QUALITATIVE PROPERTIES OF STEADY-STATE POISSON-NERNST-PLANCK SYSTEMS: MATHEMATICAL STUDY *

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Abstract. We examine qualitative properties of solutions of self-consistent Poisson-Nernst-Planck (PNP) systems, including uniqueness. In the case of vanishing permanent charge, the predominant case studied, our results unveil a rich structure inherent in these systems, one that is determined by the boundary conditions and the signs of the oppositely charged carrier fluxes. A particularly significant special case, that of simple boundary conditions, is shown to lead to uniqueness, and to a complete characterization. This case underlies the more complicated cases studied later. A contraction mapping principle is included for completeness, and allows for an arbitrary permanent charge distribution.

Key words. simple boundary conditions, uniqueness, basic symmetries, fundamental inequalities, categories

AMS subject classifications. 34A34, 34B15, 34C11, 92C05, 92C35

1. Introduction. In this paper, we investigate the properties of the solutions of steady-state Poisson-Nernst-Planck equations for charge transport in one dimension. The predominant case studied is that with vanishing permanent charge. This model has a long history within the context of electrodiffusion and semiconductor modeling (cf. [18] and [14]), and the existence of solutions of the PNP equations has been widely established, even for the more general case of the multidimensional model and variable mobilities (see [10]), as well as for arbitrary permanent charge. There also exists a rigorous Galerkin convergence theory, initiated in [13] and refined in [12]. We shall not attempt to survey the extensive literature here. The system with vanishing permanent charge consists of the Poisson electrostatic equation, coupled to particle conservation equations for oppositely charged carriers. At face value, the model describes charge transport in many basic situations, such as that of electrons and holes in pure semiconductor lattices, or anions and cations in open channels without surface charge.

The PNP equations are:

$$\lambda^2\phi_{xx} - n + p = 0, \tag{1}$$
$$n_x - n\phi_x = J_n, \tag{2}$$
$$p_x + p\phi_x = -J_p, \tag{3}$$

in $\Omega = (0,1)$, with boundary conditions,

$$p(0) = p_L > 0, \qquad n(0) = n_L > 0, \tag{4}$$
$$p(1) = p_R > 0, \qquad n(1) = n_R > 0, \tag{5}$$
$$\phi(0) = \phi_0, \qquad \phi(1) = \phi_1, \tag{6}$$
$$V = \phi_0 - \phi_1. \tag{7}$$

Here, without loss of generality, we shall often take $\phi_1 = 0$ in electrostatic applications; ϕ is the electrostatic potential, scaled by U_T, n and p the negative and

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positive carrier concentrations, scaled by S, J_n is n-current, J_p is p-current, and λ^2 is a strictly positive parameter, the squared quotient of two natural lengths, defined by

$$\lambda^2 = \epsilon_0 U_T/(d^2 eS).$$

Here, the expression $U_T \equiv kT_0/e$ is called the thermal voltage, e is the charge modulus, d is the original (dimensional) length of Ω, prior to normalization to unity, and S is the appropriate concentration scale, selected so that concentrations are on the order of unity. The expression kT_0 has its usual meaning as Boltzmann's constant k times the temperature T_0. The quantity ϵ_0 is the dielectric constant, and λd is known as the Debye length. The electrostatic flux (displacement vector) is then given by the product of the dielectric with the electric field, $-\nabla\phi$. Implicit in this formulation is the use of the Einstein relations, expressing the diffusion coefficients as thermal voltage–mobility coefficient products, which are assumed constant here. For the most part, we shall assume that the two carrier species have identical mobilities, although we shall indicate the modifications required when this does not hold. Although it is found that λ is often small, we do not require that in this paper, and have selected notation which does not suggest it.

The derivation of this system also admits interpretation in general terms, beyond the scope of charged fluids. Specifically, the system is valid whenever there exists a velocity field, derived from a potential, which induces the drift of two "competing" species. This situation can even be realized outside the province of science and engineering, e.g., as a model of cooperating and noncooperating groups in flux, where the inducement for the group to move outside any locality is measured as a "force" proportional to the excess, within that locality, of noncooperators over cooperators. In order to emphasize the general scope of the model, we remind the reader of the familiar derivation of the PNP system, based on a single conservation principle, which is presented now. Suppose a scalar quantity ρ is associated with a fluid, occupying a spatial domain G, where ρ is a volume density. Suppose that the (outward) flux of the fluid quantity across the boundary of a fixed spatial region $\mathcal{B} \subset G$ is determined as J_ρ. By means of an application of the classical divergence theorem (cf. [6]), we then have the volume balance,

$$\int_{\mathcal{B}} -\frac{\partial\rho}{\partial t}\, dV = \int_{\mathcal{B}} \{\nabla\cdot J_\rho + g\}\, dV, \tag{8}$$

where g is negatively signed for a source and positively signed for a sink. Since the region $\mathcal{B}$ is arbitrary, the integrands must agree in (8). We thus have the *conservation equation*,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot J_\rho + g = 0. \tag{9}$$

This equation holds in the entire region G of the fluid. The Poisson equation results when ρ is identified with electrostatic potential ϕ, and $J_\rho = -\epsilon\nabla\phi$. The conservation equations result when the drift components of the carrier mass fluxes have drift velocity defined by the mobility–electric field product; standard diffusion is assumed as remarked above. Here, we recall that the units of mobility are length^2/time/Volt, while the electric field is the negative gradient of the electrostatic potential. Interpretations outside the domain of charged fluids require the above formal identifications. The one-dimensional problem as studied here, however, has been formulated and studied in ([2]) and further analyzed in [5] in the case of ionic channels.

There are very few results for uniqueness or qualitative properties of solutions. Later, in §2.4, we shall survey the appropriate literature, insofar as it is related to this work. In this paper, we shall restrict our attention to two monovalent species. We have also derived a contraction principle, which can be used in boundary layers, or more globally, permitting nonzero permanent charge. This is presented in complete detail in §5.

2. Basic symmetries, definitions, and properties. In this section, we shall display two symmetries of the PNP model, and demonstrate the nonnegativity of n and p. This will be followed by a description of fundamental flux properties. We close with a discussion.

2.1. Basic symmetries.

(i) Suppose $(\phi(x), n(x), p(x))$ is a solution of (1)-(6). The first symmetry employs reflection in the physical boundary, with accompanying reversal of flux:

$$x \mapsto 1-y, \ \ (\phi(x), n(x), p(x)) \mapsto (\hat{\phi}(y), \hat{n}(y), \hat{p}(y)), \ \ (J_n, J_p) \mapsto (-J_n, -J_p),$$

in (1)-(3) and

$$(V, n_L, p_L, n_R, p_R) \mapsto (-V, n_R, p_R, n_L, p_L)$$

in (4)-(6) to obtain a new equivalent system.

(ii) Suppose $(\phi(x), n(x), p(x))$ is a solution of (1)-(6). A second symmetry uses an interchange of carriers and reversal of electric field:

$$(\phi(x), n(x), p(x)) \mapsto (-\phi(x), p(x), n(x)), \ \ (J_n, J_p) \mapsto (-J_p, -J_n),$$

in (1)-(3) and

$$(V, n_L, p_L, n_R, p_R) \mapsto (-V, p_L, n_L, p_R, n_R)$$

in (4)-(6) to obtain a new equivalent system.

Later in the paper, we shall see how these symmetries reduce the number of possible case distinctions allowed by the boundary conditions (see §4).

2.2. The positivity of n and p. We verify the expected property of positivity for the concentrations by use of the model.

