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SELF-SIMILAR SOLUTIONS FOR THE TWO-DIMENSIONAL NERNST–PLANCK–DEBYE SYSTEM

Abstract. We investigate the two-component Nernst–Planck–Debye system by a numerical study of self-similar solutions using the Runge–Kutta method of order four and comparing the results obtained with the solutions of a one-component system. Properties of the solutions indicated by numerical simulations are proved and an 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 1920s, 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 diffusion. Due to the common occurrence of electrically charged particles in the nature, NPD 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].

The NPD system is

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

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

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

Our goal is to study some numerical solutions as well as to prove the existence of some special solutions of (1.1) in the case when Ω is the entire space $\mathbb{R}^2$, so (1.1) is supplemented with the integrability conditions $u(\cdot,t), v(\cdot,t) \in L^1(\mathbb{R}^2)$, instead of no-flux boundary conditions on $\partial\Omega \times (0,T)$.

As 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 the particles themselves [9], with $\Delta\phi = v - u$. Besides electrochemistry, similar systems occur in 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 of (1.1) and their asymptotic behaviour for 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 $\Omega = \mathbb{R}^n$, $n \geq 3$, 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 performed for the one-component system in [8], is of 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 part of [10, Master Thesis] written under the supervision of Dr. Michał Olech.

It is worth mentioning that the similar model

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

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

The authors of [3] initiated a study of 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 (global 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, $M_\eta \geq 0$. Apart from the 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 the equations coupled through the potential function ϕ. One can approximate solutions of such a 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 in this study. In our case we propose to make some preliminary reductions, namely, we consider solutions which are radially symmetric and scale-invariant. Despite the simplifications, numerically solving the system (1.1) will not be a trivial task because of singular coefficients of order $1/y$ 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 the next 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, and 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 shall 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 $\Omega = \mathbb{R}^2$. They are called

- *radially symmetric* if

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

- *self-similar* (invariant under a scaling) if 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 of (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 so, we first define

$$Q(r,t)=\int_{B_r} u(x,t)\,dx,\qquad P(r,t)=\int_{B_r} v(x,t)\,dx, \tag{2.1}$$

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

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

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

In the new variables the initial conditions (1.2) imply

$$\begin{aligned} &Q(0,t)=0,\qquad P(0,t)=0,\\ &\lim_{r\to\infty} Q(r,t)=M_u\equiv\int u_0(x)\,dx,\qquad \lim_{r\to\infty} P(r,t)=M_v\equiv\int v_0(x)\,dx. \end{aligned} \tag{2.3}$$

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 their self-similarity. Applying the substitutions $Q(r,t)=2\pi\xi(r^2/t)$ and $P(r,t)=2\pi\eta(r^2/t)$, where $\xi,\eta\colon\mathbb{R}\to\mathbb{R}$ and $y=r^2/t$, we rewrite (2.2) in the form

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

with the boundary conditions at the origin

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

and the asymptotic conditions at infinity

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

In 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:

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

where a and b are nonnegative real numbers.

Now, we can numerically solve the system (2.4) with the initial conditions (2.7) using the Runge–Kutta method. Because of singularities, we use the diagonally implicit scheme of the method with variable y-step (which preserves stability properties of solutions and features reasonable computational cost) 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 for selected values of a and b.

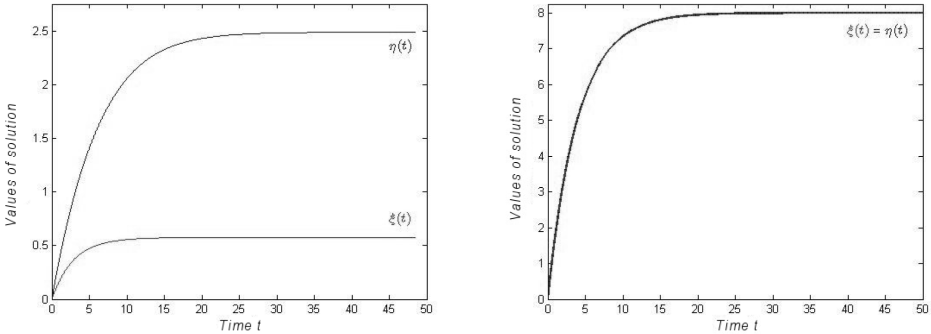


Fig. 1. Bounded solutions of (2.4)–(2.7) for $a = 0.2$, $b = 0.4$ (left) and $a = 2.0$, $b = 2.0$ (right). Notice that the functions with smaller initial data stabilise faster than those with greater initial slopes.

