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Instability in the dynamics of long DNA undergoing gel electrophoresis in a strong field

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We present a model describing reptation motion of a long DNA chain undergoing gel electrophoresis. Internal modes of the chain in an effective tube are associated with lateral loops (hernias), and the effect of the field on these lateral loops is analyzed. An equation describing reptation dynamics of the chain is derived. It is shown for fields exceeding some critical value that stationary reptation motion becomes unstable. Mobility of the chain in the weak fields is also calculated. © 1995 American Institute of Physics.

I. INTRODUCTION

One of the important problems in the dynamics of DNA undergoing gel electrophoresis is to consider the influence of the lateral loops on the reptation motion. It is well known that in a strong field a charged chain does not move in a gel by reptation along its own contour, but leaks out of the tube creating hernias.^{1–11} On the other hand, in weak fields the reptation mechanism of motion is believed to be corrected.^{12–14} This mechanism of motion can become unstable only due to lateral loops that can grow under the influence of an electric field. In this paper we investigate the influence of loops on the reptation dynamics and determine the critical conditions, at which the reptation mechanism implies instability.

The first step in our consideration is to derive the equation of motion for the charged chain, reptating in a gel under the influence of an electric field, E , in the case when the field impacts also on loops (Fig. 1). We propose that the chain elongates in the direction of the field and also that drift motion is dominant. The model we use is the following. The chain moves along its primitive path on a lattice with coordination number z . The length of a segment of the chain coincides with the lattice size and equals α . The number of segments in the chain is N_0 , $N_0 \gg 1$, and the charge of a segment is q . During reptation under the field the leading segment of the chain orients, so that all chain segments should also orient, the average orientation of the segments being $\langle \cos \theta \rangle = \delta$, where θ is the angle between the direction of field axis x and the orientation of a tube segment (i.e., the local orientation of the primitive path of the chain), δ is a parameter. Classical theories^{13,14} predict a linear dependence, $\delta \sim E$, for the weak fields. However, the detailed calculations including the effect of fluctuations resulted in $\delta \sim \sqrt{E}$.¹⁵

II. THE MODEL EQUILIBRIUM PROPERTIES

Let us divide the chain into $N = N_0/g$ blobs, each containing g segments (here $g \gg 1$ is the arbitrary large param-

eter: the final results do not depend on g). The current coordinate of the center of mass of the n th blob along the reptation line (or equivalently along the primitive path) at the time t is denoted by $y_n(t)$ (y is the length). The problem is to set an equation for this function $y_n(t)$. In order to derive this equation we have to consider the stored free energy and the dissipation.

The free energy of the chain consists of two parts, respectively: the electrostatic energy and the elastic energy. The electrostatic energy of the blob having the coordinate y_n can be written as

$$F_E(y_n) = F_0 - gqEx(y_n), \quad (1)$$

where $x(y_n)$ is the coordinate of the blob along the field, F_0 is constant. The total electrostatic energy is given by the sum over all blobs:

$$F_E(y_1 \cdots y_N) = NF_0 - gqE \int_0^N dn x(y_n). \quad (2)$$

The derivative $r(y_n) = dx(y_n)/dy_n$ coincides with the average orientation of the blob and can be written as

$$r(y_n) = \frac{1}{gk} \sum_{j=1}^{gk} \cos \theta_{n,j} = \delta + \psi(y_n), \quad (3)$$

where δ is the permanent part and ψ is the fluctuating part. Here gk is the number of segments in the primitive path of the n th blob, $\cos \theta_{n,j}$ is the orientation of the segment j along the primitive path. The orientation of the segments are statistically independent because the chain is flexible. Using this fact we can obtain correlation characteristics for the field ψ :

$$\langle \psi(y_n) \rangle = 0, \quad \langle \psi(y_{n_1}) \psi(y_{n_2}) \rangle = \frac{1}{3gk} \delta(n_2 - n_1). \quad (4)$$

Next we turn to the elastic free energy. First the free energy of a blob, containing g segments will be calculated. If the field is switched off ($E=0$), the free energy is approximately equal to^{16,17}

