Self-similar solutions for the two-dimensional Nernst-Planck-Debye system

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Abstract. We investigate the two-component Nernst-Planck-Debye system by numerical study of self-similar solutions using the Runge-Kutta method of order four and comparing the obtained results with the solutions of one-component system. Properties of the solutions raised in numerical simulations are proved and the existence result is established based on comparison arguments for singular ordinary differential equations.

1 Introduction

The Nernst–Planck–Debye (NPD) system is a mathematical model formulated by W. Nernst and M. Planck at the end of the 19th century as a basic model for electrodiffusion processes in plasmas. Later on, in the twenties of the 20th century, it was studied by P. Debye and E. Hückel in the context of electrolysis.

The model represents transport of charged particles in a continuous environment such as either ions (in plasmas or electrolytes) or electrons and holes (in semiconductors) subject to the diffusion. Due to the common occurrence of electrically charged particles in the nature, Nernst–Planck–Debye equations play an important role in computer simulations in electrochemistry and biology. They relate to simulations of ions channels in cell membranes, propagation of signals in nerves and other phenomena [1, 2, 6, 9, 12].

Our goal is to study some numerical solutions as well as to prove the existence of some special solutions for the system

$$\begin{aligned} u_t &= \Delta u + \nabla \cdot \big(u \nabla \phi_{v-u}\big) \quad \text{in} \quad \Omega \times \mathbb{R}^+, \\ v_t &= \Delta v - \nabla \cdot \big(v \nabla \phi_{v-u}\big) \quad \text{in} \quad \Omega \times \mathbb{R}^+, \\ \phi_{v-u} &= E_n * (v-u) \quad \text{in} \quad \Omega, \end{aligned} \tag{1.1}$$

where $u = u(x,t)$, $v = v(x,t) \colon \Omega \times \mathbb{R}^+ \to \mathbb{R}$ for given $\Omega \subset \mathbb{R}^n$ either a bounded subset or the entire space in the case $n \geqslant 2$, E_n is the fundamental solution of the Laplace equation, and $*$ denotes the convolution. The initial conditions for the system are

$$u(x,0) = u_0(x), \quad v(x,0) = v_0(x) \quad \text{in} \quad \Omega. \tag{1.2}$$

In this paper we assume that Ω is the entire space $\mathbb{R}^2$, so (1.1) is supplemented with the integrability conditions $u(.,t)$, $v(.,t) \in L^1(\mathbb{R}^2)$, instead of suitable no-flux boundary conditions imposed on $\partial\Omega \times (0,T)$.

As we mentioned above, such a model describes electrodiffusion processes, where $u(x,t)$ and $v(x,t)$ characterise the densities of negatively and positively charged particles, respectively. The function $\phi = \phi_{v-u}$ is the electric potential generated by particles themselves [9], $\Delta\phi = v - u$. Besides the electrochemistry similar systems occur in the semiconductors theory [7], where $u(x,t)$ and $v(x,t)$ describe the density of charge carriers, e.g. electrons and holes.

There is an extensive literature devoted to the existence of solutions and their asymptotic behaviour phenomena for the model with various boundary conditions, see e.g. [1, 2, 7, 8].

In particular, it was shown in [2] that for solutions of the Cauchy problem for (1.1) in $\Omega = \mathbb{R}^n, n \geqslant 3$, the intermediate asymptotics is determined by the Gauss–Weierstrass kernel, i.e. the diffusion prevails in the long time behaviour. In the two-dimensional case $\Omega = \mathbb{R}^2$, the solutions have genuinely nonlinear asymptotics determined by self-similar solutions. Thus, the study of self-similar solutions, as was shown for the one-component system in [8], is of immediate importance in that case.

Nevertheless, up to our best knowledge, the problem of characterising the existence range of total charges (M_ξ, M_η) of self-similar solutions has not been solved yet. A numerical study of self-similar solutions is a part of [10] Master Thesis written under the supervision of Dr. Michał Olech.

