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Electric field of dielectric cylinder with given surface charge density immersed in electrolite

D Ouroushev

Department of Condensed Matter Physics, Faculty of Physics, University of Sofia, Boul. James Bourchier 5, 1126 Sofia, Bulgaria

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Abstract. The following physical situation is investigated. A dielectric cylinder with a given surface charge density is immersed in electrolite. The electrolite is treated via the two-dimensional nonlinear Poisson–Boltzmann equation. In the case of single-line charge located on the cylindrical surface, analytical expressions for the electric field as well as for the space charge distribution in the electrolite are derived. The matter investigated here is related to the problem of the structure of the electric potential emanating from DNA.

1. Introduction

The mathematical model presented here reveals a possibility to describe the structure of the electric potential and field, and of the space charge distribution in a situation where a dielectric cylinder with a given surface charge density σ is immersed in an electrolite. These investigations point to the problem of finding the structure of the electric potential emanating from dissolved DNA and the charge distribution in surrounding electrolite.

The investigations presented in this paper are induced from [1, 2]. In these papers DNA is treated as dielectric cylinder on the surface of which are distributed point charges forming double helix. It is immersed in a dielectric media divided into two areas with different dielectric constants ε_1 and ε_2. The first one corresponds to the Manning cloud, the second corresponds to the bulk solvent.

An important feature of this model is that the helical charge distribution is decomposed into n vertical lines of charges. According to this, the investigation of the electric field in the case when the surface charge consists of vertical lines would be useful.

Some other models treat the solvent with versions of either Debye–Hűckel or Poisson–Boltzmann (PB) equations, but treat DNA as a continuous charge distribution with cylindrical symmetry [3, 4]. In our model the electrolite outside the cylinder is treated via the complete exponentially nonlinear two-dimensional PB equation. On the other hand, it is shown that the structure of the charge on the surface of DNA might be considered.

The exponentially nonlinear PB equation may reveal some new properties of the system, as we illustrated in other situations [5, 6], which remain obscure when the linearised version is used. We consider the one-component PB equation assuming that near the cylinder mainly the opposite charged ions, with respect to σ, are concentrated.

Analytical expressions for the electric potential and field inside and outside the cylinder will be obtained in the case in which the surface of the cylinder a single-line charge is located.

2. The nonlinear PB equation and its solutions

The nonlinear homogeneous PB equation in polar coordinates is

$$\frac{\partial^2\Psi}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial\Psi}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\varphi^2}=-\frac{4\pi qnN}{\varepsilon}\exp(-\frac{q\Psi}{kT}). \tag{1}$$

The dimensionless form is obtained via the transformations

$$\bar{\rho}=\rho f \qquad \bar{\Phi}=-\frac{q\Psi}{(kT)} \tag{2}$$

or

$$\frac{\partial^2\bar{\Phi}}{\partial\bar{\rho}^2}+\frac{1}{\bar{\rho}}\frac{\partial\bar{\Phi}}{\partial\bar{\rho}}+\frac{1}{\bar{\rho}^2}\frac{\partial^2\bar{\Phi}}{\partial\varphi^2}=\exp(\bar{\Phi}). \tag{3}$$

Here $f=(\frac{4\pi Nn}{\varepsilon}L)^{1/2}$, where L is the characteristic length defined by

$$L=q^2/(kT). \tag{4}$$

Also n is the normalization factor given by

$$n^{-1}=\int_{V_e}\mathrm{e}^{-q\Psi/kT}\,\mathrm{d}v \tag{5}$$

where V_e is the volume of the electrolite under consideration and N is the number of the free ions with charge q per unit axial length.

Introducing a new variable and function by

$$x=\ln\bar{\rho} \qquad \Phi=\bar{\Phi}+2x$$

we obtain the equation

$$\frac{\partial^2\Phi}{\partial x^2}+\frac{\partial^2\Phi}{\partial\varphi^2}=\exp(\Phi). \tag{6}$$

The relation between the solutions of this equation and the solutions of the Laplace equation was first mentioned by Liouville [7]. Using Bắcklund transformations the solution of (6) can be expressed through arbitrary harmonic functions. Performing such procedure the following real solution of (6) is obtained

$$\Phi=\ln\left\{\frac{2\left(\frac{\partial U(x,\varphi)}{\partial x}\right)^2+2\left(\frac{\partial U(x,\varphi)}{\partial\varphi}\right)^2}{U^2(x,\phi)}\right\}. \tag{7}$$