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FIG. 1. The model of the chain with lateral loops.

$$F_0 = k_B T \left[g \frac{\kappa_0}{2} (k - k_0)^2 - \ln \left(\frac{z}{2\sqrt{z-1}\sqrt{2\pi g}} \right) \right], \quad (5)$$

where $k_B T$ is the thermal energy, k is the normalized length of the primitive path (i.e., if $g\alpha$ is contour length of a blob, $kg\alpha$ is the length of its primitive path), $k_0 = (z-2)/z$, $\kappa_0 = z^2/4(z-1)$. The second term on the right-hand side of Eq. (5) can be omitted as it does not depend on k .

Corrections to Eq. (5) due to the influence of the electric field on loops can be calculated by perturbation theory only. For this purpose we must calculate the electrostatic correction to the free energy of one loop, containing m segments. In the first order of perturbation theory the electric field has only an influence on the distribution of the center of mass of the loop, leaving the internal conformations of the loop unchanged. In this case the free energy change is given by

$$\Delta F = -\langle m q \mathbf{R} \mathbf{E} \rangle, \quad (6)$$

where $\mathbf{R}$ is the vector connecting the coinciding loop ends and its center of mass. The mean-square distance $\langle \mathbf{R}^2 \rangle$ coincides with the equilibrium value^{16,17}

$$\langle \mathbf{R}^2 \rangle = \frac{\sqrt{2\pi}}{8} \frac{z}{z-2} \alpha^2 m^{0.5}. \quad (7)$$

Using fluctuation theorem¹⁸ the mean value of $\mathbf{R}$ induced by E is

$$\langle \mathbf{R} \rangle = \frac{\chi \mathbf{E}}{m q}, \quad (8)$$

where χ is the susceptibility, which is related to fluctuation of $\mathbf{R}$:

$$\chi = \frac{m^2 q^2}{k_B T} \langle \mathbf{R}^2 \rangle. \quad (9)$$

The correction to the free energy can now be written as

$$\Delta F = -\frac{1}{2} \chi E^2. \quad (10)$$

Thus finally we get

$$\Delta F = -k_B T \frac{\sqrt{2\pi}}{48} \frac{z}{z-2} \varepsilon^2 m^{2.5}, \quad (11)$$

where the parameter ε is given by $\varepsilon = qE\alpha/k_B T$.

Let us return to the calculation of the blob energy. If the blob has a primitive path equal to $gk\alpha$, then the number of loops in this blob is equal to gk , and the average number of segments in a loop is $\bar{m} = 1/k$. Obviously, the number of segments in loops fluctuate, so the general equation for the distribution function of number of segments in a loop is^{16,17}

$$\rho^*(m) = C^* m^{-1.5} e^{-\mu m}, \quad (12)$$

where C^* is a normalization constant, μ is the chemical potential, that can be calculated from the relation

$$\bar{m} = \int_0^\infty \rho^*(m) m dm. \quad (13)$$

After averaging Eq. (11) using the distribution function relation (12) and relation (13), the average free energy for a loop in the blob is found to be

$$\overline{\Delta F} = -k_B T \frac{1}{96} \frac{z}{z-2} \varepsilon^2 k^{-2.5}. \quad (14)$$

The full correction to the free energy of the blob due to the influence of the electric field is a product of $\overline{\Delta F}$ and the number of loops in the blob, that is gk ,

$$\Delta F_b = -k_B T g \frac{1}{96} \frac{z}{z-2} \varepsilon^2 k^{-1.5}. \quad (15)$$

The total free energy of the blob is a sum of free energies in Eq. (5) (without the constant $\ln$ term) and Eq. (15):

$$F_b = k_B T g \left(\frac{\kappa_0}{2} (k - k_0)^2 - \frac{1}{96} \frac{z}{z-2} \frac{\varepsilon^2}{k^{1.5}} \right). \quad (16)$$

Equations (15) and (16) are singular for $k=0$ because in this case the free energy is a nonlinear function of g . The discussion will be restricted to those values of k , for which the inequality $F_0 \gg \Delta F_b$ is satisfied.

