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A Solution of the Spherical Poisson-Boltzmann Equation

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Abstract

In this paper, we used a field and coordinate transformations and the Jacobi Elliptic functions, in order to solve the Spherical Poisson-Boltzman (SPB) equation. We find several families of solutions.

Keywords: Spherical Poisson-Boltzman, Jacobi Elliptic functions

1 Introduction

The spherical Poisson-Boltzmann equation (SPBEq) gives the electrical potential distribution for a charged spherical electrolyte [1]-[2]. SPB equation is a mean field theory that gives into account of the electrostatic interactions between the charges in an ionic solution [3]. Also, a such enormous theoretical effort has been done over the years, in order to provide analytical solutions to nonlinear partial differential equations. Among the most popular developed methods we can find the so called solitary wave methods. We employ the Jacobi Elliptic functions [4] and [5] solitary wave methods.

2 Spherical Poisson-Boltzmann equation

We start from the spherical Poisson-Boltzmann equation [1]-[2]:

$$\nabla^2\rho = \frac{d^2\rho}{dr^2} + \frac{2}{r}\frac{d\rho}{dr} = \kappa^2 e^{\rho} \tag{1}$$

Where $\kappa = \lambda_D^{-1}$, and λ_D is known as the Debye-Hückel screening length [1]-[2]. Using the transformation [7]

$$\rho = \psi - 2\ln(r) + \ln(2) \tag{2}$$

And [6]

$$r = e^{\zeta}, \;\; \frac{d}{dr} = e^{-\zeta}\frac{d}{d\zeta}, \;\; \frac{d^2}{dr^2} = e^{-2\zeta}(\frac{d^2}{d\zeta^2} - \frac{d}{d\zeta}) \tag{3}$$

And replacing in eq. (1)

$$\frac{\partial^2\psi}{d\zeta^2} + \frac{\partial\psi}{d\zeta} - 2 = 2\kappa^2 e^{\psi} \tag{4}$$

Now defining the variables

$$v = e^{\psi} \tag{5}$$

Then

$$\frac{d\psi}{d\zeta} = \frac{1}{v}\frac{dv}{d\zeta} \tag{6}$$

$$\frac{d^2\psi}{d\zeta^2} = -\frac{1}{v^2}(\frac{dv}{d\zeta})^2 + \frac{1}{v}\frac{d^2v}{d\zeta^2} \tag{7}$$

And replacing in eq. (4)

$$v\frac{d^2v}{d\zeta^2} - (\frac{dv}{d\zeta})^2 + v\frac{dv}{d\zeta} - 2v^2 - 2\kappa^2 v^3 = 0 \tag{8}$$

3 Solution 1

We suppose a solution given by the Jacobi elliptic functions, [4] and [5]. They hold the next relations

$$sn^2(\zeta,k) + cn^2(\zeta,k) = 1, \quad k^2 sn^2(\zeta,k) + dn^2(\zeta,k) = 1 \tag{9}$$

$$dn^2(\zeta,k) - k^2 cn^2(\zeta,k) = k'^2, \quad k'^2 sn^2(\zeta,k) + cn^2(\zeta,k) = dn^2(\zeta,k) \tag{10}$$

$$k' = \sqrt{1-k^2} \tag{11}$$

Then, we suppose the next solution

$$\begin{aligned} &v = Acn(a\zeta, k); \quad \frac{dv}{d\zeta} = -aAsn(a\zeta, k)dn(a\zeta, k); \\ &\frac{d^2v}{d\zeta^2} = Aa^2(-2k^2cn^3(a\zeta, k) - (1-2k^2)cn(a\zeta, k)) \end{aligned} \tag{12}$$

Then, replacing eqs. (12) in eq. (8)

$$\begin{aligned} &-2A^2a^2k^2cn^4(a\zeta, k) - A^2a^2(1-2k^2)cn^2(a\zeta, k) \\ &-a^2A^2sn^2(a\zeta, k)dn^2(a\zeta, k) - aA^2cn(a\zeta, k)sn(a\zeta, k)dn(a\zeta, k) \\ &-2A^2cn^2(a\zeta, k) - 2\kappa^2A^3cn^3(a\zeta, k) = 0 \end{aligned} \tag{13}$$

Equating the left hand side of eq. (13) to zero, we get:

$$\begin{aligned} &(-a^2sn(a\zeta, k)dn(a\zeta, k) - acn(a\zeta, k))A^2sn(a\zeta, k)dn(a\zeta, k) = 0 \\ &\to -asn(a\zeta, k)dn(a\zeta, k) = cn(a\zeta, k) \end{aligned} \tag{14}$$

Then

$$(-a^2(1-2k^2) - 2)A^2cn^2(a\zeta, k) = 0 \to a_{1,2} = \pm\sqrt{\frac{2}{(2k^2-1)}} \tag{15}$$

And

$$\begin{aligned} &(-2a^2k^2cn(a\zeta, k) - 2A\kappa^2)A^2cn^3(a\zeta, k) = 0 \\ &\to cn(a\zeta, k) = -\frac{A\kappa^2}{a^2k^2} \to cn^2(a\zeta, k) = \frac{A^2\kappa^4}{a^4k^4} \end{aligned} \tag{16}$$

