Radial Distribution Function of Rod-like Polyelectrolytes

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I. CONFORMATIONAL STATISTICS OF A POLYELECTROLYTE IN THE ROD-LIKE LIMIT: BACKGROUND AND GENERAL CONSIDERATIONS

Because of their fundamental importance in many key biological processes, electrostatically charged polymers, or polyelectrolytes (PE’s), have been the subject of intense research recently. These polymers often have stiff structures due to their Coulomb self-repulsion, and this structural property lies at the heart of their biological functionality. For example, the cytoskeletal network of actin filaments plays a crucial role in the recovery of eukaryotic cell shape in the face of the stresses imposed by cell movement, growth, and division. Furthermore, the storage properties and accessibility of DNA is known to be both constrained and controlled by its stiffness. Clearly, a complete study of the elastic properties of these charged biopolymers, which is now facilitated by single filament imaging and manipulation techniques, is crucial to an understanding of their role in nature.

In the case of neutral polymers, the wormlike chain (WLC) model of Kratky and Porod provides a powerful and convenient characterization of flexibility through the persistence length, which quantifies the correlations of unit tangent vectors parallel to the chain. Odijk, Skolnick, and Fixman (OSF), have applied this notion to PE’s through the introduction of an “electrostatic” persistence length \( \ell_e \). They derived the relationship

\[
\ell_e = \ell_{\text{OSF}} = \frac{\beta}{\kappa^2},
\]

(1)

where \( \kappa^{-1} \) is the Debye screening length (a measure of the ionic strength of the solvent), and \( \beta = \ell_B/b^2 \) is the strength of the electrostatic interaction. In the latter quantity \( \ell_B = e^2/\kappa g T \) is the Bjerrum length with \( e \) the dielectric constant of the ion-free solvent, and \( b \) the average separation between neighboring charges along the PE.

The notion of electrostatic persistence length, however, is believed to have shortcomings, as it replaces the many length scales in a PE by a single effective persistence length. The first note of caution is due to Odijk himself, who pointed out that if one tries to make use of the concept of an effective WLC approximation for a PE of finite length \( L \), the corresponding persistence length should be \( L \)-dependent. Barrat and Joanny later noted that, in fact, each deformation mode of a PE with a given wavelength has a different effective persistence length. Moreover, the wavevector dependence of the rigidity causes deviations from the linear dependency \( \ell \propto \beta \). These observations—which point to the complications that may arise if one insists on an effective WLC scheme for the characterization of PE’s—follow from the study of the averages \( \langle R \rangle \) and \( \langle R^2 \rangle \), where \( R = r(L) - r(0) \) is the end-to-end distance of the PE. It is not at all clear that a description based on the matching of first or second moments of the end-to-end length distribution is equivalent to a comprehensive study of conformational properties of a PE. An appealing alternative is a study of the full radial distribution function of the end-to-end distance of PE’s, which provides an excellent gauge of the conformation statistics of polymers in general and stiff chains in particular. This quantity, which can be measured experimentally through fluorescence microscopy, allows one to determine whether or not the WLC model accurately reflects the properties of the polymer segments. If the model has been shown to apply, then the fit of the distribution to the data directly yields the persistence length and, hence, the elastic modulus of the polymer.
In this article, we calculate the end-to-end distribution function of a charged inextensible chain in its rod-like limit. This distribution is then utilized to investigate the validity of a WLC with an adjusted persistence length as a model for a PE. We find that when the Coulomb interaction is only a perturbation to the mechanical stiffness of the chain, or when Debye screening is sufficiently strong, the full radial distribution of the PE can be collapsed onto that of a WLC. However, in the case of sizable Coulomb interactions and when the screening length is insufficiently short, we find that the distribution cannot be collapsed onto that of any WLC. To quantify the deviations from WLC behavior, we define an effective 

\[ \ell_{p0} \]

where \( \ell \) is the persistence length of the WLC that is most likely to have the same end-to-end distance as the PE chain. We discover strong evidence of a universal scaling function relating the electrostatic persistence length, \( \ell_{p0} \), to the intrinsic persistence length, \( \ell_p \), the Debye screening length, \( \kappa \), and the strength of electrostatic interaction, \( \beta \).

