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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 tanh and Riccati solitary wave methods in order to solve the Spherical Poisson-Boltzman (SPB) equation. We find several families of solutions.

Keywords: Spherical Poisson-Boltzman, Tanh, Riccati

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 tanh [4] and Riccati [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)

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

Now, we introduce a new independent variable:

$$Y = \tanh(\zeta) \tag{9}$$

Then, the derivatives of ζ, are:

$$\frac{d}{d\zeta} = (1-Y^2)\frac{d}{dY};\quad \frac{d^2}{d\zeta^2} = -2Y(1-Y^2)\frac{d}{dY} + (1-Y^2)^2\frac{d^2}{dY^2} \tag{10}$$

The solutions are postulated as:

$$v(u) = \sum_{i=1}^{m} a_i Y^i \tag{11}$$

Then replacing

$$\begin{aligned} & v(-2Y(1-Y^2)\frac{dv}{dY} + (1-Y^2)^2\frac{d^2v}{dY^2}) \\ & -((1-Y^2)\frac{dv}{dY})^2 + v((1-Y^2)\frac{dv}{dY}) + 2v^2 - 2\kappa^2 v^3 = 0 \end{aligned} \tag{12}$$

Now, we balance the highest-order linear derivative with the highest order nonlinear terms in eq. (12). Then

$$vY^4\frac{d^2v}{dY^2} \to v^3 \to m + 4 + m - 2 = 3m \to m = 2 \tag{13}$$

Then

$$v = a_0 + a_1 Y + a_2 Y^2 \tag{14}$$

Replacing in eq. (12)

$$\begin{aligned} & +(a_0 + a_1 Y + a_2 Y^2)(-2Y(1-Y^2)(a_1 + 2a_2 Y) + (1-Y^2)^2 2a_2) \\ & -((1-Y^2)(a_1 + 2a_2 Y))^2 + (a_0 + a_1 Y + a_2 Y^2)((1-Y^2)(a_1 + 2a_2 Y)) \\ & +2(a_0 + a_1 Y + a_2 Y^2)^2 - 2\kappa^2(a_0 + a_1 Y + a_2 Y^2)^3 = 0 \end{aligned} \tag{15}$$

$$a_{2,1} = 0, \quad a_{2,2} = -\frac{1}{2\kappa^2} \tag{16}$$

$$a_{1_1} = 0, \quad a_{1_2} = -\frac{1}{6\kappa^2}, \quad a_{0_1} = -\frac{1}{3\kappa^2} \tag{17}$$

$$\begin{aligned} a_{0_2} = \frac{1}{36}(-\frac{1}{\kappa^2} + \frac{1}{\left(-\kappa^6 - 324\kappa^8 + 18\sqrt{2}\sqrt{\kappa^{14} + 162\kappa^{16}}\right)^{1/3}} \\ + \frac{\left(-\kappa^6 - 324\kappa^8 + 18\sqrt{2}\sqrt{\kappa^{14} + 162\kappa^{16}}\right)^{1/3}}{\kappa^4}) \end{aligned} \tag{18}$$

$$a_{0_3} = -\frac{1}{36\kappa^2} - \frac{1+i\sqrt{3}}{72\left(-\kappa^6 - 324\kappa^8 + 18\sqrt{2}\sqrt{\kappa^{14}+162\kappa^{16}}\right)^{1/3}} - \frac{\left(1-i\sqrt{3}\right)\left(-\kappa^6 - 324\kappa^8 + 18\sqrt{2}\sqrt{\kappa^{14}+162\kappa^{16}}\right)^{1/3}}{72\kappa^4} \tag{19}$$

$$a_{0_4} = -\frac{1}{36\kappa^2} - \frac{1-i\sqrt{3}}{72\left(-\kappa^6 - 324\kappa^8 + 18\sqrt{2}\sqrt{\kappa^{14}+162\kappa^{16}}\right)^{1/3}} - \frac{\left(1+i\sqrt{3}\right)\left(-\kappa^6 - 324\kappa^8 + 18\sqrt{2}\sqrt{\kappa^{14}+162\,\kappa^{16}}\right)^{1/3}}{72\kappa^4} \tag{20}$$

$$a_{0_{5,6}} = \frac{-1 \pm \sqrt{1-\kappa^4}}{6\kappa^4}, \quad a_{0_7} = -\frac{1}{18\kappa^2}, \quad a_{1_3} = -\frac{1}{7\kappa^2} \tag{21}$$

defining $l_1 = -9\kappa^{12} + \sqrt{21585}\kappa^{12}$

$$a_{0_8} = -\frac{42^{2/3}\kappa^2}{21^{1/3}\left(l_1\right)^{1/3}} + \frac{\left(l_1\right)^{1/3}}{42^{2/3}\kappa^6} \tag{22}$$

