

EUROPHYSICS LETTERS

OFFPRINT

Vol. 66 • Number 5 • pp. 763–769

Barrier crossing of semiflexible polymers

* * *

P. KRAIKIVSKI, R. LIPOWSKY and J. KIERFELD



Published under the scientific responsibility of the
EUROPEAN PHYSICAL SOCIETY
Incorporating
JOURNAL DE PHYSIQUE LETTRES • LETTERE AL NUOVO CIMENTO



EUROPHYSICS LETTERS

Editor-in-Chief

Prof. Denis Jérôme
Lab. Physique des Solides - Université Paris-Sud
91405 Orsay - France
jerome@lps.u-psud.fr

Staff Editor: Yoanne Sobieski
Europhysics Letters, European Physical Society, 34 rue M. Seguin, 68060 Mulhouse Cedex, France

Editorial Director: Angela Oleandri
Production Editor: Paola Marangon

Publishers: EDP Sciences S.A., France - Società Italiana di Fisica, Italy

Taking full advantage of the service on Internet,
please choose the fastest connection:

<http://www.edpsciences.org>
<http://edpsciences.nao.ac.jp>
<http://edpsciences-usa.org>
<http://www.epletters.ch>

Director of publication: Jean-Marc Quilbé

Europhysics Letter was launched more than fifteen years ago by the European Physical Society, the Société Française de Physique, the Società Italiana di Fisica and the Institute of Physics (UK) and owned now by 17 National Physical Societies/Institutes.

Europhysics Letters aims to publish short papers containing non-trivial new results, ideas, concepts, experimental methods, theoretical treatments, etc. which are of broad interest and importance to one or several sections of the physics community.

Europhysics letters provides a platform for scientists from all over the world to offer their results to an international readership.

Subscription 2004

24 issues - Vol. 65-68 (6 issues per vol.)

ISSN: 0295-5075 - ISSN electronic: 1286-4854

- France & EU (VAT included) 1 678 €
- Rest of the World (without VAT) 1 678 €

Payment:

- Check enclosed payable to EDP Sciences
- Please send me a pro forma invoice
- Credit card:
 Visa Eurocard American Express

Valid until: [][][][][]

Card No: []

- Please send me a free sample copy

Institution/Library:

.....

Name:

Position:

Address:

.....

.....

ZIP-Code:

City:

Country:

E-mail:

Signature:

Order through your subscription agency or directly to EDP Sciences:

17 av. du Hoggar • B.P. 112 • 91944 Les Ulis Cedex A • France
Tel. 33 (0)1 69 18 75 75 • Fax 33 (0)1 69 86 06 78 • subscribers@edpsciences.org

Barrier crossing of semiflexible polymers

P. KRAIKIVSKI, R. LIPOWSKY and J. KIERFELD

*Max-Planck-Institut für Kolloid- und Grenzflächenforschung
14424 Potsdam, Germany*

(received 14 January 2004; accepted in final form 5 April 2004)

PACS. 87.15.-v – Biomolecules: structure and physical properties.

PACS. 87.15.He – Dynamics and conformational changes.

PACS. 87.15.Tt – Electrophoresis.

Abstract. – We consider the motion of semiflexible polymers in double-well potentials. We calculate shape, energy, and effective diffusion constant of kink excitations, and in particular their dependence on the bending rigidity of the semiflexible polymer. For symmetric potentials, the kink motion is purely diffusive, whereas kink motion becomes directed in the presence of a driving force on the polymer. We determine the average velocity of the semiflexible polymer based on the kink dynamics. The Kramers escape over the potential barriers proceeds by nucleation and diffusive motion of kink-antikink pairs, the relaxation to the straight configuration by annihilation of kink-antikink pairs. Our results apply to the activated motion of biopolymers such as DNA and actin filaments or synthetic polyelectrolytes on structured substrates.