It is worth mentioning that the similar model

$$\begin{aligned} u_t &= \Delta u - \nabla \cdot \big(u \nabla \phi_{v+u}\big) \quad \text{in} \quad \Omega \times \mathbb{R}^+, \\ v_t &= \Delta v + \nabla \cdot \big(v \nabla \phi_{v+u}\big) \quad \text{in} \quad \Omega \times \mathbb{R}^+, \\ \phi_{v+u} &= E_n * (v+u) \quad \text{in} \quad \Omega, \end{aligned}$$

describes the phenomena of chemotaxis, that is the evolution of particles subject to attracting forces, [5, 3]. The classical parabolic-elliptic Keller–Segel model is the above one with $v \equiv 0$. Here, the self-similar solutions exist if and only if the sum of masses is less than 8π.

The authors of [3] started a study of general two-component systems in $\mathbb{R}^2$ with general interactions between the components. In particular, they studied conditions for finite time blowup of solutions versus the existence of (globally defined in time) forward self-similar solutions which, in this case, can have finite mass/charge.

The main result in this note is Theorem 3.1 on the existence of self-similar solutions of (1.1) for *arbitrary total charges* M_ξ, $M_\eta \geqslant 0$. Apart from a proof of that statement based on comparison arguments for singular ordinary differential equations (in fact, for the system (2.4) below), we present some numerical results showing some properties of self-similar solutions which have not been rigorously treated yet.

The system (1.1) poses certain difficulties in finding numerical solutions due to the nonlinear and nonlocal character of these equations coupled through the potential function ϕ. One can approximate solutions of such problem using e.g. *the finite element* or *the finite volume method*. However, these methods are useful over a bounded domain which is not the case of this study. In that case we propose to make some preliminary reductions, namely, we consider solutions which are radially symmetric and scale-invariant functions. Despite the simplifications, solving the system (1.1) will not be a trivial task because of singular coefficients of the order $\frac{1}{y}$ in an ordinary differential equation for $y \in (0, \infty)$, cf. (2.4) below.

In numerical experiments we used *the Runge–Kutta method* of the fourth order standard for finding solutions of ordinary differential equations. In this section we shall deal with numerical investigation of solutions of (2.4). Moreover, we shall try to discover conditions for initial parameters when the solutions are bounded as well as we shall check their concavity. Our main point of reference for all numerical simulations is the one-component model described in [8] where the authors proved the existence of solutions and their properties. We shall check whether analogous properties hold in the two-component case, and then we shell prove Theorem 3.1.

2 Radially symmetric and self-similar solutions

Definition 2.1. *Let $u(x,t)$ and $v(x,t)$ be solutions of the system* (1.1) *in* $\Omega = \mathbb{R}^2$, *then*

- *the functions are called radially symmetric if*

$$u(x,t) = u(|x|,t) \quad v(x,t) = v(|x|,t),$$

- *the functions are called self-similar (invariant under a scaling), if for solutions u, v and for each $\lambda > 0$, the rescaled functions $\lambda^2 u(\lambda x, \lambda^2 t)$, $\lambda^2 v(\lambda x, \lambda^2 t)$ are also solutions to* (1.1)*.*

Using the so–called *integrated density method* (see e.g. [5]) we are able to convert (1.1) into a system of two ordinary differential equations with certain boundary conditions. To do that, first we define the functions $Q(r,t)$ and $P(r,t)$ as

$$Q(r,t) = \int_{B_r} u(x,t)\,\mathrm{d}x, \quad P(r,t) = \int_{B_r} v(x,t)\,\mathrm{d}x, \tag{2.1}$$

where B_r is the ball of current radius $r > 0$ centered at the origin.

Integrating both equations of (1.1) over the ball B_r, and changing the variables, we obtain the new system (which is no longer nonlocal)

$$\begin{aligned} Q_t &= Q_{rr} - \frac{1}{r}Q_r + \frac{1}{2\pi r}Q_r\big(P - Q\big), \\ P_t &= P_{rr} - \frac{1}{r}P_r - \frac{1}{2\pi r}P_r\big(P - Q\big). \end{aligned} \tag{2.2}$$

Then, in these new variables the initial conditions (1.2) imply

$$\begin{gathered} Q(0,t) = 0, \quad P(0,t) = 0, \\ \lim_{r\to\infty} Q(r,t) = M_u \equiv \int u_0(x)\, \mathrm{d}x, \quad \lim_{r\to\infty} P(r,t) = M_v \equiv \int v_0(x)\, \mathrm{d}x. \end{gathered} \tag{2.3}$$

Further we suppose that M_u, M_v are finite, i.e. u and v are integrable over $\mathbb{R}^2$.