$$a_{0_9} = \frac{22^{2/3}\left(1+i\sqrt{3}\right)\kappa^2}{21^{1/3}\left(l_1\right)^{1/3}} - \frac{\left(1-i\sqrt{3}\right)\left(l_1\right)^{1/3}}{242^{2/3}\kappa^6} \tag{23}$$

$$a_{0_{10}} = \frac{22^{2/3}\left(1-i\sqrt{3}\right)\kappa^2}{21^{1/3}\left(l_1\right)^{1/3}} - \frac{\left(1+i\sqrt{3}\right)\left(l_1\right)^{1/3}}{242^{2/3}\kappa^6} \tag{24}$$

$$a_{0_{11}} = \frac{343-\sqrt{319249}}{420\kappa^2}, \quad a_{0_{12}} = \frac{343+\sqrt{319249}}{420\kappa^2} \tag{25}$$

$$a_{0_{13}} = \frac{233-\sqrt{62521}}{294\kappa^2}, \quad a_{0_{14}} = \frac{233+\sqrt{62521}}{294\kappa^2} \tag{26}$$

$$a_{0_{15}} = -\frac{33}{98\kappa^4} + \frac{2}{343\kappa^2}, \quad a_{0_{16}} = \frac{13}{588\kappa^2} \tag{27}$$

	A	C	F
1	1/2	-1/2	$coth(\xi) \pm cosh(\xi)$, $tanh(\xi) \pm isech(\xi)$
2	1/2	1/2	$sec(\xi) \pm itan(\xi)$
3	-1/2	- 1/2	$csc(\xi) \pm icot(\xi)$
4	1	- 1	$tanh(\xi)$, $coth(\xi)$
5	1	1	$tan(\xi)$
6	-1	-1	$cot(\xi)$

Table 1: Solutions for eq. (30), [7] .

Then, the solutions are

$$\begin{aligned}
&f_1 \rightarrow (a_{0_1}, a_{1_1}, a_{2_1}), \quad f_2 \rightarrow (a_{0_2}, a_{1_2}, a_{2_1}) \\
&f_3 \rightarrow (a_{0_3}, a_{1_2}, a_{2_1}), \quad f_4 \rightarrow (a_{0_4}, a_{1_2}, a_{2_1}) \\
&f_5 \rightarrow (a_{0_5}, a_{1_2}, a_{2_1}), \quad f_6 \rightarrow (a_{0_6}, a_{1_2}, a_{2_1}) \\
&f_7 \rightarrow (a_{0_7}, a_{1_2}, a_{2_1}), \quad f_8 \rightarrow (a_{0_8}, a_{1_3}, a_{2_2}) \\
&f_9 \rightarrow (a_{0_9}, a_{1_3}, a_{2_2}), \quad f_{10} \rightarrow (a_{0_{10}}, a_{1_3}, a_{2_2}) \\
&f_{11} \rightarrow (a_{0_{11}}, a_{1_3}, a_{2_2}), \quad f_{12} \rightarrow (a_{0_{12}}, a_{1_3}, a_{2_2}) \\
&f_{13} \rightarrow (a_{0_{13}}, a_{1_3}, a_{2_2}), \quad f_{14} \rightarrow (a_{0_{14}}, a_{1_3}, a_{2_2}) \\
&f_{15} \rightarrow (a_{0_{15}}, a_{1_3}, a_{2_2}), \quad f_{16} \rightarrow (a_{0_{16}}, a_{1_3}, a_{2_2})
\end{aligned} \tag{28}$$

3 Solitary wave solution 2

Also, we apply $\phi(\xi)$ to find solutions, [7]

$$v(\zeta) = \sum_{i=1}^{m} a_i F^i \tag{29}$$

where F solves, table (1), the Riccati equation, i.e.

$$F^{'} = CF^2 + A. \rightarrow F^{''} = C2FF^{'} = 2CF(CF^2 + A) = 2C^2F^3 + 2ACF \tag{30}$$

here A, C are constants, table (1). Replacing in eq. (8), and taking $m = 2$ in eq. (29) and doing the algebra, we get, $v(\zeta) = a_0 + a_1F + a_2F^2$. So:
then

$$\begin{aligned}
&v^{'} = a_1F^{'} + 2a_2FF^{'} = a_1CF^2 + a_1A + 2a_2CF^3 + A2a_2F \\
&v^{''} = a_1F^{''} + 2a_2(F^{'})^2 + 2a_2FF^{''} = 2a_1C^2F^3 + 2a_1ACF \\
&+2a_2(CF^2 + A)^2 + 2a_2F(2C^2F^3 + 2ACF)
\end{aligned} \tag{31}$$

