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ORIGINAL PAPER

The exact solution to the one-dimensional Poisson–Boltzmann equation with asymmetric boundary conditions

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Abstract The exact solution to the one-dimensional Poisson–Boltzmann equation with asymmetric boundary conditions can be expressed in terms of the Jacobi elliptic functions. The boundary conditions determine the modulus of the Jacobi elliptic functions. The boundary conditions can not be solved analytically, thus a numerical scheme has been applied.

Keywords Jacobi elliptic functions · Poisson–Boltzmann equation · Boundary conditions

1 Introduction

The electric potential in a double layer system plays an important role in the description of the properties of ionic solutions, such as the behavior of battery electrodes, the stability of charged colloid solutions, membrane properties in biological cells, and various other situations [1,2]. An accurate analysis of such a double layer system requires solving the one-dimensional Poisson–Boltzmann equation. The main difficulty in solving this equation is the complicated electric boundary conditions, which generally allow the potential only to be expressed in terms of elliptic functions [3,4]. Therefore this equation usually is either linearized, in which case an analytic expression can be found, or solved by numerical schemes. The aim of this paper is to present an analytic solution to the one-dimensional Poisson–Boltzmann equation for arbitrary boundary conditions.

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2 The one-dimensional Poisson–Boltzmann equation

In terms of a dimensionless electrostatic potential, y, the one-dimensional Poisson–Boltzmann equation can be written as [1,2]:

$$y'' = \sinh y \tag{1}$$

Assume the surface potentials are of the same sign, say $y(-L) = a$ and $y(L) = b$, a and b being some positive values, and L being some dimensionless length. It should be noted, that one could equally well have used the length L_1 on the left hand side and L_2 on the right hand side, the steps are still the same. Let $y(x) = \psi(\omega \cdot x + \phi)$, where:

$$\psi(u) = \ln \frac{dn(u, k^2) + k'}{dn(u, k^2) - k'} \tag{2}$$

is a solution of the differential equation $\psi'' = k^2 \sinh \psi$ [5], and $k^2 + k'^2 = 1$ [3,4].

Thus: $y'' = \omega^2 \psi'' = \omega^2 k^2 \sinh \psi = \omega^2 k^2 \sinh y$

Therefore it follows, that $k^2 = 1/\omega^2$, and from the boundary conditions $y(-L) = a$, it follows that, $dn(\phi - \omega \cdot L, k^2) = k'\alpha$, where $\alpha = (e^a + 1)/(e^a - 1)$, and similarly with $\beta = (e^b + 1)/(e^b - 1)$ one has from the second boundary condition that, $dn(\phi + \omega \cdot L, k^2) = k'\beta$. Thus the two coupled non-linear equations to be solved are:

$$\begin{aligned} & dn\left(\phi - \omega \cdot L, \frac{1}{\omega^2}\right) = \sqrt{1 - \frac{1}{\omega^2}}\, \alpha \\ & \wedge \\ & dn\left(\phi + \omega \cdot L, \frac{1}{\omega^2}\right) = \sqrt{1 - \frac{1}{\omega^2}}\, \beta \end{aligned} \tag{3}$$

It seems impossible to solve this system of equations analytically and thus an iterative scheme has been applied ("Appendix"). In case of $L = 1$, $a = 1$, and $b = 3$ one finds the values, $\omega = 1.10756$, and $\phi = 0.678761$, so that:

$$y(x) = \ln \frac{dn\left(\omega \cdot x + \phi, \frac{1}{\omega^2}\right) + \sqrt{1 - \frac{1}{\omega^2}}}{dn\left(\omega \cdot x + \phi, \frac{1}{\omega^2}\right) - \sqrt{1 - \frac{1}{\omega^2}}} \tag{4}$$

is the exact solution. This solution, which is positive for all values of x, is plotted in Fig. 1 as the solid line and the numerical solution is shown as the dashed line. The steps would be similar if either one or both of the boundary conditions were specified by the derivative of the dimensionless potential y.

