

## Stretching Short DNAs in Electrolytes

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**Abstract:** This paper is aimed at a combined theoretical and numerical study of the force-extension relation of a short DNA molecule stretched in an electrolyte. A theoretical formula based on a recent discrete wormlike chain (WLC) model of Kierfeld *et al.* (*Eur. Phys. J. E*, Vol. 14, pp.17-34, 2004) and the classical OSF mean-field theory on electrostatic stiffening of a charged polymer is numerically verified by a set of Brownian dynamics simulations based on a generalized bead-rod (GBR) model incorporating long-ranged electrostatic interactions via the Debye-Hueckel potential (DH). The analysis indicates that the stretching of a short DNA can be well described as a WLC with a constant effective persistence length. This contrasts the behavior of long DNA chains that are known to exhibit variable persistent lengths depending on the ion concentration levels and force magnitudes.

### 1 Introduction

The elastic properties of DNA molecules play an important role in phenomena such as packing of DNA in viruses (Earnshaw and Harrison, 1977; Purohit, Konddev and Phillips, 2003) and nucleosomes (Schiessel, 2003). Considerable experiments and numerical studies have been performed on stretching DNAs in electrolytes (Smith *et al.*, 1992, Bustamante *et al.* 1994, Strick *et al.*, 1996). Bustamante *et al.* (1994) have shown that the force-extension curve of a 97004 bps DNA molecule in 10 mM Na<sup>+</sup> can be well described by a WLC model provided that the contour length  $L$  and persistence length  $p$  are treated as adjustable parameters to fit experimental data. On the other hand, quite large discrepancies were observed between theory and experiments at relatively low ion concentrations. For example, fitting the experimental data of Smith *et al.* (1992) for 97004 bps DNAs in 1 and 0.1 mM Na<sup>+</sup> to WLC theory yields an apparent persistence length that can increase over an order of magnitude as the magnitude of the stretching force is re-

duced. Marko and Siggia (1995) have attributed this phenomenon to electrostatic stiffening of negatively charged DNA molecules. They explained that, in the high-force regime, the apparent persistence length should be controlled by the intrinsic elastic properties of DNA as the elastic correlation length, defined as  $\xi \approx \sqrt{p/f}$  where  $p$  is the persistence length and  $f$  the stretching force, becomes smaller than the Debye electrostatic screening length; in the low-force regime, the electrostatic stiffening effect tends to increase the apparent persistence length as the elastic correlation length becomes comparable to or larger than the Debye length. The analysis of Marko and Siggia (1995) is valid for very long DNA chains. Does similar explanation or behavior also apply to stretching short DNAs? This question is addressed in the present paper and we find the answer to be negative.

Due to the lack of proper experimental techniques to manipulate short single molecules, numerical techniques such as Monte Carlo and Brownian dynamics simulations play an indispensable role in complementing theory and experiments. In the present study, we shall make use of a generalized bead-rod (GBR) model in conducting Brownian dynamics simulations of WLCs (Wang and Gao, 2005). The GBR model was developed for the purpose of modeling WLCs under strong stretch and confinement conditions. To simulate the dynamic behaviors of charged polymers such as DNA, a simplest approach is to incorporate electrostatic effects into the GBR model by means of an effective persistence length based on the mean-field theory of Odijk (1977) and Skolnick and Fixman (1977) (OSF). A more accurate approach is to directly incorporate electrostatic interactions into the GBR model via the Debye-Hueckel (DH) potential (Odijk, 1977; Skolnick and Fixman, 1977). The latter approach is adopted in the present paper.

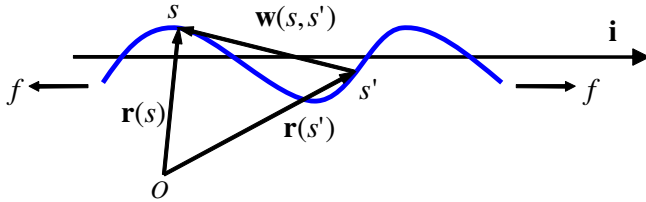
The paper is arranged as follows. In Section 2, the force-extension relation of a charged WLC is derived based on a discrete WLC model of Kierfeld *et al.* (2004) and the OSF theory. In Section 3, we discuss how the DH potential is incorporated in the GBR model. In Section

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4, we compare the simulated and theoretically predicted mean-square end-to-end distance (MSD) and the force-extension curves of short DNAs in electrolytes.

