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A Solution of the One-Dimensional Linear Quartic Poisson-Boltzmann Equation Using Lattice-Boltzmann

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Abstract

In this paper, we solve the one-dimensional linear quartic Poisson-Boltzmann equation using lattice-Boltzmann, with a $d1q3$ velocity scheme. Also, applying the He's semi-inverse method, we get several solitary wave solutions.

Keywords: 1d Quartic Poisson-Boltzmann, lattice-Boltzmann, Variational method.

1 Introduction

The Poisson-Boltzmann equation (PBEq) has been success in the physical description of electrolytes [1]. Those solutions are important in Mechanical and Chemical Engineering, with applications, e.g., in gas and oil industries [2]. This mean field theory, PBEq, can be extended to incorporate multivalent ion phenomena [3], giving rise to new and important physical phenomenology [4]-[5]. This new research field is ruled by the Poisson-Boltzmann one-dimensional quartic differential equation, whose linearized version is the main goal of our work [3]. On the other hand, lattice-Boltzmann [6] and [7], a discretized version of the Boltzmann equation, has been applied successfully to solve, such a diverse problems, as fluid dynamics, [6], till research fields such relativistic quantum mechanics [7]. In addition, variational methods have been applied successfully to obtain solitary wave solutions, [8].

2 The lattice Boltzmann model

The lattice Boltzmann equation [6] in the B.G.K. approximation [9], is:

$$f_i(x+e_i\epsilon, t+\epsilon) - f_i(x,t) = -\frac{1}{\tau}\left(f_i(x,t) - f_i^{eq}(x,t)\right) + \Xi_i(x,t) \tag{1}$$

Assuming the source term as $\Xi_i(x,t) = \epsilon^2\phi_i$, [10]. Expanding in a Taylor series, the distribution function, up to fourth order, we have:

$$\begin{aligned} f_i(x+e_i\epsilon, t+\epsilon) &- f_i(x,t) = \epsilon\left(\frac{\partial}{\partial t} + e_i\frac{\partial}{\partial x}\right) f_i + \frac{\epsilon^2}{2}\left(\frac{\partial}{\partial t} + e_i\frac{\partial}{\partial x}\right)^2 f_i \\ &+ \frac{\epsilon^3}{6}\left(\frac{\partial}{\partial t} + e_i\frac{\partial}{\partial x}\right)^3 f_i + \frac{\epsilon^4}{24}\left(\frac{\partial}{\partial t} + e_i\frac{\partial}{\partial x}\right)^4 f_i + O(\epsilon^5) \end{aligned} \tag{2}$$

Doing a perturbative expansion of the derivatives in time in powers of ϵ [6], we get:

$$f_i = f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \epsilon^3 f_i^{(3)} + \epsilon^4 f_i^{(4)} \tag{3}$$

And assuming:

$$f_i^{(0)} = f_i^{(eq)} \tag{4}$$

The temporal scales are defined as:

$$t_0 = t \quad t_1 = \epsilon t \quad t_2 = \epsilon t^2 \quad t_3 = \epsilon t^3 \quad t_4 = \epsilon t^4 \tag{5}$$

Where ϵ is a perturbative parameter [6], and a expansion in it, of the temporal derivative operator

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \epsilon^1\frac{\partial}{\partial t_1} + \epsilon^2\frac{\partial}{\partial t_2} + \epsilon^3\frac{\partial}{\partial t_3} + \epsilon^4\frac{\partial}{\partial t_4} \tag{6}$$

Replacing eqs. (2)-(6) in eq. (1), we get at first and second order in ϵ, and assuming $f_i^0 = f^{eq}$, we get the next set of equations:

$$\frac{\partial f_i^0}{\partial t_0} + e_i\frac{\partial f_i^0}{\partial x} = -\frac{1}{\tau} f_i^1 \tag{7}$$

$$\frac{\partial f_i^0}{\partial t_1} - \tau(1-\frac{1}{\tau})\left(\frac{\partial}{\partial t_0} + e_i\frac{\partial}{\partial x}\right)^2 f_i = -\frac{1}{\tau} f_i^2 + \phi_i \tag{8}$$

3 The moments of the distribution

We consider the moments of the distribution as:

$$\sum_i f_i^{(0)} = 0 = \sum_i f_i^{(eq)} \tag{9}$$

$$\sum_i e_i f_i^{(0)} = \lambda_1 \phi \tag{10}$$

$$\sum_l e_{l,i} e_{l,j} f_l^{(0)} = -\lambda_2 \frac{\partial^2 \phi}{\partial x^2} \delta_{ij} \tag{11}$$

