

POISSON-NERNST-PLANCK MODELS FOR THREE ION SPECIES: MONOTONIC PROFILES VS. OSCILLATORY PROFILES

Long Yan¹, Hongguo Xu² and Weishi Liu^{2,†}

Dedicated to Professor Jibin Li on the occasion of his 80th birthday.

Abstract We consider ionic flows through an ion channel via a quasi-one-dimensional classical Poisson-Nernst-Planck model. The specific biological setup involves ionic solutions with three ion species and the permanent charge is set to be zero. It is known that, for ionic flows with two ion species, the spatial profiles of the electric potential and the ion concentrations are monotonic, independent of boundary conditions. For ionic flows with three or more ion species with at least three different valences, depending on the boundary conditions, the profiles could be oscillatory. In this work, for ionic mixtures with two cation species of different valences and one anion species, we will provide a complete classification in terms of boundary conditions on when the profiles are monotonic and when they are oscillatory. This would be an important step for studies including nonzero permanent charges.

Keywords Ion channel, ion flow, PNP models, three ion species, monotonic vs. oscillatory spatial profiles

MSC(2010) 34A26, 34B16, 92C35.

1. Introduction

1.1. A brief background of ion channels and ionic flows

Ionic flow, migration of charged particles, is essential for living organisms. Moving through membrane channels, ionic flows provide communications between cells to coordinate with each other for biological functions (see [15–19, 40, 45]). Protein structures of ion channels can be viewed as nano valves for life (see, e.g., [5, 8, 9, 22]). Ionic flow properties are major concerns of physiological ion channels and are controlled by the nonlinear interplay among permanent charges (protein structure), transmembrane electric potential, and boundary concentrations of ion species involved. Ionic flow through ion channels is a special electrodiffusion process with a number of specifics. It is a problem with multiple interacting physical parameters and presents multi-scales too (see [1, 10, 11, 27, 28, 38, 39, 41, 42, 50]).

While experimental technology of ionic flow properties has been constantly advanced since the time of Hodgkin and Huxley, the current-voltage (I-V) relation defined in (1.5) below remains to be the major experimental measurement of ionic

[†]The corresponding author. Email: wslu@ku.edu (W. Liu)

¹School of Science, Northeast Electric Power University, Jilin 132012, China

²Department of Mathematics, University of Kansas, Lawrence, Kansas 66045, USA

flows (see, e.g., [2, 4, 7, 23]). The I-V relation is an input-output type information of an average effect of physical parameters on ionic flows; in particular, it is still not possible to “measure/observe” internal dynamical behaviors of ionic flows, such as, the spatial profiles of the electric potential and the ionic concentrations. This limitation of experiments makes it difficult for researchers to extract quantitative information or identify characteristics from experimental data that are critical for classifying general behaviors/phenomena and understanding underlying mechanisms of ionic flows.

The aforementioned challenges strongly suggest the importance and uniqueness of mathematical models and analysis and numerical simulations as complementary tools to the physiological theory and experiments. Mathematical study could provide deep correspondences from the multiple parameters involved to the internal dynamics and to properties of ion channels, at least for the simplified settings used in many biological experiments. The basic primitive models for ionic flows are the Poisson-Nernst-Planck (PNP) type models and have been analyzed and simulated extensively. The geometric singular perturbation theory, relying crucially on special structures of the PNP models, has been developed in [11, 24, 27, 28, 32], which allows a systematical study of several ion channel problems in [3, 12, 20, 25, 26, 29, 33, 34, 47, 48].

In this work, we consider a quasi-one-dimensional classical Poisson-Nernst-Planck (cPNP) system for ionic flow involving three ion species with different valences. Our focus is on basic behaviors of internal dynamics; that is, the monotonicity of the spatial profiles of the electric potential and the ion concentrations. In the case of zero permanent charge, it is known that *the spatial profile of the electric potential is monotonic (see, e.g., [28, 32]) and, for ionic flows with two ion species, the spatial profiles of the ion concentrations are also monotonic, independent of boundary conditions* (see, e.g., [1, 11, 24, 26, 27, 30, 32, 46, 49]). On the other hand, for ionic flows with three or more ion species with at least three different valences, depending on the boundary conditions, the profiles of the ionic concentrations could be oscillatory (see, e.g., [28, 32]). For ionic mixtures with three species (two cation species of different valences and one anion species), we will provide more or less explicit criteria in terms of boundary conditions for monotonic profiles and oscillatory profiles of the ionic concentrations. This would be a first step for studies including nonzero permanent charges (see, e.g., [44]).

1.2. A quasi-one-dimensional model

For ionic solution involving n types of ion species, a quasi-one-dimensional stationary PNP model is (see, e.g., [31, 35])

$$\begin{aligned} \frac{1}{\mathcal{A}(X)} \frac{d}{dX} \left(\varepsilon_r(X) \varepsilon_0 \mathcal{A}(X) \frac{d\Phi}{dX} \right) &= -e_0 \left(\sum_{s=1}^n z_s C_s + \mathcal{Q}(X) \right), \\ \frac{d\mathcal{J}_k}{dX} &= 0, \quad -\mathcal{J}_k = \frac{1}{k_B T} \mathcal{D}_k(X) \mathcal{A}(X) C_k \frac{d\mu_k}{dX}, \quad k = 1, 2, \dots, n, \end{aligned} \quad (1.1)$$

where $X \in [a, b]$ is the coordinate along the longitudinal axis of the channel, $\mathcal{A}(X)$ is the cross-section area of the channel over X , $\varepsilon_r(X)$ is the relative dielectric coefficient, ε_0 is the vacuum permittivity, e_0 is the elementary charge, $\mathcal{Q}(X)$ is the permanent charge density, k_B is the Boltzmann constant, T is the absolute temperature; Φ is the electric potential, and, for the k -th ion species, z_k is the

valence (the number of charges per particle), C_k is the concentration, $\mathcal{J}_k(X)$ is the flux density through the cross-section over X , $\mathcal{D}_k(X)$ is the diffusion coefficient, and μ_k is the electrochemical potential depending on Φ and C_k .

The electrochemical potential $\mu_k = \mu_k^{id} + \mu_k^{ex}$ consists of the ideal component μ_k^{id} and the excess component μ_k^{ex} . The ideal component μ_k^{id} is given by

$$\mu_k^{id} = z_k e_0 \Phi + k_B T \ln \frac{C_k}{C_0} \quad (1.2)$$

and accounts for point-charge effect, where C_0 is a characteristic concentration. The excess component μ_k^{ex} accounts for finite sizes of ions that is not completely understood but has been approximated and tested extensively (see, e.g., [6, 13, 14, 21, 24, 36, 37, 43]). The *classical* PNP (cPNP) model deals only with the ideal component μ_k^{id} .

Associated to system (1.1), we consider boundary conditions, for $k = 1, 2, \dots, n$,

$$\Phi(a) = \mathcal{V}, \quad C_k(a) = \mathcal{L}_k > 0; \quad \Phi(b) = 0, \quad C_k(b) = \mathcal{R}_k > 0. \quad (1.3)$$

For boundary conditions, one often imposes the electroneutrality conditions to avoid sharp boundary layers (see, e.g., [47, 48] for a reason)

$$\sum_{s=1}^n z_s \mathcal{L}_s = \sum_{s=1}^n z_s \mathcal{R}_s = 0. \quad (1.4)$$

A major quantity from lab experiments is *the I-V (current-voltage) relation* defined, in terms of solutions of the boundary value problem (BVP) (1.1) and (1.3), as follows. For fixed \mathcal{L}_k 's and \mathcal{R}_k 's, a solution $(\Phi, C_k, \mathcal{J}_k)$ of the BVP will depend on the voltage \mathcal{V} only. The stationary current (*the flow rate of charges*), \mathcal{I} , is given by

$$\mathcal{I} = \sum_{s=1}^n z_s \mathcal{J}_s(\mathcal{V}; \{\mathcal{L}_k\}, \{\mathcal{R}_k\}). \quad (1.5)$$

1.3. The dimensionless quasi-one-dimensional PNP model

For convenience of mathematical analysis of the BVP (1.1) and (1.3), we will work on a dimensionless form. Let C_0 be a characteristic concentration of the problems, for example,

$$C_0 = \max_{1 \leq k \leq n} \{ \mathcal{L}_k, \mathcal{R}_k, \sup_{X \in [a, b]} |\mathcal{Q}(X)| \}.$$

Set

$$\mathcal{D}_0 = \max_{1 \leq k \leq n} \left\{ \sup_{X \in [a, b]} \mathcal{D}_k(X) \right\} \quad \text{and} \quad \hat{\varepsilon}_r = \sup_{X \in [a, b]} \varepsilon_r(X).$$

Let

$$\begin{aligned} x &= \frac{X - a}{b - a}, \quad A(x) = \frac{\mathcal{A}(X)}{(b - a)^2}, \quad D_k(x) = \frac{\mathcal{D}_k(X)}{\mathcal{D}_0}, \quad Q(x) = \frac{\mathcal{Q}(X)}{C_0}, \\ \bar{\varepsilon}_r(x) &= \frac{\varepsilon_r(X)}{\hat{\varepsilon}_r}, \quad \varepsilon^2 = \frac{\bar{\varepsilon}_r \varepsilon_0 k_B T}{e_0^2 (b - a)^2 C_0}, \quad \bar{\mu}_k = \frac{1}{k_B T} \mu_k, \\ \phi(x) &= \frac{e_0}{k_B T} \Phi(X), \quad c_k(x) = \frac{C_k(X)}{C_0}, \quad J_k = \frac{\mathcal{J}_k}{(b - a) C_0 \mathcal{D}_0}. \end{aligned}$$