Because of the inextensibility of the PE's under consideration, we adopt the Kratky and Porod WLC model to describe the bending energy of the chain. In this model, a polymer is represented by a space curve \( r(s) \) as a function of the arc length parameter \( s \). The total energy of the chain, which is the sum of the intrinsic elasticity and the electrostatic energy can be written as

\[ \mathcal{H} = \frac{\ell_p}{k_B T} \int_0^L ds \left( \frac{d\mathbf{t}}{ds} \right)^2 + \frac{\beta}{2} \int_0^L ds ds' e^{-\kappa |r(s) - r(s')|} |r(s) - r(s')|, \]

where \( \mathbf{t}(s) \) is the unit tangent vector, and \( \ell_{p0} \) is the intrinsic persistence length of the PE. We do not take into account the fluctuations in the charges localized to the chain and in the counterion system that can give rise to attractive interactions leading to chain collapse. Because the chain is in its rod-like limit, excluded volume does not play a role. The double integral on the right hand side of Eq. (2) is cut off when \( |s - s'| < b \), where \( b \) is the spacing between charges on the PE. The quantity \( b \) also represents the intrinsic “coarse-graining” of the effective Hamiltonian, in that structure on a smaller length scale is not encompassed by the model embodied in Eq. (2). In addition, the value of \( b \) represents a lower limit on the magnitude of the intrinsic persistence length \( \ell_{p0} \), in that there is no physical meaning to a persistence length that is exceeded by the smallest length scale in the system.

The end-to-end distribution function is defined as follows:

\[ G(r) = \langle \delta(r - R) \rangle, \]

where \( R = r(L) - r(0) \). The average in (3) is over an ensemble of PE chains. The function \( G(r) \) is, then, the probability that a given chain in the ensemble will have an end-to-end distance equal to \( r \). We make use of the procedure Wilhelm and Frey have implemented to calculate the end-to-end distribution function for inextensible neutral polymers. We focus on inextensible chains with \( \ell_{p0} \sim L \) or \( \ell_{p0} \ll L \). In both cases, our study is limited to regions where the combination of intrinsic stiffness and repulsive strength of the Coulomb interaction keeps the chain in its rod-like limit. That is, the combination of intrinsic persistence length and Coulomb repulsion acts to keep the chain nearly straight over its entire length, so that its end-to-end distance does not greatly deviate from its total arc length. We parameterize the contour in terms of the tangent field:

\[ t(s) = (a_x(s), a_y(s), 1)/\sqrt{1 + a_x^2(s) + a_y^2(s)}, \]

and then retain only terms up to second order in the \( a \)'s in the measure factor, \( H \), and in the argument of the delta-function in Eq. (3), which is rewritten in terms of its Fourier representation. Expanding \( a_x(s) \) and \( a_y(s) \) in a cosine series, as mandated by the open-end boundary conditions, and making use of the relationship

\[ r(s) - r(s') = \int_s^{s'} dx \mathbf{t}(x), \]

we obtain

\[ G(r) = N \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega(1-r/L)} \prod_{n=1}^{\infty} \left( \frac{1}{\lambda_n + i\omega} \right), \]

in which \( N \) is a normalization constant. The \( \lambda_n \)'s are eigenvalues of the matrix

\[ \mathbf{T} = (n\pi)^2(\ell_{p0}/L)\mathbf{I} + \beta \mathbf{LE}, \]

where \( \mathbf{I} \) is the unity matrix and \( \mathbf{E} \) is the electrostatic energy matrix in the cosine basis set. Contour integration then yields

\[ G(r) = N \sum_n f(n) e^{-\lambda_n(1-r/L)}, \]

where

\[ f(n) = \prod_{i \neq n} 1/(\lambda_i - \lambda_n). \]