Where δ_{ij} is Kronecker's delta. Also, we suppose the higher orders of the moments distribution as:

$$\sum_i f_i^{(k)} = 0, \quad with \quad k > 0 \tag{12}$$

4 The 1d Quartic Poisson-Boltzmann equation

Summing on i in eq. (7) and using eqs. (9), (10) and (12) we get:

$$\frac{\partial \sum_i f_i^0}{\partial t_0} + \frac{\partial}{\partial x}(\sum_i e_i f_i^{(0)}) = 0 \to \lambda_1 \frac{\partial}{\partial x}(\phi) = 0 \tag{13}$$

An now, summing on i in eq. (8) and multiplying by ϵ

$$\epsilon \frac{\partial \sum_i f_i^0}{\partial t_1} - \epsilon\tau(1 - \frac{1}{\tau}) \sum_i \left(\frac{\partial}{\partial t_0} + e_i \frac{\partial}{\partial x} \right)^2 f_i = -\epsilon \frac{1}{\tau} \sum_i f_i^{(2)} + \epsilon \sum_i \phi_i \tag{14}$$

Using eqs, (10) and (13)

$$\epsilon \frac{\partial \sum_i f_i^0}{\partial t_1} - \epsilon\tau(1 - \frac{1}{\tau})(\sum_i (e_i \frac{\partial}{\partial x})^2 f_i = -\epsilon \frac{1}{\tau} \sum_i f_i^{(2)} + \epsilon \sum_i \phi_i \tag{15}$$

Also, using eq. (12), we have:

$$\epsilon \frac{\partial \sum_i f_i^0}{\partial t_1} - \epsilon\tau(1 - \frac{1}{\tau}) \left(\frac{\partial}{\partial x_k} \frac{\partial}{\partial x_j} \sum_i f_i e_{i,k} e_{i,j} \right) = \epsilon \sum_i \phi_i \tag{16}$$

Summing eq. (16) to eq. (13) and using eq. (11):

$$\frac{\partial \sum_i f_i^0}{\partial t_0} + \epsilon \frac{\partial \sum_i f_i^0}{\partial t_1} + \lambda_1 \frac{\partial}{\partial x}(\phi) + \lambda_2 \epsilon\tau(1 - \frac{1}{\tau}) \frac{\partial^4 \phi}{\partial x^4} = \epsilon \sum_i \phi_i \tag{17}$$

Figure 1: Lattice-Boltzmann velocity scheme $d1q3$.

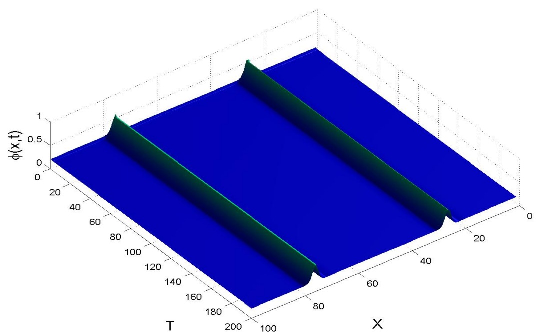

Figure 2: The spatiotemporal Lattice-Boltzmann for $\phi(x,t)$ using a $d1q3$ lattice velocity, for two initial profiles given by eq. (22).

Also, $\epsilon \sum_i \phi_i = -(b+1)\lambda_3\epsilon(\phi)$, [10]. Where b is the dimension of the discretized velocity space. Then, we get: using eqs. (6) and (9), at first order:

$$\frac{\partial(0)}{\partial t} + \lambda_1 \frac{\partial \phi}{\partial x} + \lambda_2 \epsilon\tau(1 - \frac{1}{\tau})\frac{\partial^4 \phi}{\partial x^4} + (b+1)\lambda_3\epsilon(\phi) = 0 \tag{18}$$

Defining $\xi^4 = \lambda_2\epsilon\tau(\frac{1}{\tau} - 1)$, $\lambda_1 = (2\xi^2 - 1)$ and $1 = \lambda_3(b+1)\epsilon$, we get:

$$\xi^4 \frac{\partial^4 \phi}{\partial x^4} + (2\xi^2 - 1)\frac{\partial \phi}{\partial x} + \phi = 0 \tag{19}$$

5 The equilibrium distribution function

In figure (1), we show a $d1q3$ one-dimensional velocity scheme with $e_\alpha = \{0, c, -c\}$ [6]. So, the one particle equilibrium equilibrium distribution function is:

$$f_i^{(eq)} = \left\{ \begin{array}{ccc} \frac{\lambda_2}{c^2}\frac{\partial^2\phi}{\partial x^2} & \rightarrow & i = 0 \\ \frac{\lambda_1}{2c}\phi - \frac{\lambda_2}{2c^2}\frac{\partial^2\phi}{\partial x^2} & \rightarrow & i = 1 \\ -\frac{\lambda_1}{2c}\phi - \frac{\lambda_2}{2c^2}\frac{\partial^2\phi}{\partial x^2} & \rightarrow & i = 2 \end{array} \right\} \tag{20}$$