On the basis of the free energy in Eq. (16) we can investigate the equilibrium properties of the blob. The quantitative dependence of the free energy on k for different values of ε is shown in Fig. 2. Note the critical value $\varepsilon = \varepsilon_c$: for $\varepsilon > \varepsilon_c$ the free energy has no minimum. This implies that the length of the primitive path must nearly tend to zero in this case. The calculations show that

$$\varepsilon_c = \left(\frac{128}{5} \right)^{1/2} \left(\frac{5}{7} \right)^{7/2} \kappa_0^{0.5} \left(\frac{z-2}{z} \right)^{9/4}. \quad (17)$$

At the critical point the length of the primitive path is given by

$$k_c = \frac{5}{7} \frac{z-2}{z}, \quad (18)$$

and for $0 \leq \varepsilon \leq \varepsilon_c$, $k_0 \geq k \geq 5/7 k_0$, so the field only slightly influences the length of primitive path in this range. Thus ε_c is small if formally $z \rightarrow 2$. In what follows we assume that this is the case: $z-2 \ll 1$. Although this condition is not re-

FIG. 2. The quantitative dependence of the free energy on the length of primitive path k for different values of the parameter ε : (1) $\varepsilon < \varepsilon_c$, (2) $\varepsilon = \varepsilon_c$, (3) $\varepsilon > \varepsilon_c$.

alistic, we believe that the final results can be qualitatively applied also to the general case of arbitrary z .

Let us return to the original model of the chain. The free energy of the blob with index n , $F_b(n)$, is given by Eq. (16), with

$$k = k_n = \frac{1}{\alpha g} \frac{\partial y_n(t)}{\partial n}. \quad (19)$$

The total elastic free energy is

$$F_{el} = \int_0^N dn F_b(n). \quad (20)$$

III. DYNAMIC EQUATION

In order to get an equation of motion we must calculate the dissipative function which is the function of generalized velocities and characterizes dissipative rate in the system.¹⁸ The velocity of the chain along its contour is given by

$$v_c = \alpha g \frac{\partial y_n / \partial t}{\partial y_n / \partial n}. \quad (21)$$

The friction force per blob is $f_{fr} = \xi g v_c$, where ξ is the friction coefficient of a segment. Thus the total dissipative function is

$$D = \frac{g\xi}{2} \int_0^N dn (\alpha g)^2 \frac{(\partial y_n / \partial t)^2}{(\partial y_n / \partial n)^2}. \quad (22)$$

The equation of motion can be obtained from the equality¹⁸

$$\frac{\delta(F_E + F_{el})}{\delta y_n} = - \frac{\delta D}{\delta(\partial y_n / \partial t)}, \quad (23)$$

where δ indicates a variational derivative, and F_E , F_{el} and D are defined by Eqs. (2), (20), and (22). From Eq. (23) we find that the function $y_n(t)$ obeys

$$\xi \frac{\partial y_n}{\partial t} = \frac{kT}{(\alpha g)^4} \left(\frac{\partial y_n}{\partial n} \right)^2 \left[\left(\kappa_0 - \frac{5}{128} \frac{z}{z-2} \frac{\varepsilon^2}{k_n^{3.5}} \right) \frac{\partial^2 y_n}{\partial n^2} + \alpha \varepsilon g^2 [\delta + \psi(y_n)] \right], \quad (24)$$

where k_n is defined by Eq. (19). The imposed boundary conditions correspond to equilibrium conditions for the end blobs, i.e.,

$$\frac{\partial y_n}{\partial n} = \alpha g \bar{k}, \quad n = 0, N. \quad (25)$$

Here $\bar{k}$ must be defined from minimization of the free energy (16).

