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Role of Geometrical Shape in Like-Charge Attraction of DNA

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Abstract While the phenomenon of like-charge attraction of DNA is clearly observed experimentally and in simulations, mean-field theories fail to predict it. Kornyshev et al. argued that like-charge attraction is due to DNA's helical geometry and hydration forces. Strong coupling (SC) theory shows that attraction of like-charged rods is possible through ion correlations alone at large coupling parameters, usually by multivalent counterions. However for SC theory to be applicable, counterion-counterion correlations perpendicular to the DNA strands need to be sufficiently small, which is not a priori the case for DNA even with trivalent counterions. We study a system containing infinitely long DNA strands and trivalent counterions by computer simulations employing varying degrees of coarse-graining. Our results show that there is always attraction between the strands, but its magnitude is indeed highly dependent on the specific shape of the strand. While discreteness of the charge distribution has little influence on the attractive forces, the role of the helical charge distribution is considerable: charged rods maintain a finite distance in equilibrium, while helices collapse to close contact with a phase shift of π, in full agreement with SC predictions. The SC limit is applicable because counterions strongly bind to the charged sites of the helices, so that helix-counterion interactions dominate over counterion-counterion interactions. Thus DNA's helical geometry is not crucial for like-charge DNA attraction, but strongly enhances it, and electrostatic interactions in the strong coupling limit are sufficient to explain this attraction.

1 Introduction

Macromolecules possessing dissociable groups, such as DNA, can dissociate in polar solvents and become charged. They are then surrounded by their oppositely charged counterions. At low ion concentrations, this can be described well on the mean-field level of Poisson-Boltzmann (PB) theory [1,2], but for sufficiently strong electrostatic interactions, the validity of the mean-field level approximation tends to break down. A fascinating example is like-charge attraction: attraction between any form of like-charged macroions is impossible within the framework of the well-known Poisson-Boltzmann theory [1,2,3,4]. However, attraction between rod-like macroions has been observed many times in experiments with DNA, a stiff, highly-charged polyelectrolyte which can be condensed by multivalent counterions [5,6,7]. This phenomenon has also been observed in computer simulations [8,9,10,11,12].

Experiment and simulations indicate that attraction of like-charged macroions occurs in systems with strong Coulomb interactions, e.g. at low temperatures or in presence of multivalent counterions; the failure of Poisson-Boltzmann theory is therefore not surprising. However, this means that an explanation of like-charge attraction needs to either attribute it to other effects, or go beyond the mean-field level, and thus was lacking for a long time. One possible candidate interaction that can mediate attraction are hydration forces. Indeed, Kornyshev and Leikin argued that hydration forces in combination with screened Coulomb interactions of the helical DNA are the cause of the attraction [13,14]. However, since like-charge attraction is not a DNA-specific effect and also occurs in many other charged macromolecules, an explanation based only on electrostatic interactions would be favorable.

Recently, the strong coupling (SC) theory by Moreira and Netz [15,16,17] offers a route to handle systems with strong Coulomb interactions directly, rather than extending Poisson-Boltzmann. If the DNA is modeled as an infinitely long, structureless rod, SC theory indeed predicts like-charge attraction for a wide range of parameters [18], without requiring any other interactions. For a more elaborate model taking into account the double helical charge distribution, the same holds [19]. In addition, these calculations predict that there is a favorable phase shift of π between the attracting DNA double strands. This means that the DNA strands are not intertwining as closely as possible, but rather prefer a zig-zag like pattern of close approach and nearly 4 nm charge distance. However, SC theory relies on the formation of a correlation hole around the counterions, which permits to ignore counterion-counterion correlations. In the case of DNA at physiological conditions, the lateral and perpendicular ion distances are however comparable [20]. Thus, while SC

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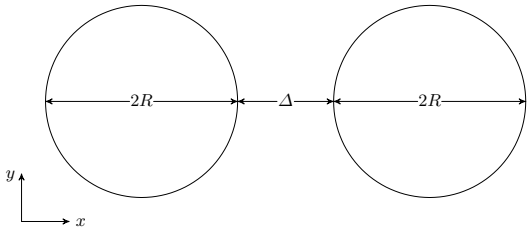

Figure 1. Schematic view of the two-rod system, viewed along the rod axis. The large circles represent the two rods of radius R and line charge density τe each, at a surface-to-surface distance Δ.

theory demonstrates that like-charge attraction is in principle possible, it does not necessarily apply to DNA.