In terms of the new variables, the BVP (1.1) and (1.3) with $\mu_k = \mu_k^{id}$ given in (1.2) becomes the following quasi-one-dimensional classical PNP:

$$\begin{aligned} \frac{\varepsilon^2}{A(x)} \frac{d}{dx} \left(\bar{\varepsilon}_r(x) A(x) \frac{d}{dx} \phi \right) &= - \sum_{s=1}^n z_s c_s - Q(x), \\ \frac{dJ_k}{dx} &= 0, \quad -J_k = D_k(x) A(x) \frac{dc_k}{dx} + D_k(x) z_k c_k A(x) \frac{d\phi}{dx}, \quad k = 1, 2, \dots, n, \end{aligned} \quad (1.6)$$

with the boundary conditions

$$\phi(0) = V = \frac{e_0}{k_B T} \mathcal{V}, \quad c_k(0) = l_k = \frac{\mathcal{L}_k}{C_0}; \quad \phi(1) = 0, \quad c_k(1) = r_k = \frac{\mathcal{R}_k}{C_0}. \quad (1.7)$$

The electroneutrality boundary conditions in (1.4) and the I - V relation (1.5) read now

$$\sum_{s=1}^n z_s l_s = \sum_{s=1}^n z_s r_s = 0 \quad \text{and} \quad I = \sum_{s=1}^n z_s J_s(V; \{l_k\}, \{r_k\}).$$

The quasi-one-dimensional cPNP system (1.6) is a simplest PNP type model for ionic flow. The purpose of this paper is to provide a detailed analysis to the BVP (1.6) and (1.7) for $n = 3$ with $z_1 > z_2 > 0 > z_3$ and with zero permanent charge $Q = 0$. This work is based on the result in [32] on the existence and uniqueness of solutions of the BVP (1.6) and (1.7) recalled below. We remark that, in [32], the authors assume $A(x) = 1$ for simplicity. The result can be easily extended to general $A(x)$ and we will provide the result without details. It should become clear from the rest of the paper that the BVP (1.6) and (1.7) even with $Q = 0$ is already quite involved. We believe that the analysis provided in this paper will become a fundamental step and be useful for further studies of more sophisticated PNP models that take into consideration of permanent charges and ion sizes for ionic solutions with three and more ion species.

The rest of the paper is organized as follows. In Section 2, we review the relevant general result in [32] that this paper is based upon and identify our main concerns in this paper in terms of zeros of a meromorphic function $g(z)$ defined by boundary conditions. Section 3 focuses on three ion species and contains the main results (Propositions 3.5, 3.6, and 3.8) as well as detailed analyses on the zeros of $g(z)$ to determine boundary conditions for monotonic or oscillatory spatial profiles of ionic concentrations. In Section 4, we provide explicit formulas for fluxes and current in terms of boundary conditions and the zeros of $g(z)$. We expect that these explicit formulas could be very useful for further studies on ionic flow properties.

2. Relevant results from [32] on the BVP (1.6) and (1.7)

We now recall some relevant results in [32]. In [32], it took a uniform cross-section area $A(x) = 1$. We will state the result for general $A(x)$ and comment on the differences it makes in the proofs in [32] at the end of this discussion. In the following, we assume

- (A1) z_1, z_2, \dots, z_n are nonzero and distinct, $\bar{\varepsilon}_r(x) = 1$, $Q(x) = 0$, and $D_k(x) = 1$ for all k ;
 (A2) $L = (l_1, l_2, \dots, l_n)^T \neq 0$, $R = (r_1, r_2, \dots, r_n)^T \neq 0$, $(l_k, r_k) \neq (0, 0)$ for any k , and $V > 0$.

Remark 2.1. Regarding the assumption that $V > 0$ in (A2), we first comment that, if $V = 0$, then the solution of the BVP (1.6) and (1.7) is given by

$$\phi(x) = 0, \quad c_k(x) = \left(1 - \frac{H(x)}{H(1)}\right)l_k + \frac{H(x)}{H(1)}r_k, \quad J_k = \frac{1}{H(1)}(r_k - l_k),$$

where $H(x) = \int_0^x A^{-1}(s)ds$. So we will not include this case in the remaining study.

Secondly, the BVP (1.6) and (1.7) has the apparent symmetry with respect to the change $x \rightarrow 1 - x$. In particular, the problem with $V < 0$ can be converted to that with $V > 0$ as in (A2). \square

For $Q = 0$, the authors of [32] applied the geometric singular perturbation framework developed in [28] to reduce the BVP (1.6) and (1.7) to a singular connecting problem and the singular connecting problem is shown to be equivalent to: determining a (column) vector $f \in \mathbb{R}^n$ so that the matrix $D(f) = \Gamma - fb^T$, where $\Gamma = \text{diag}\{z_1, z_2, \dots, z_n\}$ and $b = (z_1^2, z_2^2, \dots, z_n^2)^T$, satisfies

$$R = e^{VD(f)}L$$

and, for $C(\tau) = e^{VD(f)\tau}L \in \mathbb{R}^n$, $\tau \in [0, 1]$,

$$c_k(\tau) \geq 0 \quad \text{for } k = 1, 2, \dots, n.$$

We note that the matrix $D(f)$ determines f uniquely. It turns out the special structure of $D(f)$ allows its eigenvalues to determine f (and hence $D(f)$) uniquely too. In fact, one has

Theorem 2.1 (Theorem 3.1, [32]). *Suppose $\lambda_1, \dots, \lambda_p$ are distinct eigenvalues of $D(f)$ with algebraic multiplicities s_1, \dots, s_p (so that $s_1 + s_2 + \dots + s_p = n$). Then*

$$f_j = \frac{1}{b_j} \frac{\prod_{k=1}^p (z_j - \lambda_k)^{s_k}}{\prod_{1 \leq k \leq n, k \neq j} (z_j - z_k)} \quad \text{for } j = 1, 2, \dots, n.$$

Let $g : \mathbb{C} \rightarrow \mathbb{C}$ be the meromorphic function given by

$$g(z) = \sum_{k=1}^n \frac{z_k^2 r_k}{z_k - z} - e^{Vz} \sum_{k=1}^n \frac{z_k^2 l_k}{z_k - z}. \quad (2.1)$$

Set

$$\begin{aligned} \mathcal{P}_1 &= \{k \in \{1, 2, \dots, n\} : r_k \neq e^{Vz_k} l_k\}, \\ \mathcal{P}_2 &= \{k \in \{1, 2, \dots, n\} : r_k = e^{Vz_k} l_k\}. \end{aligned}$$

Then, \mathcal{P}_1 and \mathcal{P}_2 form a partition of $\{1, 2, \dots, n\}$, that is,

$$\mathcal{P}_1 \cap \mathcal{P}_2 = \emptyset \quad \text{and} \quad \{1, 2, \dots, n\} = \mathcal{P}_1 \cup \mathcal{P}_2.$$

For $k \in \mathcal{P}_1$, z_k is a simple pole of $g(z)$ and, for $k \in \mathcal{P}_2$, z_k is a removable singularity of $g(z)$. Let $m = \#(\mathcal{P}_1)$ be the number of elements in \mathcal{P}_1 . Then $n - m = \#(\mathcal{P}_2)$.

For any integer $p \geq 0$, define the (open) stripe S_p in \mathbb{C} as

$$S_p = \{z = x + iy : y \in (-(2p+1)\pi/V, (2p+1)\pi/V)\}.$$

Theorem 2.2 (Theorem 3.5, [32]). *The meromorphic function $g(z)$ has infinite many zeros. More precisely, for each integer $p \geq 0$, $g(z)$ has exactly $m + 2p$ zeros (counting multiplicity) in the stripe S_p ; in particular, $g(z)$ has exactly m zeros in the stripe S_0 and, for any $p \geq 1$, $g(z)$ has exactly one pair of complex conjugate zeros in $S_p \setminus S_{p-1}$, one in each connected component.*

Since $g(z)$ has exactly m zeros (counting multiplicity) in the stripe S_0 , the total number of zeros (counting the multiplicities) and removable singularities of $g(z)$ in the stripe S_0 is exactly n .

Let $\lambda_1, \lambda_2, \dots, \lambda_p$ with multiplicities s_1, s_2, \dots, s_p be all the zeros and the removable singularities of $g(z)$ in S_0 . Necessarily, $s_1 + s_2 + \dots + s_p = n$. It turns out λ_j 's (counting the multiplicities) are exactly the eigenvalues of $D := D(f)$. Then the unique singular orbit is determined by

$$\phi(\tau) = V - \tau V, \quad C(\tau) = e^{VD\tau} L, \quad H(x(\tau)) = VI^{-1} \int_0^\tau b^T C(s) ds, \quad (2.2)$$

where τ is an intermediate variable such that $x(1) = 1$. Furthermore, with $J = If$,

$$J = \frac{V}{H(1)} \int_0^1 \Gamma e^{VDs} L ds - R + L, \quad I = \sum_{s=1}^n z_s J_s = \frac{V}{H(1)} \int_0^1 b^T e^{VDs} L ds,$$

where $\Gamma = \text{dig}\{z_1, z_2, \dots, z_n\}$ and $b^T = (z_1^2, z_2^2, \dots, z_n^2)$ are introduced previously when $D(f)$ is defined.