The large eigenvalues of the matrix \( \mathbf{T} \) are dominated by the diagonal terms \( (n\pi)^2(\ell_{p0}/L) \). In other words, the effect of the electrostatic interaction is swamped by semiflexible energetics at short length scales. In the case of a neutral polymer with an intrinsic persistence length that is comparable with the total length of the polymer, the above series converges very rapidly, as noted in Ref. [13]. When the chain is charged, and in particular, when the stiffness is due predominantly to electrostatic effects, more terms in the series must be preserved in order to obtain a stable answer for \( G(r) \). In the calculations described here, we truncate the matrix \( \mathbf{T} \) at a size much greater than the number of terms needed to obtain an accurate answer for the series of Eq. (6). This is because a larger dimension of the truncated matrix leads to more accurate values for the lower eigenvalues (which...
participate in the sum), and a more accurate \( f(n) \). In practice, we increased the dimension of the matrices until the effect (on the end-to-end distribution function) of a further increase in the size of \( T \) by a factor of two was less than a part in a thousand. A restriction on the size of the matrix arises from the requirement that the coarse graining length \( b \) not exceed the smallest wavelengths appearing in the cosine basis set. If the length of the PE is \( L \), this means that the size, \( N \), of the basis set satisfies \( N \leq L/b \). At no point in our calculations was this inequality violated.

We set \( b/L = 10^{-3} \). In this case, the distribution function of PE's depends on three independent dimensionless parameters \( \ell_{p0}/L, \beta L, \) and \( \kappa L \). Figure 2 illustrates the effect of the screened electrostatic interaction on the distribution function of a chain with \( \ell_{p0}/L = 0.5 \) at different salt concentrations and, hence, different values of \( \kappa \). As illustrated in the figure, the end-to-end distance of the chain on average becomes shorter upon a decrease of the screening length (for fixed \( \beta L \)). The quantity \( \beta L \), which depends on the solvent dielectric constant and the charge density on the PE chain, is equal to 100 for all the three curves in the figure.

We now seek to determine under what conditions the end-to-end distribution function of a rod-like PE is satisfactorily reproduced by that of a WLC with an adjusted persistence length. We also scrutinize the adjusted persistence length of a WLC whose end-to-end distribution is the closest fit to that of a rod-like PE to determine whether or not this persistence length is in accord with existing predictions for the dependence of the electrostatic persistence length on properties of the PE chain. In the cases we consider here the combination of intrinsic stiffness—as parameterized by \( \ell_{p0}/L \)—and of charging—quantified by \( \beta L \)—provides enough stiffening of the PE to guarantee rod-like behavior in all length scales.

II. REGIMES IN WHICH THE PE BEHAVES LIKE A WLC

We find that there exist regimes in which the conformational statistics of a PE chain in the rod-like limit are identical to those of a WLC with an adjusted persistence length. For such cases, PE and WLC distributions are indistinguishable to the naked eye. In these regimes, the persistence length is as predicted by Eq. (8), or, when \( \kappa L \) is not significantly larger than unity, by Eq. (9). We are able to divide this regime into two different categories.

A. Intrinsically stiff chains (\( \ell_{p0} \sim L \))

Whenever the electrostatic interaction plays a perturbative role in the chain energetics, it is possible to obtain a satisfactory collapse of the PE distribution onto that of a WLC. One noteworthy feature of this regime is that the electrostatic persistence length always satisfies \( \ell_{\text{e}} < \ell_{p0} \).

These regions are associated by weak charging of chain for small values of \( \kappa L \) (\( \kappa L \sim 1 \)). As we increase screening, \( \kappa L \), the collapse of the two distributions can be achieved for higher charge density. Figure 2 illustrates two examples of this regime. In plot (a), the Debye screening length is short, while \( \beta L \), the strength of coupling, is high. In plot (b), the Debye screening length is relatively long, but the electrostatic coupling is very weak. In both cases, we find that the distribution function of the PE’s collapse onto WLC’s with adjusted persistence lengths that follows Odijk and OSF predictions (Eqs. (8) and (9)).

Our calculations verify that under physiological conditions (\( \kappa = 1 \text{nm}^{-1} \)), the distribution functions for rod-like DNA segments (\( L \leq 100 \text{nm} \)) as well as those of stiffer actin filaments also collapse onto the end-to-end distribution for neutral chains with an effective persistence length given by Eq. (8).