IV. THE STABILITY ANALYSIS AND MOBILITY

In the zeroth approximation $k_n = \bar{k}$, and the average velocity of the chain along its primitive path is given by

$$\bar{v} = \frac{gE\delta\bar{k}^2}{\xi}. \quad (26)$$

Let us investigate the stability of the motion with constant velocity $\bar{v}$, when the random field $\psi = 0$. Starting with

$$y_n(t) = \alpha g \bar{k} n + \bar{v} t + u_n(t), \quad (27)$$

one gets the equation for the deformation $u_n(t)$:

$$\frac{\partial u_n}{\partial t} = \frac{kT\bar{k}^2}{\xi\alpha^2 g^2} \kappa_0 (1 - \varepsilon^2/\varepsilon_c^2) \left(\frac{\partial^2 u_n}{\partial n^2} + \frac{2\pi\omega^*}{N} \frac{\partial u_n}{\partial n} \right), \quad (28)$$

where ε_c obey Eq. (17), $\omega^* = \varepsilon \delta N_0 \pi \kappa_0 (1 - \varepsilon^2/\varepsilon_c^2)$ with boundary conditions

$$\frac{\partial u_n}{\partial n} = 0, \quad n = 0, N. \quad (29)$$

The eigenvalue spectrum for Eq. (28) with boundary conditions (29) is given by

$$\lambda_p = - \frac{kT\bar{k}^2 \pi^2 \kappa_0 (1 - \varepsilon^2/\varepsilon_c^2)}{\xi\alpha^2 N_0^2} (p^2 + \omega^{*2}), \quad p = 0, \pm 1, \dots \quad (30)$$

In the vicinity of $\varepsilon = \varepsilon_c$ the nonlinear terms in the expansion of Eq. (24) are important. Obviously, for $\varepsilon > \varepsilon_c$ the spectrum λ_p is positive, so the reptation motion with permanent velocity becomes unstable.

Let us assume that $\varepsilon = \varepsilon_c$, and consider behavior of the function $\Delta_n = k_n - \bar{k}$, that is the local deformation of the n th blob. Using Eq. (24) we get

$$\frac{\partial \Delta_n}{\partial t} = \frac{2\bar{v}}{\alpha g \bar{k}} \frac{\partial \Delta_n}{\partial n} \left(1 + \frac{\Delta_n}{\bar{k}} \right). \quad (31)$$

This is nonlinear equation for propagation of distortion Δ_n . In the linear approximation the velocity of this wave along coordinate y relative to the moving chain is $2\bar{v}$ and is directed opposite to the velocity of the chain. Thus the deformation (or loops) moves with the velocity $-\bar{v}$ along tube relative to the gel. This implies that the fluctuations of deformation have a tendency to be pushed out of the chain. Non-

linear terms in Eq. (31) only change the shape of the wave, but cannot change the total behavior, and does not influence the stability.

The next problem is to take into account the fluctuating part of the electric force, namely the field ψ_n . As it has been shown for the model of a Rouse chain moving in a gel by reptation under electric field,¹⁹ the time average of the non-linear random field ψ_n is not equal to zero and depends on n . The same effect exists in the model under consideration, and it must result in a renormalization of the average velocity $\bar{v}$ and in an additional deformation of the chain. The local deformation becomes a function of n .

Let us assume that the chain moves with a renormalized velocity v^* , and has local deformation Δ_n , so that $k_n = \bar{k} + \Delta_n$. The averaged deformation is $\bar{\Delta} = (1/N) \times \int_0^N \Delta_n dn$. It is assumed that the deformation is small, $\bar{\Delta} \ll \bar{k}$. Now the problem can be considered self-consistently. Rewrite Eq. (24) approximately as follows:

$$\xi \frac{\partial y_n}{\partial t} = \frac{kT}{(\alpha g)^4} \left(\frac{\partial y_n}{\partial n} \right)^2 \left[\left(\kappa_0 - \frac{5}{128} \frac{z}{z-2} \frac{\varepsilon^2}{(\bar{k} + \bar{\Delta}_n)^{3.5}} \right) \frac{\partial^2 y_n}{\partial n^2} + a \varepsilon g^2 [\delta + \psi(y_n)] \right]. \quad (32)$$