Note that if $A(x) = 1$, then $H(x) = x$ and (2.2) is nothing but the formula (2.16) in [32]. For general $A(x)$, the only difference is, for example, in display (2.14) in [32], there is an extra factor $A^{-1}(w)$ on the left-hand side of the w -equation, which leads to the function $H(x(\tau))$ on the left-hand side of (2.2).

3. Zeros of the function $g(z)$ in (2.1) for $n = 3$

It is noticed that $\lambda = 0$ is always a zero of $g(z)$ (and hence, an eigenvalue of D) due to the electroneutrality boundary conditions $\sum_{s=1}^n z_s l_s = \sum_{s=1}^n z_s r_s = 0$. For $n = 2$, the other eigenvalue of D must be real too – in fact it is $V^{-1}(\ln r_1 - \ln l_1)$. This is the reason for the spatial profiles of ionic concentrations to be monotonic for $n = 2$. It is thus interesting to know, for $n \geq 3$, when there are complex conjugate eigenvalues and, most importantly, what the implications are to ionic flows. Our interest for $n = 3$ in this paper is reduced to determine when the other two eigenvalues are real and when they are complex (necessarily as a conjugate pair).

As mentioned above, we will consider $n = 3$ with $z_1 > z_2 > 0 > z_3$, which includes the cases for ion mixtures with Ca^{++} , Na^+ and Cl^- , and with Ca^{++} , K^+ and Cl^- . We will work with the function $g(z)$.

3.1. Preparations

For easy of notation, we introduce

$$P_z = \prod_{j=1}^3 z_j, \quad S_l = \sum_{j=1}^3 l_j, \quad S_r = \sum_{j=1}^3 r_j, \quad \Lambda_l = \sum_{j=1}^3 z_j^2 l_j, \quad \Lambda_r = \sum_{j=1}^3 z_j^2 r_j.$$

We first make some technical preparations.

Lemma 3.1. *The function $g(z)$ in (2.1) can be written as*

$$g(z) = z\tilde{g}(z) \quad \text{where} \quad \tilde{g}(z) = \sum_{j=1}^3 \frac{z_j r_j}{z_j - z} - e^{Vz} \sum_{j=1}^3 \frac{z_j l_j}{z_j - z}.$$

Proof. It follows from the electroneutrality boundary conditions

$$\sum_{j=1}^3 z_j r_j = \sum_{j=1}^3 z_j l_j = 0$$

that

$$\sum_{j=1}^3 \frac{z_j^2 r_j}{z_j - z} = \sum_{j=1}^3 \frac{z_j(z_j - z)r_j + z z_j r_j}{z_j - z} = z \sum_{j=1}^3 \frac{z_j r_j}{z_j - z}$$

and

$$\sum_{j=1}^3 \frac{z_j^2 l_j}{z_j - z} = z \sum_{j=1}^3 \frac{z_j l_j}{z_j - z}.$$

The statement is a direct consequence. \square

Obviously, the other zeros λ_2 and λ_3 of $g(z)$ under consideration are just those of $\tilde{g}(z)$. We introduce

$$h(z) = \frac{1}{\Lambda_l} \tilde{g}(z) \prod_{j=1}^3 (z - z_j).$$

Note that, for $k \in \{1, 2, 3\}$, z_k is a removable singularity of g (an eigenvalue of D) if $r_k = e^{Vz_k} l_k$. In this case, z_k is a zero of $h(z)$. Thus,

Proposition 3.2. *The other two eigenvalues λ_2 and λ_3 of D are exactly the zeros of $h(z)$ in the stripe S_0 .*

Lemma 3.3. *The function h can be expressed as*

$$h(z) = (z - m_l) e^{Vz} - \rho(z - m_r), \quad (3.1)$$

where

$$m_l = -\frac{S_l}{\Lambda_l} P_z > 0, \quad m_r = -\frac{S_r}{\Lambda_r} P_z > 0, \quad \rho = \frac{\Lambda_r}{\Lambda_l} > 0.$$

Proof. First of all,

$$\prod_{j=1}^3 (z_j - z) \sum_{j=1}^3 \frac{z_j r_j}{z_j - z}$$

$$\begin{aligned}
&= z_1(z_2 - z)(z_3 - z)r_1 + z_2(z_1 - z)(z_3 - z)r_2 + z_3(z_1 - z)(z_2 - z)r_3 \\
&= \prod_{j=1}^3 z_j \sum_{j=1}^3 r_j - z(z_1(z_2 + z_3)r_1 + z_2(z_1 + z_3)r_2 + z_3(z_1 + z_2)r_3) + z^2 \sum_{j=1}^3 z_j r_j.
\end{aligned}$$

Since $\sum_{j=1}^3 z_j r_j = 0$ and

$$z_1(z_2 + z_3)r_1 + z_2(z_1 + z_3)r_2 + z_3(z_1 + z_2)r_3 = \sum_{j=1}^3 z_j \sum_{j=1}^3 z_j r_j - \sum_{j=1}^3 z_j^2 r_j = -\Lambda_r,$$

one has

$$\prod_{j=1}^3 (z_j - z) \sum_{j=1}^3 \frac{z_j r_j}{z_j - z} = P_z S_r + \Lambda_r z.$$

Similarly,

$$\prod_{j=1}^3 (z_j - z) \sum_{j=1}^3 \frac{z_j l_j}{z_j - z} = P_z S_l + \Lambda_l z.$$

The formula (3.1) for $h(z)$ then follows. \square

Lemma 3.4. *The following relations hold.*

$$\begin{bmatrix} l_1 \\ l_2 \\ l_3 \end{bmatrix} = \begin{bmatrix} \frac{z_1 \Lambda_l + P_z S_l}{z_1(z_1 - z_2)(z_1 - z_3)} \\ \frac{z_2 \Lambda_l + P_z S_l}{z_2(z_2 - z_1)(z_2 - z_3)} \\ \frac{z_3 \Lambda_l + P_z S_l}{z_3(z_3 - z_1)(z_3 - z_2)} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} \frac{z_1 \Lambda_r + P_z S_r}{z_1(z_1 - z_2)(z_1 - z_3)} \\ \frac{z_2 \Lambda_r + P_z S_r}{z_2(z_2 - z_1)(z_2 - z_3)} \\ \frac{z_3 \Lambda_r + P_z S_r}{z_3(z_3 - z_1)(z_3 - z_2)} \end{bmatrix},$$

or equivalently,

$$\begin{bmatrix} l_1 \\ l_2 \\ l_3 \end{bmatrix} = \Lambda_l \begin{bmatrix} \frac{z_1 - m_l}{z_1(z_1 - z_2)(z_1 - z_3)} \\ \frac{z_2 - m_l}{z_2(z_2 - z_1)(z_2 - z_3)} \\ \frac{z_3 - m_l}{z_3(z_3 - z_1)(z_3 - z_2)} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \Lambda_r \begin{bmatrix} \frac{z_1 - m_r}{z_1(z_1 - z_2)(z_1 - z_3)} \\ \frac{z_2 - m_r}{z_2(z_2 - z_1)(z_2 - z_3)} \\ \frac{z_3 - m_r}{z_3(z_3 - z_1)(z_3 - z_2)} \end{bmatrix}.$$

In particular, if $z_1 > z_2 > 0 > z_3$, then $z_2 \leq m_l, m_r \leq z_1$.

Proof. It is clear that

$$\begin{bmatrix} S_l \\ 0 \\ \Lambda_l \end{bmatrix} = W \begin{bmatrix} l_1 \\ l_2 \\ l_3 \end{bmatrix}, \quad \begin{bmatrix} S_r \\ 0 \\ \Lambda_r \end{bmatrix} = W \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix},$$

where

$$W = \begin{bmatrix} 1 & 1 & 1 \\ z_1 & z_2 & z_3 \\ z_1^2 & z_2^2 & z_3^2 \end{bmatrix}.$$

Simple calculations yield

$$W^{-1} = \begin{bmatrix} \frac{1}{(z_1 - z_2)(z_1 - z_3)} & 0 & 0 \\ 0 & \frac{1}{(z_2 - z_1)(z_2 - z_3)} & 0 \\ 0 & 0 & \frac{1}{(z_3 - z_1)(z_3 - z_2)} \end{bmatrix} \begin{bmatrix} z_2 z_3 - (z_2 + z_3) 1 \\ z_1 z_3 - (z_1 + z_3) 1 \\ z_1 z_2 - (z_1 + z_2) 1 \end{bmatrix}.$$

The relations claimed then follow directly. The range for m_l and m_r is a consequence of $l_j \geq 0$ and $r_j \geq 0$. \square

3.2. Roots of $h(z) = 0$ in the stripe S_0

Recall that we assume $V > 0$. To characterize λ_2 and λ_3 , we consider three cases:

Case (a): $m_r = m_l$; Case (b): $m_r < m_l$; Case (c): $m_r > m_l$.

