LETTER TO THE EDITOR

Duality mapping and unbinding transitions of semiflexible and directed polymers

Jan Kierfeld and Reinhard Lipowsky

MPI für Kolloid und Grenzflächenforschung, D-14424 Potsdam, Germany

Received 9 November 2004, in final form 17 January 2005
Published 16 February 2005
Online at stacks.iop.org/JPhysA/38/L155

Abstract
Directed polymers (strings) and semiflexible polymers (filaments) are one-dimensional objects governed by tension and bending energy, respectively. They undergo unbinding transitions in the presence of a short-range attractive potential. Using transfer matrix methods we establish a duality mapping for filaments and strings between the restricted partition sums in the absence and the presence of a short-range attraction. This allows us to obtain exact results for the critical exponents related to the unbinding transition, the transition point and transition order.

PACS numbers: 05.70.Fh, 64.60.Fr, 82.35.Gh, 87.15.Aa

1. Introduction
Directed polymers (or 'strings' in the following) are one-dimensional objects governed by their tension which tends to minimize the contour length of the polymer. Semiflexible polymers (or 'filaments' in the following), on the other hand, are governed by their bending energy which tends to straighten the polymer. In the presence of a short-range attractive potential, these objects undergo unbinding or desorption transitions which represent a number of important critical phenomena [1, 2]. The unbinding of strings describes wetting [1], polymer adsorption [3], pinning of flux lines in type-II superconductors [4] or roughening of crystal surfaces [5]. The unbinding of filaments describes adsorption and bundling of many biopolymers (DNA, F-actin, microtubules) and polyelectrolytes with large persistence lengths [6].

In this letter we use transfer matrix (TM) methods to derive a duality mapping for filaments and strings between the restricted partition sums in the absence and the presence of a short-range attractive potential. This allows us to obtain the unbinding and desorption transition point, the order of the transition and a set of scaling relations for the critical exponents of bound and unbound filaments and strings.
2. Model

We consider strings or filaments in $1 + d_{\perp}$ dimensions which are oriented along the $x$-axis such that we can parametrize the contour by a $d_{\perp}$-dimensional field $z(x)$ of displacements perpendicular to the $x$-axis with $0 < x < L$, where $L$ is the projected length of the string or filament. The Hamiltonian for strings is given by the sum of the tension energy $\int_0^L dx (\sigma/2)(\partial_x z)^2$ with a string tension $\sigma$ and the potential energy $\int_0^L V(z(x))$, where $V(z)$ contains an attractive potential well of range $\ell_a$ which favours the configuration $z = 0$.

The Hamiltonian for filaments is given by the sum of the bending energy $\int_0^L dx (\kappa/2)(\partial_x^2 z)^2$ and the potential energy $\int_0^L V(z(x), \partial_x z)$. $\kappa$ is the bending rigidity of the filament and $L_p = 2\kappa / T$ is the persistence length at temperature $T$. The expression for the bending energy in the parametrization by the projected length is appropriate if either the total length $L$ or the longitudinal correlation length $\xi_L$ to be defined below is small compared to $L_p$. In contrast to the string, the filament has a well-defined tangent vector at each point, and therefore, also the external potential $V(z, v)$ can depend on the tangent vector $v \equiv \partial_x z$.

Generic potentials are of the form $V = V_r + V_a + V_p$ and contain a hard-core potential $V_r$, a short-range attractive potential $V_a$ and eventually a long-range power-law potential $V_p$. The hard-core potential $V_r$ is given by $V_r(z) = \infty$ for $|z| < \ell_r$, and $V_r(z) = 0$ otherwise. The short-range attractive potential $V_a$ attains the asymptotic form $V_a(z) \sim G \ell_a^{-d_{\perp}} \Phi(v) \delta(z)$ in the limit of small $\ell_a$ where $G \equiv W \pi^{d_{\perp}/2} / \Gamma(1 + d_{\perp}/2) < 0$. Finally, we can also include attractive long-range power-law potentials $V_p(z) = w|z|^{-p}$ for $|z| > \ell_a$. Our results apply to potentials $V_a$ that decay sufficiently fast, i.e., potentials $V_p$ with $p \geq 2$ for strings and $p \geq 2/3$ for filaments [7].