Introduction. – The Kramers problem [1] of thermally activated escape of an object over a potential barrier is one of the central problems of stochastic dynamics. It has been extensively studied not only for point particles [2], but also for extended objects such as elastic strings which occur in a variety of contexts in condensed-matter physics such as dislocation motion in crystals [3], motion of flux lines in type-II superconductors [4], or charge-density waves [5]. Elastic strings activate over potential barriers by nucleation and subsequent separation of soliton-antisoliton pairs which are localized kink excitations [6, 7]. An analogous problem is the activated motion of a flexible polymer over a potential barrier [8].

However, the thermally activated escape of a semiflexible polymer, which is a filament governed by its bending energy rather than entropic elasticity or tension, remained an open question that we want to address in this paper. Semiflexible polymers such as DNA or actin filaments have a large bending stiffness and, thus, a large persistence length, L_p . On scales exceeding L_p , the orientational order of the polymer segments decays exponentially, and the polymer effectively behaves as a flexible chain with a segment size set by L_p . In contrast, on length scales which are small compared to L_p , the bending energy of the semiflexible polymer strongly affects the behaviour of the polymer. The persistence lengths of the most prominent biopolymers range from 50 nm for DNA [9], to the 10 μ m range for actin [10, 11] or even up to the mm range for microtubules [11] and becomes comparable to typical contour lengths of these polymers. Whereas the adsorption of such semiflexible polymers onto homogeneous adhesive

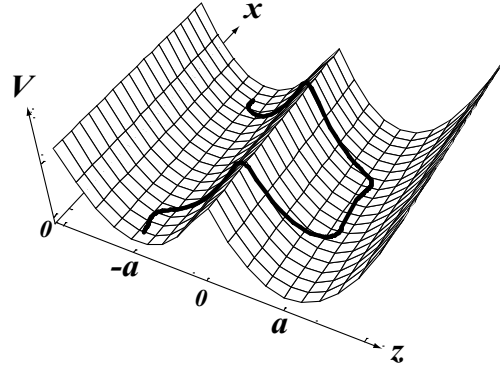


Fig. 1 – Typical conformation of a semiflexible polymer (thick line) with a kink-antikink pair in a double-well potential V which depends on the coordinate z and is independent of the coordinate x .

surfaces has been studied previously in [12–14], much less is known about the behaviour of a semiflexible polymer adsorbed on a *structured* surface.

In this article we focus on the escape of a semiflexible polymer over a translationally invariant potential barrier as shown in fig. 1, which can be realized on chemically or lithographically structured surfaces. The behaviour of semiflexible biopolymers on such structured substrates is of interest, *e.g.*, for electrophoresis applications [15]. Another important class of semiflexible polymers are synthetic polyelectrolytes, whose self-assembly and dynamic behaviour on structured substrates has only been studied recently [16]. In this article we consider homogeneous driving forces across the potential barriers as they can be easily realized on structured substrates by electric fields for charged polymers as in electrophoresis or by hydrodynamic flow. Alternatively, escape over a barrier can be driven by entropic forces arising from asymmetric shapes of the potential valleys [17].

Our main results are as follows. As for flexible polymers, the activated dynamics of semiflexible polymers is governed by the nucleation of localized kink-like excitations shown in fig. 1. We find, however, that the activated dynamics of semiflexible polymers is different from that of flexible polymers as kink properties are not governed by entropic elasticity of the polymer chain but rather by the bending energy of the semiflexible polymer. This enables us to determine the persistence length from kink properties. Furthermore, we calculate time scales for barrier crossing and the mean velocity of the semiflexible polymer for all regimes of driving forces: i) nucleation and purely diffusive motion of single kinks, ii) nucleation and driven diffusive motion of single kinks and iii) for large driving force dynamic equilibrium between nucleation and recombination in a kink ensemble.