3.2.1. Cases (a) and (b)

For these two cases, λ_2 and λ_3 are real; more precisely, we have

Proposition 3.5. *For Case (a) where $m_l = m_r$, one has*

$$h(z) = (z - m_l)(e^{Vz} - \rho)$$

and it has two real zeros

$$\lambda_2 = m_l \quad \text{and} \quad \lambda_3 = \frac{\ln \rho}{V} \begin{cases} > 0, & \text{if } \rho > 1 \\ = 0, & \text{if } \rho = 1 \\ < 0, & \text{if } \rho < 1 \end{cases}.$$

For Case (b) where $m_r < m_l$, $h(z)$ has two distinct real roots λ_2 and λ_3 satisfying

$$\begin{cases} \lambda_2 < 0, & \text{if } \rho m_r < m_l \\ \lambda_2 = 0, & \text{if } \rho m_r = m_l \\ 0 < \lambda_2 < m_r, & \text{if } \rho m_r > m_l \end{cases} \quad \text{and} \quad \lambda_3 > m_l.$$

Proof. For Case (a), one has $h(z) = (z - m_l)(e^{Vz} - \rho)$. The claim then follows. For Case (b), we rewrite $h(z) = 0$ as $h_l(z) = h_r(z)$ where

$$h_l(z) = \frac{1}{\rho} e^{Vz} \quad \text{and} \quad h_r(z) = \frac{z - m_r}{z - m_l}.$$

The statement follows easily from the graphs of $h_l(z)$ and $h_r(z)$ shown in Figure 1. \square

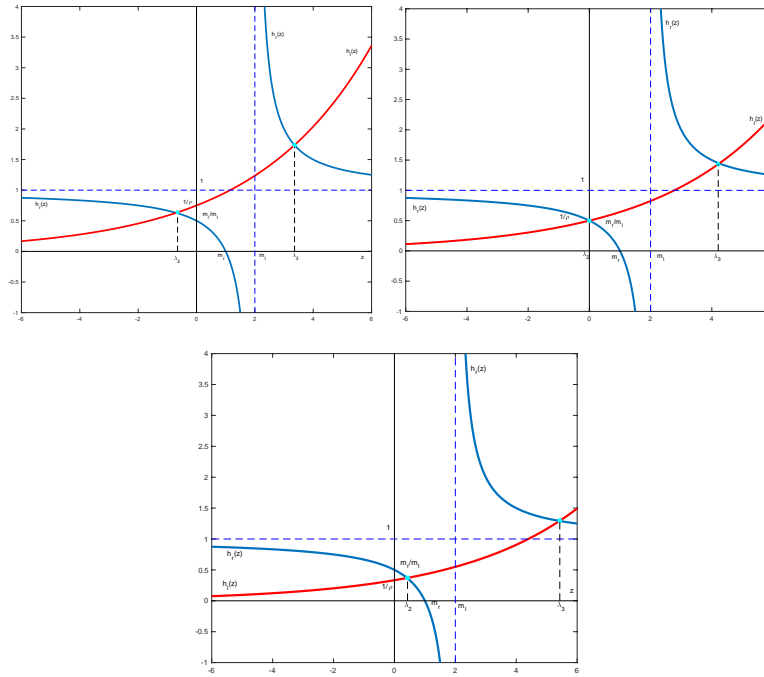


Figure 1. Graphs in Case (b) $m_r < m_l$: first for $\rho m_r < m_l$, second for $\rho m_r = m_l$, third for $\rho m_r > m_l$

3.2.2. Case (c) where $m_r > m_l$

We split this case into three subcases:

$$(c1) \quad \rho m_r < m_l; \quad (c2) \quad \rho m_r = m_l; \quad \text{and} \quad (c3) \quad \rho m_r > m_l.$$

For Subcases (c1) and (c2), we have the following result.

Proposition 3.6. For Subcase (c1), $h(z) = 0$ has two real roots λ_2 and λ_3 with

$$\lambda_2 < 0 < \lambda_3 < m_l.$$

For Subcase (c2), $h(z) = 0$ has two real roots λ_2 and λ_3 with

$$\begin{cases} \lambda_2 < 0 \quad \text{and} \quad \lambda_3 = 0, & \text{if } V < \frac{1}{m_l} - \frac{1}{m_r} \\ \lambda_2 = 0 \quad \text{and} \quad \lambda_3 = 0, & \text{if } V = \frac{1}{m_l} - \frac{1}{m_r} \\ \lambda_2 = 0 \quad \text{and} \quad 0 < \lambda_3 < m_l, & \text{if } V > \frac{1}{m_l} - \frac{1}{m_r} \end{cases}.$$

Proof. For Subcase (c1) where $m_r > m_l$ and $\rho m_r < m_l$, the graphs of $h_l(z)$ and $h_r(z)$ are plotted in Figure 2. Due to the fact that $1/\rho > m_r/m_l$, in this subcase $h(z) = 0$ always has two real roots λ_2 and λ_3 with $\lambda_2 < 0 < \lambda_3 < m_l$.

For Subcase (c2) where $m_r > m_l$ and $\rho m_r = m_l$, the graphs of $h_l(z)$ and $h_r(z)$ are plotted in Figure 3. In this subcase $h(z) = 0$ has two real roots, at least one of

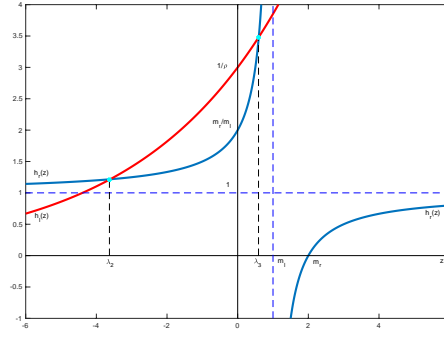


Figure 2. Graphs of Subcase (c1) $m_r > m_l$ and $\rho m_r < m_l$

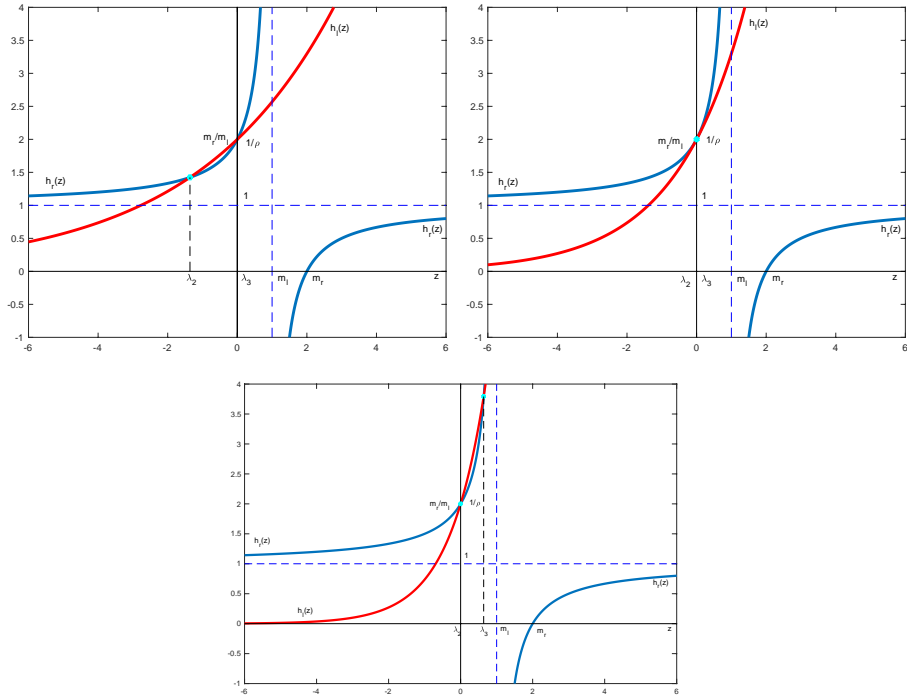


Figure 3. Graphs in Subcase (c2) $m_r > m_l$ and $\rho m_r = m_l$: first for $V < \frac{1}{m_l} - \frac{1}{m_r}$, second for $V = \frac{1}{m_l} - \frac{1}{m_r}$, third for $V > \frac{1}{m_l} - \frac{1}{m_r}$

which must be zero. Now

$$h'_l(0) = \frac{V}{\rho} = \frac{Vm_r}{m_l}, \quad h'_r(0) = \frac{m_r - m_l}{m_l^2}.$$

Clearly, if $h'_l(0) < h'_r(0)$, then another root is negative, if $h'_l(0) = h'_r(0)$, then 0 is a double root, and if $h'_l(0) > h'_r(0)$, then another root is positive. The statement then follows. \square

It remains to consider Subcase (c3) where $m_r > m_l$ and $\rho m_r > m_l$. To state

the result for this subcase, we introduce several quantities:

$$\begin{aligned} t &= \frac{2 + V(m_r - m_l) + \sqrt{(2 + V(m_r - m_l))^2 - 4}}{2}, \\ \rho(t) &= \frac{1}{t} \exp \left(\frac{t^2 - \left(1 + \frac{m_r}{m_l}\right)t + \frac{m_r}{m_l}}{\left(\frac{m_r}{m_l} - 1\right)t} \right). \end{aligned} \quad (3.2)$$

Recall that we assume $V > 0$. The next result can be established easily.