3. Transfer matrix equations

In order to simplify the notation, we introduce rescaled quantities measuring energies in units of the temperature $T$ and lengths in units of $T / 2\sigma$ for strings and in units of the persistence length $L_p = 2\kappa / T$ for filaments. In rescaled units the restricted partition sum for strings with fixed initial point $z_0 \equiv z(0)$ and end point $z \equiv z(L)$ takes the form

$$Z_L(z|z_0) = \int_{(z_0;0)}^{(z;L)} Dz(x) \exp \left\{ -\int_0^L dx \left[ \frac{1}{4} (\partial_x z)^2 + V(z(x)) \right] \right\}. \quad (1)$$

In analogy with quantum mechanics, this path-integral fulfils a Schrödinger equation in imaginary time, the partial differential TM equation given by

$$\partial_t Z_L = \nabla^2_z Z_L - V(z) Z_L \quad (2)$$

with the boundary condition $Z_0(z|z_0) = \delta(z - z_0)$ at $L = 0$. The Laplace transform of the restricted partition sum with respect to $L$, $\tilde{Z}_s = \int_0^\infty dL e^{-sL} Z_L$, fulfils the differential TM equation

$$s \tilde{Z}_s = \nabla^2_{\tilde{z}} \tilde{Z}_s - V(z) \tilde{Z}_s + \delta(z - z_0) \quad (3)$$

where the last term on the right-hand side represents the boundary condition at $L = 0$.

For a sufficiently attractive potential, there exist bound states for which we make the ansatz $Z_L(z|z_0) \sim \psi_L(z) \exp(-E L)$, where $E < 0$ is the free energy difference between the bound
state and the free state (obtained for $V = 0$). The eigenfunction $\psi_E(z)$ for the energy level $E$ then solves the stationary Schrödinger equation (2)

$$-E\psi_E = \nabla_z^2 \psi_E - V(z)\psi_E$$

with $E < 0$ for a bound state. We impose the normalization $\int \psi_E^2(z) = 1$. Then the solution satisfying the proper boundary condition is obtained by summing over all energy levels $E_n$, $Z_L(z|z_0) = \sum_n \psi_{E_n}(z)\psi_{E_n}(z_0) e^{-E_n L}$, where the ground state $E_0$ dominates the sum for lengths $L$ exceeding the correlation length $\xi_1 = 1/|E_0|$ (assuming that binding is weak such that the continuous scattering spectrum starts at $E_1 = 0$).

For filaments we can proceed similarly starting from the restricted partition sum in rescaled units, in which we additionally fix initial tangent $v_0 = \partial_z z(0)$ and end tangent $v = \partial_z z(L)$. This partition function is given by

$$Z_L(z, v|z_0, v_0) = \int_{(z_0, v_0; 0)} \mathcal{D}z(x) \exp \left\{ -\int_0^L dx \left[ \frac{1}{4}(\nabla_z^2 z)^2 + V(z(x), \partial_z z) \right] \right\}$$

and again fulfills a Schrödinger-like differential TM equation [8, 9]

$$\partial_z Z_L = -v \cdot \nabla_z Z_L + \nabla_v^2 Z_L - V(z, v) Z_L$$

with the boundary condition $Z_0(z, v|z_0, v_0) = \delta(z - z_0)\delta(v - v_0)$ at $L = 0$. As for strings we can consider the Laplace transform which fulfills the differential TM equation

$$s \tilde{Z}_s = -v \cdot \nabla_z \tilde{Z}_s + \nabla_v^2 \tilde{Z}_s - V(z, v) \tilde{Z}_s + \delta(z - z_0)\delta(v - v_0)$$

where the last term on the right-hand side stems from the boundary condition at $L = 0$. For sufficiently strong attractive potential, there exist bound states for which we make the ansatz $Z_L(z, v|z_0, v_0) \sim \psi_E(z, v) \exp(-E L)$, where $E < 0$ is the free energy difference between the bound and the free state. The eigenfunction $\psi_E(z, v)$ for the energy level $E$ then solves the stationary version of the Schrödinger-like equation (6),

$$-E\psi_E = -v \cdot \nabla_z \psi_E + \nabla_v^2 \psi_E - V(z, v)\psi_E$$

with $E < 0$ for a bound state. As for strings, we impose a normalization $\int \int \psi_E^2(z, v) = 1$, and the solution satisfying the proper boundary condition is obtained by summing over all energy levels $E_n$. For lengths $L$ exceeding the correlation length $\xi_1 = 1/|E_0|$, the ground state dominates and $Z_L(z, v|z_0, v_0) \approx \psi_{E_0}(z, v)\psi_{E_0}(z_0, v_0) e^{-E_0 L}$.