Model. – We consider the dynamics of a semiflexible polymer in $1 + 1$ dimensions in a double-well potential that is translationally invariant in one direction, say the x -axis as in fig. 1. The semiflexible polymer has a bending rigidity κ and persistence length $L_p = 2\kappa/T$, where T is the temperature in energy units. We focus on the regime where the potential is sufficiently strong that the semiflexible polymer is oriented along the x -axis and can be parameterized by displacements $z(x)$ perpendicular to the x -axis with $-L/2 < x < L/2$, where L is the projected length of the polymer. The Hamiltonian of the semiflexible polymer is given by

$$\mathcal{H} = \int_{-L/2}^{L/2} dx \left[\frac{\kappa}{2} (\partial_x^2 z)^2 + V(z) \right], \quad (1)$$

i.e., the sum of its bending and potential energy. We consider a piecewise harmonic double-well potential $V(z) = \frac{1}{2}V_0(|z| - a)^2 - Fz$ that is independent of x and thus translationally invariant in the x -direction, where V_0 is the depth of the potential and F an external driving force density. Below the critical force $F_c \equiv aV_0$, the potential has two minima at $z_{\min}^{\pm} = \pm a + F/V_0$. The Hamiltonian (1) can be made dimensionless by measuring energies in units of a characteristic energy $E_{sc} = a^2\kappa^{1/4}V_0^{3/4}$, the x -coordinate in units of a characteristic length $x_{sc} = (\kappa/V_0)^{1/4}$ and the z -coordinate in units of a .

We consider an overdamped dynamics of the semiflexible polymer with an equation of motion

$$\gamma\partial_t z = -\frac{\delta\mathcal{H}}{\delta z} + \zeta(x, t) = -\kappa\partial_x^4 z - V'(z) + \zeta(x, t), \quad (2)$$

where γ is the damping constant and ζ is a Gaussian distributed thermal random force with $\langle\zeta\rangle = 0$ and $\langle\zeta(x, t)\zeta(x', t')\rangle = 2\gamma T\delta(x - x')\delta(t - t')$.

Static kink. – At first, we construct the static kink for $F = 0$, which is a localized metastable excitation. The static kink $z_k(x)$ is defined as the configuration that minimizes the energy (1), *i.e.*, is a time-independent solution of (2) in the absence of thermal noise ($\zeta = 0$) for boundary conditions $z_k(\pm L/2) = \pm a$ and $\partial_x z_k|_{\pm L/2} = 0$. For $F = 0$, the potential is symmetric and $V(z) = V(-z)$ such that the kink configuration is anti-symmetric with $z_k(x) = -z_k(-x)$ and centered at $x = 0$ (*i.e.* $z_k(0) = 0$). For our piecewise defined potential we have to fulfill five matching conditions at $x = 0$ which connect the two parts $x < 0$ and $x > 0$ of the kink: $z_k(-0) = z_k(+0) = 0$, $\partial_x^n z_k|_{-0} = \partial_x^n z_k|_{+0}$ for $n = 1, 2, 3$. Both parts $z_k(x) + a$ for $x < 0$ and $z_k(x) - a$ for $x > 0$ of the static kink are linear combinations of the four functions $e^{\pm x/w_k}$, $e^{\pm ix/w_k}$, where the eight linear expansion coefficients are determined from the boundary and matching conditions. The width w_k of the kink and the energy E_k of a single static kink in the thermodynamic limit of large L are given by

$$w_k = \sqrt{2}x_{sc} = \sqrt{2}(\kappa/V_0)^{1/4} \quad \text{and} \quad E_k = E_{sc}/\sqrt{2} = a^2\kappa^{1/4}V_0^{3/4}. \quad (3)$$

We expect our results for the kink energy $E_k \sim E_{sc}$ and width $w_k \sim x_{sc}$ to hold for all potentials with a barrier height $\sim V_0 a^2$ and potential minima separation $\sim a$ independent of the particular potential form; only numerical prefactors will differ. We want to point out that measurements of the kink width w_k and the critical force density F_c or the kink energy E_k are sufficient to determine the bending rigidity $\kappa = F_c w_k^4/4a = E_k w_k^3/2a^2$ and thus the persistence length $L_p = 2\kappa/T$ if the distance $2a$ between potential minima is known.