Lemma 3.7. *One has*

$$t > 1, \quad V = \frac{(t-1)^2}{(m_r - m_l)t} \quad \text{and} \quad \rho(t) < \rho(1/t).$$

Furthermore,

- (i) if $0 < V < 1/m_l - 1/m_r$, then $1 < t < m_r/m_l$ and $\rho(t)$ is strictly decreasing;
- (ii) if $V > 1/m_l - 1/m_r$, then $t > m_r/m_l$ and $\rho(t)$ is strictly increasing.
- (iii) For $t > 1$, $\rho(1/t)$ is strictly increasing in t , and

$$\lim_{t \rightarrow \infty} \rho(1/t) = \infty \quad \text{and} \quad \lim_{t \rightarrow 1} \rho(1/t) = 1.$$

The main result contained in the next proposition is on the nature of λ_2 and λ_3 for this subcase.

Proposition 3.8. *Consider Subcase (c3) where $m_r > m_l$ and $\rho m_r > m_l$.*

(I) *Concerning double roots $\lambda_2 = \lambda_3$, one has*

- (i) For $V \in \left(0, \frac{1}{m_l} - \frac{1}{m_r}\right)$ or $t \in \left(1, \frac{m_r}{m_l}\right)$, if $\rho = \rho(t)$, then $\rho \in \left(\frac{m_l}{m_r}, 1\right)$ and there is a negative double root; if $\rho = \rho(1/t)$, then $\rho \in \left(1, \frac{m_r}{m_l} e^{\frac{m_r}{m_l} - \frac{m_l}{m_r}}\right)$ and there is a double root in the interval $(m_r + m_l, \infty)$.
- (ii) For $V \in \left(\frac{1}{m_l} - \frac{1}{m_r}, \infty\right)$ or $t \in \left(\frac{m_r}{m_l}, \infty\right)$, if $\rho = \rho(t)$, then $\rho \in \left(\frac{m_l}{m_r}, \infty\right)$ and there is a positive double root in the interval $(0, m_l)$; also, there exists $t_0 > \frac{m_r}{m_l}$ such that $\rho \in \left(\frac{m_l}{m_r}, 1\right)$ when $t \in \left(\frac{m_r}{m_l}, t_0\right)$ and $\rho \in [1, \infty)$ when $t \in [t_0, \infty)$; if $\rho = \rho(1/t)$, then $\rho \in \left(\frac{m_r}{m_l} e^{\frac{m_r}{m_l} - \frac{m_l}{m_r}}, \infty\right)$ and there is a double root in the interval $(m_r, m_r + m_l)$;
- (iii) For $V = \frac{1}{m_l} - \frac{1}{m_r}$ or $t = \frac{m_r}{m_l}$, if $\rho = \rho(t) = m_l/m_r$, then $\lambda_2 = \lambda_3 = 0$, which is shown in Subcase (c2); if $\rho = \rho(1/t) = \frac{m_r}{m_l} e^{\frac{m_r}{m_l} - \frac{m_l}{m_r}}$, then the double root is $m_r + m_l$.

(II) *If $\rho \in (\rho(t), \rho(1/t))$, then $h(z) = 0$ has a pair of complex conjugate roots.*

(III) *Concerning distinct real roots λ_2 and λ_3 , one has*

- (i) for $\rho > \rho(1/t)$, $h(z) = 0$ has two distinct positive roots $\lambda_2, \lambda_3 > m_r$;
- (ii) if $\frac{m_l}{m_r} < \rho < \rho(t)$, then $h(z) = 0$ has two negative roots for $0 < V < \frac{1}{m_l} - \frac{1}{m_r}$ and two positive roots in $(0, m_l)$ for $V > \frac{1}{m_l} - \frac{1}{m_r}$.

Proof. (I). We first consider the possible double root situation of $h(z) = 0$. This happens when z satisfies

$$h_l(z) = h_r(z), \quad h'_l(z) = h'_r(z),$$

that is,

$$\frac{1}{\rho}e^{Vz} = \frac{z - m_r}{z - m_l}, \quad \frac{V}{\rho}e^{Vz} = \frac{m_r - m_l}{(z - m_l)^2}.$$

Substituting the first equation into the second one, we have

$$V \frac{z - m_r}{z - m_l} = \frac{m_r - m_l}{(z - m_l)^2}$$

or

$$z^2 - (m_r + m_l)z + m_l m_r - \frac{m_r - m_l}{V} = 0,$$

which has two roots

$$\zeta_{1,2} = \frac{m_r + m_l \pm \sqrt{(m_r + m_l)^2 - 4 \left(m_l m_r - \frac{m_r - m_l}{V} \right)}}{2}.$$

In order to have $\lambda_2 = \lambda_3 = \zeta_j$ for $j = 1$ or 2 , ζ_j must satisfy

$$\frac{1}{\rho}e^{V\zeta_j} = \frac{\zeta_j - m_r}{\zeta_j - m_l} \quad \text{and} \quad \frac{V}{\rho}e^{V\zeta_j} = \frac{m_r - m_l}{(\zeta_j - m_l)^2}. \quad (3.3)$$

Let us first consider the smaller root ζ_1 .

$$\zeta_1 = \frac{m_r + m_l - \sqrt{(m_r + m_l)^2 - 4 \left(m_l m_r - \frac{m_r - m_l}{V} \right)}}{2} = m_l - \frac{1}{V} \left(1 - \frac{1}{t} \right) \quad (3.4)$$

where t is given in (3.2).

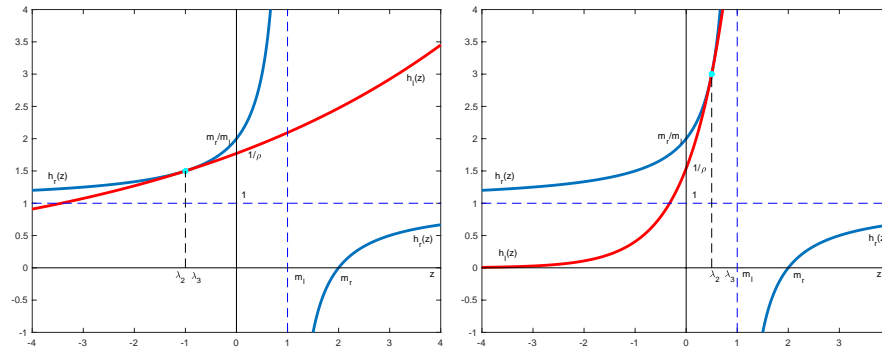


Figure 4. Graphs in Subcase (c3) $m_r > m_l$ and $\rho m_r > m_l$ in smaller double root situation: first for $V < \frac{1}{m_l} - \frac{1}{m_r}$, second for $V > \frac{1}{m_l} - \frac{1}{m_r}$.

From the graphs of $h_l(z)$ and $h_r(z)$ in Figure 4, one has $\zeta_1 < m_l$, which is also obvious from the last expressions in (3.4). From the first expression in (3.4), one

has

$$\begin{cases} \zeta_1 < 0, & \text{if } V < \frac{1}{m_l} - \frac{1}{m_r} \\ \zeta_1 = 0, & \text{if } V = \frac{1}{m_l} - \frac{1}{m_r} \\ 0 < \zeta_1 < m_l, & \text{if } V > \frac{1}{m_l} - \frac{1}{m_r} \end{cases}.$$

It follows from the first condition in (3.3) that, if $\zeta_1 = 0$, then $\rho = m_l/m_r$, which contradicts to $\rho m_r > m_l$. Therefore, for $V = 1/m_l - 1/m_r$, $h(z) = 0$ cannot have double roots. Note that this situation is covered in Subcase (c2).

Next we analyze the other two situations: $V < \frac{1}{m_l} - \frac{1}{m_r}$ and $V > \frac{1}{m_l} - \frac{1}{m_r}$. From Lemma 3.7,

$$V = \frac{(t-1)^2}{(m_r - m_l)t}. \quad (3.5)$$

Hence, using the second relation in (3.3) with ζ_1 and (3.4),

$$\rho = \frac{1}{t} \exp \left(\frac{m_l t^2 - (m_l + m_r)t + m_r}{(m_r - m_l)t} \right) = \frac{1}{t} \exp \left(\frac{t^2 - \left(1 + \frac{m_r}{m_l}\right)t + \frac{m_r}{m_l}}{\left(\frac{m_r}{m_l} - 1\right)t} \right) =: \rho(t),$$

which is the same as the one defined in (3.2). Clearly if $t := t(V)$ is viewed as a function of V , it is strictly increasing.

When $0 < V < 1/m_l - 1/m_r$, from Lemma 3.7, one has $1 < t < m_r/m_l$, and $\rho(t)$ is a strictly decreasing function of t as well as V on the given interval. Moreover, one has $m_l/m_r < \rho(t) < 1$. Therefore, we have the following one-to-one relations

$$\rho \in \left(\frac{m_l}{m_r}, 1 \right) \longleftrightarrow V \in \left(0, \frac{1}{m_l} - \frac{1}{m_r} \right) \longleftrightarrow t \in \left(1, \frac{m_r}{m_l} \right).$$

Using (3.4) and (3.5), one can write

$$\zeta_1 = m_l - \frac{m_r - m_l}{t - 1} = m_l \frac{t - \frac{m_r}{m_l}}{t - 1} =: \zeta_1(t), \quad (3.6)$$

that is, ζ_1 can be viewed as a strictly increasing function of t , therefore also a strictly increasing function of V . This shows the first part of (i).