In this article, we compute the interactions between two infinitely long DNA molecules as well as the counterion distributions around the DNA molecules by means of computer simulations. We model the DNA as charged rigid rods, lines of discrete charges, and double-helices of discrete charges, only taking into account bare Coulomb and steric interactions. By gradually increasing the geometric accuracy we show that, while the strength of the interaction depends on the specific model, DNA always attracts in the presence of multivalent counterions, independent of the model. In all cases, SC predictions agree well with our computer simulations, showing that like-charge attraction can indeed be explained by electrostatic interactions in strong coupling without the need for additional, DNA-specific interactions.

2 Theory

In the following, we briefly introduce PB and SC theory for the classical DNA model geometry of a charged, structureless rod. In this model, the DNA is a cylinder with line charge density τe and radius R, surrounded by counterions of charge qe, where e denotes the unit charge. Our interest is to compute the force between two parallel rods as a function of the surface-to-surface distance Δ (or, equivalently, the axial separation is $2R + \Delta$). The geometry is illustrated in Figure 1.

2.1 Poisson-Boltzmann Theory

Treatment of electrostatic interactions at a mean-field level as in the standard PB theory is only valid in the absence of electrostatic correlations, i.e. for weak surface charges, low counterion valencies and small Bjerrum lengths. This condition can be quantified by the *coupling parameter* [21]

$$\Xi = 2\pi q^3 l_B^2 \sigma_s, \tag{1}$$

where q is the counterion valency and $\sigma_s = \tau/(2\pi R)$ is the surface charge density of the charged cylinders. The *Bjerrum length* is defined as

$$l_B = \frac{e^2}{4\pi\varepsilon k_B T} \tag{2}$$

with the unit charge e, dielectric permittivity ε, Boltzmann constant k_B, and temperature T. The Bjerrum length is the distance at which the electrostatic interaction energy of two unit charges equals thermal energy. A high Bjerrum length corresponds to a low temperature or, more generally, strong Coulombic interactions. PB theory is asymptotically valid for $\Xi \to 0$, where ion correlations are weak.

In the PB regime, the force per unit length acting on the two parallel cylinders with radius R, linear charge density τ and surface-to-surface distance Δ is [11]

$$\frac{F}{k_B T} = \frac{2 l_B \tau^2}{2R + \Delta}. \tag{3}$$

This force is repulsive; in fact, it has been proven rigorously that Poisson-Boltzmann will always predict repulsion between like-charged objects, independently of their shape [1,2,3,4]. Thus, PB theory is not adequate to describe like-charge DNA attraction, and this attraction is necessarily due to ion correlations.

2.2 Strong Coupling Theory

The limit of $\Xi \gg 1$, i.e. the opposite of the limit taken by PB theory, is the realm of Strong Coupling theory, where the free energy of the system is expanded in terms of inverse powers of the coupling parameter Ξ [15]. While for planar surfaces the coupling parameter Ξ sufficiently characterizes the system, rod-shaped macroions require a second parameter, the *Manning parameter* [22]

$$\xi = q l_B \tau, \tag{4}$$

where τ is the cylinders' line charge density. ξ describes the degree to which counterions condense onto the rod surface. For $\xi > 1$, a certain fraction of the counterions are bound to the rod, which allows for attraction between multiple rods if Ξ is also sufficiently large [18].