So, using eqs. (9) and (14), we get

$$k^2sn^4(a\zeta, k) - sn^2(a\zeta, k) + \frac{A^2\kappa^4}{a^6k^4} = 0 \tag{17}$$

Solving for $sn^2(a\zeta, k)$

$$sn^2(a\zeta,k) = \frac{1 \pm \sqrt{1-4k^2\frac{A^2\kappa^4}{a^6k^4}}}{2k^2} \tag{18}$$

Again, using eqs. (16), (18) and (9), we have

$$\frac{1 \pm \sqrt{1-4k^2\frac{A^2\kappa^4}{a^6k^4}}}{2k^2} + \frac{A^2\kappa^4}{a^4k^4} = 1 \tag{19}$$

$$a^8k^4 - 4a^2k^2A^2\kappa^4 = (2k^2a^4k^2 - a^4k^2 - 2A^2\kappa^4)^2 \tag{20}$$

If we define in eq. (20) $E = 4\kappa^8$, $F = (4a^2k^2\kappa^4 + 8a^4k^2\kappa^4 - 8a^4k^4\kappa^4)$ and $G = +3a^8k^4 - 8a^8k^6 + 4a^8k^8$, we get

$$EA^4 + FA^2 + G = 0 \tag{21}$$

solving for A

$$A_1 = -\frac{\sqrt{-\frac{F}{E} - \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{22}$$

$$A_2 = \frac{\sqrt{-\frac{F}{E} - \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{23}$$

$$A_3 = -\frac{\sqrt{-\frac{F}{E} + \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{24}$$

$$A_4 = \frac{\sqrt{-\frac{F}{E} + \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{25}$$

So, we find eight families of solutions

$$v = A_i cn(a_j\zeta, k) \tag{26}$$

4 Solution 2

Also, we suppose a solution

$$v = Asn(a\zeta,k); \quad \frac{dv}{d\zeta} = aAcn(a\zeta,k)dn(a\zeta,k); \tag{27}$$
$$\frac{d^2v}{d\zeta^2} = Aa^2(2k^2sn^3(a\zeta,k) - (1+k^2)sn(a\zeta,k))$$

Then, replacing eq. (27) in eq. (8)

$$\begin{aligned} &2A^2a^2k^2sn^4(a\zeta,k) - a^2(1+k^2)A^2sn^2(a\zeta,k) \\ &-a^2A^2cn^2(a\zeta,k)dn^2(a\zeta,k) + aA^2sn(a\zeta,k)cn(a\zeta,k)dn(a\zeta,k) \\ &-2A^2sn^2(a\zeta,k) - 2\kappa^2A^3sn^3(a\zeta,k) = 0 \end{aligned} \tag{28}$$

Equating the left hand side of eq. (28) to zero, we get:

$$\begin{aligned} &(-a^2cn(a\zeta,k)dn(a\zeta,k) + asn(a\zeta,k))A^2cn(a\zeta,k)dn(a\zeta,k) = 0 \\ &\to acn(a\zeta,k)dn(a\zeta,k) = sn(a\zeta,k) \end{aligned} \tag{29}$$

Also

$$(-a^2(1+2k^2) - 2)A^2sn^2(a\zeta,k) = 0 \to a_{1,2} = \pm i\sqrt{\frac{2}{(2k^2+1)}} \tag{30}$$

And

$$\begin{aligned} &(2a^2k^2sn(a\zeta,k) - 2A\kappa^2)A^2sn^3(a\zeta,k) = 0 \\ &\to sn(a\zeta,k) = \frac{A\kappa^2}{a^2k^2} \to sn^2(a\zeta,k) = \frac{A^2\kappa^4}{a^4k^4} \end{aligned} \tag{31}$$

So, using eqs. (29), (31) and eq. (9), we have

$$cn^2(a\zeta,k) = \frac{A^2\kappa^4}{a^6k^4(1-\frac{A^2\kappa^4}{a^4k^2})} \tag{32}$$

Using eqs. (31), (32) and (9), we get

$$EA^4 - FA^2 + G = 0 \tag{33}$$

where, we define $E = \kappa^8$, $F = (a^2k^2\kappa^4(1 + k^2 + a^2k^2)$ and $G = a^8k^6$ in eq. (33) , and solving

$$A_5 = -\frac{\sqrt{\frac{F}{E} - \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{34}$$

$$A_6 = \frac{\sqrt{\frac{F}{E} - \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{35}$$

$$A_7 = -\frac{\sqrt{\frac{F}{E} + \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{36}$$

$$A_8 = \frac{\sqrt{\frac{F}{E} + \frac{\sqrt{F^2-4EG}}{E}}}{\sqrt{2}} \tag{37}$$

So, we get eight families of solutions

$$v = A_i sn(a_j\zeta, k) \tag{38}$$

5 Conclusions

We solved the spherical Poisson Boltzmann equation using the Jacobi Elliptic functions. We obtain sixteen families of solutions. As a future work, we can extend the method to investigate other charge configurations and other geometric symmetries.

$$\rho(r) = \ln\left(A_i cn(a_j \ln(r), k)\right) - 2\ln(r) + \ln(2) \tag{39}$$

$$\rho(r) = \ln\left(A_i sn(a_j \ln(r), k)\right) - 2\ln(r) + \ln(2) \tag{40}$$

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