A static single kink in a polymer of length L is equivalent to one half of a symmetric kink-antikink pair configuration with kink-antikink separation $d = L$ in a polymer of length $2L$, as shown in fig. 1. The kink-antikink interaction energy $E_{\text{int}}(d) = 2(E_k(d) - E_k(\infty))$ can thus be found by determining the single kink energy in a polymer of length $L = d$. For large separation $d/w_k \gg 1$, we find an exponential decay $E_{\text{int}}(d) \sim \exp[-2d/w_k]$.

A semiflexible polymer will stay localized to the potential wells even if we set $V(z) = 0$ for $|z| > 2a$ as long as $V_0 > V_{0,c}$ with $V_{0,c} a^2 \simeq (T/L_p)(L_p/a)^{2/3}$ according to [14]. This condition is equivalent to $E_k \gg T$ and thus a small density of thermally induced kink excitations. A small kink density in combination with the condition $L_p \gg a$ also ensures that the semiflexible polymer stays oriented along the x -axis so that the Hamiltonian (1) stays valid. The condition $E_k \gg T$ of a small kink density is equivalent to $L_p \gg w_k^3/a^2$. For sufficiently strong substrate potentials, this gives a much wider range of applicability of the Hamiltonian (1) than in the absence of a potential where the condition $L_p > L$ of weak bending has to be fulfilled for a semiflexible polymer to be oriented.

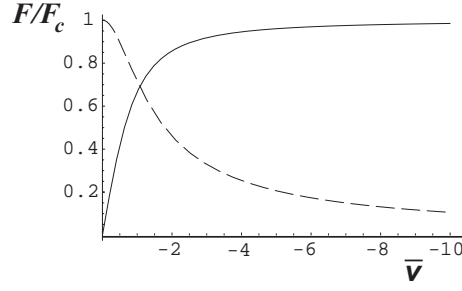


Fig. 2 – Force density F (in units of F_c , solid line) and friction constant η_k (in units of $3F_c a/2^{3/2}v_{sc} = 3a^2\gamma/w_k$, dashed line) as a function of velocity $\bar{v} = 3^{3/4}v/4v_{sc}$ for a moving kink.

Moving kink. – A driving force density F leads to an asymmetry in the potential and an effective force on kinks. Moving a kink by $-\Delta x$ increases the polymer length in the lower potential minimum by Δx and leads to an energy gain $-2aF\Delta x$ and thus a constant force $\mathcal{F}_k = -2aF$ on a kink. As argued above, deviations from kink interactions are exponentially small for separations $d \gg w_k$. The force \mathcal{F}_k leads to kink motion so that we also have to consider moving kink solutions. For constant kink velocity v , the kink configuration assumes a form $z_k(x, t) = z_k(x - vt)$ that solves (2) for $\zeta = 0$. Introducing the coordinate $y \equiv x - vt$ for the comoving frame, eq. (2) reduces to