## 2 Theory



**Figure 1** : Coordinate system of a stiff wormlike chain (WLC) under stretch.

The DH potential (Marko and Siggia, 1995; Odijk, 1977; Skolnick and Fixman, 1977) for a charged wormlike polymer chain (**Figure 1**) can be written as

$$U_e = \frac{1}{2} k_B T l_B \sigma_0^2 \int_0^L ds \int_0^L ds' \left[ \frac{\exp(-\kappa |\mathbf{r}(s) - \mathbf{r}(s')|)}{|\mathbf{r}(s) - \mathbf{r}(s')|} - \frac{\exp(-\kappa |s - s'|)}{|s - s'|} \right] \quad (1)$$

where  $s, s'$  are two arc length positions along the chain,  $\mathbf{r}(s), \mathbf{r}(s')$  are the corresponding position vectors,  $\sigma_0$  is the number of effective electron charges per unit length of the chain. Furthermore,

$$l_B = e^2 / 4\pi\epsilon\epsilon_0 k_B T \quad (2)$$

is the so-called Bjerrum length at which the electrostatic interaction between two ions of unit charge  $e$  is equal to the thermal energy  $k_B T$ ,  $\epsilon$  is the dielectric constant of the medium and  $\epsilon_0$  is the vacuum permittivity. The parameter  $\kappa$  corresponds to the inverse of the Debye screening length (Skolnick and Fixman, 1977)

$$\kappa = \sqrt{4000 N_A \pi v (v + 1) l_{BCs}}, \quad (3)$$

where  $N_A$  is the Avogadro number,  $c_s$  the mole concentration of salt and  $v$  the counterion valence for a 1: $v$  salt. For a stiff WLC with a straight rod reference configuration along direction  $\mathbf{i}$ , we define the relative position vector along the contour of the chain as

$$\mathbf{w}(s, s') \equiv \mathbf{r}(s) - \mathbf{r}(s') = \alpha(s, s') \mathbf{i} + \beta(s, s') \mathbf{j} + \gamma(s, s') \mathbf{k}. \quad (4)$$

Using Taylor expansion around  $s' = s$  and noting  $(\partial_s^2 \mathbf{r} / \partial s^2)^2 \approx (\partial_s^2 \beta / \partial s^2)^2 + (\partial_s^2 \gamma / \partial s^2)^2$ , Skolnick and Fixman (1977) derived the following approximate formula,

$$\mathbf{w}(s, s') \approx \left[ (s' - s) - \frac{(s' - s)^3}{6} \left( \frac{\partial_s^2 \mathbf{r}}{\partial s^2} \right)^2 \right] \mathbf{i} + \frac{(s' - s)^2}{2} \frac{\partial_s^2 \beta}{\partial s^2} \mathbf{j} + \frac{(s' - s)^2}{2} \frac{\partial_s^2 \gamma}{\partial s^2} \mathbf{k}, \quad (5)$$

which leads to

$$|\mathbf{r}(s) - \mathbf{r}(s')| = |\mathbf{w}(s, s')| \approx |s' - s| \sqrt{1 - \frac{(s' - s)^2}{12} \left( \frac{\partial_s^2 \mathbf{r}}{\partial s^2} \right)^2}. \quad (6)$$

Expanding  $|\mathbf{r}(s) - \mathbf{r}(s')|$  and  $\exp(-\kappa |\mathbf{r}(s) - \mathbf{r}(s')|)$  in a Taylor series about  $s' = s$  and perform integration in terms of Eqs. (1) and (6) by assuming the electrostatic interaction is sufficiently short ranged yields (Skolnick and Fixman, 1977; Ariel and Andelman, 2003)

$$U_e \approx \frac{k_B T}{8v^2 \kappa^2 l_B} \int_0^L \left( \frac{\partial_s^2 \mathbf{r}}{\partial s^2} \right)^2 ds \quad (7)$$

for a 1: $v$  salt.