The field ψ can be expended in two parts, namely the permanent $\langle \psi_n \rangle$ and the fluctuating $\psi'_n = \psi_n - \langle \psi_n \rangle$. Similarly, the coordinate $y_n(t)$ can also be represented by a sum of a permanent part of a fluctuating part $u_n(t)$:

$$y_n(t) = \alpha g \left(\bar{k}n + \int_0^n \bar{\Delta}_{n'} dn' \right) + v^*t + u_n(t), \quad (33)$$

where $\bar{\Delta}_n$ is the time-average local deformation. The equation for the permanent deformation Δ_n and the fluctuating field u_n are derived from Eq. (32) and are given by

$$\xi v^* = \frac{k_B T}{\alpha g} (\bar{k} + \bar{\Delta}_n)^2 \left[h(\varepsilon, \bar{\Delta}_n) \frac{d\bar{\Delta}_n}{dn} + g \varepsilon (\delta + \langle \psi_n \rangle) \right], \quad (34)$$

where

$$h(\varepsilon, \bar{\Delta}) = \kappa_0 - \frac{5}{128} \frac{z}{z-2} \frac{\varepsilon^2}{(\bar{k} + \bar{\Delta}_n)^{3.5}},$$

with boundary conditions

$$\Delta_n = 0, \quad n = 0, N \quad (35)$$

and

$$\xi \frac{\partial u_n}{\partial t} = \frac{kT}{(\alpha g)^2} \left[(\bar{k} + \bar{\Delta}_n)^2 h(\varepsilon, \bar{\Delta}_n) \frac{\partial^2 u_n}{\partial n^2} + 2g\varepsilon \delta (\bar{k} + \bar{\Delta}_n) \frac{\partial u_n}{\partial n} + \alpha g^2 \varepsilon (\bar{k} + \bar{\Delta}_n)^2 \psi'_n \right], \quad (36)$$

with boundary conditions

$$\frac{\partial u_n}{\partial n} = 0, \quad n = 0, N. \quad (37)$$

From Eq. (34) we obtain the average velocity

$$v^* = \frac{qE\delta\bar{k}^2}{\xi} (1 + 2\bar{\Delta}/\bar{k} + \bar{\psi}/\delta), \quad (38)$$

where

$$\bar{\psi} = \frac{1}{N} \int_0^N \langle \psi[y_n(t)] \rangle dn.$$

Our perturbation scheme is valid, if $\bar{\Delta}/\bar{k} \ll 1$, $\bar{\psi}/\delta \ll 1$.

In the first approximation the average $\langle \psi[y_n(t)] \rangle$ is given by¹⁹

$$\langle \psi[y_n(t)] \rangle = \frac{1}{\alpha g \bar{k}} \left\langle u_n(t) \frac{\partial \psi_n(t)}{\partial n} \right\rangle. \quad (39)$$

For the random field $\psi'_n(t)$ using Eq. (4) we obtain the following characteristics:

$$\begin{aligned} \langle \psi'_n(t) \rangle &= 0, \\ \langle \psi'_{n_1}(t_1) \psi'_{n_2}(t_2) \rangle &= \frac{1}{3g\bar{k}} \delta \left[n_2 - n_1 - \frac{v^*}{\alpha g \bar{k}} (t_1 - t_2) \right]. \end{aligned} \quad (40)$$

Equation (36) with boundary conditions (37) can be solved by using the Laplace transform method. After some calculations the final equation for $\langle \psi[y_n(t)] \rangle$ is found to be

$$\begin{aligned} \langle \psi_n \rangle &= - \frac{2\pi\omega}{3N_0\delta\bar{k}} \left(\frac{\exp\left(-\frac{2\pi\omega(N-n)}{N}\right)}{1 - \exp(-2\pi\omega)} \right. \\ &\quad - \frac{1}{\pi_{q \neq 0}} \sum \frac{\left(q \cos \frac{\pi q n}{N} + \omega \sin \frac{\pi q n}{N} \right)}{(q^2 + \omega^2)(q^2 + \omega_1^2)} \\ &\quad \times \left[\frac{1}{\omega} (q^2 + \omega^2) q (-1)^q \exp\left(-\frac{\pi q^2(N-n)}{\omega N}\right) \right. \\ &\quad \left. \left. + (q^2 + \omega_1^2) \sin \frac{\pi q n}{N} + q(\omega_1 - \omega) \cos \frac{\pi q n}{N} \right] \right), \end{aligned} \quad (41)$$

where

$$\omega = \frac{\varepsilon \delta N_0}{\pi \bar{k} h(\varepsilon, \delta)}, \quad \omega_1 = \omega \frac{v^* - \bar{v}}{\bar{v}} = \omega (2\bar{\Delta}/\bar{k} + \bar{\psi}/\delta). \quad (42)$$