$$\kappa \partial_y^4 z_k - v\gamma \partial_y z_k + V'(z_k) = 0, \quad (4)$$

which has to be solved with boundary conditions analogously to the static kink. However, in the asymmetric potential the kink is no longer symmetric but centered at $y_0 \neq 0$ with $z_k(y_0) = 0$, where we also have to evaluate the matching conditions. Equation (4) can be made dimensionless by measuring time in units of a characteristic time $t_{sc} = \gamma/V_0$ and velocities in units of $v_{sc} = x_{sc}/t_{sc} = \kappa^{1/4}V_0^{3/4}/\gamma$. For a moving kink both parts $z_k(y) - z_{\min}^-$ for $y < 0$ and $z_k(y) - z_{\min}^+$ for $y > 0$ are linear combinations of four functions $e^{K_n y}$, where K_n ($n = 1, \dots, 4$) are the four roots of the equation $\kappa K_n^4 - v\gamma K_n + V_0 = 0$, the real part of which determines the width of the kink: $w_k(v) \sim 1/|\text{Re}(K_n)|$. We find $K_n w_k = \pm H^{1/2}(\bar{v}) \pm (-H(\bar{v}) \pm 2^{3/2}3^{-3/4}\bar{v}H^{-1/2}(\bar{v}))^{1/2}$ (the first and third signs have to be identical), where $\bar{v} = 3^{3/4}v/4v_{sc}$ is a dimensionless velocity and $H(\bar{v}) = 3^{-1/2}((\bar{v}^2 + \sqrt{\bar{v}^4 - 1})^{1/3} + (\bar{v}^2 + \sqrt{\bar{v}^4 - 1})^{-1/3})$ an increasing, real function with $H(\bar{v}) \geq H(0) = 1$ and $H(\bar{v}) \sim \bar{v}^{2/3}$ for $\bar{v} \gg 1$. The width of the moving kink decreases with velocity as $w_k(\bar{v}) = w_k H^{-1/2}(\bar{v})$ (for $\bar{v} < 1$). In the limit of large polymer length, $L \gg w_k(v)$, a moving kink solution, fulfilling all boundary and matching conditions, must satisfy the force-velocity relation

$$F(\bar{v}) = -F_c \bar{v} \frac{3^{1/4} 2^{-1/2} H^{3/2}(\bar{v})}{H^3(\bar{v}) + 3^{-3/2} \bar{v}^2}. \quad (5)$$

For small force densities, we find a linear relation $F \approx -3^{1/4} 2^{-1/2} F_c \bar{v}$; close to the critical force density F_c the velocity diverges as $-\bar{v} \sim (1 - F/F_c)^{-3/2}$, see fig. 2.

The result (5) can also be used to obtain the friction constant η_k of a moving kink by equating the friction force $v\eta_k$ with the driving force $\mathcal{F}_k = -2aF$, which gives the relation $\eta_k = 2a|F(v)|/v$, see fig. 2. η_k is also related to the energy dissipation rate dE/dt due to kink motion which is defined as the product of the friction force $-v\eta_k$ and velocity: $dE/dt = -v^2\eta_k$. On the other hand, dE/dt can be calculated directly using the equations of motion (2) and (4)

in the limit of large L :

$$\frac{dE}{dt} = \int_{-\infty}^{+\infty} dx \frac{\delta \mathcal{H}}{\delta z_k} \partial_t z_k = -\gamma v^2 \int_{-\infty}^{+\infty} dy (\partial_y z_k)^2, \quad (6)$$

and we read off a kink friction constant $\eta_k = \gamma \int_{-\infty}^{+\infty} dy (\partial_y z_k)^2$. Integration in the limit of small driving forces gives $\eta_k \approx 3\gamma a^2/2w_k$ and equating the friction force with the driving force $-2aF = v\eta_k$ gives a linear relation $v = -4Fw_k/3\gamma a$ which agrees to leading order with our above result (5), see also fig. 2.

Thermal noise and kink motion. – For a more detailed analysis of the effect of noise on the kink motion we consider noise-induced perturbations of shape and velocity of a kink moving with constant velocity v . For a time-dependent kink center at $x_k(t)$, the comoving frame coordinate is given by $\bar{y} \equiv x - x_k(t)$. Adding shape perturbations to the corresponding kink solution $z_k(\bar{y})$ of (4), we arrive at the decomposition

$$z(x, t) = z_k(x - x_k(t)) + \sum_{p=1}^{\infty} X_p(t) \phi_p(x - x_k(t), t). \quad (7)$$