According to Eq. (7), the Hamiltonian of a charged stiff WLC under stretch becomes

$$H \approx \frac{1}{2} (p_0 + p_e) k_B T \int_0^L ds \left( \frac{\partial_s^2 \mathbf{r}}{\partial s^2} \right)^2 - \mathbf{f} \cdot [\mathbf{r}(L) - \mathbf{r}(0)] \quad (8)$$

where  $\mathbf{f}$  is the stretching force,  $p_0$  is the intrinsic elastic persistence length and

$$p_e = \frac{1}{4v^2 \kappa^2 l_B} \quad (9)$$

represents contribution of electrostatic interactions to the persistent length. In Eq. (8), the bending rigidity due to elasticity of the chain is decoupled from that due to electrostatic interactions. We note that Eq. (8) is strictly valid only for stiff polymers with rodlike configurations, namely, the contour length  $L$  should be comparable to the elastic persistence length. In this case, the force-extension relation obtained by Marko and Siggia (1995) for a long WLC

$$\frac{fp}{k_B T} = \langle x \rangle + \frac{1}{4(1 - \langle x \rangle)^2} - \frac{1}{4}, \quad (10)$$

where  $\langle x \rangle$  denotes the average extension of the chain along the force direction, is no longer valid. In addition, the elastic correlation length, usually defined as  $\xi \approx \sqrt{p/f}$ , is subject to uncertain interpretations for short stiff chains. A formula for stretching of discrete WLCs consistent with the Hamiltonian of Eq. (8) has been derived by Kierfeld *et al* (2004) as

$$\begin{aligned} \frac{fp}{k_B T} = & \frac{1}{2B} \left[ \left( 1 + \frac{B}{(1 - \langle x \rangle)^2} \right)^{1/2} - (1+B)^{1/2} \right] \\ & + \frac{p}{L} \left( \frac{1}{1 - \langle x \rangle} - 1 \right) \\ & + \left( -\frac{1}{2\sqrt{1+B}} - \frac{p}{L} + \frac{3}{2} \frac{1}{\Phi(p/L)} \right) \langle x \rangle \end{aligned} \quad (11)$$

where  $\Phi(x) = 1 - x + xe^{-1/x}$  and  $B = (b/2p)^2$ ,  $b$  being the length of a unit bond in the discrete chain. This equation suggests that a constant effective persistent length  $p = p_0 + p_e$  may be sufficient to describe stretching of short DNAs in electrolytes, a behavior which would deviate from that of long DNA molecules with apparent persistent lengths varying according to on the force magnitude at low ion concentrations. In the following, we use the GBR model to verify this difference between short and long DNAs.

### 3 GBR model incorporating DH potential

In the GBR model of a WLC under strong confinements (Wang and Gao, 2005), a semiflexible polymer or filament is described as  $N$  identical virtual beads of radius  $a$  connected by  $N - 1$  inextensible rods of length  $b$  with the unit tangent vectors  $\mathbf{u}_j$  ( $|\mathbf{u}_j| = 1$ ,  $j = 1, 2, \dots, N - 1$ ). The contour length of the chain is  $L = (N - 1)b$ . The  $N$  virtual beads with coordinates  $\mathbf{r}_j = (x_j, y_j, z_j)$  ( $j = 1, 2, \dots, N$ ) are introduced for modeling hydrodynamic interactions between different chain segments. The Brownian dynamics of a discrete WLC involves the collective motion of  $N$  identical beads in solution. After the hard rod constraint is implemented via the so-called linear constraint solver (LINCS), the new position vector  $\mathbf{r}_{(n+1)}$  of the  $N$  beads is determined from

$$\begin{aligned} \mathbf{r}_{(n+1)} = & (\mathbf{I} - \mathbf{T}_{(n)} \mathbf{B}_{(n)}) (\mathbf{r}_{(n)} + \frac{\Delta t}{k_B T} \mathbf{D}_{(n)} \mathbf{F}_{(n)} + \boldsymbol{\xi}_{(n)}) \\ & + \mathbf{T}_{(n)} \mathbf{d} \end{aligned} \quad (12)$$

where  $\mathbf{r}_{(n)}$  ( $3N$  vector) is the current position of the

beads;  $\mathbf{F}_{(n)}$  is the collective vector of internal (inter-beads) and external forces;  $\boldsymbol{\xi}_{(n)}$  is the random force generated at each time step from a Gaussian distribution with zero mean and variance equal to

$$\langle \boldsymbol{\xi}_{(n)} \boldsymbol{\xi}_{(n')} \rangle = 2\mathbf{D}_{(n)} \Delta t \delta_{nn'} \quad (13)$$