SC theory predicts that, for Manning parameters above $\frac{2}{3}$, the force $F/k_B T$ between two parallel charged rods becomes constant and attractive at large distances [23,18], that is, SC theory predicts like-charge attraction. More precisely, SC theory predicts an equilibrium surface-to-surface distance of

$$\Delta_0 = \frac{2}{3}\mu + \mathcal{O}(\xi^{-1}), \tag{5}$$

where the *Gouy-Chapman length* is

$$\mu = \frac{1}{2\pi q l_B \sigma_s}, \tag{6}$$

which gives the distance at which the thermal energy equals the counterion-DNA surface interaction energy. The exact ξ-dependence can be obtained by numerical integration [23], which also needs to applied for more complex geometries, such as double helices [19]. In this case, Kanduc et al. showed that the optimal phase shift for double-stranded DNA is π, i. e., the strands form a zig-zag pattern [19].

The applicability of SC theory however also depends on the geometry. The reason for this is that in the strong coupling limit, counterion-counterion correlations perpendicular to the rod are negligible compared to those parallel to the rods. At the same time, the ions are strongly attracted to the rod surfaces. Therefore perpendicular counterion-counterion correlations are suppressed and can be ignored. At finite coupling however, this only holds if the lateral particle distance is much larger than the perpendicular extent of the system.

This requirement can be quantified by two more parameters: the *Rouzina-Bloomfield parameters*

$$\gamma_{\mathrm{RB}} = \frac{q}{\tau \Delta}, \tag{7}$$

which compares the average distance along the rods between neighboring counterions with the gap between the rods, and

$$\gamma_z = \frac{q}{\tau R}, \tag{8}$$

which compares the average distance between neighboring counterions with the rod diameter. Previous simulations [18,20] have demonstrated good agreement between SC theory and simulations of rods indeed only for large values of γ_{RB} and γ_z. γ_{RB} is inversely proportional to the equilibrium surface-to-surface distance, which in the interesting case of attraction is sufficiently small and thus does not impose much of a restriction. γ_z however is a constant that only depends on the size of the considered molecule. Because the radius of the DNA double helix is rather large, γ_z is small and SC theory does not necessarily apply even to the typical case of DNA condensation by trivalent ions [20]. Nevertheless, SC theory has shown that like-charge attraction is possible without invoking additional interactions such as specific or hydration forces.

3 Simulation Method

As we have seen, the geometry plays an important role in strong coupling. On the other hand, a fundamental explanation of like-charge attraction that does not require DNA-specific interactions would be desirable. Therefore, we investigate the attraction of different basic DNA models using Molecular Dynamics computer simulations. *Basic* refers to that we take into account only electrostatic and steric interactions. We thus ignore the screening due to the additional monovalent co- and counterions which are necessary to stabilize DNA. We also do not take into account hydration forces, which are quite strong as we consider multivalent ions. Finally, DNA has a much lower dielectric constant than the surrounding water, which weakens the electrostatic DNA-ion interaction [24]. But since like-charge attraction has been observed in many different setups with DNA and other polyelectrolytes, our goal is to elucidate whether the always present electrostatic interaction alone is sufficient to explain this effect.

Model parameters were chosen to match DNA in a salt-free environment, which has two charges per base pair when fully dissociated, so the line charge density is $\tau = 6/\mathrm{nm}$ and the radius is $R = 10\,\text{Å}$. The surface-to-surface distance Δ of the two polymers was varied between 0 and 10 Å as in previous simulations [18], where the equilibrium distance for two structureless rods at DNA parameters was found to be approximately $\Delta_0 = 0.5\,\text{Å}$. For the helical models, Δ may become negative until the helices are actually in contact as the radius R is the outer bounding radius and two helices can overlap.