The parameter ω is proportional to the ratio of the Rouse relaxation time to the time of tube renewal due to field. From Eq. (41) we can get the average force $\bar{\psi}$. In the limiting cases

$$\bar{\psi} = - \frac{1}{3N_0\delta\bar{k}}, \quad |\omega_1| \ll \omega \ll 1, \quad (43a)$$

$$\bar{\psi} = \frac{\pi\omega}{3N_0\delta\bar{k}}, \quad |\omega_1| \ll 1 \ll \omega, \quad (43b)$$

$$\bar{\psi} = \frac{1}{3N_0\delta\bar{k}} \left(\frac{2\omega}{\omega_1} - \pi\omega_1 \right), \quad 1 \ll |\omega_1| \ll \omega. \quad (43c)$$

Let us consider the distribution of deformations along the chain. This function can be obtained from Eq. (34):

$$\Delta_n = \frac{g\varepsilon}{h(\varepsilon, \bar{\Delta})} \left(n\bar{\psi} - \int_0^n \langle \psi_{n'} \rangle dn' \right). \quad (44)$$

After substitution of Eq. (41) in Eq. (44) and averaging $\bar{\Delta}_n$ along the chain we get the self-consistent equation for $\bar{\Delta}$:

$$\bar{\Delta} = \frac{2\pi\varepsilon\beta(\omega, \omega_1)}{3\delta\bar{k}h(\varepsilon, \bar{\Delta})}, \quad (45)$$

where

$$\begin{aligned} \beta(\omega, \omega_1) = & \omega \left\{ -\frac{1}{4\pi\omega} + \frac{1}{2\pi\omega} \left(\frac{1}{1 - \exp(2\pi\omega)} + \frac{1}{2\pi\omega} \right) \right. \\ & + \frac{1}{2\pi^2} \sum_{q \neq 0} \frac{\omega^2 - q^2}{(q^2 + \omega_1^2)(q^2 + \omega^2)} \left[1 + (-1)^q \right. \\ & \times \exp \left(-\frac{\pi q^2}{\omega} \right) \left. \right] + \frac{\omega}{\pi^3} \sum_{q \neq 0} \frac{q^2 - 3\omega^2}{(q^2 + \omega_1^2)(q^2 + \omega^2)^2} \\ & \times \left[1 - (-1)^q \exp \left(-\frac{\pi q^2}{\omega} \right) \right] + \frac{1}{2\pi^2} \\ & \times \sum_{q \neq 0} \frac{q^2 - \omega^2 + \omega_1\omega + \omega_1^2}{(q^2 + \omega_1^2)(q^2 + \omega^2)} \left. \right\}. \end{aligned} \quad (46)$$

The function $\beta(\omega, \omega_1)$ has the following asymptotics:

$$\beta(\omega, \omega_1) = -\omega^2/6, \quad |\omega_1| \ll \omega \ll 1, \quad (47a)$$

$$\beta(\omega, \omega_1) = -9/4\pi + \pi^2\omega_1^2\omega/240, \quad |\omega_1| \ll 1 \ll \omega, \quad (47b)$$

$$\beta(\omega, \omega_1) = \omega/(4\pi\omega_1), \quad 1 \ll |\omega_1| \ll \omega. \quad (47c)$$

From Eqs. (43a) and (43b) we can conclude that our perturbation scheme is valid when the inequalities

$$N_0 \gg N_1 = 1/\bar{k}\delta^2, \quad \mu = \varepsilon/\delta\bar{k}^2\kappa_0 \ll 1 \quad (48)$$

are satisfied.