ϕ_p are normal modes of the kinked polymer which we will determine below and $X_p(t)$ are expansion coefficients; the zero mode of kink translation is explicitly taken into account by positioning the kink center at $x_k(t)$. Substituting (7) into the equation of motion (2) and expanding about the kink, we obtain

$$\gamma(v - \dot{x}_k) \left(\partial_{\bar{y}} z + \sum_{p=1}^{\infty} X_p \partial_{\bar{y}} \phi_p \right) + \gamma \sum_{p=1}^{\infty} \dot{X}_p \phi_p = \zeta \quad (8)$$

if the normal modes $\phi_p(\bar{y}, t) = f_p(\bar{y})e^{-\omega_p t}$ fulfill the eigenvalue equation

$$\kappa \partial_{\bar{y}}^4 f_p - \gamma v \partial_{\bar{y}} f_p + V''(z_k(\bar{y})) f_p = \omega_p \gamma f_p, \quad (9)$$

where $V''(z) = V_0(1 - 2a\delta(z))$. Equation (9) has to be solved with boundary conditions $f_p(-L/2) = f_p(L/2) = 0$ and $f'_p(-L/2) = f'_p(L/2) = 0$, where we consider the limit $L/2 \gg x_k(t)$ and neglect the shift of boundaries in the comoving frame. Equation (9) has a set of eigenvalues ω_p with orthonormal eigenfunctions $f_p(\bar{y})$ (with respect to the scalar product $\langle f|g \rangle \equiv \int d\bar{y} f(\bar{y})g(\bar{y})$). The translation mode $f_0 = \partial_{\bar{y}} z_k(\bar{y})/C$ of the kink has zero eigenvalue $\omega_0 = 0$. C is a normalization constant determined by $C^2 = \langle \partial_{\bar{y}} z_k | \partial_{\bar{y}} z_k \rangle$. Multiplying eq. (8) with the translation mode f_0 and integrating yields an equation of motion for the kink:

$$\dot{x}_k = v + \zeta_k \left[1 + C^{-1} \sum_{p=1}^{\infty} X_p e^{-\omega_p t} \langle f_0 | \partial_{\bar{y}} f_p \rangle \right]^{-1}, \quad (10)$$

where $\zeta_k(t) = -(C\gamma)^{-1} \int d\bar{y} f_0(\bar{y}) \zeta(\bar{y} + x_k(t), t)$ is an effective Gaussian thermal noise for the kink with correlations $\langle \zeta_k(t) \zeta_k(t') \rangle = \delta(t - t') (2T/C^2\gamma)$ (where we used $\langle f_0 | f_0 \rangle = 1$). The sum in (10) represents terms from kink-phonon scattering, neglect of which leads to the overdamped Langevin equation $\dot{x}_k(t) = v + \zeta_k(t)$ describing Brownian motion with drift. From the noise correlations we can read off the corresponding diffusion constant of the kink as $D_k = T/C^2\gamma$. Note that the corresponding kink friction constant $\eta_k = T/D_k$ is identical to our above result (6) obtained from complementary energetic considerations.

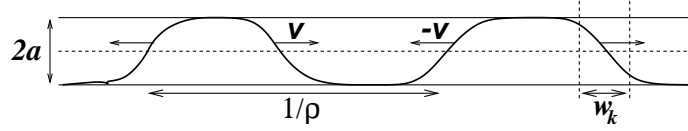


Fig. 3 – An ensemble of well-separated kinks and antikinks which move with velocity v and $-v$, respectively.

If kink-phonon scattering is neglected, the kink is performing a Brownian motion with drift. The polymer crosses the potential barrier by moving a kink over the entire length L of the polymer. Thus, the average crossing time is $t_{\text{cr}} \sim L/v$ for the case of directed diffusion with $v > 0$ under the influence of a driving force density F . For $F = 0$ and $v = 0$, the kink performs an unbiased random walk with $\langle x_k^2 \rangle \sim D_k t$ from which we estimate the average crossing time as $t_{\text{cr}} \sim L^2 \eta_k / T \sim L^2 \gamma a^2 / T w_k$. For $F = 0$ and at low temperatures t_{cr} gives the relaxation time from a kinked state as in fig. 1 to a kinkless state. The diffusive part of the kink motion can be neglected for forces $F \gg 2T/La$.