Here,  $\Delta t$  is the time step and  $\delta_{nn'}$  is the Kronecker delta symbol;  $\mathbf{D}_{(n)}$  is the translational diffusion matrix consisting of  $3 \times 3$  sub-blocks  $\mathbf{D}^{jk}$ ,  $j, k = 1, \dots, N$ . The hydrodynamic interaction tensor between beads  $j$  and  $k$ , the Rotne-Prager tensor, is used for  $\mathbf{D}^{jk}$ . For  $N - 1$  time-independent constraint equations

$$g_i(\mathbf{r}) = \|\mathbf{r}_i - \mathbf{r}_{i+1}\| - d_i = 0, \quad i = 1, 2, \dots, N - 1 \quad (14)$$

the  $(N - 1) \times 3N$  gradient matrix  $\mathbf{B}$  of Eq. (12) can be expressed as

$$\mathbf{B} = \left\{ \frac{\partial g_i(\mathbf{r})}{\partial \mathbf{r}}, \quad i = 1, 2, \dots, N - 1 \right\}; \quad (15)$$

$\mathbf{T}_{(n)} = \mathbf{D}_{(n)} \mathbf{B}_{(n)}^T (\mathbf{B}_{(n)} \mathbf{D}_{(n)} \mathbf{B}_{(n)}^T)^{-1}$  and  $\mathbf{I} - \mathbf{T}_{(n)} \mathbf{B}_{(n)}$  is a projection matrix which sets the constraints. In order to avoid matrix inversion in the computation, an order  $N$  algorithm has been introduced in the work of Wang and Gao (2005). Defining  $\mathbf{A}_{(n)} \equiv \mathbf{I} - \mathbf{B}_{(n)} \mathbf{B}_{(n)}^T / 2$  and following a strategy of truncated series expansion of matrices, one can write

$$\mathbf{T}_{(n)} \approx \mathbf{B}_{(n)}^T + \mathbf{B}_{(n)}^T \sum_{j=1}^K \mathbf{A}_{(n)}^j \quad (16)$$

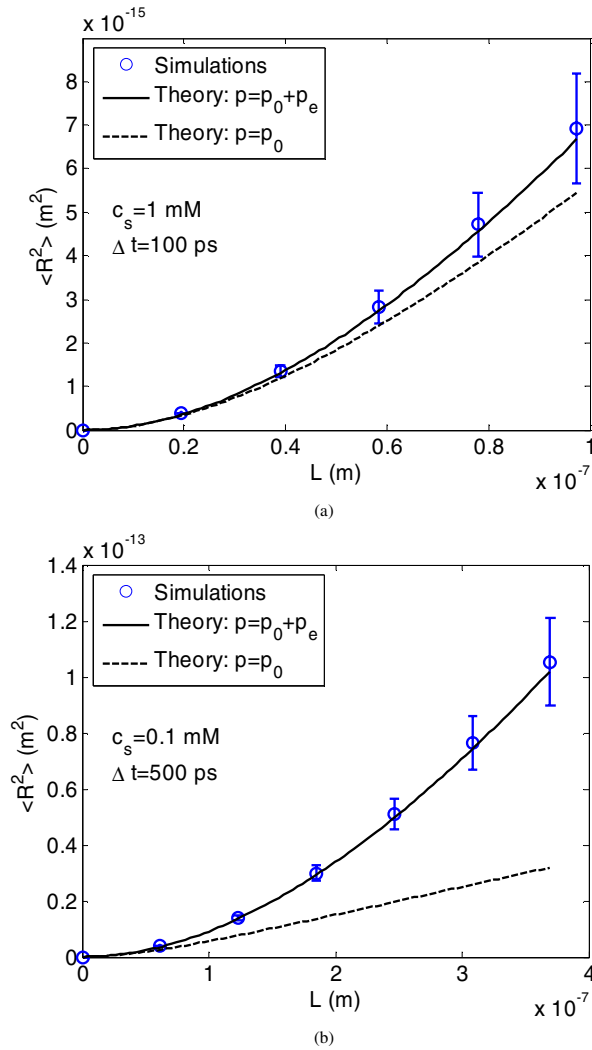
where  $K$  denotes the order of approximation.