4. Scaling behaviour and exponents

Strings and filaments differ in the scaling of free mean-square displacements, i.e., $\langle |z|^2 \rangle \sim L^{2\xi}$ for $V = 0$ where $\xi$ is the roughness exponent. Strings show diffusive behaviour with $\xi = 1/2$, whereas filaments have $\xi = 3/2$. Tangent vector fluctuations scale as $\langle |v|^2 \rangle \sim L^{2(\xi-1)}$ and show diffusive behaviour for filaments, whereas tangent vector fluctuations are finite and thus irrelevant for the scaling behaviour of strings. In the presence of a potential $V = V_r + V_a + V_p$, the scaling behaviour of unbound segments of a string or filament is governed by the same roughness exponents (provided $p \geq 2$ for strings and $p \geq 2/3$ for filaments [7]).

For unbound strings and filaments, i.e., in the absence of a sufficiently strong attractive potential $V_a$, this leads to the scaling form

$$Z_L = L^{-\xi_{\theta}^0} |z|^{\theta_{\theta}^0/2} \Omega_{\theta}(|z|L^{-\xi}, |v|L^{1-\xi})$$

in the limit of small $|z_0|$ and $|v_0|$. For strings, the tangent $v$ is an irrelevant scaling variable. We introduced exponents $\chi_{\theta}$ characterizing the return probability and $\theta_{\theta}$ characterizing the
Kolmogorov relations come from small scales of the polymer segment distribution at $z \approx 0$, and a shape function $\Omega_u(y, u)$ (with finite $\Omega_u(0,0)$) giving the shape of the polymer segment distribution.

For strings and filaments bound by the attractive potential $V_a$, the longitudinal correlation length $\xi = 1/|E_0|$ gives the characteristic length of unbound segments and enters the scaling behaviour,

$$Z_L = \xi^{-\chi_u} |z|^{\theta_u/2} \Omega_u(z, |z|^{1-\chi_u}) e^{L/\xi}$$

with analogous exponents $\chi_b$ and $\theta_b$, which differ from the unbound case in general.

For a given potential, the two exponents $\chi$ and $\theta$ are not independent as can be seen by using the above scaling forms in the Chapman–Kolmogorov relations

$$Z_L(\mathbf{z}, \mathbf{v}|\mathbf{z}_0, \mathbf{v}_0) = Z_{2L}(\mathbf{z}_1, \mathbf{v}_1|\mathbf{z}_0, \mathbf{v}_0)$$

and

$$Z_L(\mathbf{z}, \mathbf{v}|\mathbf{z}_0, \mathbf{v}_0) = Z_{2L}(\mathbf{z}_1|\mathbf{z}_0) Z_L(\mathbf{z}_1|\mathbf{z}_0)$$

for strings. This leads to scaling laws

$$\chi = \max(d_L/2 + \theta/2, 0) \quad \text{(strings)}, \quad \chi = \max(2d_L + 3\theta/2, 0) \quad \text{(filaments)}$$

holding for both $\chi_u, \theta_u$ and $\chi_b, \theta_b$. Exponents $\chi < 0$ are not possible because they correspond to an unphysical increase of contacts as the length $\xi$ of unbound segments increases. If $d_L/2 + \theta/2 < 0$ for strings or $2d_L + 3\theta/2 < 0$ for filaments a finite fraction of all polymer segments is bound at $z = 0$ and the main contributions to the $z$-integrals in the Chapman–Kolmogorov relations come from small scales $|z| \sim \ell_a$ leading to $\chi = 0$ in (11).