Thermally activated barrier crossing. – For sufficiently large F , thermally activated barrier crossing proceeds by the nucleation and subsequent separation of a kink-antikink pair, see fig. 3. Each passing kink or antikink increases the polymer position by $\Delta z = 2a$. For an ensemble of ρL kinks and ρL antikinks with kink density $\rho \ll 1/w_k$ as in fig. 3, the fraction of moving polymer segments is given by $2\rho L w_k / L = 2\rho w_k$. These polymer segments move with velocity $2av/w_k$ in the z -direction which leads to the average velocity $v_z \equiv \langle \partial_t z \rangle = 4av\rho$. The kink density ρ is determined by the dynamical equilibrium of kink nucleation with rate j (per length) that we will calculate below, see (11), and kink-antikink recombination with rate $2\rho^2 v$ [6]. Equating both rates gives a steady-state density $\rho^2 = j/2v$ and thus an average polymer velocity $v_z = 2a(2vj)^{1/2}$.

In order to find the nucleation rate j , we use Kramers theory. In the following, we only give the main results of this calculation; details will be described elsewhere. As for flexible strings [6], the dynamics of the nucleation is governed by the critical nucleus representing the saddle point in the multi-dimensional energy landscape. The critical-nucleus configuration $z_n(x)$ is the analogon of the static kink-antikink pair for $F > 0$ and fulfills the same saddle-point equation $\delta\mathcal{H}/\delta z = 0$, see (2). For the critical nucleus we obtain an excess energy $\Delta E_n \approx 2E_k(1 - F/F_c)^2$ that enters the nucleation current $j \sim \exp[-\Delta E_n/T]$. The prefactor depends on the corresponding attempt frequencies and, thus, the spectra $\omega_{n,p}$ and $\omega_{s,p}$ of fluctuations around the the critical nucleus and the straight polymer, respectively. For the straight polymer we find a spectrum of stable phononic modes $\omega_{s,0} = V_0/\gamma$ and $\omega_{s,p} \approx V_0/\gamma + \kappa((\pi/2 + p\pi)/L)^4/\gamma$ ($p \geq 1$). For the critical nucleus, the spectrum consists of an unstable mode $\omega_{n,0} < 0$ representing the collective coordinate along which the nucleation proceeds, a zero mode $\omega_{n,1} = 0$ corresponding to the translation of the nucleus, and a sequence of stable phononic modes $\omega_{n,2} = V_0/\gamma$ and $\omega_{n,p} \approx V_0/\gamma + \kappa((b + p\pi)/L)^4/\gamma$ ($p \geq 3$), where b is a numerical constant. Using Kramers theory in the regime $F > T/2aw_k$ [18], we finally obtain the nucleation rate

$$j = (2\pi)^{-3/2} \gamma^{1/2} G T^{-1/2} Q_n \exp[-\Delta E_n/T], \quad (11)$$

where $Q_n^2 \equiv |\omega_{n,0}| \omega_{s,0} \omega_{s,1} \prod_{p>1} \omega_{s,p} / \omega_{n,p} \approx |1 - 2^{4/3}(1 - F/F_c)^{-8/3}| (V_0/\gamma)^3$ contains all attempt frequencies, and $G \equiv L^{-1} \int dx_n [\int dx (\partial_x z_n(x))^2]^{1/2} \approx a(1 - F/F_c) / \sqrt{w_k}$ is the Jacobian for the change of coordinates from the amplitude of the translational mode $\partial_x z_n$ to the nucleus position x_n .

For small driving force densities $F \ll 2\rho T/a$, the kink motion is diffusive, and the above approach breaks down as kink-antikink pairs cannot separate but tend to recombine. For $E_k \gg T$, the system reaches thermodynamic equilibrium with a low kink density $\rho_{\text{eq}} \sim \exp[-E_k/T]$ given by the Boltzmann distribution and with $v_z = 4av\rho_{\text{eq}}$. For intermediate driving forces $2\rho T/a \ll F < F/2aw_k$, the critical nucleus is in quasi-equilibrium [18], and we find again $j \sim \exp[-\Delta E_n/T]$ as in the high-force expression (11) but with a different parameter dependence of the prefactor.