LEMMA 2.1. *If n and p satisfy (1)-(6), then they are strictly positive.*

Proof. Multiply the continuity equations (2) and (3) by $e^{-\phi}$ and e^{ϕ}, respectively, to obtain the following equations:

$$\Big(n(x)e^{-\phi(x)}\Big)' = J_n \cdot e^{-\phi(x)}, \tag{10}$$

$$\Big(p(x)e^{\phi(x)}\Big)' = -J_p \cdot e^{\phi(x)}. \tag{11}$$

Integrating these equations, we have, respectively,

$$J_n \cdot \int_0^x e^{-\phi(y)} dy = n(x)e^{-\phi(x)} - n_L e^{-\phi_0}, \tag{12}$$

$$-J_p \cdot \int_0^x e^{\phi(y)} dy = p(x)e^{\phi(x)} - p_L e^{\phi_0}. \tag{13}$$

From the above equations, we eliminate J_n and J_p, and that gives

$$n(x)e^{-\phi(x)} = n_R f(x) + n_L e^{-\phi_0}(1 - f(x)),$$
$$p(x)e^{\phi(x)} = p_R g(x) + p_L e^{\phi_0}(1 - g(x)),$$

where $f(x)$ and $g(x)$ are two functions of x which increase monotonically from 0 to 1. Specifically,

$$f(x) = \frac{\int_0^x \exp(-\phi(y))dy}{\int_0^1 \exp(-\phi(y))dy},$$
$$g(x) = \frac{\int_0^x \exp(\phi(y))dy}{\int_0^1 \exp(\phi(y))dy}.$$

This proves the positivity of n and p. □

2.3. Basic flux properties. We introduce the physical current, I, the negative of the total (particle) flux, J, and the bias, V, by $I = J_n + J_p$, $J = J_n - J_p$ and, as before, $V = \phi_0 - \phi_1$. Consider the equations (12) and (13) at $x = 1$. Then we have

$$J_n = \frac{n_R e^V - n_L}{\int_0^1 e^{\phi_0 - \phi(x)}dx}, \tag{14}$$

$$J_p = -\frac{p_R e^{-V} - p_L}{\int_0^1 e^{-\phi_0 + \phi(x)}dx}. \tag{15}$$

An important identity, allowing flux representation solely in terms of the parameters of the problem and the (differences in the) specified boundary conditions, is given by the following.

THEOREM 2.2. *J can be expressed by the equation,*

$$J = (n+p)(1) - (n+p)(0) - \frac{\lambda^2}{2}(\phi_x^2(1) - \phi_x^2(0)). \tag{16}$$

Proof. To derive the identity (16), we add (2) and (3) and integrate with respect to x to obtain the following:

$$J = (n+p)(1) - (n+p)(0) - \int_0^1 (n-p)\phi_x dx. \tag{17}$$

Using the Poisson equation, we have (16). This concludes the proof. □

2.4. Discussion and general uniqueness results. The reason we shall begin our in depth study in the next section with the special case of simple boundary conditions is its central role in more general case studies. The results of §3 will be used in a fundamental way in §4 which follows it. Indeed, we can give a complete resolution of the uniqueness question in this case. In the case when permanent charge is present, uniqueness is not expected in general. The classic counterexample is that of the thyristor, with three or more junctions [19]. We therefore review the uniqueness results presently available. One class of uniqueness results is valid for a restricted range of an appropriate parameter; this type of result is based either explicitly or implicitly upon a contraction principle. Thus, the first uniqueness result with nonvanishing permanent charge was obtained by Mock [15], under the provision that $|n_L e^{-\phi_0} - n_R e^{-\phi_1}|$ and $|p_L e^{\phi_0} - p_R e^{\phi_1}|$ are sufficiently small (or equivalently, provided that $|V = \phi_0 - \phi_1|$ is sufficiently small). His proof is based on a monotonicity operator property, and ultimately upon resolvent contractiveness. Unfortunately, this argument does not hold if $|V|$ is not small. More recently, Brezzi et al [4] studied this model with nonvanishing permanent charge, which changes its sign once (so it is a junction), with specific boundary conditions, as a singular perturbation problem, and proved that the solution is unique if the value of the singular perturbation parameter is small enough. Also, Gajewski [7] proved the uniqueness of the solution for a given V, if λ is sufficiently large, and Jerome [11] proved the uniqueness theorem with nonvanishing permanent charge, using the contraction mapping principle of the Gummel map in a two dimensional setting. The diameter of the device and the energy band bending are the critical parameters in the latter approach. Recently, Alabau [1] introduced a new method which is based on a decoupling of the linearized system and on maximum principle arguments. The main interest in that method is the proof of global uniqueness, even for large V. In this paper, we shall derive a new uniqueness result (Theorem 3.8), which extends Alabau's result in the case of simple boundary conditions. We shall also present a sharp form of the contraction mapping principle (Theorem 5.1), which is especially effective in any boundary layer theory.

3. PNP system: simple boundary conditions. We introduce a new notation in terms of dimensionless ratios. Set

$$\rho_L = \frac{p_L}{n_L},\ \rho_R = \frac{p_R}{n_R}. \tag{18}$$

We shall say that the nonlinear system (1)-(6) has simple boundary values if $\rho_L = \rho_R = 1$. In this case, the electroneutral case, as a biologist, chemist, or electrical engineer might call it, we denote the common values by c_L, c_R, respectively. In the language of quasi-Fermi levels, the electrostatic potential equals the mean value of the quasi-Fermi levels, associated with the oppositely charged carriers, at each boundary of the device. In terms of these Fermi levels, denoted v and w,

$$n = c\exp(\phi - v), \quad p = c\exp(w - \phi),$$

for an appropriate constant c. Although we shall not have occasion to make direct use of these logarithmic variables, they arise implicitly in many of the calculations of this paper.

3.1. The fundamental inequalities. Recall that the orientation of J is opposite to the mass flux. One might anticipate a flow law, stipulating that such flux seeks lower concentration levels. In a global sense, such a law is valid.

THEOREM 3.1 (Flux Law). *In the case of simple boundary conditions, J satisfies the following inequality:*

$$J(c_R - c_L) \geq 0. \tag{19}$$

Thus, net particle flow is directed from higher to lower concentrations, and a modified Fick's law holds. Equality holds if and only if both factors are zero, and, in this equilibrium case, $n \equiv p \equiv const$.

Proof. We begin by multiplying (2) by n_x and then integrate with respect to x. After a few manipulations, we get

$$J_n \cdot (n - c_L) = \int_0^x (n_x)^2 dy - \frac{1}{2} n^2 \phi_x|_0^x + \frac{1}{2}\int_0^x n^2 \phi_{xx} dy. \tag{20}$$

A similar expression can be obtained by starting from (3), viz.,

$$-J_p \cdot (p - c_L) = \int_0^x (p_x)^2 dy + \frac{1}{2} p^2 \phi_x|_0^x - \frac{1}{2}\int_0^x p^2 \phi_{xx} dy. \tag{21}$$

If we add these two expressions, and use the Poisson equation (1), we see that

$$\begin{aligned} &J_n(n - c_L) - J_p(p - c_L) \\ &= \int_0^x (p_x^2 + n_x^2) dy + \frac{1}{2\lambda^2}\int_0^x (p+n)(p-n)^2 dy + \frac{1}{2}(p^2 - n^2)(x)\phi_x(x). \end{aligned} \tag{22}$$

Note that this identity simplifies whenever $n(x) = p(x)$. In particular, for $x = 1$, we have

$$J(c_R - c_L) = \int_0^1 (p_x^2 + n_x^2) dy + \frac{1}{2\lambda^2}\int_0^1 (p+n)(p-n)^2 dy. \tag{23}$$

We shall refer to either of the above equations as the first fundamental identity. Note that the right hand side of (23) is nonnegative, and therefore we immediately conclude that

$$J(c_R - c_L) \geq 0.$$

Thus, although Fick's law in the strict sense does not hold, in that flux is not proportional to the negative concentration gradient, this extended version does hold. The final statement follows from (23) and (2)-(3). □

The next result involves a quantity, viz., IV, which might be called the power dissipation by an electrical engineer. We find that it is always nonegative.

THEOREM 3.2 (Power Dissipation Law). *In the case of simple boundary conditions, IV satisfies the following inequality:*

$$IV \geq 0. \tag{24}$$

Equality holds if and only if both factors are zero, and, in this case, $n \equiv p$ and $\phi \equiv const$. Thus, power is strictly dissipated, except in the trivial situation when there is no electric field and no current flow.