When $V > 1/m_l - 1/m_r$, from Lemma 3.7, one has $t > m_r/m_l > 1$ and $\rho(t)$ is a strictly increasing function of t as well as V , satisfying $\frac{m_l}{m_r} < \rho(t) < \infty$. Again, this exhibits the one-to-one relations

$$\rho \in \left(\frac{m_l}{m_r}, \infty \right) \longleftrightarrow V \in \left(\frac{1}{m_l} - \frac{1}{m_r}, \infty \right) \longleftrightarrow t \in \left(\frac{m_r}{m_l}, \infty \right).$$

On the given interval of V , ζ_1 is the double root of $h(z) = 0$, that is,

$$\lambda_2 = \lambda_3 = \zeta_1 \in (0, m_l).$$

Again, ζ_1 is a strictly increasing function of t as well as V .

Because $m_l/m_r < 1$ and $\rho(t)$ is increasing for $t > m_r/m_l$, there must be a unique $t_0 \in (m_r/m_l, \infty)$ such that $\rho(t_0) = 1$. Thus, t_0 must be a root of the equation

$$t = \exp \left(\frac{\left(t - \frac{m_r}{m_l}\right)(t-1)}{\left(\frac{m_r}{m_l} - 1\right)t} \right). \quad (3.7)$$

It is obvious that $\frac{m_l}{m_r} < \rho(t) < 1$ when $\frac{m_r}{m_l} < t < t_0$ and $1 \leq \rho(t) < \infty$ when $t_0 \leq t < \infty$. This proves the first part of (ii).

Note that (3.7) has two roots, one is t_0 and the other is 1. Note that both ρ and ζ_1 can be considered as functions of V as well. Since

$$\frac{dV}{dt} = \frac{t^2 - 1}{(m_r - m_l)t^2},$$

one has

$$\frac{d\rho}{dV} = \frac{m_l \left(t - \frac{m_r}{m_l}\right)}{t(t-1)} \exp \left(\frac{\left(t - \frac{m_r}{m_l}\right)(t-1)}{\left(\frac{m_r}{m_l} - 1\right)t} \right), \quad \frac{d\zeta_1}{dV} = \frac{\frac{d\zeta_1}{dt}}{\frac{dV}{dt}} = \frac{(m_r - m_l)^2 t^2}{(t-1)^3(t+1)}.$$

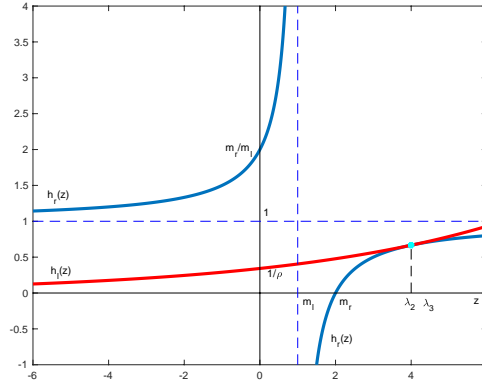


Figure 5. Graphs in Subcase (c3) $m_r > m_l$ and $\rho m_r > m_l$ in larger double root situation

Now for the larger root ζ_2 , we have

$$\zeta_2 = m_l + \frac{t-1}{V} = m_r + \frac{1}{V} \left(1 - \frac{1}{t}\right),$$

where t is defined in (3.2). Since $t > 1$ (Lemma 3.7), one has $\zeta_2 > m_r$ (see also Figure 5). From the first relation of (3.3) and using (3.5) one has

$$\rho = t \exp \left(\frac{(m_r t - m_l)(t-1)}{(m_r - m_l)t} \right) = t \exp \left(\frac{\left(\frac{m_r}{m_l} t - 1\right)(t-1)}{\left(\frac{m_r}{m_l} - 1\right)t} \right) = \rho(1/t),$$

where $\rho(t)$ is defined in (3.2) as well.

Observe that with (3.5),

$$\zeta_2 = m_r + \frac{m_r - m_l}{t - 1} = \frac{m_r t - m_l}{t - 1} = \zeta_1(1/t),$$

where $\zeta_1(t)$ is defined in (3.6). From Lemma 3.7, $\rho(1/t)$ is strictly increasing for $t > 1$, or equivalently for $V > 0$, and $1 < \rho(1/t) < \infty$ for $1 < t < \infty$. This shows the one-to-one relations

$$\rho \in (1, \infty) \quad \longleftrightarrow \quad V \in (0, \infty) \quad \longleftrightarrow \quad t \in (1, \infty).$$

The second parts of both (i) and (ii) then follow from the properties of $\rho(1/t)$ and $\zeta_1(1/t)$.

Also, we have $d\zeta_2/dt = d\zeta_1(1/t)/dt = -(m_r - m_l)/(t - 1)^2$ and

$$\frac{d\rho(1/t)}{dV} = \frac{m_l t \left(\frac{m_r}{m_l} t - 1 \right)}{t - 1} \exp \left(\frac{\left(\frac{m_r}{m_l} t - 1 \right) (t - 1)}{\left(\frac{m_r}{m_l} - 1 \right) t} \right), \quad \frac{d\zeta_2}{dV} = -\frac{(m_r - m_l)^2 t^2}{(t - 1)^3 (t + 1)}.$$

To summarize, for $h(z) = 0$ to have a nonzero double real root, that is, $\lambda_2 = \lambda_3 \neq 0$, it is necessary that $m_r > m_l$ and $\rho m_r > m_l$.

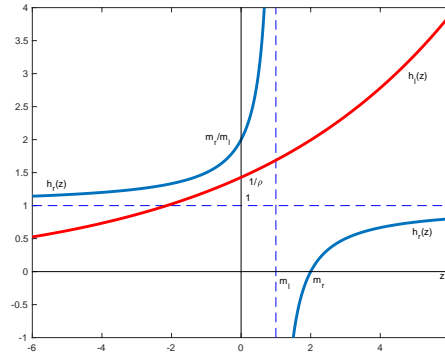


Figure 6. Graphs in Subcase (c3) $m_r > m_l$ and $\rho m_r > m_l$ with $\rho(t) < \rho < \rho(1/t)$: roots in complex conjugate pair

(II) From Lemma 3.7, one has $\rho(t) < \rho(1/t)$ for $t > 1$ or $V > 0$. For ρ and V in the region given by the inequalities $\rho(t) < \rho < \rho(1/t)$, the equation $h(z) = 0$ does not have a real root. See Figure 6. So it has a pair of complex conjugate roots λ_2 and $\bar{\lambda}_2$.

(III) It can be seen from Figure 7 that, if

$$\frac{m_l}{m_r} < \rho < \rho(t),$$

then $h(z) = 0$ has two real roots, either both are negative or both are positive, depending on whether $V < \frac{1}{m_l} - \frac{1}{m_r}$ or $V > \frac{1}{m_l} - \frac{1}{m_r}$. The properties also follow from the continuity of the roots of $h_l(z) = h_r(z)$ corresponding to ρ and the results in (i) and (ii) of Subcase (I) when $\rho = \rho(t)$. Note that 0 cannot be a root of $h_l(z) = h_r(z)$ when $\rho > \frac{m_l}{m_r}$.

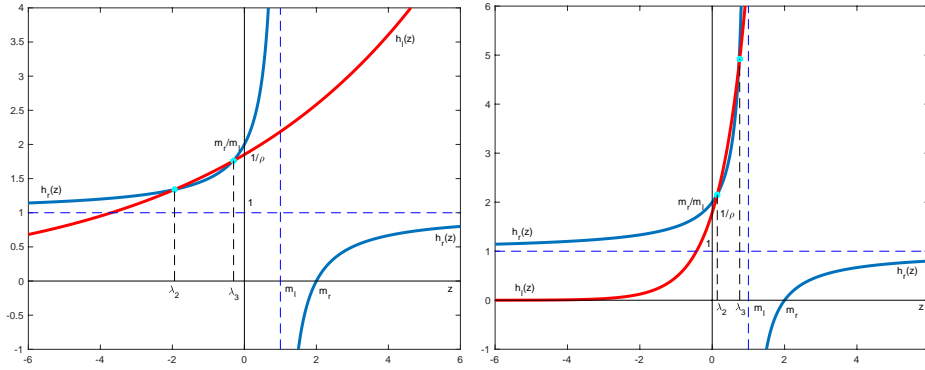


Figure 7. Graphs in Subcase (c3) $m_r > m_l$ and $\rho m_r > m_l$ with $m_l/m_r < \rho < \rho(t)$: real roots with same sign

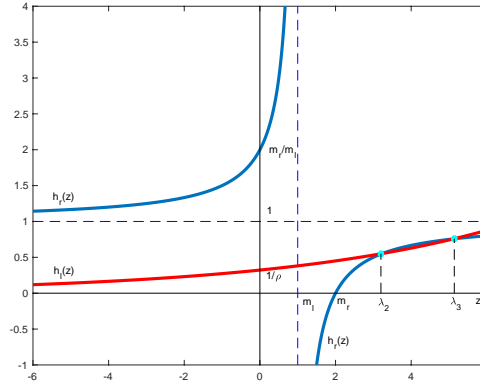


Figure 8. Graphs in Subcase (c3) $m_r > m_l$ and $\rho m_r > m_l$ with $\rho > \rho(1/t)$: real roots $\lambda_2, \lambda_3 > m_r$

Similarly, in the case that $\rho > \rho(1/t)$, one can show that $h(z) = 0$ has two positive real roots $\lambda_2, \lambda_3 > m_r$. See also Figure 8. \square

For Case (c), the relations between ρ and V as well as the roots of $h(z) = 0$ are plotted in Figure 9.