Let us calculate the average chain velocity along the field direction and average chain deformation in the limiting cases. The condition $|\omega_1| \ll \omega \ll 1$ is valid for the chain whose length obeys inequality $N_1 \ll N_0 \ll N_2$, where $N_2 = \bar{k}\kappa_0/\varepsilon\delta$. The average deformation in this case is given by [from Eqs. (45) and (47a)]

$$\bar{\Delta} = -\pi\bar{k}\mu\omega^2/9. \quad (49)$$

Using Eqs. (38), (43a), and (48) we can calculate the velocity of the chain, $v_E = v^*\delta$, along the field (axis x):

$$v_E = \frac{qE\delta^2\bar{k}^2}{\xi} \left(1 - \frac{2\pi}{9}\mu\omega^2 - \frac{1}{3\pi}\frac{\mu}{\omega} \right). \quad (50)$$

From this equation we can conclude, that the velocity increase with increasing the chain length ($\omega \sim N_0$, and the last correction term is dominant).

FIG. 3. The quantitative dependence of the average deformation $\bar{\Delta}$ and velocity v_E vs the parameter $\omega \sim N_0$.

Now let us investigate the other limiting case, when $|\omega_1| \ll 1 \ll \omega$. The self-consistent equation for ω_1 can be derived from Eqs. (42), (43b), and (47b) and is given by

$$\frac{\pi^2\omega_1^2\omega}{480} - \frac{3\omega_1}{8\mu\omega} - 1 = 0. \quad (51)$$

After solving this equation we can calculate the average velocity along the field direction and the average deformation. The average velocity

$$v_E = \frac{qE\delta^2\bar{k}^2}{\xi} \left[1 + \frac{90}{\pi^2\mu\omega^3} \left(1 - \sqrt{1 + \frac{8\pi^2}{135}\mu^2\omega^3} \right) \right] \quad (52)$$

also increases with increasing chain length and for $N_0 \rightarrow \infty$ varies as $\bar{v}\delta(1 - \text{const } N_0^{-3/2})$. The average deformation being negative and is given by

$$\bar{\Delta} = \frac{\bar{k}}{2} \left[-\frac{\pi}{3}\mu + \frac{90}{\pi^2\mu\omega^3} \left(1 - \sqrt{1 + \frac{8\pi^2}{135}\mu^2\omega^3} \right) \right]. \quad (53)$$

The last asymptotic case [Eqs. (43c) and (47c)] cannot be realized, therefore, Eqs. (52) and (53) are valid for $N_0 \gg N_2$. The quantitative dependencies of the velocity v_E and the deformation $\bar{\Delta}$ vs the parameter ω are shown in Fig. 3.

Obviously, when the parameter $\mu \sim 1$ or $\varepsilon \sim \bar{k}^4$, the deformation $\bar{\Delta} \sim -\bar{k}$ and the reptation mechanism of motion is violated. Our perturbation scheme fails in this case and we cannot investigate the details of the transition to the new type of motion.

Thus the model taking into account lateral loops predicts instability of the reptation and a complicated dependence of the mobility of the chain on its length in the range of the band effect, compared with Refs. 19–21. The calculations [see Eq. (53)] show that the chain for which $\omega \sim 1$ is the most compressed under the field.

V. DISCUSSION AND CONCLUSIONS

In conclusion we point out the new effects that emerge in the model with lateral loops. First, this model gives instability of the reptation motion in the strong fields. The critical conditions of this transition are determined by the random part of the electric force, associated with fluctuations of the tube. The calculations showed that this force gives an additional compression of the chain and, thus, decreases the critical electric field. When the electric field achieves the critical value, the chains for which the Rouse relaxation time is the order of the tube renewal time ($N_0 \sim \bar{k} \kappa_0 / \varepsilon \delta$) are characterized by the maximum compression. Therefore, these chains must collapse before the others. With increasing the electric field the other chains also transform to the collapsed state. Our perturbation scheme cannot be used for investigation of the transition point, because the deformations in this case are large.

After the transition to the collapsed regime the motion of DNA chains becomes unstable, and rather complicated:¹⁻¹¹ The chain conformation changes from extended to coiled, passing a few intermediate stages. The tube concept is not directly applicable in this regime.

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