So far we have been using only the assumption that the solutions of (1.1) are radially symmetric. Now, we use another property of the solutions, namely the self-similarity. Applying the substitutions $Q(r,t) = 2\pi\xi(\frac{r^2}{t})$ and $P(r,t) = 2\pi\eta(\frac{r^2}{t})$, where ξ, $\eta\colon \mathbb{R} \to \mathbb{R}$, and $y = \frac{r^2}{t}$, we rewrite the system (2.2) in the following form

$$\begin{aligned} \xi''(y) + \frac{1}{4}\xi'(y) + \frac{1}{2y}\xi'(y)\big(\eta(y) - \xi(y)\big) = 0, \\ \eta''(y) + \frac{1}{4}\eta'(y) - \frac{1}{2y}\eta'(y)\big(\eta(y) - \xi(y)\big) = 0, \end{aligned} \tag{2.4}$$

with the boundary conditions at the origin

$$\xi(0) = 0, \quad \eta(0) = 0, \tag{2.5}$$

and the asymptotic conditions at the infinity

$$\lim_{y\to\infty} \xi(y) = M_\xi(= \frac{1}{2\pi}M_u), \quad \lim_{y\to\infty} \eta(y) = M_\eta(= \frac{1}{2\pi}M_v). \tag{2.6}$$

For solving the system (2.4) numerically such boundary conditions are hardly applicable. Therefore, using the *shooting method*, we change these boundary conditions into the following initial conditions

$$\begin{aligned} \xi(0) = 0, \quad \eta(0) = 0, \\ \xi'(0) = a, \quad \eta'(0) = b, \end{aligned} \tag{2.7}$$

where a i b are nonnegative real numbers.

Now, we can solve the system (2.4) with the initial conditions (2.7) numerically using *the Runge–Kutta method*. Because of singularities, we use *the diagonally implicit scheme* of the method (which meets stability of solutions and costs of their computations) with variable y-step instead of the classical well-known procedure, see e.g. [11]. Such a scheme together with variable time step has been implemented using Matlab software. The time step changes dynamically according to the rate of change of the solution. We present below some solutions determined by some values of the parameters a and b.

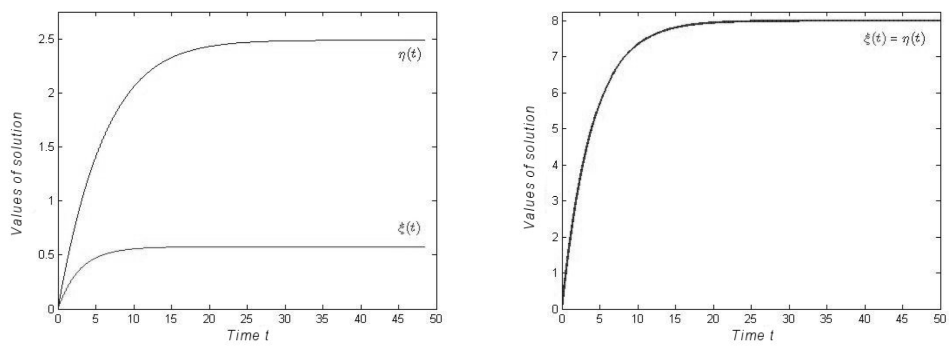

Figure 1: Bounded solutions of (2.4)–(2.7) for the parameters $a = 0.2$, $b = 0.4$ (on the left) and $a = 2.0$, $b = 2.0$ (on the right). We can notice that functions with smaller initial conditions stabilise faster than those with bigger initial slopes.