Proof. Multiply (2)-(3) by ϕ_x, and integrate over (0,1). Then we have

$$J_n \int_0^1 \phi_x \, dx = \int_0^1 n_x \phi_x \, dx - \int_0^1 n(\phi_x)^2 \, dx,$$

$$-J_p \int_0^1 \phi_x \, dx = \int_0^1 p_x \phi_x \, dx + \int_0^1 p(\phi_x)^2 \, dx.$$

Subtract the second of these two equations from the first:

$$I \int_0^1 \phi_x \, dx = \int_0^1 (n_x - p_x)\phi_x \, dx - \int_0^1 (n+p)(\phi_x)^2 \, dx, \tag{25}$$

so that, via integration by parts,

$$-IV = (n-p)\phi_x|_0^1 - \frac{1}{\lambda^2} \int_0^1 (n-p)^2 \, dx - \int_0^1 (n+p)(\phi_x)^2 \, dx. \tag{26}$$

The right hand side of this equation is nonpositive, so we have the inequality,

$$IV \geq 0.$$

The final statement follows from (26). This establishes the theorem. □

The next two results explore the relationship of the electric field to concentrations and current, respectively.

PROPOSITION 3.3. *In the case of simple boundary conditions, the following inequality is satisfied:*

$$(c_R - c_L) \int_0^1 (p-n)\phi_x dy \geq 0. \tag{27}$$

In particular, the endpoint difference evaluation of the squared electric field values is opposite in sign to the difference in concentrations. If equality is satisfied, $n \equiv p$ *are linear functions.*

Proof. Even though we have some knowledge about the fluxes $J_n,\ J_p$, it is advantageous to eliminate them. We can accomplish this by integrating the original N-P equations (2)-(3) from 0 to x, viz.,

$$J_n x = n - c_L - \int_0^x n\phi_x dy, \tag{28}$$

$$-J_p x = p - c_L + \int_0^x p\phi_x dy. \tag{29}$$

Substituting the above expressions in the first fundamental identity (22), we deduce that

$$\frac{1}{x}\left[(p-c_L)^2 + (p-c_L)\int_0^x p\phi_x dy\right] + \frac{1}{x}\left[(n-c_L)^2 - (n-c_L)\int_0^x n\phi_x dy\right]$$
$$= \int_0^x (p_x^2 + n_x^2) dy + \frac{1}{2}(p^2 - n^2)\phi_x + \frac{1}{2\lambda^2}\int_0^x (n+p)(n-p)^2 dy. \tag{30}$$

But

$$
\begin{aligned}
&\int_0^x \left\{ \left(p_x - \frac{p(x) - c_L}{x} \right)^2 + \left(n_x - \frac{n(x) - c_L}{x} \right)^2 \right\} dy \\
&= \int_0^x (n_x^2 + p_x^2) dy - \frac{(p(x) - c_L)^2}{x} - \frac{(n(x) - c_L)^2}{x}.
\end{aligned} \tag{31}
$$

Therefore,

$$
\begin{aligned}
&\frac{1}{x}(p - c_L) \int_0^x p\phi_x dy - \frac{1}{x}(n - c_L) \int_0^x n\phi_x dy \\
&\qquad = \int_0^x \left\{ \left(p_x - \frac{p(x) - c_L}{x} \right)^2 + \left(n_x - \frac{n(x) - c_L}{x} \right)^2 \right\} dy \\
&\qquad + \frac{1}{2}(p^2 - n^2)\phi_x + \frac{1}{2\lambda^2} \int_0^x (n + p)(n - p)^2 dy.
\end{aligned} \tag{32}
$$

Setting $x = 1$, we obtain the second fundamental identity, viz.,

$$
\begin{aligned}
(c_R - c_L) \int_0^1 (p - n)\phi_x dy &= \int_0^1 \{(p_x - c_R + c_L)^2 + (n_x - c_R + c_L)^2\} dy \\
&+ \frac{1}{2\lambda^2} \int_0^1 (n + p)(n - p)^2 dy.
\end{aligned} \tag{33}
$$

This implies (27). Since the left hand side of (33) is nonnegative, one obtains

$$
(c_R - c_L) \int_0^1 -\phi_{xx}\phi_x dy = \frac{1}{2}(c_R - c_L)(\phi_x^2(0) - \phi_x^2(1)) \geq 0,
$$

from which the next statement follows. The final statement follows from (33), and the proposition is established. ∎

The next result shows the relation between total current and the electric field. More precisely, they have the same orientation.

Proposition 3.4 (Current-Field Alignment). *In the case of simple boundary conditions, the following inequality is satisfied:*

$$
I\phi_x(x) \leq 0. \tag{34}
$$

In particular, the current and the electric field are similarly directed. If equality holds at a point, then it holds at each point on Ω, and, necessarily, $I = 0$ and $\phi_x \equiv 0$. In this case, the final conclusion of Theorem 3.2 holds.

Proof. We can prove this by the maximum principle. Suppose $I \geq 0$. Differentiate (1) and use the continuity equations (2) and (3) to obtain the following equation:

$$
\lambda^2 \phi_{xxx} - (n + p)\phi_x = I.
$$

If ϕ_x has a positive maximum at an interior point in the unit interval, then by the maximum principle ([17, Theorem 3]), $\phi_x \equiv const$. However, the above equation shows that this constant must be zero. The next possibility is that ϕ_x has its maximum at either end point. But again, by the maximum principle ([17, Theorem 4]), we should have

$$\phi_{xx}(0) < 0, \quad \phi_{xx}(1) > 0,$$

respectively, at the relevant endpoint. This contradicts the simple boundary condition property, $\phi_{xx}(0) = 0, \phi_{xx}(1) = 0$. Therefore, we have shown the nonpositivity of ϕ_x when $I \geq 0$.

Suppose $I \leq 0$. A repetition of the above argument leads to $\phi_x \equiv 0$ if a negative minimum of ϕ_x occurs at an interior point, while

$$\phi_{xx}(0) > 0, \phi_{xx}(1) < 0,$$

hold, respectively, if the minimum occurs at an endpoint, $x = 0$ or $x = 1$. This contradiction ensures $\phi_x \geq 0$ in this case. If the left hand side of (34) is zero at a point, then either $I = 0$, or $\phi_x(x) = 0$, which constitutes either a maximum or minimum. The same argument just given, based upon the maximum principle, shows that $\phi_x \equiv 0$ and the proof is complete. □

Theorem 3.5 (Noncrossing Graphs). *In the case of simple boundary conditions, the curves for n and p do not cross. Specifically, we have the following inequality:*

$$IJ(n - p) \geq 0. \tag{35}$$

Proof. We may assume without loss of generality that $IJ \neq 0$. We consider a representative case distinction within this class: $I > 0$, $J > 0$. By Theorem 3.1, we may assume that $c_L \leq c_R$, $I > 0$. We show that $n - p \geq 0$. This holds immediately if $c_L = c_R$ by (33), so we may assume that $c_L < c_R$. In this case, if the result does not hold, there exists an interval, say (x_1, x_2), in which

$$p(x) > n(x) \quad \text{for} \quad x \in (x_1, x_2). \tag{36}$$

Of course, one or both of these end points could coincide with the end of the channel itself. To fix our ideas, let us say that

$$\begin{aligned} n(x_1) &= p(x_1) = c_1, \\ n(x_2) &= p(x_2) = c_2. \end{aligned}$$

Now, Theorem 3.1 implies that $J(c_2 - c_1) \geq 0$. Since $J > 0$, we conclude that

$$c_2 \geq c_1. \tag{37}$$

On the other hand, the identity (32) gives

$$\begin{aligned} \frac{c_2 - c_1}{x_2 - x_1} \int_{x_1}^{x_2} (p - n)\phi_x dy = \int_{x_1}^{x_2} \left\{ \left(p_x - \frac{c_2 - c_1}{x_2 - x_1} \right)^2 + \left(n_x - \frac{c_2 - c_1}{x_2 - x_1} \right)^2 \right\} dy \\ + \frac{1}{2\lambda^2} \int_{x_1}^{x_2} (n + p)(n - p)^2 dy. \end{aligned} \tag{38}$$

Now, by (36), $p(x) > n(x)$ on (x_1, x_2). Also, by the inequality, $c_2 \geq c_1$, and the fact that $\phi_x \leq 0$, we conclude that both sides of (38) are zero. In particular, we have $n(x) = p(x)$ for all $x \in (x_1, x_2)$. This is the desired contradiction. Similarly, we can prove $n - p \leq 0$ when $I < 0$, and we can prove as well the statements for $J < 0$. This proves the theorem. ▯

3.2. Monotone behavior of n and p. We begin by showing that the ranges of n and p are contained in the intervals defined by their endpoint evaluations. This is preliminary to the monotonicity theorems.