6 He's semi-inverse method

According to He's semi inverse method [8], we postulate one functional that satisfy eq. (19). So:

$$J(\phi, \frac{d\phi}{dx}, \frac{d^2\phi}{dx^2}) = \int \left((2\xi^4 \left(\frac{d^2\phi}{dx^2}\right)^2 + (\xi^2 - 1)\left(\frac{d\phi}{dx}\right)^2 + \frac{1}{2}\phi^2 \right) dx \tag{21}$$

We have the field, ϕ, to be determined, and we select:

$$\phi = psech^2(qx) \tag{22}$$

Then, the entire action is:

$$J(q,p) = \xi^4 \frac{64p^4q^3}{21} + (\xi^2 - 1)\frac{8p^2q}{15} + \frac{p^2}{3q} \tag{23}$$

J must be stationary, then $\frac{\partial J}{\partial p} = 0$, $\frac{\partial J}{\partial q} = 0$:

$$\xi^4 \frac{16p^2q^3}{21} + (\xi^2 - 1)\frac{16q}{15} + \frac{2}{3q} = 0, \;\; \xi^4 \frac{64p^2q^2}{7} + (\xi^2 - 1)\frac{8}{15} - \frac{1}{3q^2} = 0 \tag{24}$$

So, the solutions are:

$$p_1 = -\frac{\sqrt{3696 - 7392\xi^2 + 3696\xi^4}}{125\xi^2}, q_1 = -5i\sqrt{\frac{5}{-176 + 176\xi^2}} \tag{25}$$

$$p_2 = \frac{\sqrt{3696 - 7392\xi^2 + 3696\xi^4}}{125\xi^2}, q_2 = -5i\sqrt{\frac{5}{-176 + 176\xi^2}} \tag{26}$$

$$p_3 = -\frac{\sqrt{3696 - 7392\xi^2 + 3696\xi^4}}{125\xi^2}, q_3 = +5i\sqrt{\frac{5}{-176 + 176\xi^2}} \tag{27}$$

$$p_4 = \frac{\sqrt{3696 - 7392\xi^2 + 3696\xi^4}}{125\xi^2}, q_4 = +5i\sqrt{\frac{5}{-176 + 176\xi^2}} \tag{28}$$

We found four families of solutions for eq. (22). Also, we select ϕ as:

$$\phi = psech(qx) \tag{29}$$

The action is:

$$J(q,p) = \xi^4 \frac{7p^4q^3}{15} + (\xi^2 - 1)\frac{p^2q}{3} + \frac{p^2}{2q} \tag{30}$$

Also, J must be stationary, then $\frac{\partial J}{\partial p} = 0$, $\frac{\partial J}{\partial q} = 0$:

$$\xi^4 \frac{28p^2q^3}{15} + (\xi^2 - 1)\frac{2q}{3} + \frac{1}{q} = 0, \quad \xi^4 \frac{7p^2q^2}{5} + (\xi^2 - 1)\frac{1}{3} - \frac{1}{2q^2} = 0 \tag{31}$$

Then, we get

$$p_1 = -\frac{\sqrt{\frac{1}{105}\left(4 - 8\xi^2 + 4\xi^4\right)}}{\xi^2}, q_1 = -i\sqrt{\frac{15}{-2 + 2\xi^2}}, \tag{32}$$

$$p_2 = \frac{\sqrt{\frac{1}{105}\left(4 - 8\xi^2 + 4\xi^4\right)}}{\xi^2}, q_2 = -i\sqrt{\frac{15}{-2 + 2\xi^2}} \tag{33}$$

$$p_3 = -\frac{\sqrt{\frac{1}{105}\left(4 - 8\xi^2 + 4\xi^4\right)}}{\xi^2}, q_3 = i\sqrt{\frac{15}{-2 + 2\xi^2}}, \tag{34}$$

$$p_4 = \frac{\sqrt{\frac{1}{105}\left(4 - 8\xi^2 + 4\xi^4\right)}}{\xi^2}, q_4 = i\sqrt{\frac{15}{-2 + 2\xi^2}} \tag{35}$$

We found four families of solutions for eq. (29).

7 Conclusions

Then, this paper presents a solution to the linear quartic Poisson-Boltzmann equation in one dimension using lattice-Boltzmann and He's semi inverse methods. Figure (2), presents the LB result given by two initial profiles, eq. (22). The solutions are:

$$\phi(x)_i = p_i sech^2(q_i x), \quad \phi(x)_j = p_j sech(q_j x) \tag{36}$$

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