If the surface potentials are of opposite sign, say $y(-L) = a$ and $y(L) = b$, a being negative and b being positive, and again assuming the dimensionless potential of the

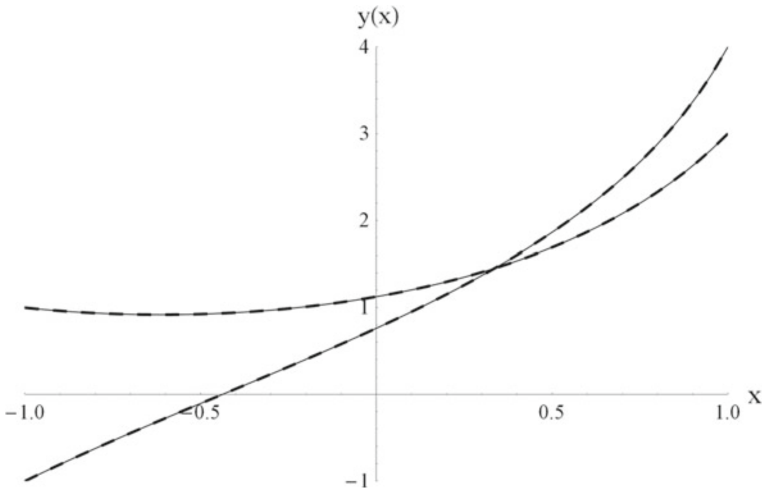

Fig. 1 Comparison of the exact (*solid line*) and numerical (*dashed line*) solutions to the Poisson–Boltzmann equation. The *lines positive* at the *left hand side* refer to Eq. (4), whereas the *lines negative* at the *left hand side* refer to Eq. (7). As can be seen exact and numerical solutions coincides

form $y(x) = \psi(\omega \cdot x + \phi)$, being a solution of the differential equation $y'' = \sinh y$, then since there is a sign change one should instead chose [5]:

$$\psi(v) = \ln \frac{1 + sn(v, k'^2)}{1 - sn\left(v, k'^2\right)} \tag{5}$$

as a solution of the differential equation $\psi'' = k^2 \sinh \psi$. Following the same steps as before the two coupled non-linear equations to be solved would be:

$$\begin{aligned} & sn\left(\phi - \omega \cdot L\ ,\ 1 - \frac{1}{\omega^2}\right) = \alpha \\ & \wedge \\ & sn\left(\phi + \omega \cdot L\ ,\ 1 - \frac{1}{\omega^2}\right) = \beta \end{aligned} \tag{6}$$

where $\alpha = (e^a - 1)/(e^a + 1)$ and $\beta = (e^b - 1)/(e^b + 1)$. In case of $L = 1$, $a = -1$, and $b = 4$ one finds that, $\omega = 0.842611$, and $\phi = 0.369168$, so that:

$$y(x) = \ln \frac{1 + sn\left(\omega \cdot x + \phi\ ,\ 1 - \frac{1}{\omega^2}\right)}{1 - sn\left(\omega \cdot x + \phi\ ,\ 1 - \frac{1}{\omega^2}\right)} \tag{7}$$

is the exact solution, which is plotted in Fig. 1 as the solid line. The dashed line is the numerical solution. As can be seen the exact and numerical solutions coincides.

3 Conclusions

It has been demonstrated how the exact solution to the one-dimensional Poisson–Boltzmann equation with asymmetric boundary conditions can be found in a straightforward manner. The boundary conditions determine the modulus of the Jacobi elliptic functions of the solution. Since it is impossible to solve these boundary conditions analytically a simple numerical method has been applied.

Appendix

In this appendix a numerical scheme for solving a non-linear system of equations of the form:

$$\vec{f}(\omega,\varphi) = (f_1(\omega,\varphi), f_2(\omega,\varphi)) = \vec{0}$$

is presented. Usually one would think of applying Newton's method. However, in the present case this method becomes very complicated due to the fact, that partial derivatives have to be calculated in each step and that the partial derivatives of the Jacobi elliptic functions are not only with respect to the variable but also with respect to the elliptic modulus of the functions. If, however, an iterative secant method is applied, one circumvents this complication. The method is as follows:

$$\begin{aligned} \varphi_{n+1} &= \varphi_n - \lambda \frac{f_1(\omega_n,\varphi_n)(\varphi_n-\varphi_{n-1})}{f_1(\omega_n,\varphi_n)-f_1(\omega_n,\varphi_{n-1})} \\ \omega_{n+1} &= \omega_n - \lambda \frac{f_2(\omega_n,\varphi_{n+1})(\omega_n-\omega_{n-1})}{f_2(\omega_n,\varphi_{n+1})-f_2(\omega_{n-1},\varphi_{n+1})} \end{aligned}$$

where new values are applied as soon as they are calculated. A convergence factor λ is included in these equation in order to ensure stability of the algorithm. A value of $\lambda = 0.1$ has been applied in all the calculations and works well.

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