LEMMA 3.6 (Endpoint Extrema). *n and p take on their extremal values at the boundaries, e.g., if $V \leq 0$ and $c_L \leq c_R$, then*

$$c_L \leq n \leq p \leq c_R. \tag{39}$$

The other cases are similar, and lead to results summarized in the next subsection.

Proof. Differentiate the continuity equation (3) to obtain the following second order differential equation:

$$p_{xx} + \phi_x p_x + \phi_{xx} p = 0.$$

This equation is used for the cases when $\phi_{xx} \leq 0$, with the equation (2) used otherwise. By the maximum principle ([8, Corollary 3.2]),

$$c_L \leq p \leq c_R. \tag{40}$$

Next, to prove $c_L \leq n$ in this subcase, we proceed as follows. Assume the existence of an interval, say (x_1, x_2), such that

$$n(x) < c_L \text{ for } x \in (x_1, x_2), \tag{41}$$

$$n(x_1) = c_L, \; n(x_2) = c_L. \tag{42}$$

Then, the equation (2), written for x_1 and x_2, reads:

$$\begin{aligned} n_x(x_1) - c_L \phi_x(x_1) &= J_n, \\ n_x(x_2) - c_L \phi_x(x_2) &= J_n. \end{aligned}$$

If we subtract these two equations, we see that

$$n_x(x_2) - n_x(x_1) - c_L(\phi_x(x_2) - \phi_x(x_1)) = 0. \tag{43}$$

But the left hand side of the above equation is strictly positive by the assumptions (41), (42), and the monotone decrease of ϕ_x. This is the desired contradiction. Hence $c_L \leq n$ holds. This concludes the proof. ▯

Next, we shall prove that n and p are monotonic functions. We provide the proof in a typical case, viz., that described in the previous lemma.

THEOREM 3.7 (Monotonicity). *For the case of simple boundary conditions,*

$$IJn_x \leq 0,\ \ IJp_x \leq 0, \text{ if } V \leq 0;\ IJn_x \geq 0,\ \ IJp_x \geq 0, \text{ if } V \geq 0. \tag{44}$$

In particular, n and p are monotonic functions of x.

Proof. Consider the subcase, $V \leq 0$ and $c_L \leq c_R$. If $V = 0$ or $I = 0$, then ϕ is constant by Theorem 3.2. By use of Proposition 3.3 it follows that n and p are (monotone) linear functions. If $c_L = c_R$, then n and p are constant by Theorem 3.1. Suppose that $I < 0$ and $c_L < c_R$ (thus, $J > 0$ by Theorem 3.1). Suppose also that p has an extremum in $(0, 1)$. Then, by Lemma 3.6, p must have at least two extrema, say at x_1, x_2. Without loss of generality, we can pick x_1, x_2 such that

$$p(x_1) \geq p(x_2). \tag{45}$$

Then the equation (3), written at these two points, and the nonnegativity of ϕ_x (see Theorem 3.2 and Proposition 3.4) lead to $\phi_x(x_1) \leq \phi_x(x_2)$. But, by Theorem 3.5, $n - p \leq 0$, so that we have $\phi_x(x) = const$ for any $x \in (x_1, x_2)$. If $p(x_1) = p(x_2)$, then $J = 0$ by Theorem 3.1. Thus, this possibility is disallowed. It follows that $\phi_x(x) = 0$ for any $x \in (x_1, x_2)$. From the simultaneous nonnegativity of ϕ_x and its decrease, we obtain $\phi_x(x) = 0$ for any $x \in [x_1, 1]$. With this result and equation (3), we conclude that

$$p_x(x) = p_x(y)\ \forall x, y \in [x_1, 1]. \tag{46}$$

This leads to the representation of $p(x)$ as a straight line segment in $[x_1, 1]$. This is the desired contradiction. It follows that p is increasing. Similarly, we can prove the monotonicity of n. This concludes the proof. □

3.3. Summary of properties for simple boundary values. The effect of the mass flux law, the power dissipation law, and the current-field principle, when combined with the monotonicity properties of the concentrations, allows for a complete categorization of the possible modes of behavior. Properties of solutions with corresponding simple boundary conditions, $n_R = p_R = c_R$, $n_L = p_L = c_L$, are thus summarized.

Case 1. $c_L \leq c_R$, $V \geq 0$.

(1) $IV \geq 0$, $J \geq 0$; (2) $\phi_x \leq 0$; (3) $n \geq p$, *i.e.*, $\phi_{xx} \geq 0$; (4) n_x, $p_x \geq 0$.

Case 2. $c_L \leq c_R$, $V \leq 0$.

(1) $IV \geq 0$, $J \geq 0$; (2) $\phi_x \geq 0$; (3) $n \leq p$, *i.e.*, $\phi_{xx} \leq 0$; (4) n_x, $p_x \geq 0$.

Case 3. $c_L \geq c_R$, $V \leq 0$.

(1) $IV \geq 0$, $J \leq 0$; (2) $\phi_x \geq 0$; (3) $n \geq p$, *i.e.*, $\phi_{xx} \geq 0$; (4) n_x, $p_x \leq 0$.

Case 4. $c_L \geq c_R$, $V \geq 0$.

(1) $IV \geq 0$, $J \leq 0$; (2) $\phi_x \leq 0$; (3) $n \leq p$, *i.e.*, $\phi_{xx} \leq 0$; (4) n_x, $p_x \leq 0$.

Remark. In cases 1 and 2, if $c_L < c_R$, then $J_n < 0$, $J_p > 0$ cannot occur simultaneously. In cases 3 and 4, if $c_L > c_R$, then $J_n > 0$, $J_p < 0$ cannot occur simultaneously.

3.4. Uniqueness of solutions for simple boundary values. We state and prove our uniqueness theorem without any restriction on V. The proof is based on the IV relation of Theorem 3.2, and the current-field relation of Proposition 3.4. The result of Alabau [1] does not cover the ranges, of greatest biological, chemical, and engineering interest,

$$\ln\left(\frac{c_L}{c_R}\right) \leq V \leq \ln\left(\frac{c_R}{c_L}\right) \quad (c_R \geq c_L),$$

$$\ln\left(\frac{c_R}{c_L}\right) \leq V \leq \ln\left(\frac{c_L}{c_R}\right) \quad (c_R \leq c_L).$$

THEOREM 3.8 (Uniqueness). *For any applied bias $V \in (-\infty, \infty)$, the nonlinear system of P-N-P equations with simple boundary conditions has a unique solution $(\phi, n, p, J_n, J_p) \in \left(H^2([0,1])\right)^3 \times R^2$. The first three components are actually arbitrarily smooth.*

Prior to the actual proof, we shall develop some basic results, which will later be drawn on in the course of the proof. We start by assuming the existence of two solutions, say $U = (\phi, n, p, J_n, J_p)$ and $\tilde{U} = (\tilde{\phi}, \tilde{n}, \tilde{p}, \tilde{J}_n, \tilde{J}_p)$. Let

$$\psi = \phi - \tilde{\phi},\ \omega = p - \tilde{p},\ \nu = n - \tilde{n},\ j_n = J_n - \tilde{J}_n,\ j_p = J_p - \tilde{J}_p. \tag{47}$$

Then the equations for the 'difference' fields are:

$$-\lambda^2 \psi_{xx} = \omega - \nu,, \tag{48}$$

$$j_n = \nu_x - \nu\Phi_x - N\psi_x, \tag{49}$$

$$-j_p = \omega_x + \omega\Phi_x + P\psi_x. \tag{50}$$

In these equations, P, N and Φ are averages of the two solutions, viz. ,

$$\Phi = \frac{1}{2}(\phi + \tilde{\phi}),\ P = \frac{1}{2}(p + \tilde{p}),\ N = \frac{1}{2}(n + \tilde{n}). \tag{51}$$

