exponent. Finally, the relative number of monomers attached to the substrate vanishes linearly as the transition is approached.

In summary, we considered a simple RSOS model for a semiflexible polymer in $1 + 1$ dimensions. The fluctuations of the chain are controlled by bending rigidity. All the statistical and thermodynamic properties of the chain can be calculated exactly. In particular, the phase diagram and the relevant critical exponents at the second-order unbinding transition have been determined. The exponent values are the same as for the unbinding (wetting) transition of an interface driven by surface tension. In the plastic phase, however, the two models differ substantially. A similar model has been studied, using a variety of approximate methods in [7], where the restrictions of the RSOS model have been imposed on the slope variables, instead of the height variables. In that model the authors found a first order unbinding transition in the limit of infinite rigidity. In the present model this rather peculiar transition is not present.

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