Conclusion. – In conclusion, we described the activated dynamics of semiflexible polymers which is governed by kink excitations. The static kink has the energy E_k and the width w_k as given by (3). Both kink properties are governed by the bending rigidity of the semiflexible polymer. In the presence of a driving force density F , there is a force \mathcal{F}_k acting on the kink that leads to moving-kink solutions which satisfy the force-velocity relation (5). In the absence of kink-phonon scattering, the kink performs Brownian motion with drift for which we have calculated the friction constant η_k and the diffusion constant D_k . This leads to estimates for the crossing times $t_{\text{cr}} \sim L/v$ for large forces $F \gg 2T/La$ and $t_{\text{cr}} \sim L^2\eta_k/T$ for small forces $F \ll 2T/La$. For large forces, the nucleation of kinks proceeds by activation over the saddle point which represents the critical nucleus. Application of Kramers theory leads to the nucleation rates (11) which determine the average velocity $\langle \partial_t z \rangle$ of the polymer. Our results are not only relevant to the dynamics of semiflexible polymers but can be extended to kink excitations in fluid membranes [19].

REFERENCES

- [1] KRAMERS H. A., *Physica (Utrecht)*, **7** (1940) 284.
- [2] HÄNGGI P., TALKNER P. and BORKOVEC M., *Rev. Mod. Phys.*, **62** (1990) 251.
- [3] HIRTH J. P. and LOTHE J., *Theory of Dislocations* (McGraw-Hill, New York) 1968.
- [4] BLATTER G., FEIGELMAN M. V., GESHKENBEIN V. B., LARKIN A. I. and VINOKUR V. M., *Rev. Mod. Phys.*, **66** (1994) 1125.
- [5] RICE M. J., BISHOP A. R., KRUMHANSL J. A. and TRULLINGER S. E., *Phys. Rev. B*, **36** (1976) 432.
- [6] BÜTTIKER M. and LANDAUER R., *Phys. Rev. Lett.*, **43** (1979) 1453; *Phys. Rev. A*, **23** (1981) 1397.
- [7] CURRIE J. F., KRUMHANSL J. A., BISHOP A. R. and TRULLINGER S. E., *Phys. Rev. B*, **22** (1980) 477.
- [8] SEBASTIAN K. L., *Phys. Rev. E*, **61** (2000) 3245; SEBASTIAN K. L. and PAUL A. K. R., *Phys. Rev. E*, **62** (2000) 927.
- [9] TAYLOR W. H. and HAGERMAN P. J., *J. Mol. Biol.*, **212** (1990) 363.
- [10] KÄS J., STREY H. and SACKMANN E., *Nature*, **368** (1994) 226.
- [11] GITTES F., MICKEY B., NETTLETON J. and HOWARD J., *J. Cell Biol.*, **120** (1993) 923.
- [12] NETZ R. N. and JOANNY J.-F., *Macromolecules*, **32** (1999) 9013.
- [13] GOMPPER G. and BURKHARDT T. W., *Phys. Rev. A*, **40** (1989) 6124.
- [14] KIERFELD J. and LIPOWSKY R., *Europhys. Lett.*, **62** (2003) 285.
- [15] HAN J., TURNER S. W. and CRAIGHEAD H. G., *Phys. Rev. Lett.*, **83** (1999) 1688.
- [16] KURTH D. G., SEVERIN N. and RABE J. P., *Angew. Chem.*, **114** (2002) 3833.
- [17] COSTANTINI G. and MARCHESONI F., *Phys. Rev. Lett.*, **87** (2001) 114102.
- [18] HAENGGI P., MARCHESONI F. and SODANO P., *Phys. Rev. Lett.*, **60** (1988) 2563.
- [19] AMMANN A. and LIPOWSKY R., *J. Phys. II*, **6** (1996) 255.