$$a_2 = C^2/\kappa^2, \quad a_1 = C/\kappa^2 \tag{32}$$

$$a_{0_{17}} = \frac{+6a_1^2 a_2 \kappa^2 - 2a_2^2 - 3a_1 a_2 C - a_1^2 C^2}{6(a_2 C^2 - a_2^2 \kappa^2)} \tag{33}$$

$$a_{0_{18}} = \frac{4a_1 a_2 + 2Aa_2^2 + a_1^2 C + 2Aa_1 a_2 C - 2a_1^3 \kappa^2}{(12a_1 a_2 \kappa^2 - 2a_1 C^2 - 2a_2 C)} \tag{34}$$

defining $m_1 = (a_1 C + 4a_2 + 8Aa_2 C - 6a_1^2 \kappa^2)^2 + 24a_2 \kappa^2 (2a_1^2 + 3Aa_1 a_2 - 2A^2 a_2^2)$

$$a_{0_{19,20}} = \frac{(a_1 C + 4a_2 + 8Aa_2 C - 6a_1^2 \kappa^2) \pm \sqrt{m_1}}{12 a_2 \kappa^2} \tag{35}$$

defining $m_2 = (Aa_2 + 2a_1 + Aa_1 C)^2 + 12a_1 \kappa^2 (Aa_1^2 - 2A^2 a_1 a_2)$

$$a_{0_{21,22}} = \frac{(Aa_2 + 2a_1 + Aa_1 C) \pm \sqrt{m_2}}{6a_1 \kappa^2} \tag{36}$$

Defining $l_2 = 16 + 36Aa_1\kappa^2 + 72A^2 a_2 \kappa^2 - 108A^2 a_1^2 \kappa^4 + (4(-4 - 6Aa_1\kappa^2 - 12A^2 a_2 \kappa^2)^3 + (16 + 36Aa_1\kappa^2 + 72A^2 a_2\kappa^2 - 108A^2 a_1^2 \kappa^4)^2)^{1/2}$

$$a_{0_{23}} = \frac{1}{3\kappa^2} - \frac{-4 - 6Aa_1\kappa^2 - 12A^2 a_2 \kappa^2}{32^{2/3}\kappa^2 \left(l_2\right)^{1/3}} + \frac{\left(l_2\right)^{1/3}}{62^{1/3} K^2} \tag{37}$$

$$a_{0_{24}} = \frac{1}{3\kappa^2} + \frac{\left(1 + i\sqrt{3}\right)\left(-4 - 6Aa_1\kappa^2 - 12A^2 a_2\kappa^2\right)}{62^{2/3}\kappa^2 \left(l_2\right)^{1/3}} - \frac{\left(1 - i\sqrt{3}\right)\left(l_2\right)^{1/3}}{122^{1/3}\kappa^2} \tag{38}$$

$$a_{0_{25}} = \frac{1}{3\kappa^2} + \frac{\left(1 - i\sqrt{3}\right)\left(-4 - 6Aa_1\kappa^2 - 12A^2 a_2\kappa^2\right)}{62^{2/3}\kappa^2 \left(l_2\right)^{1/3}} - \frac{\left(1 + i\sqrt{3}\right)\left(l_2\right)^{1/3}}{122^{1/3}\kappa^2} \tag{39}$$

$$\begin{aligned} &f_{17} \to (a_{0_{17}}, a_1, a_2), \quad f_{18} \to (a_{0_{18}}, a_1, a_2) \\ &f_{19} \to (a_{0_{19}}, a_1, a_2), \quad f_{20} \to (a_{0_{20}}, a_1, a_2) \\ &f_{21} \to (a_{0_{21}}, a_1, a_2), \quad f_{22} \to (a_{0_{22}}, a_1, a_2) \\ &f_{23} \to (a_{0_{23}}, a_1, a_2), \quad f_{24} \to (a_{0_{24}}, a_1, a_2) \\ &f_{25} \to (a_{0_{25}}, a_1, a_2) \end{aligned} \tag{40}$$

Then, we get 54 solutions using Riccati method.

4 Conclusions

We solved the spherical Poisson Boltzmann equation using the tanh and Riccati methods. We obtain sixteen families of solutions for the tanh method and fifty six solutions using Riccati solutions. As a future work, we can extend the method to investigate other charge configurations and other geometric symmetries.

$$\rho(r) = \ln\left(a_0 + a_1 \tanh(\ln r) + a_2 \tanh(\ln r)^2\right) - 2\ln(r) + \ln(2) \tag{41}$$

$$\rho(r) = \ln\left(a_0 + a_1 F(\ln r) + a_2 F(\ln r)^2\right) - 2\ln(r) + \ln(2) \tag{42}$$

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