For semiflexible polymers, the discrete version of DH potential in Eq. (1) is given by (Jian *et al.*, 1997)

$$U^e = \sum_{j>i+1} \frac{\sigma_0^2 e^2 b^2 \exp(-\kappa |\mathbf{r}_i - \mathbf{r}_j|)}{4\pi\epsilon\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} \quad (17)$$

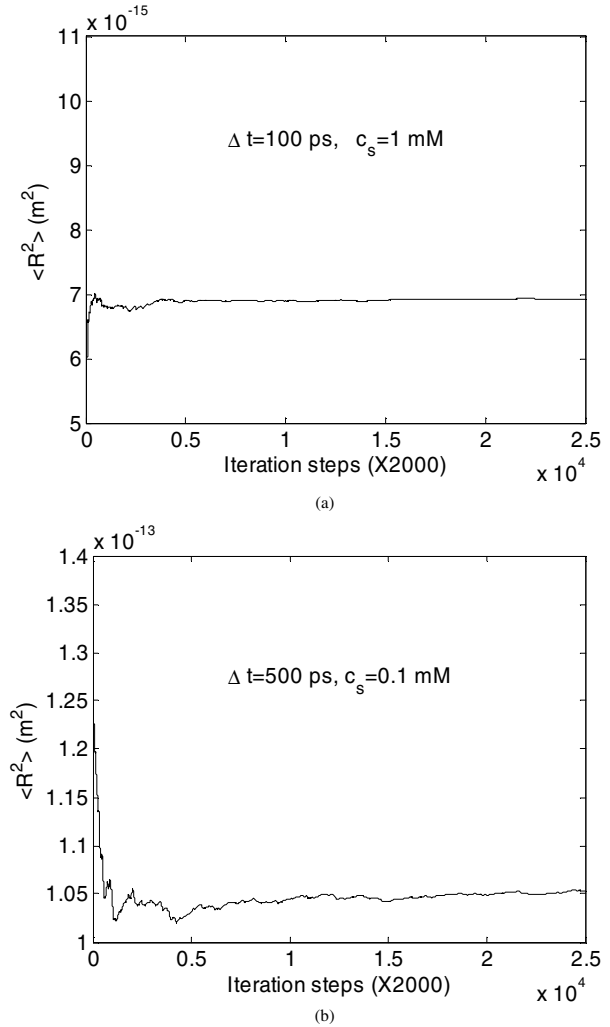
For DNA chains in an aqueous medium, one usually takes  $\sigma_0 = 0.243/A$  and  $\epsilon = 80$  (Jian *et al.*, 1997; Vologodskii and Cozzarelli, 1995). The interaction force corresponding to Eq. (17) is

$$\begin{aligned} \mathbf{F}_n^e = & -\nabla_{\mathbf{r}_n} U^e = -\frac{\sigma_0^2 e^2 b^2}{4\pi\epsilon\epsilon_0} \times \\ & \sum_{j=1, |j-n|>1}^N (1 + \kappa |\mathbf{r}_j - \mathbf{r}_n|) \exp(-\kappa |\mathbf{r}_j - \mathbf{r}_n|) \frac{\mathbf{r}_j - \mathbf{r}_n}{|\mathbf{r}_j - \mathbf{r}_n|^3} \end{aligned} \quad (18)$$



**Figure 2 :** Comparison of the simulated and theoretical MSD of DNA chains in dilute electrolytes with different ion concentrations. The theoretical predictions are plotted using different values of persistence lengths,  $p = p_0$  and  $p = p_0 + p_e$ , respectively, and the simulations are conducted under the parameter choices of  $b = 2/\kappa$  with total iteration steps of 50 million. Different ion concentrations and simulation time steps are used in each subplot: (a)  $c_s = 1.0 \text{ mM}$ ,  $\Delta t = 100 \text{ ps}$  and (b)  $c_s = 0.1 \text{ mM}$ ,  $\Delta t = 500 \text{ ps}$ .

In the Brownian dynamics simulations conducted in the present work, we are primarily interested in equilibrium properties of a short DNA under stretch. In this case, the time consuming hydrodynamic interactions are not necessary and only diagonal terms of the Rotne-Prager tensor (equal to  $k_B T / 6\pi\eta a$  where  $a$  is the radius of each



**Figure 3 :** Convergence of the MSD of DNA chains under the parameter choices of (a)  $c_s = 1.0 \text{ mM}$ ,  $\Delta t = 100 \text{ ps}$ ,  $L = 10/\kappa$  and (b)  $c_s = 0.1 \text{ mM}$ ,  $\Delta t = 500 \text{ ps}$ ,  $L = 12/\kappa$ .