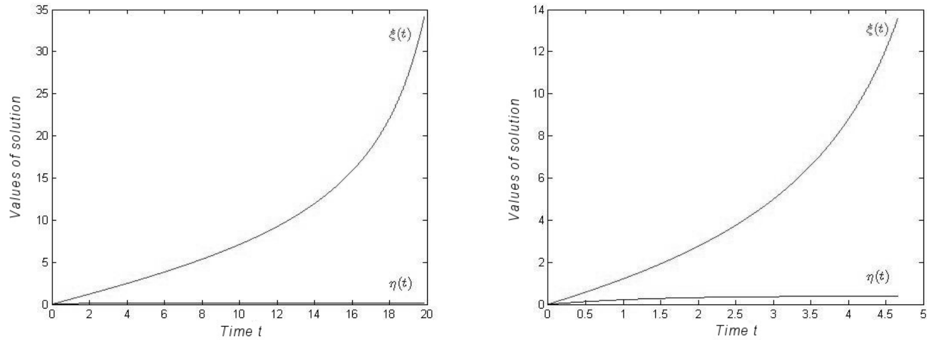


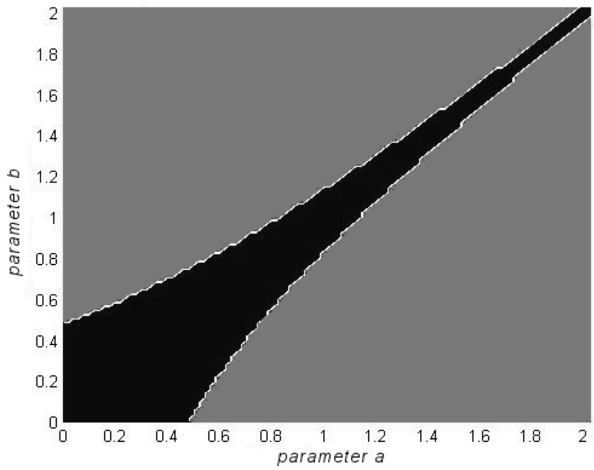
Fig. 2. Unbounded solutions of (2.4)–(2.7) for $a = 0.6$, $b = 0.1$ (left) and $a = 1.1$, $b = 0.3$ (right). Notice that the functions increase much faster for greater initial data.

Looking at these plots, the first conclusion is that solutions of (2.4)–(2.7) satisfy the boundary conditions (2.6) not for all 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 solutions are bounded if and only if they are concave, as was the case 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 the solution in the following way:

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

As long as the solution changes rapidly, the time step becomes smaller and smaller. Conversely, if the solution stabilises then the time step becomes greater. 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 the following theorem using a series of simple a priori properties of solutions of the problem (2.4)–(2.6)

THEOREM 3.1. *For all $M_\xi, M_\eta > 0$ 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 $M_\xi, M_\eta \in (0, \infty)$ and consider a solution (ξ, η) of (2.4). First we note that $\xi, \eta \in C^\infty(0, \infty)$ by (2.4). Since $M_\xi > 0$ there exists a point $y_1 > 0$ such that $\xi'(y_1) > 0$. Now 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 $w(y) = \xi(y) - \eta(y) \sim (a-b)y$ 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 the boundary conditions, it is positive and concave. Similarly, the same holds for 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. It is obvious that for $a = b$ the unique solution of (2.4)–(2.7) is $\xi(y) = \eta(y) = 4a(1 - e^{-y/4})$ 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 uniqueness, observe that the system (2.4)–(2.7) (of the first order in ξ' and η', with $\frac{1}{y}w(y) = \frac{1}{y}(\xi(y) - \eta(y)) \sim (a-b)$ as $y \to 0$) is, in fact, not singular and enjoys the property of uniqueness of solutions to the Cauchy problem.

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

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

with the boundary conditions

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

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 assume for a contradiction that there exists 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

$$\int_0^y \left(zw''(z) + \frac{1}{4}zw'(z) - \frac{1}{2}(\xi'(z) + \eta'(z))w(z) \right) dz = 0.$$

After simple calculations we have

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

Now letting $y = y_0$, as the integrands are positive, we obtain

$$0 \geq y_0 w'(y_0) = \frac{1}{4}\int_0^{y_0} w(z)\,dz + \frac{1}{2}\int_0^{y_0} (\xi'(z) + \eta'(z))w(z)\,dz > 0,$$

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

To prove the second part of the lemma, multiply (3.1) by $e^{y/4}$ to get

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

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

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

which ends the proof. ∎

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

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

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

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

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

for some positive real constant a. Herczak and Olech [8, Theorem 4.1] proved the existence of solutions for (3.3) as well as the following properties:

- if $\psi'(0) > \frac{1}{2}$ then $\psi'(y) > \frac{1}{2}$ for all $y > 0$,
- $\psi'(0) = a < \frac{1}{2}$ implies $0 < \psi'(y) < a$ and $\psi''(y) < 0$ for all $y > 0$,
- if $\psi'(0) < \frac{1}{2}$ 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 $a \geq 0$ but the limiting values $\lim_{y\to\infty}\phi(y)$ fill up 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 $M_\xi, M_\eta > 0$. We can assume that $M_\xi > M_\eta$, and as previously we define $w(y) = \xi(y) - \eta(y)$. Then w satisfies (3.1) and (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 second order ordinary differential equations to prove the existence of w with a given value of $\lim_{y\to\infty} w(y) \in (0,\infty)$. Keeping in mind Lemma 3.2 it is easy to check that w is a subsolution of (3.3),

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

Thanks to the existence result in [8] for the above equation, we have the existence of a solution w to (3.1) with any 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 a given function w and boundary conditions $\xi(0)$ and $\xi(\infty) > w(\infty)$. So this equation can be solved explicitly:

$$\xi(y) = C\int_0^y \exp\left(\int_0^t \left(\frac{w(s)}{2s} - \frac{1}{4}\right) ds\right) dt$$

with the constant

$$C = M_\xi\left(\int_0^\infty \exp\left(\int_0^t \left(\frac{w(s)}{2s} - \frac{1}{4}\right) ds\right) dt\right)^{-1}.$$

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

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