The simulations were performed using the ESPResSo [25,26] molecular dynamics (MD) simulation package, which features the MMM1D method [27] to calculate the electrostatic interactions in one-dimensionally periodic systems. Each periodic image contains $N = 84$ counterions and the appropriate charges on the polymer to neutralize the system. To prevent the trivalent counterions from escaping the simulation box, they were confined to a cylinder with a diameter of $D = 4(2R + \Delta)$ around the polymers. To simulate the hard-core repulsion the counterions experience from the polymers and the confinement cylinder, a shifted Weeks-Chandler-Anderson (WCA) potential [28] was used. This is a Lennard-Jones potential,

$$V(r) = 4\epsilon \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + c_{\mathrm{shift}} \right), \tag{9}$$

cut off at the minimum ($r_{\mathrm{cut}} = \sqrt[6]{2}\sigma$) and shifted to be continuous at the cutoff ($c_{\mathrm{shift}} = \frac{1}{4}$). $\sigma = 0.5\,\text{Å}$ was chosen so that the potential was only in effect on close contact. There is no excluded volume interaction between the counterions in addition to their electrostatic repulsion.

To thoroughly sample accessible system configurations at a Bjerrum length of $l_B = 7\,\text{Å}$ (corresponding to water at room temperature), parallel tempering [29] was used with 10 temperatures spaced exponentially so that l_B ranged between 0.7 nm and 0.1 nm. For each data point, 500 000 time steps were simulated and the forces from 500 of the resulting configurations were averaged. Additionally, for the simulations with helical geometries, results from 15 or more simulation runs were averaged to further improve sampling.

The parameters used correspond to the following values of the parameters of the theoretical models: surface charge density of macroions $\sigma_s = 0.95e/\mathrm{nm}^2$, coupling parameter $\Xi = 79$, Gouy-Chapman length $\mu = 0.079\,\mathrm{nm}$, Manning parameter $\xi = 13$, Rouzina-Bloomfield parameters $\gamma_{\mathrm{RB}} = \frac{0.51\,\mathrm{nm}}{\Delta}$ and $\gamma_z = 0.5$.

4 Results

4.1 Continuous Rods

The simplest model, consisting of rods with continuous line charge and WCA repulsion, was studied by SC theory and corresponding simulations in Refs. [18,20]. The results agreed between simulations and the strong coupling theory for the same geometry in the limit of large coupling parameter, and the quality of the agreement was

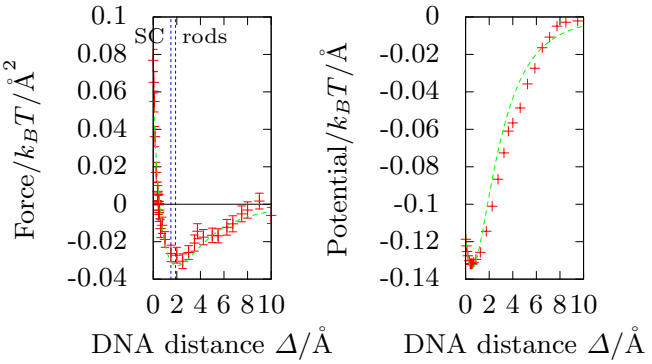

Figure 2. Forces acting on the rod-shaped polymer at DNA parameters and different gap sizes, as well as the corresponding potential obtained by numerical integration. The curve is only a guide to the eye. The equilibrium distance reproduces results from [18], but is larger than predicted by SC theory.