Here $U(x,\varphi)$ is a real arbitrary harmonic function. Consequently for the self-consistent electric potential, which is a solution of the nonlinear PB equation, from (7) we have

$$\Psi=-\frac{kT}{q}\ln\left\{\frac{2\left(\bar{\rho}\frac{\partial U(\bar{\rho},\varphi)}{\partial\bar{\rho}}\right)^2+2\left(\frac{\partial U(\bar{\rho},\varphi)}{\partial\varphi}\right)^2}{\bar{\rho}^2U^2(\bar{\rho},\phi)}\right\}. \tag{8}$$

3. Boundary conditions and approach for solving the problem

The physical situation described below is the following. A dielectric cylinder with radius b and given surface charge density $\sigma(\varphi)$ is immersed in electrolite. We have the electrostatic boundary-value problem, where outside the cylinder the electric potential is described by the nonlinear PB equation and inside the cylinder by the Laplace equation. The boundary conditions at $\rho = b$ are

$$(\boldsymbol{D}_2 - \boldsymbol{D}_1) \cdot \hat{\rho} = 4\pi\sigma(\varphi) \tag{9}$$
$$(\boldsymbol{E}_2 - \boldsymbol{E}_1) \times \hat{\rho} = 0 \tag{10}$$

where $\varepsilon(\rho)$ is

$$\varepsilon(\rho) = \begin{cases} \varepsilon_1 & 0 \leqslant \rho < b \\ \varepsilon_2 & b \leqslant \rho \leqslant \rho_0. \end{cases} \tag{11}$$

Here $\hat{\rho}$ is the outward unit radial vector. The value of ρ_0 will be determined after the normalization of the solution of the PB equation. Here the indexes 1 and 2 refer to the areas inside and outside the cylinder.

Also charge neutrality condition is imposed

$$Nq = \int_{S'} \sigma(\varphi)\, \mathrm{d}s \tag{12}$$

where S' is the boundary surface ($\rho = b$). We specialize to the concrete problem when on the boundary surface ($\rho = b$) a single-line charge is located. In this geometry the position of the charge is arbitrary, so we chose the boundary point ($\rho = b, \varphi = 0$). In this situation $\sigma(\varphi)$ has the form

$$\sigma(\varphi) = \frac{\gamma}{b}\delta(\varphi) \tag{13}$$

or

$$\sigma(\varphi) = \frac{\gamma}{\pi b}\left[\frac{1}{2} + \sum_{m=1}^{\infty}\cos(m\varphi)\right]. \tag{14}$$

Here γ is the line charge density.

To solve this electrostatic boundary-value problem we shall use a similar technique from [1, 2]. Using the representation of the Green function in polar coordinates we can write down a general ansatz which solve the Laplace equation inside the cylinder ($\rho < b$) [8]

$$\Psi_1 = \sum_{m=0}^{\infty} \bar{A}_m^1 (\rho/b)^m \cos(m\varphi). \tag{15}$$

The same ansatz might be used for the harmonic function $U(\bar{\rho}, \varphi)$, which determines the solution of PB equation. In the concrete problem investigated here the boundary conditions (9)–(11) and the charge neutrality condition (12) can be satisfied by keeping just three terms in $U(\bar{\rho}, \varphi)$. This important possibilty is due to the nonlinearity of the PB equation. It leads to relatively simple expressions for the electric field and the space charge distribution outside the cylinder. We set

$$U(\bar{\rho}, \varphi) = C\ln(\rho_1\rho) + (\bar{A}/\bar{\rho} + \bar{B}\bar{\rho})\cos\varphi. \tag{16}$$

In this situation from the boundary conditions we will obtain a finite system of equations for the expansion coefficients C, $\bar{A}$, $\bar{B}$, $\bar{A}_1^1$ and $\bar{A}_2^1$ together with a recurrent relation for the other coefficients $\bar{A}_m^1$. From (16) we obtain for the solution of the PB equation

$$\Psi_2 = -\frac{kT}{q} \ln \left\{ 2 \frac{[C + (-\bar{A}/\bar{\rho} + \bar{B}\bar{\rho}) \cos\varphi]^2 + [(\bar{A}/\bar{\rho} + \bar{B}\bar{\rho}) \sin\varphi]^2}{\bar{\rho}^2 [C \ln(\rho_1 \rho) + (\bar{A}/\bar{\rho} + \bar{B}\bar{\rho}) \cos\varphi]^2} \right\}. \tag{17}$$