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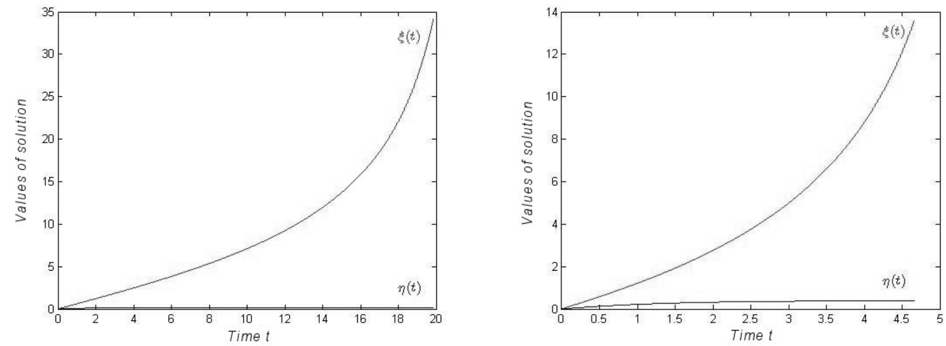


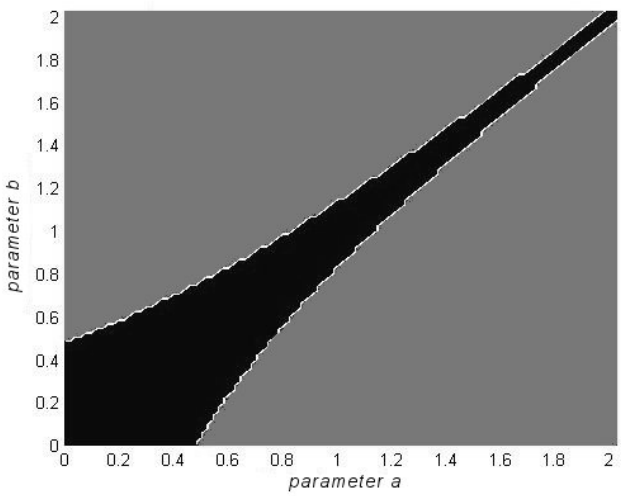
Figure 2: Unbounded solutions of (2.4)–(2.7) for the parameters $a = 0.6$, $b = 0.1$ (on the left) and $a = 1.1$, $b = 0.3$ (on the right). On the right picture,

we can also notice that the functions increase much faster for bigger initial conditions.

Looking at these plots, the first conclusion is that solutions of (2.4)–(2.7) satisfy the boundary conditions (2.6) not for every parameters a, b. Therefore, we are interested in finding pairs of parameters for which the solutions are simultaneously bounded, otherwise they could not satisfy the boundary conditions (2.6). The second observation is that the functions are bounded if and only if they are concave, similarly as was in the one-component model in [8]. To determine such values of parameters, we again use the *Runge–Kutta method* but this time we focus on the stopping conditions. As we have already mentioned, the change of the time step depends on the changes of solution in the following way

$$\frac{\text{actual time step} \times \text{accuracy}}{\text{distance between values of solutions}}.$$

As long as the solution changes rapidly, the time step becomes smaller and smaller. Conversely, if the solution stabilizes then the time step becomes bigger. When the time step is of order 10 we assume that a bounded solution is found.



The black region represents the pairs of parameters (a, b) for which solutions of (2.4) satisfy the boundary conditions (2.7) and (2.6). It is thus reasonable to conjecture that $|a - b|$ is small compared to $\max(a, b)$.

3 Existence of solutions

In this section we prove using a series of simple *a priori* properties of solutions of the problem (2.4)–(2.6), the following theorem

Theorem 3.1. *For all M_ξ, $M_\eta > 0$ there exists a unique solution of* (2.4) *satisfying the conditions* (2.5) *and* (2.6)*.*

Lemma 3.2. *Whenever solutions exist for finite positive constants M_ξ, M_η, the functions ξ and η are positive, strictly increasing and concave.*