4. Fluxes and current for $n = 3$ in terms of λ_j 's

In this section, we will provide formulas for the fluxes and the total current for convenience of future study on dependences of these key quantities on the boundary conditions, etc.

Recall that, under the electroneutrality boundary conditions, $\lambda_1 = 0$ is always a root of $g(z) = 0$. Let λ_2 and λ_3 be the other two roots of $g(z) = 0$ in the stripe

$$S_0 = \{z = x + iy : y \in (-\pi/V, \pi/V)\}.$$

As given at the end of Section 2, we have $J = If$, and from Theorem 2.1, $f =$

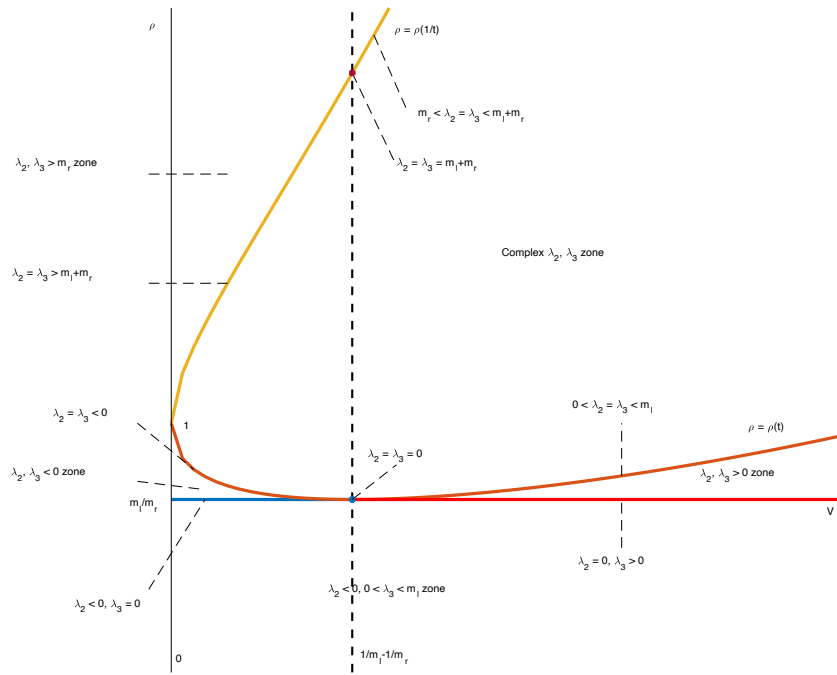


Figure 9. Case (c) ($m_r > m_l$): relation between ρ and V and zeros of $h(z)$

$(f_1, f_2, f_3)^T$ with

$$\begin{aligned} f_1 &= \frac{1}{z_1} \frac{(z_1 - \lambda_2)(z_1 - \lambda_3)}{(z_1 - z_2)(z_1 - z_3)}, \\ f_2 &= \frac{1}{z_2} \frac{(z_2 - \lambda_2)(z_2 - \lambda_3)}{(z_2 - z_1)(z_2 - z_3)}, \\ f_3 &= \frac{1}{z_3} \frac{(z_3 - \lambda_2)(z_3 - \lambda_3)}{(z_3 - z_1)(z_3 - z_2)}. \end{aligned}$$

From Proposition 3.13 in [32], one has

- if $\lambda_2 \neq 0$ and $\lambda_3 \neq 0$, then

$$I = \frac{1}{H(1)\lambda_2\lambda_3}(S_l - S_r)P_z; \quad (4.1)$$

- if 0 is a double eigenvalue and the third eigenvalue is $\lambda \neq 0$, then

$$I = -\frac{1}{H(1)\lambda} \left(\sum_{j=1}^3 \frac{l_j - r_j}{z_j} + VS_l \right) P_z.$$

The second formula can be simplified as follows. Note that, when 0 is a double eigenvalue, in addition to $\sum_{j=1}^3 z_j l_j = \sum_{j=1}^3 z_j r_j = 0$, one has $\rho m_r = m_l$, or equivalently, $S_l = S_r$, and together, they imply that

$$P_z \sum_{j=1}^3 \frac{l_j - r_j}{z_j} = z_2 z_3 (l_1 - r_1) + z_1 z_3 (l_2 - r_2) + z_1 z_2 (l_3 - r_3)$$

$$\begin{aligned}
&= (z_1 z_2 + z_1 z_3 + z_2 z_3)(S_l - S_r) - z_1(z_2(l_2 - r_2) + z_3(l_3 - r_3)) \\
&\quad - z_2(z_1(l_1 - r_1) + z_3(l_3 - r_3)) - z_3(z_1(l_1 - r_1) + z_2(l_2 - r_2)) \\
&= z_1^2(l_1 - r_1) + z_2^2(l_2 - r_2) + z_3^2(l_3 - r_3) = \Lambda_l - \Lambda_r.
\end{aligned}$$

Therefore,

$$I = -\frac{1}{H(1)\lambda} (\Lambda_l - \Lambda_r + V S_l P_z).$$

Furthermore, using $h(\lambda) = 0$ with $S_l = S_r$, one has

$$S_l P_z = \frac{\lambda}{e^{V\lambda} - 1} \Lambda_r - \frac{\lambda e^{V\lambda}}{e^{V\lambda} - 1} \Lambda_l,$$

which gives, from the previous formula,

$$I = \frac{V}{H(1)} \left((1 - p(V\lambda)) \Lambda_l + p(V\lambda) \Lambda_r \right), \quad (4.2)$$

where

$$p(x) = \frac{e^x - x - 1}{x(e^x - 1)}.$$

Since

$$p'(x) = -\frac{(e^x - 1)^2 - x^2 e^x}{x^2 (e^x - 1)^2} = -(e^x + e^{-x} - 2 - x^2) \frac{e^x}{x^2 (e^x - 1)^2}$$

and $e^x + e^{-x} - 2 - x^2 \geq 0$ with the equality holding true only when $x = 0$, $p(x)$ is a strictly decreasing function. By defining

$$p(0) = \lim_{x \rightarrow 0} p(x) = \frac{1}{2},$$

the function $p(x)$ is continuous on $(-\infty, \infty)$. Since $p(x)$ is strictly decreasing and $p(-\infty) = 1$, $p(\infty) = 0$, one has $0 < p(x) < 1$ for any x .

One simple consequence of (4.2) is that I and V have the same sign and the value of I lies between $\frac{V\Lambda_r}{H(1)}$ and $\frac{V\Lambda_l}{H(1)}$.

Since $\lim_{x \rightarrow 0} p(x) = 1/2$, by taking the limit with $\lambda \rightarrow 0$ in (4.2) we have the formula for the case when 0 is a triple eigenvalue of D :

$$I = \frac{V}{2H(1)} (\Lambda_l + \Lambda_r).$$

A different form of representation for I is given as follows.

Proposition 4.1. *Suppose the other two eigenvalues λ_2 and λ_3 are nonzero and $\lambda_2 \neq \lambda_3$. Then,*

$$I = \frac{V}{H(1)} \left(\frac{\frac{e^{V\lambda_2} - 1}{V\lambda_2} - \frac{e^{V\lambda_3} - 1}{V\lambda_3}}{e^{V\lambda_2} - e^{V\lambda_3}} \Lambda_r + \frac{e^{V\lambda_2} \frac{e^{V\lambda_3} - 1}{V\lambda_3} - e^{V\lambda_3} \frac{e^{V\lambda_2} - 1}{V\lambda_2}}{e^{V\lambda_2} - e^{V\lambda_3}} \Lambda_l \right).$$

Proof. Note that, for $j = 2, 3$,

$$e^{V\lambda_j} = \frac{\Lambda_r \lambda_j + S_r P_z}{\Lambda_l \lambda_j + S_l P_z}.$$

Then, one has the identity

$$\frac{(S_l - S_r)P_z}{V\lambda_2\lambda_3} = \frac{\frac{e^{V\lambda_2}-1}{V\lambda_2} - \frac{e^{V\lambda_3}-1}{V\lambda_3}}{e^{V\lambda_2} - e^{V\lambda_3}}\Lambda_r + \frac{e^{V\lambda_2}\frac{e^{V\lambda_3}-1}{V\lambda_3} - e^{V\lambda_3}\frac{e^{V\lambda_2}-1}{V\lambda_2}}{e^{V\lambda_2} - e^{V\lambda_3}}\Lambda_l. \quad (4.3)$$

The claimed formula then follows from (4.1). \square

Note that if we multiply the common denominator on both sides of (4.3), then the resulting identity holds true for any two zeros of $g(z)$, not necessarily those inside the stripe S_0 .

Acknowledgment. LY was partially supported by National Natural Science Foundation China # 12101112. WL was partially supported by Simons Foundation Mathematics and Physical Sciences-Collaboration Grants for Mathematicians 581822.