The boundary conditions can be rewritten in the form

$$1/\rho \frac{\partial \Psi_1}{\partial \varphi} = 1/\rho \frac{\partial \Psi_2}{\partial \varphi} \bigg|_{\rho=b} \tag{18}$$

$$\varepsilon_1 \frac{\partial \Psi_1}{\partial \rho} - \varepsilon_2 \frac{\partial \Psi_2}{\partial \rho} = 4\pi\sigma(\varphi)|_{\rho=b}. \tag{19}$$

We introduce the relations

$$\bar{A}_m^1 = \frac{kT}{q} A_m^1 \tag{20}$$

and

$$\bar{A}/(bf) = A \qquad \bar{B}(bf) = B \qquad A + B = A_1^2 \qquad A_0^2 = C \ln(\rho_1 b). \tag{21}$$

Using expressions (13), (15) and (17) for $\sigma(\varphi)$, Ψ_1 and Ψ_2 from the boundary conditions (18) and (19) we obtain the following system of algebraic equations

$$A_0^2 A_1^1 + A_1^2 A_2^1 = 2A_1^2 \tag{22}$$

$$m A_0^2 A_1^m + 1/2 A_1^2 [(m-1) A_{m-1}^1 + (m+1) A_{m+1}^1] = 0 \tag{23}$$

$$\varepsilon_1 [A_0^2 A_1^1 + A_1^2 A_2^1] - 4\varepsilon_2 B = \frac{4q\gamma}{kT} (A_0^2 + A_1^2) \tag{24}$$

$$\frac{\varepsilon_1}{2} A_1^2 A_1^1 - 2\varepsilon_2 \left[\frac{A_0^2}{\ln(\rho_1 b)} + A_0^2 \right] = \frac{2q\gamma}{kT} (A_0^2 + A_1^2) \tag{25}$$

$$m A_0^2 A_1^m + 1/2 A_1^2 [(m-1) A_{m-1}^1 + (m+1) A_{m+1}^1] = \frac{4q\gamma}{kT} (A_0^2 + A_1^2). \tag{26}$$

The system of equations (22)–(26) has the non-trivial solutions

$$A_1^1 = 4\varepsilon_2/\varepsilon_1 [1/\ln(\rho_1 b) + 1] \qquad A_2^1 = 2 + 4\varepsilon_2/\varepsilon_1 [1/\ln(\rho_1 b) + 1] \tag{27}$$

$$A = B(2\varepsilon_2/\varepsilon_1 - 1) \qquad A_0^2 = C \ln(\rho_1 b) = -2B\varepsilon_2/\varepsilon_1 \tag{28}$$

$$m A_m^1 = 1/2 [(m-1) A_{m-1}^1 + (m+1) A_{m+1}^1]. \tag{29}$$

The constant ρ_1 will be determined in the next section from the normalization condition (5).

4. Structure of the electric potential and field and normalization of the solution

Expressions (27)–(29) determine the expansion coefficients and consequently the electric potential and field inside and outside the cylinder. We will use the notations

$$\alpha := \varepsilon_2/\varepsilon_1 \qquad \beta := 2\varepsilon_2/\varepsilon_1 - 1 \qquad D := \frac{2\varepsilon_2/\varepsilon_1}{\ln(\rho_1 b)} \qquad r := \rho/b. \tag{30}$$

The self-consistent potential Ψ_2, which is a solution of the PB equation for $\rho \geqslant b$ is

$$\Psi_2 = -\frac{kT}{q} \ln \left\{ 2 \frac{[D + (\beta/r - r) \cos\varphi]^2 + [(\beta/r + r) \sin\varphi]^2}{b^2 f^2 r^2 [-2\alpha - D \ln r + (\beta/r + r) \cos\varphi]^2} \right\}. \tag{31}$$

From expression (31) for Ψ_2 and the relation $\boldsymbol{E}_2 = -\mathrm{grad}\,\Psi_2$ for the components $E_{2\rho}$ and $E_{2\varphi}$ of the electric field we obtain

$$E_{2\rho} = \frac{kT}{qb}\left\{\frac{4\cos\varphi - 2[D + 2\alpha + D\ln r]/r}{-2\alpha - D\ln r + (\beta/r + r)\cos\varphi}\right\} \tag{32}$$

$$E_{2\varphi} = -\frac{kT}{qbr}\left\{\frac{2(\beta/r + r)\sin\varphi}{-2\alpha - D\ln r + (\beta/r + r)\cos\varphi}\right\}. \tag{33}$$