The boundary conditions for the system (48)-(50) are:

$$\omega(0) = \nu(0) = \psi(0) = 0, \tag{52}$$

$$\omega(1) = \nu(1) = \psi(1) = 0. \tag{53}$$

Of course, for simple boundary conditions, we also have

$$P(0) = N(0) = c_L, \qquad \Phi(0) = V, \tag{54}$$

$$P(1) = N(1) = c_R, \qquad \Phi(1) = 0. \tag{55}$$

In the proof, there is no loss of generality in limiting the analysis to the cases,

$$j_n \leq 0,\ \ j_p \leq 0; \tag{56}$$

$$j_n \leq 0,\ \ j_p > 0, \tag{57}$$

since an interchange of U and $\tilde{U}$ can always achieve this. Within the scope of these cases, we distinguish the following principal categories:

(i) Category A:

$$i := j_n + j_p \leq 0; \tag{58}$$

(ii) Category B:

$$i > 0. \tag{59}$$

Within the two categories, A and B, we distinguish subcategories:

1. Category A1:

$$\psi_x(0) \geq 0, \quad \psi_x(1) \geq 0; \tag{60}$$

2. its logical complement, Category A2.
3. Category B1:

$$\psi_x(0) \leq 0, \quad \psi_x(1) \leq 0; \tag{61}$$

4. its logical complement, Category B2.

The following lemma is critical to the proof.

LEMMA 3.9. *Let $[0, x_0] = G_0$ and $[x_1, 1] = G_1$ be two intervals such that $\psi_x(x_0) = \psi_x(x_1) = 0$, and such that ψ_x is of one sign on G_0 and (a possibly different sign) on G_1. Then, if $j_n \psi_x \geq 0$ on these intervals,*

$$\nu \leq \text{(resp. } \geq \text{) } 0 \text{ on } G_0 \text{ (respectively on } G_1\text{);} \tag{62}$$

and, if $j_p \psi_x \geq 0$ on these intervals,

$$\text{sign}(j_p)\omega \leq \text{(resp. } \geq \text{) } 0 \text{ on } G_0 \text{ (respectively on } G_1\text{).} \tag{63}$$

Proof. When integrating factors are used in (49) and (50), we obtain

$$(\exp(-\Phi)\nu)' = \exp(-\Phi)(N\psi_x + j_n), \tag{64}$$

$$(\exp(\Phi)\omega)' = -\exp(\Phi)(P\psi_x + j_p). \tag{65}$$

The result follows by integration over G_0 and G_1. □

Proof. (Theorem 3.8) Cases A1 and B1 require an application of an "energy" argument to a second order equation for ψ_x. This is quite different from the approach of [1], though the basic approach of [1] is used for the other subcases. We proceed to derive this equation now. We are indebted to Victor Barcilon for the details of the derivation.

Differentiating the Poisson equation (48) and eliminating ω and ν whenever possible, we write

$$\begin{aligned} -\lambda^2 \psi_{xxx} &= \omega_x - \nu_x \\ &= -(j_n + j_p) - (\omega + \nu)\Phi_x - (P + N)\psi_x \end{aligned} \tag{66}$$

i.e. ,

$$-\lambda^2\psi_{xxx} + (P+N)\psi_x = -i - (\omega+\nu)\Phi_x. \tag{67}$$

In order to eliminate $\omega+\nu$, we integrate the Nernst-Planck equations (49)-(50), viz.,

$$\begin{aligned} -j_p x &= \omega + \int_0^x \omega\Phi_x\,dx + \int_0^x P\psi_x\,dx, \\ j_n x &= \nu - \int_0^x \nu\Phi_x\,dx - \int_0^x N\psi_x\,dx. \end{aligned} \tag{68}$$

Adding these equations yields

$$\begin{aligned} (-j_p + j_n)x &= \omega + \nu + \int_0^x (\omega-\nu)\Phi_x\,dx + \int_0^x (P-N)\psi_x\,dx \\ &= \omega + \nu - \lambda^2\int_0^x \psi_{xx}\Phi_x\,dx - \lambda^2\int_0^x \Phi_{xx}\psi_x\,dx \\ &= \omega + \nu - \lambda^2\big[\psi_x\Phi_x - \Phi_x(0)\psi_x(0)\big]. \end{aligned} \tag{69}$$

In summary, the third order ordinary differential equation is:

$$-\lambda^2\psi_{xxx} + \big[(P+N) + \lambda^2(\Phi_x)^2\big]\psi_x = -i - \big[jx - \lambda^2\Phi_x(0)\psi_x(0)\big]\Phi_x, \tag{70}$$

where

$$j = j_n - j_p. \tag{71}$$

If we define

$$f = \psi_x, \tag{72}$$

then the above equation becomes

$$-\lambda^2 f_{xx} + a^2 f = -i + \big[-jx + \lambda^2\Phi_x(0)\psi_x(0)\big]\Phi_x, \tag{73}$$

with

$$f_x(0) = f_x(1) = 0, \tag{74}$$

and

$$a^2 = \big[(P+N) + \lambda^2(\Phi_x)^2\big]. \tag{75}$$

This is the desired equation. We note that the sign of Φ_x is constant (and opposite to that of V) on $[0,1]$ by Theorem 3.2 and Proposition 3.4, and that $-jx + \lambda^2\Phi_x(0)\psi_x(0)$ does not change sign on $[0,1]$ if $\psi_x(0)\psi_x(1) \geq 0$, since $-j+\lambda^2\Phi_x(0)\psi_x(0) =$

$\lambda^2\Phi_x(1)\psi_x(1)$. In particular, the right hand side of (73) is nonnegative in case A1, and nonpositive in case B1.

Defining $f^- = \min(f, 0)$ and $f^+ = \max(f, 0)$, we multiply (73) by f^- in case A1 and by f^+ in case B1, then integrate over $[0, 1]$. We obtain, in case A1, $f^- \equiv 0$, and, in case B1, $f^+ \equiv 0$. These results are immediate from $0 \le \int_0^1 (\lambda^2 (f_x^-)^2 + a^2 (f^-)^2)\, dx \le 0$, and a similar relation for f^+. Simple calculus implies that the only conclusion compatible with $\psi(0) = \psi(1) = 0$ and $f^- \equiv 0$ is $f \equiv 0$, which implies $\psi \equiv 0$. A similar statement holds in regard to $f^+ \equiv 0$. This yields "uniqueness" in cases A1 and B1.

The approach in cases A2 and B2 is similar. We note that one or both of the subintervals G_0, G_1 of Lemma 3.9 exist in these cases since $\psi(0) = \psi(1) = 0$. We must distinguish between the subcases when $j_p \le 0$ and when $j_p > 0$ ($j_n \le 0$ always). When $j_p \le 0$, we note that case A2 alone occurs, and we use Lemma 3.9 and (48) to deduce that $\psi_{xx} \le 0$ on G_0 (or ≥ 0 on G_1). Either instance of this behavior of ψ_{xx} is incompatible with ψ_x vanishing at x_0 or x_1. Thus, we consider: Categories A2 and B2,

$$j_p > 0. \tag{76}$$

It is important to notice that $j < 0$ when $j_p > 0$. This ensures the inequality,

$$-jx + \lambda^2\Phi_x(0)\psi_x(0) < -jy + \lambda^2\Phi_x(0)\psi_x(0), \quad 0 < x < y < 1. \tag{77}$$

Now the following two equations can be derived from (48) and (69):

$$\begin{aligned} -\lambda^2\psi_{xx} + \lambda^2\Phi_x\psi_x &= 2\omega - jx + \lambda^2\Phi_x(0)\psi_x(0), \\ \lambda^2\psi_{xx} + \lambda^2\Phi_x\psi_x &= 2\nu - jx + \lambda^2\Phi_x(0)\psi_x(0). \end{aligned}$$

These equations can be used in conjunction with Lemma 3.9 to prove the following fundamental inequalities. For $\pi_0 = -\mathrm{sign}[\psi_x(0)],\ \pi_1 = -\mathrm{sign}[\psi_x(1)]$,

$$\pi_0\lambda^2(\psi_x \exp(\pi_0\Phi))' \le [-jx_0 + \lambda^2\Phi_x(0)\psi_x(0)]\exp(\pi_0\Phi) \text{ on } G_0, \tag{78}$$

$$[-jx_1 + \lambda^2\Phi_x(0)\psi_x(0)]\exp(\pi_1\Phi) \le \pi_1\lambda^2(\psi_x \exp(\pi_1\Phi))' \text{ on } G_1. \tag{79}$$