5. Duality mapping

Inspecting the Laplace transformed TM equation (3) and the stationary TM equation (4) for strings, we observe a formal similarity if we identify $\delta(\mathbf{z} - \mathbf{z}_0)$ in the stationary TM equation (4) plays the role of the initial condition in the Laplace transformed TM equation (3) for a potential $V - V_a$, i.e., in the absence of the short-range attraction $V_a$. A similar observation can be made for the corresponding TM equations (7) and (8) for filaments where a short-range attractive potential $V_a(\mathbf{z}, \mathbf{v}) \propto -\delta(\mathbf{z} - \mathbf{z}_0) \delta(\mathbf{v} - \mathbf{v}_0)$ in the stationary TM equation (8) plays the role of the initial condition in the Laplace transformed TM equation (7) for a potential $V - V_a$. This is the main idea of the present letter and will allow us to establish a duality mapping between the stationary TM equation for bound states (characterized by the set of exponents $\theta_b$ and $\chi_b$) in a generic potential $V = V_r + V_a + V_p$ and the Laplace transformed TM equation for unbound states (characterized by the set of exponents $\theta_u$ and $\chi_u$) in a potential $V - V_a$ = $V_r + V_p$ lacking the short-range attractive part.

A string in a bound state $\psi_E^V(\mathbf{z})$ fulfils the stationary TM equation (4) for a potential $V$ containing the short-range attraction $V_a(\mathbf{z}) = G \delta(\mathbf{z} - \mathbf{z}_0)$ where we consider the limit of small $|z_0|$. We compare the stationary TM equation (4) with the Laplace transformed TM equation (3) for $\tilde{Z}^{V-V_a}(\mathbf{z}|\mathbf{z}_0)$ with $s = -E$ and for a potential $V - V_a$ without the short-range attraction. If we rewrite

$$\delta(\mathbf{z} - \mathbf{z}_0) = \delta(\mathbf{z} - \mathbf{z}_0) \tilde{Z}^{V-V_a}(\mathbf{z}|\mathbf{z}_0)/Z^{V-V_a}(\mathbf{z}|\mathbf{z}_0)$$

we find that both equations are equivalent and solutions have the same normalization if the following two conditions are fulfilled:

$$\psi_E^V(\mathbf{z}) = N_E^V \tilde{Z}^{V-V_a}(\mathbf{z}|\mathbf{z}_0)$$

with

$$N_E^{V-V_a} = \int_\mathbf{z} \left[ \tilde{Z}^{V-V_a}(\mathbf{z}|\mathbf{z}_0) \right]^2$$

and

$$-G^{-1} = \tilde{Z}^{V-V_a}(\mathbf{z}|\mathbf{z}_0) = \psi_E^V(\mathbf{z}_0) / N_E.$$

These two conditions define the duality mapping for strings between TM equations for potentials $V$ and $V - V_a$.

For filaments we proceed analogously for a bound state $\psi_E^V(\mathbf{z}, \mathbf{v})$ which fulfils the stationary TM equation (8) for a potential $V$ containing the short-range attraction...
\[ V_s(z, v) = G \delta(z - z_0) \delta(v - v_0), \]
where we consider the limit of small \(|z_0|\) and \(|v_0|\). We compare the stationary TM equation (8) with the Laplace transformed TM equation (7) for \(Z_s^{-V_s}(z, v|z_0, v_0)\) with \(s = -E\) and for a potential \(V - V_s\) without short-range attraction.

Following analogous steps as outlined for strings above, we find the following duality mapping for filaments,

\[ \psi^V_E(z, v) = N_E Z_s^{-V_s}(z, v|z_0, v_0) \quad \text{with} \quad N_E^{-2} = \int_{z, v} \left[ Z_s^{-V_s}(z, v|z_0, v_0) \right]^2, \]

relating the TM equations for potentials \(V\) and \(V - V_s\). This exact mapping can be generalized to the more general class of potentials \(V_a = G \Phi(v) \delta(z)\) if we use the additional assumption that \(Z_s^{-V_s}(z_0, v_0|z_0, 0) \sim \delta(v_0)\) is a strongly localized function of \(v_0\) in the limit \(z_0 \approx 0\). This assumption is justified if the scaling function \(\Omega_a(y, u)\) is exponentially decaying for \(u \gg 1\) such that \(Z_s^{-V_s}(z_0, v_0|z_0, 0) \approx 0\) for tangents \(|v_0| \gg |z_0|^{|V_s|/3}\). Then we can integrate both sides of (7) with a kernel \(\int_{v_0} \Phi(v_0) Z_s^{-V_s}(z_0, v_0|z_0, 0) \ldots\), which finally leads to a generalized duality mapping