Whenever there is a virtually perfect collapse of the distribution function of a PE onto that of a neutral chain, the persistence length of the neutral chain follows Odijk’s prediction in that, \( \ell_{\text{p}} = \ell_{\text{e}} + \ell_{p0} \), where \( \ell_{\text{p}} \) is the effective persistence length of the charged chain, and \( \ell_{\text{e}} = \ell_{\text{OsF}} \).

\[
\ell_{\text{Odijk}} = \frac{\beta L^2}{12} \left[ e^{-\kappa L} \left( \frac{1}{\kappa L} + \frac{5}{(\kappa L)^2} + \frac{8}{(\kappa L)^3} \right) + \frac{3}{(\kappa L)^2} - \frac{8}{(\kappa L)^3} \right].
\]

which reduces to \( \ell_{\text{OsF}} \equiv \beta/4\kappa^2 \) for large \( \kappa L \). It is important to note that the expression for \( \ell_{\text{Odijk}} \) was derived under the assumption that the contour length of the chain, \( L \), is of the order of its intrinsic persistence length, \( \ell_{p0} \) and that the electrostatic interaction has the limited effect of only “perturbing” the WLC shape of the chain. Our results confirm the validity of OSF and Odijk formulas in the regime in which they are expected to be correct.

B. Intrinsically flexible chains (\( \ell_{p0} \ll L \))

We are also able to identify regimes in which the radial distribution function of a PE that is long compared to its intrinsic persistence length (\( \ell_{p0}/L \ll 1 \)) collapses almost perfectly onto that of an uncharged WLC. Substantial charging is required to enforce the rod-like limit for such chains. It is important to note that despite the substantial charging of the chain, the ratio of the length of the PE to the screening length, \( \kappa L \), must be sufficiently large. This requirement is essential in order to minimize the strong influence of the end effects on conformational statistics of charged chains.

The important characteristic of this regime is that \( \ell_{p0} \ll \ell_{\text{e}} \) and thus electrostatic energy no longer plays a perturbative role. Nevertheless, if \( \kappa L \) is sufficiently
large we observe collapse of the two distributions. Furthermore, we also find that Odijk’s formula works to near perfection in those cases. For example, in the extreme instance of a very short intrinsic persistence length, $\ell_p/L = 0.01$, a high degree of charging $\beta L = 36000$, and a screening length that is short compared to the chain length, $\kappa L = 100$, we obtain an end-to-end distribution that is nearly identical with that of a WLC with an appropriate $\ell_e$. The accuracy of Odijk’s formula when $\ell_e > \ell_p$ is not at all obvious, as OSF was derived in the regime where electrostatic interaction plays a perturbative role.

We emphasize that the reason for the high quality of the match with OSF in this regime is different from the reason for the corresponding result obtained by Khokhlov and Khachaturian $^{[16]}$ for weakly charged flexible chains. In our case, the chain is stiff in all length scales; the possibility of renormalizing the length and/or charge is thus excluded in our formulation.

III. REGIMES IN WHICH THE CONFORMATIONAL STATISTICS OF A PE DIFFER FROM THOSE OF A WLC

No matter how short the range of electrostatic interactions is as the result of Debye screening, at sufficiently strong charging, the PE end-to-end distribution differs significantly from that of a WLC. The emergence of a difference between the two distribution is accompanied by a divergence between the effective persistence length characterizing the conformational statistics and the predictions of either Eq. (4) or (9). Figure 3 displays the PE end-to-end distribution (solid curves) along with the modified WLC distribution (dashed curves) in a case in which it is possible to obtain a nearly perfect fit (plot b) and in a case in which the best fit not nearly as good (plot a). In both cases fit was obtained by matching the location of the maxima of the two distributions, and the electrostatic persistence length attributed to the PE distribution is that of the WLC associated with the dashed curve. The ratio of electrostatic persistence length extracted from the distribution function to Odijk’s persistence length is, $\ell_e/\ell_{\text{Odijk}} = 0.99$ in the case of plot b. For the inset graph, plot a, in which the two distributions differ noticeably, this ratio is $\ell_e/\ell_{\text{Odijk}} = 0.89$.