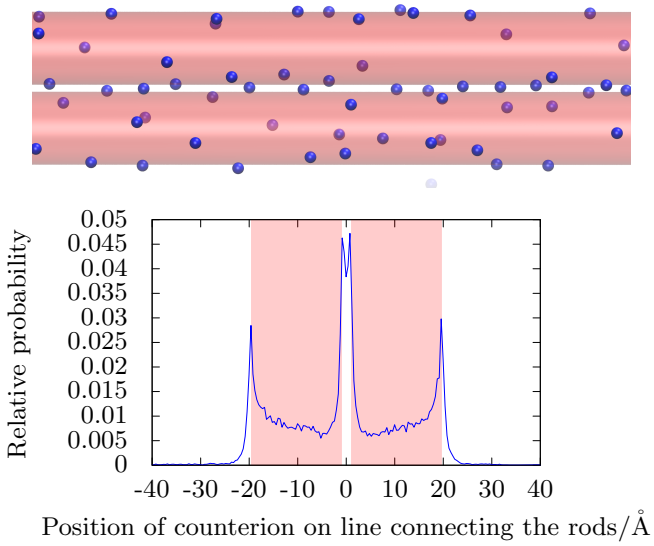

Figure 3. Top: Snapshot of the rod geometry simulated. This example has a surface-to-surface distance of the rods of $\Delta = 2$ Å. For clearer visibility, the counterions are not drawn to scale. Bottom: Histogram of the counterion distribution along the line connecting the two rods, whose width is shaded. All of the counterions arrange in close contact with one of the rods, primarily in the gap between the two rods, but also on the opposite sides of the rods and, to a lesser extent, on the entire rod surface.

indeed controlled by the two Rouzina-Bloomfield parameters γ_{RB} and γ_{z}.

Figure 2 shows the resulting forces per simulation box length for our specific parameters, which mimick DNA in salt-free solution with trivalent counterions. Attraction is indeed observed and is strongest at a distance of $\Delta_{\max} = 2.2$ Å. Repulsion is observed for $\Delta < 0.5$ Å, which is consistent with the equilibrium distance found before in simulations [18]. However, this also means that $\gamma_{\mathrm{RB}} \approx 1$, so that both Rouzina-Bloomfield parameters indicate that SC theory is unsuitable to describe attraction in this model.

This can also be verified by Figure 3, which shows that the ions concentrate not only between the rods as predicted for strong coupling, but also on the opposite sides of the rods. The latter positions are only favorable due to non-negligible counterion-counterion interactions perpendicular to the rods. On the other hand, most ions are well condensed onto the rod surfaces as expected in the SC limit, which is due to the large Manning parameter of DNA. The latter effect seems to to be dominating, since the SC approximation (Equation (5)) predicts the same equilibrium distance for these parameters, and also the more accurate numerical minimization of the SC free energy results in an only 20% lower equilibrium distance of $\Delta_0 = 0.4$ Å [18]. Thus, like-charge attraction exists even in the simple rod-like model, and SC theory works surprisingly well for predicting the effect and even quantitatively determining the equilibrium separation.

4.2 Lines of Discrete Particles

As a first refinement, we consider the DNA as composed of discrete particles; more precisely, lines of varying numbers of discrete fixed particles placed equidistantly at the centers of the rods to model the DNA. Each one of the particles making up the rod now carries both a charge and interacts individually via WCA with the counterions. The particles on the two rods were placed at the same positions along the rod axes as well as shifted relative to each other by half a particle. The particle radius as set by the WCA potential is identical to the radius of the continuous rods used in the previous section. Due to the large diameter of the double helix, the fixed rod charges thus heavily overlap.

For all but the coarsest discretizations, the force has the same general dependency on the gap size as before and looks mostly identical to Figure 2: it is strongly repulsive on contact, becomes attractive at a small distance and drops to a shallow but broad attraction maximum. The position of equilibrium and maximum attraction is shown in Figure 4, and differs from the ideal rod only for discretizations that are much coarser than that of actual DNA. Even for these discretizations, a relative shift of the two lines of particles does not appreciably influence the force. At charge discretizations comparable to DNA, the agreement between continuous and discretized rods is excellent. This shows that a continuous charge distribution is well suited to represent the DNA. Thus, it remains to check whether the helical spatial geometry of DNA plays a role.

4.3 Double helices

DNA dissociates charges mostly at its backbone, so that double-stranded DNA has a double-helical charge distribution that coincides with its helical spatial geometry. As discussed above, this helical distribution has been consid-