\[ \psi^V_E(z, v) = N_E Z_s^{-V_s}(z, v|z_0, 0) \quad \text{with} \quad N_E^{-2} = \int_{z, v} \left[ Z_s^{-V_s}(z, v|z_0, 0) \right]^2, \]

\[ -G^{-1} = \int_{v_0} \Phi(v_0) Z_s^{-V_s}(z_0, v_0|z_0, 0) = \int_{v_0} \Phi(v_0) \psi^V_E(z_0, v_0)/N_E, \]

which is valid in the limit \(z_0 \approx 0\).

The validity of the duality mappings can be confirmed for a number of potentials by direct TM calculations for strings [11] and filaments [6, 12]. The mappings allow us to obtain results for the full potential \(V\) by solving the Laplace transformed problem for the simpler potential \(V - V_s\) and give direct information on the partition sums \(\psi^V_E(z, v)\) and \(Z_s^{-V_s}(z, v|z_0, 0)\ldots\), and thus the segment distributions. The duality mappings generalize exponent relations that have been found previously, as we will show in the following section. Furthermore, relations (13), (15) and (17) allow us to determine the transition point, i.e., the critical potential strength \(G_c\), and the exponent \(v_f\) describing the divergence of the correlation length close to the transition, \(\xi_1 \propto |G - G_c|^{-v_f}\).

6. Exponent relations

Without working out explicit solutions of the TM equations, we can use the duality mapping to derive various exact exponent relations. To derive the exponent relation for \(\chi_u\) and \(\chi_b\) for strings we study the limit of small \(|E|\) in (12).

The scaling form (9) for the unbound string determines the \(s\)-dependence of the singular part of \(\tilde{Z}_s^{-V_s}\) for small \(s\) according to \(\tilde{Z}_s^{-V_s} \sim s^{\phi_u-1}\). For \(\chi_u < 1\) the singular part is the leading-order contribution; for \(\chi_u > 1\) the leading-order contribution is finite, \(\tilde{Z}_s^{-V_s} \sim \text{const}\). Using the Chapman–Kolmogorov relation, we find from (12) the singular behaviour \(N_E^{-1} \sim |E|^{\chi_u/2}\) for \(\chi_u < 2\) for small \(|E|\) and \(N_E \sim \text{const}\) for \(\chi_u > 2\). Furthermore, \(\psi^V_E \sim |E|^{\chi_b/2}\) for small \(|E|\) according to the scaling form (10). Equating powers of \(|E|\) in (12) we arrive at the exponent relation

\[ \chi_b = \begin{cases} \max(2 - \chi_u, 0) & \text{for } \chi_u > 1 \\ \chi_u & \text{for } \chi_u < 1 \end{cases} \]

for strings. For filaments, an analogous analysis of relation (14) at small \(|E|\) gives the same exponent relation (18). For strings, relation (18) agrees with direct calculations using the
TM equations [11] and also applies in the presence of a long-range power-law potential $V_2 \sim w|z|^{-2}$ ($p = 2$), where the exponents $\chi$ depend continuously on $w$, as can be checked using the results of [10]. Also for filaments, (18) agrees with direct TM calculations for potentials $V = V_2$ and $V = V_s + V_a$ [6, 12]. This exponent relation has been formulated in [13] based on a mapping between the renormalization group equations for strings and filaments of different dimensionality. An equivalent exponent relation has been confirmed numerically in [8].