For the space charge distribution ρ_{sc} outside the cylinder we obtain

$$\rho_{sc} = qnN\exp\left(-\frac{q\Psi_2}{kT}\right)$$
$$= \frac{[D + (\beta/r - r)\cos\varphi]^2 + [(\beta/r + r)\sin\varphi]^2}{\frac{b^2 2\pi q}{\varepsilon_2 kT} r^2[-2\alpha - D\ln r + (\beta/r + r)\cos\varphi]^2}. \tag{34}$$

The denominator in expressions (31)–(34) is non-zero in the interval

$$1 \leqslant r \leqslant r_0 \tag{35}$$

if r fulfils the inequality

$$2\alpha + D\ln r > \frac{\beta}{r} + r. \tag{36}$$

Condition (36) determines the area in which the solution of the PB equation does not possess unphysical singularities and the value of r_0. Consequently the N opposite charged ions are distributed in a finite area ($r \leqslant r_0$). The value of r_0 depends on $\varepsilon_1, \varepsilon_2$ and still undetermined constant D. The value of D can be obtained from the normalization condition (5). According to (12) we demand charge neutrality or

$$Nq = \gamma. \tag{37}$$

The both conditions (5) and (37) are fulfilled if

$$\int_{V_e} qnN\mathrm{e}^{-q\Psi_2/kT}\,\mathrm{d}v = \gamma. \tag{38}$$

The normalization of the solution can be performed on any curve $r(\varphi)$, determining V_e, such that $r(\varphi) \leqslant r_0$ for $0 \leqslant \varphi \leqslant 2\pi$. This is in some sense a self-consistent procedure, because the value of D or r_0 is determined after the integration in (38).

If we demand homogeneous space charge density at the upper boundary of the area V_e we will obtain

$$qnN\mathrm{e}^{-q\Psi_2/kT} = \rho_{sc}^0 = \text{constant}. \tag{39}$$

Condition (39) gives an equation for the function $r(\varphi)$ determining this boundary

$$[D + (\beta/r - r)\cos\varphi]^2 + [(\beta/r + r)\sin\varphi]^2$$
$$= \rho_{sc}^0\frac{b^2 2\pi q}{\varepsilon_2 kT} r^2[-2\alpha - D\ln r + (\beta/r + r)\cos\varphi]^2. \tag{40}$$

The constant D is determined again from (38).

The components of the electric field $E_{1\rho}$ and $E_{2\rho}$ inside the cylinder are obtained by using the relation $\boldsymbol{E}_1 = -\mathrm{grad}\,\Psi_1$ and expressions (27) and (29) for the expansion coefficients. So we obtain

$$E_{1\rho} = -1/b\sum_{m=1}^{\infty} m\bar{A}_m^1 r^{m-1}\cos(m\varphi) \tag{41}$$

$$E_{1\varphi} = 1/b\sum_{m=1}^{\infty} m\bar{A}_m^1 r^{m-1}\sin(m\varphi). \tag{42}$$

For the expansion coefficients $\bar{A}^1_m$ we have

$$\bar{A}^1_1 = 4\frac{\varepsilon_2}{\varepsilon_1}[(\ln(\rho_1 b)^{-1} + 1]kT/q \quad (43)$$

$$\bar{A}^1_2 = \left\{2 + 4\frac{\varepsilon_2}{\varepsilon_1}[(\ln(\rho_1 b))^{-1} + 1]\right\} kT/q \quad (44)$$

and

$$m\bar{A}^1_m = 1/2[(m-1)\bar{A}^1_{m-1} + (m+1)\bar{A}^1_{m+1}]. \quad (45)$$

The constant $\ln(\rho_1 b)$ is determined after the normalization of the solution of the PB equation ($D = 2\frac{\varepsilon_2}{\varepsilon_1}(\ln(\rho_1 b))^{-1}$) as it is explained above.

5. Conclusion

The mathematical model and results given above reveal a possibility to develop the model of dissolved DNA presented in [1, 2] treating the surrounding electrolite via the nonlinear PB equation. Considering the two-dimensional nonlinear PB equation is also a step forward because the DNA is not treated as a homogeneous charged cylinder as in some previous models [3, 4]. The mathematical model presented here is more general and can be successfully applied in the cases when the surface charge density consists of several vertical or non-vertical lines. Bearing this in mind the results will be made closer to the real problem of DNA, by considering more complicated forms of σ, which is the subject of our future work.

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