If inequality (77) is employed in conjunction with integration of inequalities (78) and (79) over G_0 and G_1, one obtains the conclusion, for some positive constants C_0 and C_1,

$$C_0|\psi_x(0)| < -C_1|\psi_x(1)|. \tag{80}$$

In categories A2 and B2 this leads to a contradiction, showing that these categories are vacuous. This concludes the proof of the theorem. □

4. General boundary conditions. In this section, we permit a choice of general boundary conditions. We find it convenient to introduce categories, defined by the comparison of their numerical values. Because all ionic solutions that can be made are nearly electroneutral, general boundary conditions describe a situation in which additional ions are present that do not enter the domain Ω, and do not modify its boundary conditions. Such ions are called "impermanent ions" in physiology and "supporting electrolytes" in electrochemistry. There does not appear to be a common term in semiconductor theory, due to the fact that simple boundary conditions with nonvanishing permanent charge (doping) define the canonical problem in this subject for so-called Ohmic contacts. Nonetheless, electroneutral boundary conditions need not hold for other contacts, and are worth consideration even in semiconductor theory.

The number of possible subcategories is large, sixteen in all, though these are reduced by one-half via the symmetries introduced in §2.1. The distinctions are both natural and necessary to distinguish different modes of behavior of the system solutions.

4.1. The relations between fluxes and boundary conditions. Thus, we define the following categories, distinguished primarily by boundary conditions, and secondarily by fluxes.

$$\text{(BC1)} \quad 0 < p_L \le n_L, \ 0 < n_R \le p_R. \tag{81}$$

(1.1) $J_n \ge 0, J_p \ge 0$;
(1.2) $J_n \ge 0, J_p < 0$;
(1.3) $J_n < 0, J_p \ge 0$;
(1.4) $J_n < 0, J_p < 0$.

$$\text{(BC2)} \quad 0 < p_L \le n_L, \ 0 < p_R \le n_R. \tag{82}$$

(2.1) $J_n \ge 0, J_p \ge 0$;
(2.2) $J_n \ge 0, J_p < 0$;
(2.3) $J_n < 0, J_p \ge 0$;
(2.4) $J_n < 0, J_p < 0$.

$$\text{(BC3)} \quad 0 < n_L \le p_L, \ 0 < p_R \le n_R. \tag{83}$$

$$\text{(BC4)} \quad 0 < n_L \le p_L, \ 0 < n_R \le p_R. \tag{84}$$

In terms of the numbers introduced in (18), the primary categories can be described by

$$\text{(BC1)}: \ \rho_L \le 1, \rho_R \ge 1; \tag{85}$$
$$\text{(BC2)}: \ \rho_L \le 1, \rho_R \le 1; \tag{86}$$
$$\text{(BC3)}: \ \rho_L \ge 1, \rho_R \le 1; \tag{87}$$
$$\text{(BC4)}: \ \rho_L \ge 1, \rho_R \ge 1. \tag{88}$$

The coordinates ρ_L and ρ_R do not characterize the current and flux.

PROPOSITION 4.1 (Redundancy of Categories Three and Four). *Categories (BC3) and (BC4) are logically equivalent to (BC1) and (BC2), respectively.*

Proof. If we employ the first symmetry of §2.1, we find that the equations are structurally unchanged, but (BC1) and (BC3) have been interchanged, together with the flux subcategories. This means that (BC3) is logically included in (BC1). If we employ the second symmetry, we find that, again, the equations are unchanged, but (BC2) and (BC4) have been interchanged, together with the flux subcategories. This means that (BC4) is logically included in (BC2). The reverse implications are also valid. □

From the equations for J_n and J_p, we can derive the following relations between the signs of the fluxes and the boundary conditions, i.e.,

(i) $J_n > 0,\ J_p > 0$, if and only if

$$\max\left(\ln\left(\frac{n_L}{n_R}\right), \ln\left(\frac{p_R}{p_L}\right)\right) < V; \tag{89}$$

(ii) $J_n > 0,\ J_p < 0$, if and only if

$$\ln\left(\frac{n_L}{n_R}\right) < V < \ln\left(\frac{p_R}{p_L}\right); \tag{90}$$

(iii) $J_n < 0,\ J_p > 0$, if and only if

$$\ln\left(\frac{p_R}{p_L}\right) < V < \ln\left(\frac{n_L}{n_R}\right); \tag{91}$$

(iv) $J_n < 0,\ J_p < 0$, if and only if

$$V < \min\left(\ln\left(\frac{p_R}{p_L}\right), \ln\left(\frac{n_L}{n_R}\right)\right). \tag{92}$$

By the above relations and the boundary conditions, we can derive the following lemma easily.

LEMMA 4.2. *With (BC1), if we assume $p_L > p_R$, then $J_n > 0,\ J_p < 0$ cannot occur simultaneously. Also, if $n_R > n_L$, then $J_n < 0,\ J_p > 0$ cannot occur simultaneously. With (BC2), if $p_L > n_R$, then $J_n > 0,\ J_p < 0$ cannot occur simultaneously. Also, if $p_R > n_L$, then $J_n < 0,\ J_p > 0$ cannot occur simultaneously.*

4.2. Properties of solutions with (BC1). In this subsection, we shall show, in the case of (BC1), that the curves for n and p cross exactly once, and we shall demonstrate monotonicity properties of n and p. We shall also generalize the current–field alignment property of Proposition 3.4.

PROPOSITION 4.3 (Single Crossing). *Consider nonlinear system (1)-(6) with (BC1), with $\rho_L \neq 1$ and $\rho_R \neq 1$. Then the curves for n and p cross each other exactly once in Ω.*

Proof. If the conclusion does not hold, there exist intervals $[x_1, x_2]$, $[x_3, x_4]$, such that

$$\begin{aligned}
&n(x_1) = p(x_1) = c_1,\\
&n(x_2) = p(x_2) = c_2,\\
&(p - n)(x) > 0 \quad \text{for } x \in (x_1, x_2),
\end{aligned}$$

and

$$\begin{aligned}
&n(x_3) = p(x_3) = c_3,\\
&n(x_4) = p(x_4) = c_4,\\
&(p-n)(x) < 0 \quad \text{for } x \in (x_3, x_4).
\end{aligned}$$

First, assume that $IJ > 0$. The conjunction of this property, with the description of the interval $[x_1, x_2]$ as one on which simple boundary conditions are satisfied, contradicts Theorem 3.5. If $IJ < 0$, this again contradicts Theorem 3.5 in relation to the interval $[x_3, x_4]$. The case $IJ = 0$ requires separate consideration of $I = 0$ and $J = 0$. We may consider the interval $[x_1, x_2]$. $I = 0$ contradicts the final statement of Theorem 3.2, while $J = 0$ contradicts the final statement of Theorem 3.1. The proof is concluded. □

Lemma 4.4 (Generalized Current–Field Property). *Consider the nonlinear system (1)-(6) with (BC1). If $I \geq 0$, then $\phi_x(x) \leq 0$, $\forall x \in \Omega$. No claim is made if $I \leq 0$.*

Proof. The proof follows that of Proposition 3.4, with one change. The conclusions,

$$\phi_{xx}(0) < 0, \quad \phi_{xx}(1) > 0,$$

at the relevant endpoints, contradict the (BC1) property, $\phi_{xx}(0) \geq 0, \phi_{xx}(1) \leq 0$. Otherwise, the nonpositivity of ϕ_x when $I \geq 0$ follows as before. □

Proposition 4.5 (Restricted Monotonicity). *Consider the nonlinear system (1)-(6) with (BC1).*

$$\begin{aligned}
&(a) \text{ If } I \geq 0,\ J_p \leq 0, \text{ then } p_x \geq 0.\\
&(b) \text{ If } I \geq 0,\ J_n \leq 0, \text{ then } n_x \leq 0.
\end{aligned}$$

Proof. We can prove (a) and (b) from the continuity equations and the nonpositivity of ϕ_x, which follows from Lemma 4.4. This concludes the proof. □

Remark. It follows from the first part of Lemma 4.2 that, if both $p_L > p_R$ and $n_R > n_L$, then the hypotheses of (a) and (b) do not hold. Clearly, the conclusions cannot hold either, in this case.