In order to derive the corresponding exponent relation for $\theta_s$ and $\theta_b$ for strings and filaments, we analyse the scaling behaviour of the Laplace transform $\tilde{Z}_V^{V_s-V_a}$ of the unbound string or filament for small $|z|$ in (12) and (14), respectively. Using the scaling form (9) for the unbound string or filament we find $\tilde{Z}_V^{V_s-V_a} \sim |z|^{(1-\chi_s)/\nu_s+\theta_s/2}$ for $\chi_s > 1$ and $\tilde{Z}_V^{V_s-V_a} \sim |z|^\theta_s$ for $\chi_s < 1$. According to the scaling form (10) for the bound string or filament we have $\psi_s^{V_s-V_a} \sim |z|^\nu_s$ for small $|z|$. Equating powers of $|z|$ in (12) or (14) we arrive at the exponent relation

$$
\theta_b = \begin{cases} 
\theta_a + 2(1 - \chi_a)/\zeta & \text{for } \chi_a > 1 \\
\theta_a & \text{for } \chi_a < 1,
\end{cases}
$$

which holds for strings with $\zeta = 1/2$ and $\chi_a = d_s/2 + \theta_b/2$ and filaments with $\zeta = 3/2$ and $\chi_a = 2d_s + 3\theta_b/2$, according to the scaling laws (11) (note that $\chi_a > 0$ for the unbound case). Again, it can be checked that relation (19) agrees with direct TM calculations both for strings [10, 11] and for filaments [6, 8, 12, 13].

Now we address the transition point, transition order and the correlation length exponent $\nu_1$ by analysing the dependence of the bound state energy $E$ on the potential strength $G$ in relations (13) and (15). Setting $E = 0$ on the right-hand side we find the transition point $G_c$. As the singular part of $\tilde{Z}_V^{V_s-V_a}$ for small $s$ is $\tilde{Z}_V^{V_s-V_a} \sim s^{\chi_s-1}$, we find $G_c = 0$ for $\chi_s < 1$; thus, there is no unbinding transition for $\chi_s < 1$ and strings and filaments are always in a bound state. Expanding around $E = 0$ for $\chi_s > 1$ gives $|G_c^{-1} - G^{-1}| \propto |E|^{1/\nu_1} = \xi_\parallel^{1/\nu_1}$ with

$$
1/\nu_1 = \max(\chi_a - 1, 1) \quad \text{for } \chi_0 > 1.
$$

We also used that the linear order dominates the singular contribution to $\tilde{Z}_V^{V_s-V_a}$ for $\chi_a > 2$ such that the transition becomes first order with $\nu_1 = 1$. For $1 < \chi_a < 2$, we find $\nu_1 > 1$ and a continuous transition. The result (20) agrees with those of the necklace model [14]. For filaments, relation (20) can be generalized for a class of tangent-dependent potentials $V_a = G\Phi_s(v)\delta(z)$, satisfying a homogeneity relation $\Phi_s(bv) = b^{-\Delta}\Phi_s(v)$, which has been considered also in [6]. Performing the analogous expansion in (17) we find

$$
1/\nu_1 = \min(\tilde{\chi}_a - 1, 1) \quad \text{for } \tilde{\chi}_a > 1 \quad \text{where } \tilde{\chi}_a \equiv \chi_a - d_s(1 - \Delta)/2.
$$

For this class of potentials there is no transition for $\tilde{\chi}_a < 1$, a first-order transition for $\tilde{\chi}_a > 2$ and a continuous transition for $1 < \tilde{\chi}_a < 2$. The result (20) is recovered for $\Delta = 1$ and $\Phi_s(v) = \delta(v)$.

The exponent relations (18) and (20) or (21), together with the scaling law (11), allow us to calculate all critical exponents of the unbinding problem if only one exponent ($\chi_a$ or $\theta_a$) of the unbound string or filament in the absence of the short-range attractive potential is known. These exponents are often known analytically, or can be easily obtained numerically. For $V = 0$, we have $\theta_a = \theta_b = 0$ for strings and filaments. For $V = V_s$ and $d_s = 1$, we can make use of another exponent relation, $\chi_a = \chi_r = 1 + \zeta$ [15], which is also valid for both strings and filaments.
7. Conclusions

In conclusion we derived a duality mapping between bound and unbound states of one-dimensional strings and filaments. This mapping allows us to determine the transition point and the order of unbinding and desorption transitions of strings and filaments. We derived exponent relations for the return probability exponents $\chi$, the segment distribution exponents $\theta$ and the correlation length exponent $\nu$ from the mapping. These relations allow us to determine all critical exponents related to the unbinding and desorption transitions of both filaments and strings from a single exponent characterizing the unbound string or filament.

References