Proof. Fix M_ξ, $M_\eta \in (0, \infty)$ and consider a solution (ξ, η) of (2.4). First we note that ξ, $\eta \in C^\infty(0, \infty)$ by (2.4). Since $M_\xi > 0$ there exists a point $y_1 > 0$ such that $\xi'(y_1) > 0$. Now let us assume for a contradiction that the function ξ is not strictly increasing. Then, there exists $y_0 > 0$ such that $\xi'(y_0) = 0$. The *Cauchy–Lipschitz theorem* (applied to the first order equation in ξ'

$$\xi''(y) + \frac{1}{4}\xi'(y) - \frac{1}{2y}w(y)\xi'(y) = 0$$

with a coefficient $w(y) = \xi(y) - \eta(y) \sim (a - b)y$ as $y \to 0$) implies that $\xi'(y) = 0$ for $y > 0$. Hence $\xi(y) = \xi(y_0) > 0$ for each $y > 0$ which contradicts the boundary conditions (2.5). Since ξ is increasing and satisfies boundary conditions, then ξ is immediately positive and concave. Similarly, this holds for the function η. ∎

Lemma 3.3. *Whenever solutions exist for finite positive constants M_ξ, M_η such that $M_\xi > M_\eta$, then $\xi(y) > \eta(y)$ and $\xi'(y) > \eta'(y)$ for all $y > 0$.*

Proof. Note that for $a = b$ the obvious (and unique) solution of (2.4)–(2.7) is $\xi(y) = \eta(y) = 4a\big(1 - e^{-y/4}\big)$ with $M_\xi = M_\eta = 4a$, which represents the electroneutrality case of charged particles that do not interact on the average (in the mean field approximation). Concerning the uniqueness, observe that the system (2.4)–(2.7) (of the first order in ξ' and η', with the coefficient $\frac{1}{y}w(y) = \frac{1}{y}(\xi(y) - \eta(y)) \sim (a - b)$ as $y \to 0$) is, in fact, not singular and enjoys the property of the uniqueness of solutions to the Cauchy problem.

Let us define a new function $w(y) = \xi(y) - \eta(y)$. Then w satisfies the following equation

$$w''(y) + \frac{1}{4}w'(y) - \frac{1}{2y}(\xi'(y) + \eta'(y))w(y) = 0 \tag{3.1}$$

with the boundary conditions

$$w(0) = 0, \quad w(\infty) = M_\xi - M_\eta > 0. \tag{3.2}$$

By the previous uniqueness property $a \neq b$, i.e. $w'(0) \neq 0$. Therefore, either $w = \xi - \eta$ or $w = \eta - \xi$ is strictly positive for $y > 0$ in a neighbourhood of the origin. Now let us assume for a contradiction that there exists a point y_0 such that $w(y_0) = 0$, and take the minimal $y_0 > 0$ with this property. Multiplying (3.1) by y and integrating it from 0 to y we obtain

$$\int_0^y \Big(zw''(z) + \tfrac{1}{4}zw'(z) - \tfrac{1}{2}\big(\xi'(z) + \eta'(z)\big)w(z) \Big)\, \mathrm{d}z = 0.$$

After simple calculations we have

$$yw'(y) - w(y) + \frac{1}{4}yw(y) = \frac{1}{4}\int_0^y w(z)\, \mathrm{d}z + \frac{1}{2}\int_0^y \big(\xi'(z) + \eta'(z)\big)w(z)\, \mathrm{d}z.$$

Now letting $y = y_0$, due to the fact that the functions under the integrals are positive, we obtain

$$0 \geqslant y_0 w'(y_0) = \frac{1}{4}\int_0^{y_0} w(z)\, \mathrm{d}z + \frac{1}{2}\int_0^{y_0} \big(\xi'(z) + \eta'(z)\big)w(z)\, \mathrm{d}z > 0$$

which is a contradiction. Therefore, $w > 0$ over the positive half-line. Since $\xi(y) > \eta(y)$ for large y, hence $\xi(y) > \eta(y)$ holds for all $y > 0$.