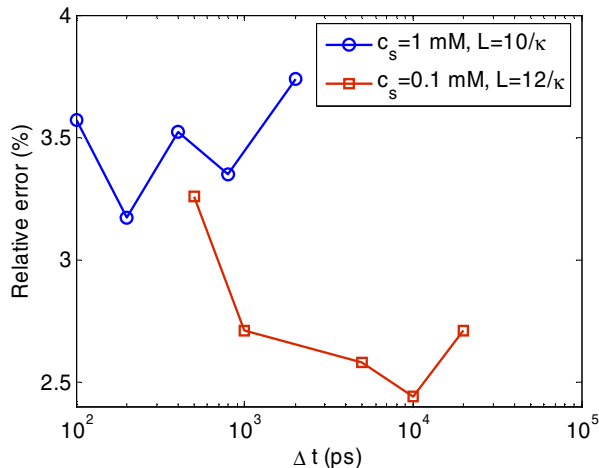
bead and  $\eta$  the viscosity of solvent) in Eq. (12) need to be considered.

## 4 Results and discussions

### 4.1 Mean-square end-to-end distance

One of the quantities that play an important role in characterizing the conformation of a polymer is the mean-square end-to-end distance (MSD), which for the WLC model is given by

$$\langle \mathbf{R}^2 \rangle = 2pL - 2p^2(1 - e^{-L/p}). \quad (19)$$



**Figure 4** : Relative errors for the simulated MSD when different time steps are used.

For a short, charged WLC,  $p = p_0 + p_e$  according to the Hamiltonian of Eq. (8).

We have tested the efficiency of the GBR model with DH potential by comparing the simulated MSD and Eq. (19) with  $p = p_0 + p_e$ . In each simulation, after the trajectory of each bead  $\mathbf{r}_j(t)$  is determined via Eq. (12), the MSD is obtained from

$$\langle \mathbf{R}^2 \rangle = \langle \|\mathbf{r}_1(t) - \mathbf{r}_N(t)\|^2 \rangle. \quad (20)$$

The initial configurations of chains are taken to be straight in all simulations. **Figure 2** shows the comparison of simulated and theoretical MSD of DNA chains in dilute electrolytes with different ion concentrations. The two theoretical MSDs in the figure are obtained using different values of the persistence length,  $p = p_0 = 50 \text{ nm}$  and  $p = p_0 + p_e$ , respectively. The simulations are conducted under the parameter choices of  $b = 2/\kappa$  with total iteration steps of 50 million. Different ion concentrations and simulation time steps are considered in each subplot: (a)  $c_s = 1.0 \text{ mM}$ ,  $\Delta t = 100 \text{ ps}$  and (b)  $c_s = 0.1 \text{ mM}$ ,  $\Delta t = 500 \text{ ps}$ . The simulation results appear to be in good agreement with the theoretical prediction of Eq. (19) when  $p = p_0 + p_e$  (instead of  $p = p_0$ ) for electrolytes at ion concentrations of 0.1 mM and 1 mM.

The results shown in **Figure 3** confirm that the simulations have been performed long enough to have reached steady state.

In order to test the influence of time steps on the simulations results, we can take a look at the relative error of

the simulated MSD:

$$100\% \times \frac{(\langle \mathbf{R}^2 \rangle_{\text{simulation}} - \langle \mathbf{R}^2 \rangle_{\text{theory}})}{\langle \mathbf{R}^2 \rangle_{\text{theory}}}, \quad (21)$$

where  $p = p_0 + p_e$  is used in the evaluation of the theoretical MSD. **Figure 4** shows that the error is within 4% for time steps up to 20 ns. The large time step corresponds to the large rod length  $b = 2/\kappa$  chosen to be twice of the Debye length. As the ion concentration  $c_s$  decreases, both the Debye length and the rod length  $b = 2/\kappa$  tend to increase.

We conclude from these results that the GBR model with DH potential is capable of capturing electrostatic interactions of a charged DNA chain.