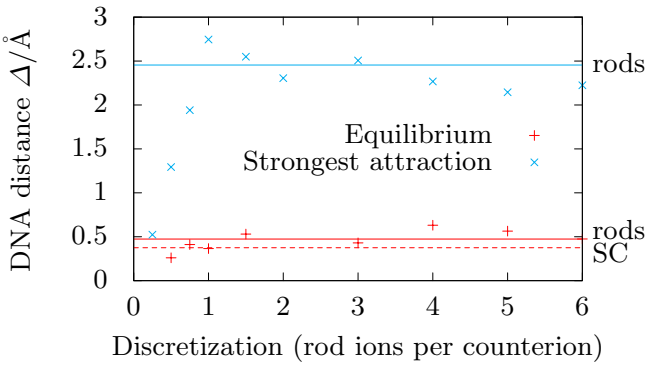

Figure 4. Equilibrium distance and distance of greatest attraction for the various levels of discretization of the linear model, compared with the corresponding distances for the continuous rods. For rods, the result from Ref. [18] is reproduced (solid lines), while the theoretical SC prediction is about 20% smaller (dashed line). The equilibrium distance of the rods is reproduced for discretizations of at least 3 bases per counterion (i.e. the natural charge distribution of DNA considering trivalent counterions). The distance of strongest attraction however is slightly smaller for the discrete lines of charges than for continuous rods.

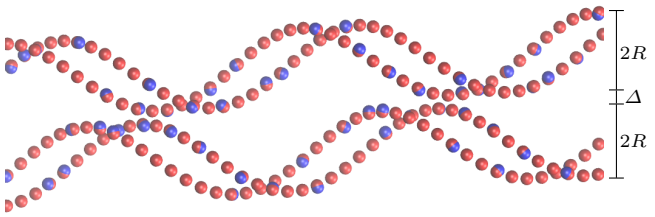

Figure 5. Snapshot of the double helix geometry simulated. This example has a relative shift of the two double helices of 5.25 base pairs and a surface-to-surface distance of $\Delta = 2\,\text{Å}$. For clearer visibility, the ions are not drawn to scale. All of the counterions arrange in close contact with one of the charges making up the double helices.

ered theoretically before, both in the framework of Poisson-Boltzmann [13,14,19] and strong coupling theory [19]. In our model, the bead diameter and the pitch (the height of a single turn of each helix) are again chosen to match those of DNA: the bead size is 3 Å and the pitch 34 Å, i.e. there are 10.5 base pairs per turn as in B-DNA, compare Figure 5. The main difference between our model and the one considered in Ref. [19] is that our counterions are point-like, while they have an extent of 0.2 nm in Ref. [19]. Another difference is that Ref. [19] considers the DNA molecules as coiled around a cylinder impenetrable to the counterions, while in our model ions can penetrate the helices. However, this difference is negligible because the ions are strongly bound to the helix charges and thus barely explore the accessible volume.

Forces obtained with different phase shifts between the two double helices are shown in Figure 6, and compare rather well to the forces predicted by SC theory [19] at distances above 0.5 nm. Large deviations at distances below 0.5 nm are due to the counterion excluded volume that we do not take into account.

For all phase shifts the forces hardly resemble the forces acting on plain rods even at moderate distances, thus the helical structure indeed plays a crucial role. More importantly, the forces tend to almost always be attractive, so that the equilibrium position is on contact, in contrast to the finite equilibrium distance for plain rods. At small distances, where the attraction is strongest, the strength varies strongly with the phase shift between the helices: For helices running in phase, the attraction is negligible except when they are almost in contact, while helices shifted 180° relative to each other have a strong attraction up to close contact. If free to move, helices will thus align at close contact with a 180° phase shift relative to each other as depicted in Figure 5. Again, this is in full agreement with the SC predictions.

The reason for this good agreement with SC theory lies in the different ion distribution, which is drastically different from the loose distribution over the surface of the continuous rod model: the ions approach the DNA charges much closer and practically fully condense onto the double helices. Thus counterion-counterion correlations perpendicular to the strands are drastically reduced, as required for SC theory to work. This distribution also explains why the equilibrium phase shift is 180°: as we have seen in the rod model, counterion-counterion interactions are still too strong to line up all counterions between the rods. The phase shift allows the counterions to occupy positions both between the rods at the contact positions, where they mediate the attraction, and positions that are further away, reducing the counterion-counterion repulsion.