To prove the second part of the lemma let us multiply the equation (3.1) by the function $e^{y/4}$. Then

$$\big(w'(y)e^{y/4}\big)' = e^{y/4}\frac{1}{2}\big(\xi'(y) + \eta'(y)\big)w(y).$$

Integrating the above equation over the interval $(0, y)$ we obtain

$$w'(y) = e^{-y/4}w'(0) + \frac{1}{2}e^{-y/4}\int_0^y e^{z/4}\big(\xi'(z) + \eta'(z)\big)w(z)\,\mathrm{d}z > 0,$$

which ends the proof. ∎

Before we prove Theorem 3.1 let us recall the main statements related to self-similar solutions for the one-component Debye system

$$\psi''(y) + \frac{1}{4}\psi'(y) - \frac{1}{2y}\psi(y)\psi'(y) = 0, \tag{3.3}$$

$$\psi(0) = 0, \quad \lim_{y\to\infty}\psi(y) = M. \tag{3.4}$$

Like in the two-component problem it is more convenient to consider the equation with the initial conditions

$$\psi(0) = 0, \quad \psi'(0) = a,$$

for some positive real constant a. The authors in [8, Theorem 4.1] proved the existence of solutions for (3.3) as well as the following properties

- $\psi'(0) > \frac{1}{2}$ then $\psi'(y) > \frac{1}{2}$ for all $y > 0$,
- $\psi'(0) = a < \frac{1}{2}$ implies that $0 < \psi'(y) < a$ and $\psi''(y) < 0$ for all $y > 0$,
- $\psi'(0) < \frac{1}{2}$ then $\lim_{y\to\infty}\psi(y)$ exists, and the values of that limit fill up the half-line $[0, \infty)$.

A similar analysis of the equation

$$\phi'' + \frac{1}{4}\phi' + \frac{1}{2y}\phi\phi' = 0$$

arising in chemotaxis and gravitationally attracting particles theory is in [4]. Here, the solutions with $\phi(0) = 0$, $\phi'(0) = a$, exist for each $a \geqslant 0$ but the limiting values $\lim_{y\to\infty}\phi(y)$ fill up exactly the finite interval $[0, 4)$.

Now, knowing the main result for (3.3)–(3.4), namely the existence of solutions with a given $M > 0$, we are able to prove Theorem 3.1.

Proof of Theorem 3.1. Fix M_ξ, $M_\eta > 0$. We can assume with no loss of generality that $M_\xi > M_\eta$, and we define as previously the function $w(y) = \xi(y) - \eta(y)$. Then w satisfies (3.1) with the conditions (3.2). We have proved in previous lemmas (which are in fact *a priori* estimates for any possible solution of (2.4)) that $w(y) > 0$ and $w'(0) > 0$ for all $y > 0$. Therefore, we can apply the comparison principle for a second order ordinary differential equation to prove the existence of the function w with a given value of $\lim_{y\to\infty} w(y) \in (0, \infty)$. Keeping in mind the results of Lemma 3.2 it is easy to check that w is a subsolution of (3.3)

$$w''(y) + \frac{1}{4}w'(y) - \frac{1}{2y}w'(y)w(y) \geqslant 0.$$

Thanks to the existence result in [8] on the above equation, we have the existence of function w to (3.1) with any arbitrarily given $\lim_{y\to\infty} w(y) \in (0, \infty)$. Now the function ξ satisfies the linear equation

$$\xi''(y) + \frac{1}{4}\xi'(y) - \frac{1}{2y}\xi'(y)w(y) = 0$$

with some given function w and given boundary conditions $\xi(0)$ and $\xi(\infty) > w(\infty)$. So this equation can be solved explicitly

$$\xi(y) = C \int_0^y \exp\Big(\int_0^t \big(\frac{w(s)}{2s} - \frac{1}{4}\big)\, \mathrm{d}s\Big)\, \mathrm{d}t$$

with the following constant

$$C = M_\xi \Big(\int_0^\infty \exp\Big(\int_0^t \big(\frac{w(s)}{2s} - \frac{1}{4}\big)\, \mathrm{d}s\Big)\, \mathrm{d}t\Big)^{-1}.$$

Then we calculate $\eta(y) = \xi(y) - w(y)$ and check its properties, which ends the proof. ■

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