4.3. Some properties of solutions with (BC2). Since the values of n dominate those of p at the endpoints in this case, it is natural to investigate whether this holds over the entire interval. The following theorem provides a partial answer.

Theorem 4.6 (Domination of Concentrations). *Consider the nonlinear system (1)-(6) with (BC2), with $\rho_L \neq 1$ and $\rho_R \neq 1$. Assume that $IJ \geq 0$. Then the following properties hold.*

$$\begin{aligned}
&(a) \ n - p \geq 0.\\
&(b) \ \min(p_L, p_R) \leq p \leq n \leq \max(n_L, n_R).
\end{aligned}$$

Proof. If (a) fails, there exists an interval $[x_1, x_2]$ such that

$$\begin{aligned}
&n(x_1) = p(x_1) = c_1,\\
&n(x_2) = p(x_2) = c_2,\\
&(p-n)(x) > 0 \quad \text{for } x \in (x_1, x_2).
\end{aligned}$$

Note that this contradicts Theorem 3.5 if $IJ \geq 0$, so that $n - p \geq 0$ in this case.

To prove (b), we use the maximum principle on n and part (a). For simplicity, let $n_R \leq n_L,\ p_R \leq p_L$. We differentiate the continuity equation for n once, and then we have the following second order equation:

$$n_{xx} - n_x\phi_x - n\phi_{xx} = 0.$$

By the maximum principle ([8, Cor. 3.2]) and (a) (so that $\phi_{xx} \geq 0$), we conclude that

$$p \leq n \leq n_L, \tag{93}$$

which establishes the second inequality of (b) in a typical subcase. Next, to prove $p \geq p_R$ in this subcase, we proceed as follows. Assume the existence of an interval, say (x_1, x_2), such that

$$p(x) < p_R \text{ for } x \in (x_1, x_2), \tag{94}$$

$$p(x_1) = p_R,\ p(x_2) = p_R. \tag{95}$$

Then, the equation (3), written for x_1 and x_2, reads:

$$\begin{aligned}
p_x(x_1) + p_R\phi_x(x_1) = -J_p,\\
p_x(x_2) + p_R\phi_x(x_2) = -J_p.
\end{aligned}$$

If we subtract these two equations, we see that

$$p_x(x_2) - p_x(x_1) + p_R(\phi_x(x_2) - \phi_x(x_1)) = 0. \tag{96}$$

But the left hand side of the above equation is strictly positive by the assumptions (94), (95), and the monotonicity of ϕ_x. This is the desired contradiction. Hence (b) holds. The other subcases are similar. This completes the proof. $\square$

4.4. Non-uniformly diffusing systems of multiple species. We can extend the results in this paper to three species, e.g., one negative ion, and two positive ions. Then the system becomes

$$\begin{aligned}
\lambda^2\phi_{xx} - n + p_1 + p_2 &= 0,\\
n_x - n\phi_x &= J_n,\\
D_1(p_1^{'} + p_1\phi_x) &= -J_{p_1},\\
D_2(p_2^{'} + p_2\phi_x) &= -J_{p_2},
\end{aligned}$$

in $\Omega = (0,1)$, where we have normalized the diffusion coefficient of the negative ion species, and permitted distinct diffusion coefficients D_1, D_2 for the positive ion species. We have also chosen units in which $kT_0 = 1$. Let $J_p = \frac{J_{p_1}}{D_1} + \frac{J_{p_2}}{D_2}$ and $p = p_1 + p_2$. Then the system for three species reduces to the two species system, with the scaled quantities J and I. Thus, we can extend all the results in this paper to systems of three and more species, with the scalings indicated.

5. Contraction mapping alternative. We consider a more general form of the nonlinear system of PNP equations, with nonvanishing permanent charge $N(x)$, on an interval of length d. Such permanent charge governs the qualitative properties of transistors and is thought to be important in channels [9]. The length parameter d is correlated with the dimensionless parameter λ, and satisfies $d = \theta\lambda$. In this section, we shall analyze the system on the left layer $[0, d]$, and we shall explicitly estimate the condition on θ to ensure that the system possesses a strictly contractive fixed point mapping. This means that successive approximation is a valid numerical procedure on such an interval. The boundary conditions at the left endpoint are those given, while those at the right endpoint are determined by some other method. This includes, for example, the boundary condition used to compute the boundary layer solution associated with the perturbation solution, analyzed at length in [3]. The complete system is given by

$$\lambda^2\phi_{xx} = n - p + N(x), \tag{97}$$
$$J_n = n_x - n\phi_x, \tag{98}$$
$$J_p = -p_x - p\phi_x, \tag{99}$$

on $\Omega_b = (0, d)$, with

$$n(0) = n_L,\ n(d) = n_d, \tag{100}$$
$$p(0) = p_L,\ p(d) = p_d, \tag{101}$$
$$\phi(0) = \phi_0,\ \phi(d) = \phi_d. \tag{102}$$

Let ϕ_* be the intrinsic potential, which is the constant system potential in the case of electroneutrality. We introduce the Slotboom variables, ν, ω, customary in semiconductor theory, so that n and p are given by

$$n = e^{\phi-\phi_*}\nu,\ \ p = e^{\phi_*-\phi}\omega. \tag{103}$$

Then the PNP model is expressed by the system of differential equations,

$$\lambda^2\phi_{xx} - e^{\phi-\phi_*}\nu + e^{\phi_*-\phi}\omega - N = 0, \tag{104}$$
$$(e^{\phi-\phi_*}\nu_x)_x = 0, \tag{105}$$
$$(e^{\phi_*-\phi}\omega_x)_x = 0, \tag{106}$$

with the boundary conditions,

$$\nu(0) = \nu_0,\ \nu(d) = \nu_d, \tag{107}$$
$$\omega(0) = \omega_0,\ \omega(d) = \omega_d, \tag{108}$$
$$\phi(0) = \phi_0,\ \phi(d) = \phi_d. \tag{109}$$

In our analysis, we employ the contraction mapping framework. We define a fixed point mapping after introducing the following terminology. Let

$$K = \{\tilde{\nu} | \alpha_\nu \le \tilde{\nu} \le \beta_\nu\} \times \{\tilde{\omega} | \alpha_\omega \le \tilde{\omega} \le \beta_\omega\}, \tag{110}$$

where

$$\alpha_\nu = \inf(\nu_0, \nu_d),\ \beta_\nu = \sup(\nu_0, \nu_d),\ \alpha_\omega = \inf(\omega_0, \omega_d),\ \beta_\omega = \sup(\omega_0, \omega_d).$$

Also, set

$$\begin{aligned}
\alpha &= \min(\alpha_\nu, \alpha_\omega),\\
\beta &= \max(\beta_\nu, \beta_\omega),\\
\gamma &= \min(\inf(\phi_0, \phi_d), \gamma^{'}),\\
\delta &= \max(\sup(\phi_0, \phi_d), \delta^{'}),
\end{aligned}$$

where $\gamma^{'}$ and $\delta^{'}$ are uniquely defined by

$$e^{\gamma^{'} - \alpha} - e^{\alpha - \gamma^{'}} - \inf N = 0,$$

and

$$e^{\delta^{'} - \beta} - e^{\beta - \delta^{'}} - \sup N = 0.$$

Define

$$T_s : K \to (H^1(\Omega_b))^2, \tag{111}$$

$T_s(\tilde{\nu}, \tilde{\omega}) = [\nu, \omega]$, where $\nu,\ \omega$ solve the following equations:

$$(e^{\tilde{\phi} - \phi_*} \nu_x)_x = 0, \tag{112}$$

$$(e^{\phi_* - \tilde{\phi}} \omega_x)_x = 0, \tag{113}$$

with $\tilde{\phi} = \phi(\tilde{\nu}, \tilde{\omega})$.