#### 4.2 Stretching short DNAs in electrolytes

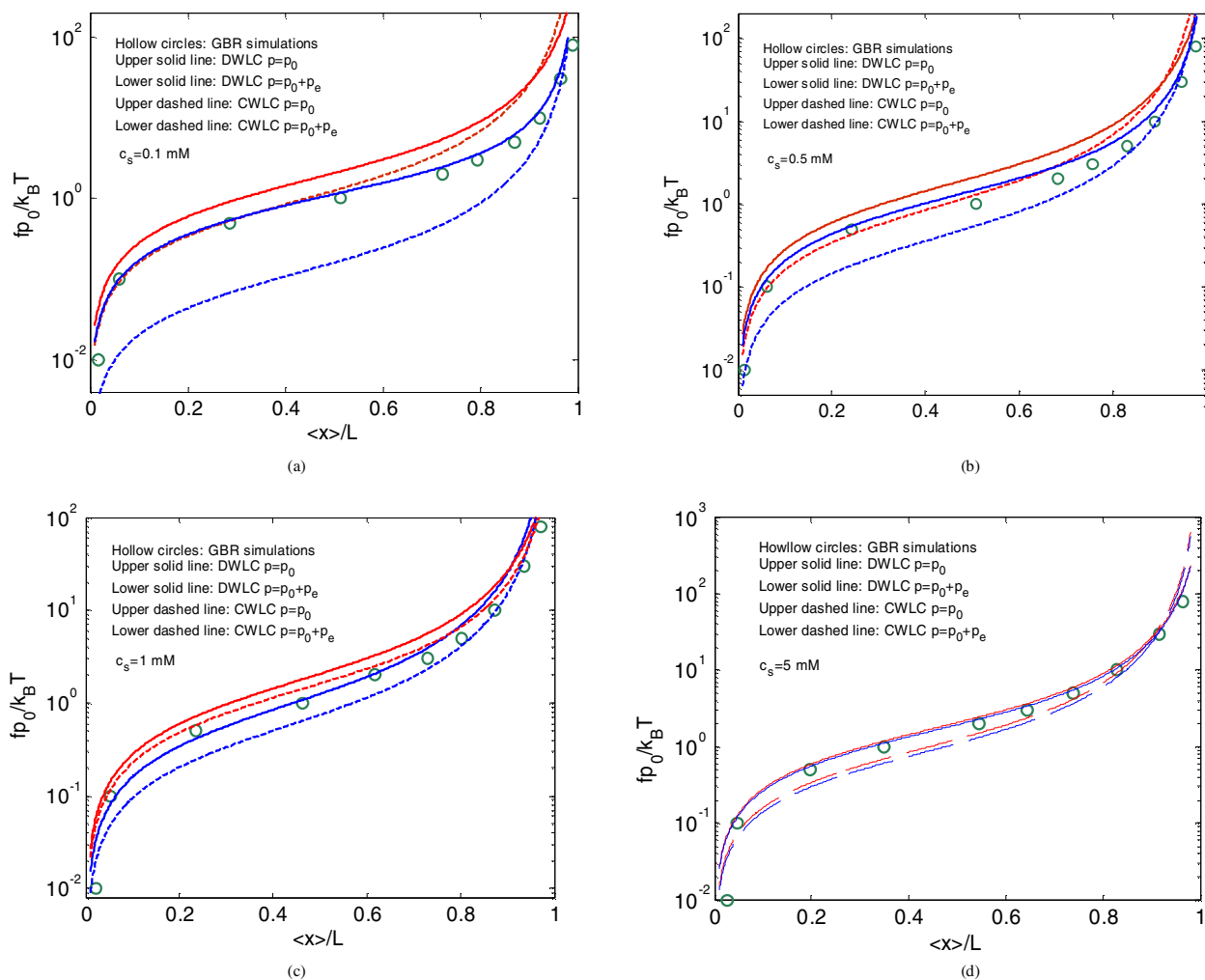
For a charged DNA subjected to a constant tensile force  $f$  on both ends of the chain in the  $x$ -direction, the force vector  $\mathbf{F}_{(n)}$  in Eq. (11) consists of

$$\mathbf{F}_{(n)} = \mathbf{F}_{(n)}^b + \mathbf{F}_{(n)}^e + \mathbf{F}^t \quad (22)$$

where  $\mathbf{F}^t$  is the tensile force.