Besides the simulations with natural minor and major groove sizes of the DNA, corresponding to a shift of 3 and 7.5 base pairs between the two helices in each double helix, simulations with symmetric grooves were also performed to determine the effect of torsion applied to the DNA molecule, which partially separates the strands. While the resulting forces differed slightly, they were mostly within error bars of those shown in Figure 6. This is not unexpected, since the pattern of alternating touching of the DNA strands is unchanged by shifting the grooves.

5 Conclusion

We have performed computer simulations to elucidate the role of geometry in the like-charge attraction between double-stranded DNA molecules in the presence of trivalent ions. The simulations show that the frequently-used rod approximation is sufficient to explain like-charge attraction, but does not apply to DNA very well because its helical structure changes the electrostatic forces between DNA molecules drastically. While plain charged rods maintain a finite equilibrium distance, helices attract up to close contact. The equilibrium phase shift is π, meaning that the two DNA strands assume a zig-zag configuration which allows the counterions to maximize their perpendicular distance. These findings are in good agreement with predictions based on the strong coupling theory [19]. As our

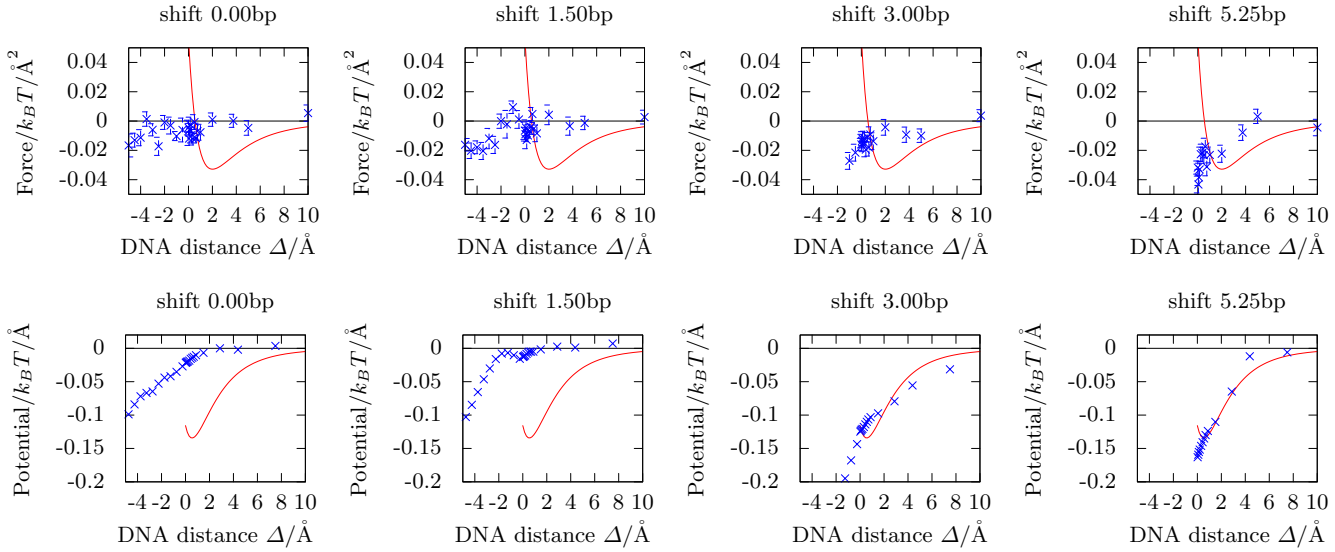

Figure 6. Forces and corresponding potential acting on the polymer modeled as a double helix with different shifts between the two polymers. Crosses mark the helix results, while solid lines correspond to the results for rods with comparable parameters. The simulations were only performed for Δ large enough for the two double helices not to interpenetrate each other.

simulations do not include interactions other than electrostatics and excluded volume, we conclude that like-charge attraction of DNA is indeed a purely electrostatic effect that does not require additional interactions such as hydration forces and can be well described by SC theory.

Author contribution statement

All authors have contributed equally to this paper.

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