THEOREM 5.1 (Contraction Constant). *Assume that the boundary data $n_L,\ n_d,\ p_L,\ p_d,\ \phi_0,\ \phi_d$ are given, and $N \in L^\infty(\Omega_b)$. Then the Gummel map T_s is well defined and K is invariant under T_s. Also, on K, there exists a constant C such that T_s satisfies*

$$\int_{\Omega_b} \{|\nu_1 - \nu_2|^2 + |\omega_1 - \omega_2|^2\} dx \le C \int_{\Omega_b} \{|\tilde{\nu_1} - \tilde{\nu_2}|^2 + |\tilde{\omega_1} - \tilde{\omega_2}|^2\}, \tag{114}$$

where $[\nu_i, \omega_i] = T_s(\tilde{\nu_i}, \tilde{\omega_i}),\ i = 1, 2,$ and, if $d = \theta\lambda$, C is given by

$$C = 4 e^{8(\delta - \gamma)} \theta^4 \max\{|n_d e^V - n_L|^2, |p_d e^{-V} - p_L|^2\}. \tag{115}$$

Remark. If $C < 1$, then we can choose $[\nu_0, \omega_0]$ arbitrarily in K, and the Picard iterates, $(\nu_m, \omega_m) = T_s^m(\nu_0, \omega_0)$, will converge to the unique fixed point of T_s in K as $m \to \infty$, i.e., the PNP model has a unique solution.

To prove Theorem 5.1, we need several lemmas.

Lemma 5.2. *We have the inequality,*

$$\int_{\Omega_b} \{|(\nu_1-\nu_2)_x|^2 + |(\omega_1-\omega_2)_x|^2\}dx \le 2e^{2(\delta-\gamma)} \int_{\Omega_b} |\tilde{\phi_1}-\tilde{\phi_2}|^2 W dx, \tag{116}$$

where W is an apriori bound for $|(\nu_2)_x|^2,\ |(\omega_2)_x|^2$.

Proof. Consider the weak solution of the PNP equations. Then

$$\int_{\Omega_b} e^{\tilde{\phi}-\tilde{\phi}_*}\nu_x\psi_x dx = 0, \tag{117}$$

where $\forall\psi\in H_0^1(\Omega_b)$. We successively rewrite the above equation with $\tilde{\phi}=\tilde{\phi_i},\ i=1,2$. If we subtract these equations, let $\psi=\nu_1-\nu_2$, and use Young's inequality, we have the following:

$$\int_{\Omega_b} \{|(\nu_1-\nu_2)_x|^2 \le e^{2(\delta-\gamma)} \int_{\Omega_b} |\tilde{\phi_1}-\tilde{\phi_2}|^2|\nu_x|^2 dx. \tag{118}$$

Similarly, we have same inequality on ω. □

Lemma 5.3. *We have the inequality,*

$$\int_{\Omega_b} |(\tilde{\phi_1}-\tilde{\phi_2})_x|^2 dx \le c\cdot d^2 \left\{\int_{\Omega_b} |\tilde{\nu_1}-\tilde{\nu_2}|^2 dx + \int_{\Omega_b} |\tilde{\omega_1}-\tilde{\omega_2}|^2 dx\right\} \tag{119}$$

for any $[\tilde{\nu_1},\tilde{\omega_1}]$, $[\tilde{\nu_2},\tilde{\omega_2}]$ in K, where

$$c = \frac{2}{\lambda^4}\max(e^{2(\delta-\phi_*)},\ e^{2(\phi_*-\gamma)}).$$

Proof. We begin by noting the weak form of Poisson's equation,

$$\lambda^2\int_{\Omega_b}\phi_x\psi_x dx + \int_{\Omega_b}(e^{\phi-\phi_*}\nu - e^{-(\phi-\phi_*)}\omega - N)\psi = 0, \tag{120}$$

$\forall\psi\in H_0^1(\Omega_b)$. Given $\nu=\tilde{\nu_i},\ \omega=\tilde{\omega_i},\ i=1,2$, we consider two equations for $\tilde{\phi_i}$, subtract them, and set $\psi=\phi_1-\phi_2$. Then we obtain, using Young's inequality,

$$\begin{aligned}
&\lambda^2\int_{\Omega_b}|(\tilde{\phi_1}-\tilde{\phi_2})_x|^2dx + \int_{\Omega_b} e^{\tilde{\phi_2}-\phi_*}(e^{\tilde{\phi_1}-\tilde{\phi_2}}-1)\tilde{\nu_1}(\tilde{\phi_1}-\tilde{\phi_2})dx \\
&+\int_{\Omega_b} e^{-(\tilde{\phi_2}-\phi_*)}(1-e^{-(\tilde{\phi_1}-\tilde{\phi_2})})\tilde{\omega_1}(\tilde{\phi_1}-\tilde{\phi_2})dx \\
&\le \max(e^{2(\delta-\phi_*)},\ e^{2(\phi_*-\gamma)})\frac{d^2}{\lambda^2}\int[|\tilde{\nu_1}-\tilde{\nu_2}|^2+|\tilde{\omega_1}-\tilde{\omega_2}|^2]dx + \frac{\lambda^2}{2d^2}\int_{\Omega_b}|\tilde{\phi_1}-\tilde{\phi_2}|^2dx.
\end{aligned}$$

By the Poincaré inequality, we have

$$\int_{\Omega_b}|(\tilde{\phi_1}-\tilde{\phi_2})_x|^2dx \le \frac{2d^2}{\lambda^4}\max(e^{2(\delta-\phi_*)},\ e^{2(\phi_*-\gamma)})\int_{\Omega_b}[|\tilde{\nu_1}-\tilde{\nu_2}|^2+|\tilde{\omega_1}-\tilde{\omega_2}|^2]dx.$$

□

Proof. (Theorem 5.1). The invariance of K under T_s is easily proved by maximum principles. To prove the inequality, we use the Poincaré inequality and Lemmas 5.2 and 5.3. Thus,

$$\begin{aligned}
&\int_{\Omega_b} \{|\nu_1 - \nu_2|^2 + |\omega_1 - \omega_2|^2\} dx \\
&\leq d^2 \int_{\Omega_b} \{|(\nu_1 - \nu_2)_x|^2 + |(\omega_1 - \omega_2)_x|^2\} dx \\
&\leq 4e^{4(\delta-\gamma)} W \frac{d^6}{\lambda^4} \int_{\Omega_b} \{|\tilde{\nu_1} - \tilde{\nu_2}|^2 + |\tilde{\omega_1} - \tilde{\omega_2}|^2\} dx.
\end{aligned}$$

From (112) and (113) we have the bounds,

$$|(\nu)_x| \leq |J_n| e^{\phi_* - \gamma}, \tag{121}$$

$$|(\omega)_x| \leq |J_p| e^{\delta - \phi_*}. \tag{122}$$

Also from (14), (15), which do not depend upon vanishing permanent charge, we have

$$|J_n| \cdot d \leq |n_d e^V - n_L| \cdot e^{\delta - \phi_0},$$
$$|J_p| \cdot d \leq |p_d e^{-V} - p_L| \cdot e^{\phi_0 - \gamma}.$$

Therefore,

$$C = 4e^{8(\delta-\gamma)} \frac{d^4}{\lambda^4} \max\{|n_d e^V - n_L|^2, |p_d e^{-V} - p_L|^2\}. \tag{123}$$

The substitution $d = \theta\lambda$ completes the proof. □

Remark. Note that, when

$$2e^{4(\delta-\gamma)} \max\{|n_d e^V - n_L|, |p_d e^{-V} - p_L|\} < \frac{1}{\theta^2}, \tag{124}$$

we have the unique solution of the PNP model in the one dimensional case. Here the uniqueness depends on the interval $[0, \theta\lambda]$, and the boundary values. Since successive approximation is known to converge in this case from any starting value in the domain of T_s, we may begin with the boundary layer solution (or modification thereof), introduced in [3], as an excellent starting guess. The paper [3] to follow illustrates in detail many of the possible modes of behavior associated with the general boundary conditions described earlier. Comparisons and contrasts with behavior predicted by a singular perturbation analysis, in terms of the paramater λ, are provided in detail.

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