References

- [1] N. Abaid, R. S. Eisenberg and W. Liu, *Asymptotic expansions of I-V relations via a Poisson-Nernst-Planck system*, SIAM J. Appl. Dyn. Syst., 2008, 7, 1507–1526.
- [2] V. Barcion, D. Chen, R. S. Eisenberg and J. W. Jerome, *Qualitative properties of steady-state Poisson-Nernst-Planck systems: Perturbation and simulation study*, SIAM J. Appl. Math., 1997, 57, 631–648.
- [3] P. Bates, Z. Wen and M. Zhang, *Small permanent charge effects on individual fluxes via Poisson-Nernst-Planck models with multiple cations*, J. Nonl. Sci., 2021, 31(3), Paper No. 55, 62 pp.
- [4] M. Bazant, K. Chu and B. Bayly, *Current-Voltage relations for electrochemical thin films*, SIAM J. Appl. Math., 2005, 65, 1463–1484.
- [5] F. Bezanilla, *The voltage sensor in voltage-dependent ion channels*, Phys. Rev., 2000, 80, 555–592.
- [6] J. J. Bikerman, *Structure and capacity of the electrical double layer*, Philos. Mag., 1942, 33, 384–397.
- [7] D. Chen and R. S. Eisenberg, *Charges, currents and potentials in ionic channels of one conformation*, Biophys. J., 1993, 64, 1405–1421.
- [8] R. S. Eisenberg, *Ion channels as devices*, J. Comp. Electro., 2003, 2, 245–249.
- [9] R. S. Eisenberg, *Proteins, channels, and crowded ions*, Biophys. Chem., 2003, 100, 507–517.
- [10] B. Eisenberg, Y. Hyon and C. Liu, *Energy variational analysis of ions in water and channels: Field theory for primitive models of complex ionic fluids*, J. Chem. Phys., 2010, 133, 104104(1–23).
- [11] B. Eisenberg and W. Liu, *Poisson-Nernst-Planck systems for ion channels with permanent charges*, SIAM J. Math. Anal., 2007, 38, 1932–1966.

- [12] B. Eisenberg, W. Liu and H. Xu, *Reversal permanent charge and reversal potential: Case studies via classical Poisson-Nernst-Planck models*, Nonlinearity, 2015, 28, 103–128.
- [13] D. Gillespie, W. Nonner and R. S. Eisenberg, *Coupling Poisson-Nernst-Planck and density functional theory to calculate ion flux*, J. Phys.: Condens. Matter, 2002, 14, 12129–12145.
- [14] D. Gillespie, W. Nonner and R. S. Eisenberg, *Density functional theory of charged, hard-sphere fluids*, Phys. Rev. E, 2003, 68, 0313503(1–10).
- [15] B. Hille, *Ion Channels of Excitable Membranes* (3rd ed.), Sinauer Associates Inc., 2001.
- [16] A. L. Hodgkin, *The ionic basis of electrical activity in nerve and muscle*, Biol. Rev., 1951, 26, 339–409.
- [17] A. L. Hodgkin and A. F. Huxley, *Currents carried by sodium and potassium ions through the membrane of the giant axon of Loligo*, J. Physiol., 1952, 116, 449–472.
- [18] A. L. Hodgkin, A. F. Huxley and B. Katz, *Ionic currents underlying activity in the giant axon of the squid*, Arch. Sci. Physiol., 1949, 3, 129–150.
- [19] A. L. Hodgkin and B. Katz, *The effect of sodium ions on the electrical activity of the giant axon of the squid*, J. Physiol., 1949, 108, 37–77.
- [20] W. Huang, W. Liu and Y. Yu, *Permanent charge effects on ionic flow: A numerical study of flux ratios and their bifurcation*, Commun. Comput. Phys., 2021, 30, 486–514.
- [21] Y. Hyon, B. Eisenberg and C. Liu, *A mathematical model for the hard sphere repulsion in ionic solutions*, Commun. Math. Sci., 2010, 9, 459–475.
- [22] W. Im, D. Beglov and B. Roux, *Continuum solvation model: Electrostatic forces from numerical solutions to the Poisson-Boltzmann equation*, Comp. Phys. Comm., 1998, 111, 59–75.
- [23] S. Ji, B. Eisenberg and W. Liu, *Flux ratios and channel structures*, J. Dynam. Differential Equation, 2019, 31, 1141–1183.
- [24] S. Ji and W. Liu, *Poisson-Nernst-Planck systems for ion flow with density functional theory for hard-sphere potential: I-V relations and critical potentials. Part I: Analysis*, J. Dynam. Differential Equations, 2012, 24, 955–983.
- [25] S. Ji, W. Liu and M. Zhang, *Effects of (small) permanent charge and channel geometry on ionic flows via classical Poisson-Nernst-Planck models*, SIAM J. Appl. Math., 2015, 75, 114–135.
- [26] G. Lin, W. Liu, Y. Yi and M. Zhang, *Poisson-Nernst-Planck systems for ion flow with a local hard-sphere potential for ion size effects*, SIAM J. Appl. Dyn. Syst., 2013, 12, 1613–1648.
- [27] W. Liu, *Geometric singular perturbation approach to steady-state Poisson-Nernst-Planck systems*, SIAM J. Appl. Math., 2005, 65, 754–766.
- [28] W. Liu, *One-dimensional steady-state Poisson-Nernst-Planck systems for ion channels with multiple ion species*, J. Differential Equations, 2009, 246, 428–451.

- [29] W. Liu, *A flux ratio and a universal property of permanent charges effects on fluxes*, Comput. Math. Biophys., 2018, 6, 28–40.
- [30] W. Liu, X. Tu and M. Zhang, *Poisson-Nernst-Planck systems for ion flow with density functional theory for hard-sphere potential: I-V relations and critical potentials. Part II: Numerics*, J. Dynam. Differential Equations, 2012, 24, 985–1004.
- [31] W. Liu and B. Wang, *Poisson-Nernst-Planck systems for narrow tubular-like membrane channels*, J. Dynam. Differential Equations, 2010, 22, 413–437.
- [32] W. Liu and H. Xu, *A complete analysis of a classical Poisson-Nernst-Planck model for ionic flow*, J. Differential Equations, 2015, 258, 1192–1228.
- [33] H. Mofidi, B. Eisenberg and W. Liu, *Effects of diffusion coefficients and permanent charge on reversal potentials in ionic channels*, Entropy, 2020, 22, 325(1–23).
- [34] H. Mofidi and W. Liu, *Reversal potential and reversal permanent charge with unequal diffusion coefficients via classical Poisson-Nernst-Planck models*, SIAM J. Appl. Math., 2020, 80, 1908–1935.
- [35] W. Nonner and R. S. Eisenberg, *Ion permeation and glutamate residues linked by Poisson-Nernst-Planck theory in L-type Calcium channels*, Biophysical J., 1998, 75, 1287–1305.
- [36] Y. Rosenfeld, *Free-energy model for the inhomogeneous hard-sphere fluid mixture and Density-Functional Theory of freezing*, Phys. Rev. Lett., 1989, 63, 980–983.
- [37] Y. Rosenfeld, *Free energy model for the inhomogeneous fluid mixtures: Yukawa-charged hard spheres, general interactions, and plasmas*, J. Chem. Phys., 1993, 98, 8126–8148.
- [38] I. Rubinstein, *Multiple steady states in one-dimensional electrodiffusion with local electroneutrality*, SIAM J. Appl. Math., 1987, 47, 1076–1093.
- [39] I. Rubinstein, *Electro-Diffusion of Ions*, SIAM Studies in Applied Mathematics, SIAM, Philadelphia, PA, 1990.
- [40] B. Sakmann and E. Neher, *Single Channel Recording* (2nd ed.), Plenum, 1995.
- [41] A. Singer and J. Norbury, *A Poisson-Nernst-Planck model for biological ion channels—an asymptotic analysis in a three-dimensional narrow funnel*, SIAM J. Appl. Math., 2009, 70, 949–968.
- [42] A. Singer, D. Gillespie, J. Norbury and R. S. Eisenberg, *Singular perturbation analysis of the steady-state Poisson-Nernst-Planck system: applications to ion channels*, Eur. J. Appl. Math., 2008, 19, 541–560.
- [43] L. Sun and W. Liu, *Non-localness of excess potentials and boundary value problems of Poisson-Nernst-Planck systems for ionic flow: A case study*, J. Dynam. Differential Equations, 2018, 30, 779–797.
- [44] N. Sun and W. Liu, *Flux ratios for effects of permanent charges on ionic flows with three ion species: New phenomena from a case study*, J. Dynam. Differential Equations, 2022. <https://doi.org/10.1007/s10884-021-10118-x>.
- [45] H. H. Ussing, *Interpretation of the exchange of radio-sodium in isolated muscle*, Nature, 1947, 160, 262–263.

- [46] X. Wang, D. He, J. Wylie and H. Huang, *Singular perturbation solutions of steady-state Poisson-Nernst-Planck systems*, Phys. Rev. E, 2014, 89, 022722(1–14).
- [47] L. Zhang, B. Eisenberg and W. Liu, *An effect of large permanent charge: Decreasing flux with increasing transmembrane potential*, Eur. Phys. J. Special Topics, 2019, 227, 2575–2601.
- [48] L. Zhang and W. Liu, *Effects of large permanent charges on ionic flows via Poisson-Nernst-Planck models*, SIAM J. Appl. Dyn. Syst., 2020, 19, 1993–2029.
- [49] M. Zhang, *Asymptotic expansions and numerical simulations of I - V relations via a steady-state Poisson-Nernst-Planck system*, Rocky Mountain J. Math., 2015, 45, 1681–1708.
- [50] Q. Zheng and G. Wei, *Poisson-Boltzmann-Nernst-Planck model*, J. Chem. Phys., 2011, 134, 194101(1–17).