It is important to note that a rescaling of the backbone length of the PE is not an acceptable stratagem for improving the agreement between the PE radial distribution and that of a WLC. This is because the backbone length is essentially fixed by the rod-like chain condition. The shortening and thickening that is associated with intermediate blob-like structures $^{[17]}$ will not occur. In fact, we have observed that a reduction in the effective value of $L$ actually degrades the quality of the correspondence between the conformational statistics of a PE and those of the corresponding WLC.

Our general observation is that the ratio of $\ell_e$ extracted from the effective WLC distribution to Odijk’s persistence length correlates with the quality of the fit of an effective WLC end-to-end distribution to that of a PE. When this ratio is equal to one, the PE is described to a high degree of accuracy in terms of a WLC. As this ratio decreases, the deviation becomes more pronounced. Figure 4 displays a diagram which delineates the quality of the fit. The line that is used in the Figure to separate the two regimes corresponds to $\ell_e/\ell_{\text{Odijk}} = 0.58$. As indicated in this Figure, for fixed $\kappa L$, when $\beta L$ is below a certain value the PE behaves like a WLC, while for larger $\beta L$ there is a substantial difference between the electrostatic persistence length of a rod-like PE and Odijk’s prediction. As illustrated in Fig. 4, the deviation of $\ell_e/L$ from $\ell_{\text{Odijk}}/L$, with increasing $\beta L$ is more pronounced at lower values of $\kappa L$. The Figure also shows that the electrostatic persistence length of a rod-like PE, $\ell_e/L$, depends on $\ell_p/L$. This dependence is not present in Odijk’s formula.

IV. UNIVERSAL BEHAVIOR

Our general observation of the curves of $\ell_e/L$ versus $\beta L$ is that they asymptote to a power law of the form $\ell_e \propto (\beta L)^{1-x}$ where the exponent $x(\kappa L)$ lies between zero and one. In search of a possible universal behavior, which might relate $\ell_p/L$, $\beta L$ and $\kappa L$ to $\ell_e/L$, we have rescaled our graphs for different values of the parameters. The details of rescaling will be presented in a forthcoming publication $^{[21]}$. The dependence on charging, $\beta$, of the ratio of the persistence length of a WLC and the prediction for that quantity embodied in Eq. (9) can be systematized in terms of a universal formula $^{[18]}$. This formula points to the existence of a scaling mechanism. At this point, we are not able to provide an explanation for this mechanism or indicate a possible underlying basis for it. Figure 5 contains plots of the ratio of the electrostatic persistence length of PE distributions to the predictions of Odijk in Eq. (4). As shown in the figure, all rescaled plots collapse on to a single curve corresponding to the following crossover formula for $\ell_e$:

$$\ell_e = \frac{\ell_{\text{Odijk}}}{1 + (\beta/\beta_0)^x} \quad (10)$$

This formula provides a remarkable fit to our data when the exponent $x \approx 0.4$, as exemplified in Fig. 5. The quantity $\beta_0$ is an increasing function of $\ell_p$ and $\kappa$. Our most striking result is that for all investigated values of $\kappa L$ and/or $\ell_p/L$, the exponent $x$ remains fixed at $\approx 0.4$, independent of all the other parameters. This function encompasses all the regimes described above. We are able to obtain the value of $\beta_0$ from our data. The crossover discussed in the previous section occurs when $\beta \approx 0.446\beta_0$ which corresponds to $\ell_e \approx 0.58\ell_{\text{Odijk}}$ in Eq. (4). The curve in Fig. 5 indicates the values of $\beta_0 L$ at different $\kappa L$’s for $\ell_p/L = 0.5$. Similar curves have been
generated for other, smaller, values of $\ell_p / L$. The behavior of these other curves is the same as the one plotted in Fig. 4.

V. CONCLUSIONS

We conclude with a few brief comments. To fit the PE and WLC distributions we have matched the maxima of the two. A fit can also be effected by matching moments, or by a least-squares procedure. Alternate fitting approaches have been explored by us, but the results obtained were entirely consistent with the conclusions set forth above. The reason for the present choice was the strong correlation between Odijk’s prediction and the fit of the distributions. If we match the maxima of the two distributions, the electrostatic persistence length departs from Odijk’s predictions when the distributions cease to closely resemble each other, and thus the ratio of $\ell_e / \ell_{\text{Odijk}}$ is a good measure of the similarity of the two distributions. However, if we used a matching of the first or second moment to calculate the effective persistence length, the two distributions are clearly distinguishable from each other well within the regime in which Odijk’s formula for the persistence length remains accurate.