Brownian dynamics simulations based on the GBR model with force vector (22) have been performed for a charged 100-nm-long DNA chain. **Figure 5** compares the simulated results with different theoretical predictions. The chain is simulated for a total time of 25 ms with the GBR bond length chosen as 10 nm and the time step as 500 ps. The abbreviation ‘‘DWLC’’ stands for the discrete WLC model in Eq. (11), and ‘‘CWLC’’ stands for the continuous WLC model in Eq. (10). The simulations are conducted at different ion concentrations: (a)  $c_s = 0.1 \text{ mM}$ , (b)  $c_s = 0.5 \text{ mM}$ , (c)  $c_s = 1.0 \text{ mM}$  and (d)  $c_s = 5.0 \text{ mM}$ , respectively. **Figure 5** shows that the simulation results are in good agreement with those of the DWLC predictions with a constant effective persistence length,  $p = p_0 + p_e$ , in both low-force and high-force regimes. These results are consistent with the experimental observations of Smith et al. (1992) for stretching of long DNA molecules in an electrolyte at high ion concentrations but deviate from the behaviors of long DNA at low ion concentrations.

**Figure 6** shows the normalized end-to-end distance over a total simulation time of 25 ms under parameters of  $b = 10 \text{ nm}$ ,  $\Delta t = 500 \text{ ps}$ ,  $f p_0 / k_B T = 0.01$  and  $c_s = 5 \text{ mM}$ .



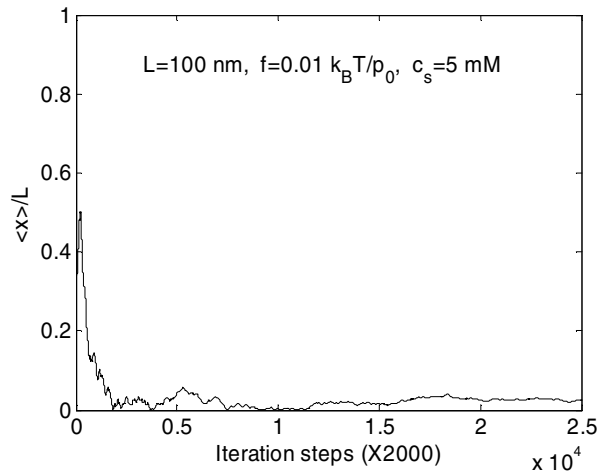
**Figure 5** : Comparison of the simulated force-extension curves with different theoretical predictions for a 100 nm-long DNA. The chain is simulated for a total time of 25 ms with the bond length in the GBR model chosen as 10 nm and the time step as 500 ps. The abbreviation “DWLC” stands for the discrete WLC model in Eq. (11), and “CWLC” stands for the continuous WLC model in Eq. (10). Different ion concentrations are used in each subplot: (a)  $c_s = 0.1\text{mM}$ , (b)  $c_s = 0.5\text{mM}$ , (c)  $c_s = 1.0\text{mM}$  and (d)  $c_s = 5.0\text{mM}$ .

The results indicate that equilibrium is reached within several milliseconds. The larger the force, the faster the equilibration.

The numerical simulation results based on GBR indicates that the behavior of a short DNA chain stretched in an electrolyte can be well described by the discrete WLC model of Eq. (11) with a constant effective persistent length  $p = p_0 + p_e$ , for the entire range of ionic concentrations and force magnitudes investigated here.

## 5 Conclusion

We have investigated the force-extension relation of a short DNA chain stretched in an electrolyte under different ion concentrations and force magnitudes. Using the newly developed GBR model (Wang and Gao, 2005) incorporating electrostatic interactions via the Debye-Hueckel potential, we find that the behavior of short DNAs can be well described by the discrete WLC model of Kierfeld et al. (2004) with a constant effective persistent length  $p = p_0 + p_e$ . This conclusion is at variance with the behavior of long DNA chains that are known to



**Figure 6** : Convergence of the normalized MSD of a 100-nm-long DNA chain under stretch under parameter choices of  $b = 10$  nm,  $\Delta t = 500$  ps,  $f p_0 / k_B T = 0.01$  and  $c_s = 5$  mM.

exhibit variable apparent persistent lengths depending on the ion concentration levels and force magnitudes.

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