Our results indicate that the difference between the radial distribution of the PE and the WLC can be attributed, at least in part, to the influence of end effects. In fact, we believe that the behavior of the persistence length is substantially controlled by end effects. One way of understanding this is in terms of Odijk’s derivation of the expression (8) for the electrostatic persistence length $\ell_e$. This derivation is based on a calculation of the energy of a bent segment of a charged rod. A key assumption in this derivation is that the segment takes the form of an arc of a circle. End effects are readily associated with the difference between the shape of a real bent rod and the circular arc assumed in Odijk’s derivation. An exploration of these effects in this context will be described in forthcoming work [19].

As noted above, the effect of counterion condensation has been ignored throughout the above work. It has been shown that counterion condensation modifies the bending rigidity of a semiflexible chain [14, 20] and may result in the collapse of the PE chain [14]. We have performed a calculation of the distribution function taking into account the attractive interaction due to counterion fluctuations and observed the signature of collapse. We are currently investigating these effects [21].

In summary, we have been able to verify that the modified WLC as a model of a rod-like PE works in the regime in which electrostatic effects play a perturbative role, and that the Odijk and OSF forms for the electrostatic persistence length are quantitatively accurate in this regime. We have also found that the above model and formulas are accurate in non-perturbative regimes if Debye screening is sufficiently strong. In the regimes in which the above model fails, we have discovered evidence for a scaling form, exhibited in Eq. (10), for the correction to the Odijk result for the persistence length. As yet, no model provides a theoretical basis for the scaling exhibited by this formula.

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FIG. 1: End-to-end distributions of charged semiflexible chains. The thin solid lines are plots of $G(r)$ for PE's with $\kappa L = 12, 6, 3$ from left to right. In all cases $\beta L = 100$ and $\ell_{\phi 0}/L = 0.5$. The dashed line is the end-to-end distribution of a neutral semiflexible chain with $\ell_{\phi 0}/L = 0.5$.

FIG. 2: The distribution for a polyelectrolyte with $\ell_{\phi 0} = 0.5$, $\beta L = 2400$, and $\kappa L = 50$, compared to that of a wormlike chain with $\ell_p = 0.74$ (two superimposed curves and perfect match with Eq. (1)). Inset: the distribution for a polyelectrolyte with $\ell_{\phi 0} = 0.5$, $\beta L = 5$, and $\kappa L = 5$, compared to that of a wormlike chain with $\ell_p = 0.524$ (two superimposed curves and perfect match with Eq. (9)).

FIG. 3: The distribution for a polyelectrolyte with $\ell_{\phi 0} = 0.5$, $\beta L = 600$, and $\kappa L = 10$, compared to that of a wormlike chain with $\ell_p = 1.3$. Inset: the distribution for a polyelectrolyte with $\ell_{\phi 0} = 0.5$, $\beta L = 60$, and $\kappa L = 10$, compared to that of a wormlike chain with $\ell_p = 0.6$ (two superimposed curves).
FIG. 4: The diagram delineating the quality of a WLC fit for $\ell_0/L = 0.5$. The curve separating the two regimes corresponds to $\ell_e/\ell_{\text{Odijk}} = 0.58$. This line also indicates the values of $\beta L$ in Eq. (10) at different $\kappa L$'s.

FIG. 5: Comparison of our results for the electrostatic persistence length with Odijk's finite size formula [13] (solid line) at $\kappa L = 2$ with $\ell_0/L = 0.5$ (filled circles) and $\ell_0/L = 0.01$ (hollow circles). The inset is for $\kappa L = 17$ and $\ell_0/L = 0.5$.

FIG. 6: Log-log plot of a comparison of our data, suitably rescaled, to the expression in Eq. (10). The points correspond to our rescaled plots of $\ell_e/L$ versus $\beta L$ at $\kappa L = 6, 8, 10, 12$. 