# A complete analysis of a classical Poisson-Nernst-Planck model for ionic flow

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**Abstract**

In this work, we examine the stationary one-dimensional *classical Poisson-Nernst-Planck* (cPNP) model for ionic flow – a singularly perturbed boundary value problem (BVP). For the case of zero permanent charge, we provide a complete answer concerning the existence and uniqueness of the BVP. The analysis relies on a number of ingredients: a geometric singular perturbation framework for a reduction to a singular BVP, a reduction of the singular BVP to a matrix eigenvalue problem, a relation between the matrix eigenvalues and zeros of a meromorphic function, and an application of the Cauchy Argument Principle for identifying zeros of the meromorphic function. Once the zeros of the meromorphic function in a stripe are determined, an explicit solution of the singular BVP is available. It is expected that this work would be useful for studies of other PNP systems.

**Key words. Ionic flow, Boundary value problem, Geometric singular perturbation**

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## 1 Introduction

In this work, we revisit the one-dimensional steady-state *classical Poisson-Nernst-Planck* (cPNP) system for ionic flow studied in [31] by one of the

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authors. For $n$ types of ion species, the cPNP model is, for $k = 1, 2, \cdots, n$,

$$\begin{aligned} &\frac{\varepsilon^2}{h(x)}\frac{d}{dx}\left(h(x)\frac{d}{dx}\phi\right) = -\sum_{s=1}^{n}\alpha_s c_s - Q(x), \\ &\frac{dJ_k}{dx} = 0, \quad h(x)\frac{dc_k}{dx} + \alpha_k c_k h(x)\frac{d\phi}{dx} = -J_k, \end{aligned} \tag{1.1}$$

$x \in (0,1)$ with the boundary conditions

$$\phi(0) = \mathcal{V},\ c_k(0) = l_k \geq 0; \quad \phi(1) = 0,\ c_k(1) = r_k \geq 0, \tag{1.2}$$

where the unknown variables are the electric potential $\phi$, the concentration (number density) $c_k$ and the flux density $J_k$ of the $k$th ion species. The interval $[0, 1]$ is the scaled one-dimensional ion channel with $x = 0$ and $x = 1$ representing the two open ends of the channel, $\varepsilon^2 \ll 1$ is a dimensionless parameter, $h(x)$ represents the cross-section area of the ion channel over $x$, $Q(x)$ is the permanent charge, and, for the $k$th ion species, $\alpha_k \neq 0$ is its valence (number of charges per particle), $l_k$ and $r_k$ are its concentrations at the boundaries (left and right baths).

An important quantity for characterizing ion channel properties is the so-called *I-V (current-voltage)* relation defined as follows. For fixed $l_k$'s and $r_k$'s, a solution $(\phi, c_k, J_k)$ of the boundary value problem (BVP) (1.1) and (1.2) will depend on the voltage $\mathcal{V}$ only, and the current $\mathcal{I}$, *the flow rate of charges*, is thus related to the voltage $\mathcal{V}$ by

$$\mathcal{I} = \sum_{s=1}^{n}\alpha_s J_s(\mathcal{V}). \tag{1.3}$$

A related quantity $\mathcal{F}$, *the flow rate of matter*, is defined by

$$\mathcal{F} = \sum_{s=1}^{n} J_s. \tag{1.4}$$

The purpose of this paper is to provide a complete analysis to the BVP (1.1) and (1.2) with zero permanent charge $Q = 0$. For simplicity, we also assume $h(x) = 1$. Roughly speaking, we will show that,

*For $Q = 0$ and for $\varepsilon > 0$ small, there is a unique solution of the BVP (1.1) and (1.2) satisfying $c_k(x) \geq 0$ for $x \in [0,1]$ and for $1 \leq k \leq n$; in fact, $c_k(x) > 0$ for $x \in (0,1)$ if $(l_k, r_k) \neq (0,0)$.*

We remark that the cPNP system (1.1) is a simplest PNP type model for ionic flow. It should become clear from the rest of the paper that the BVP

(1.1) and (1.2) even with $Q = 0$ is already quite involved. Yet, our study shows rich properties of the problem, and its delicate and elegant path from the conditions to its solution. 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.

The research on ion channel problems, most using PNP type models, becomes an extremely active area. We refer readers to the following partial list [1, 2, 3, 4, 7, 8, 9, 10, 11, 13, 14, 15, 17, 18, 19, 20, 21, 23, 26, 27, 28, 30, 31, 32, 33, 39, 40, 41, 42, 43, 44, 47, 49, 50, 55, 56, 57, 58, 59] and references therein for more details on ion channel problems, general PNP type models, and some numerical and analytical results. The closely related semiconductor problems have been extensively analyzed and are better understood. For semiconductors, there are two ($n = 2$) types of ion species (electrons and holes) involved but boundary conditions are more complicated and also recombination rates are involved. For analysis of this problem, we refer readers to [5, 6, 22, 34, 35, 36, 45, 46, 48, 51, 52] and reference therein.

In direct connection to results in this work, we mention those in [31] and [54]. In [31], a geometric singular perturbation framework for the BVP (1.1) and (1.2) with piecewise constant permanent charges $Q(x)$ was developed, extending that in [11] where two ion species was considered. Two special features underlined in the nonlinearity of the problem were identified which play crucial roles for the geometric construction of a solution: a complete set of first integrals for the limiting fast system and a blow-up for the limiting slow system together with a nonlinear rescaling. As the result, the problem of existence and uniqueness of singular orbits for the BVP (1.1) and (1.2) is reduced to that of a system of algebraic equations. In Example 5.1 in [31], for $n = 3$ and $Q = 0$, coexistence of a spatially monotone solution and a spatially vibrating solution was claimed. Unfortunately, the spatially vibrating solution is not physical since it yields negative ion concentrations over a certain spatial region, as correctly pointed out in a recent work [54]. The authors of [54] also considered the problem with $Q = 0$. They applied the classical asymptotic expansion approach and provided a better reduction of the zeroth order problem to a scalar transcendental equation. Based on the reduction, for $n = 3$, they established the existence and uniqueness result for the BVP (1.1) and (1.2).

The result on existence and uniqueness for a general $n$ established in this paper is clean and sounds simple but the proof is highly nontrivial. There is a number of difficulties that one has to overcome. For example, the region $\{c_k \geq 0,\ 1 \leq k \leq n\}$ is NOT invariant; indeed, there are infinitely many solutions of the reduced BVP but only one satisfying $c_k(x) \geq 0$ for $x \in [0, 1]$

and $1 \leq k \leq n$. The actual proof presents a thorough understanding of the problem. To provide a guideline for readers, we summarize the main steps of our proof and the organization of the paper below.

(1) First of all, we apply the geometric singular perturbation framework to reduce the BVP (1.1) and (1.2) to a singular connecting problem. With the help of a special structure of the problem at hand, the singular connecting problem is shown to be equivalent to: determining a (column) vector $f \in \mathbb{R}^n$ so that,

   (i) for the matrix $D(f) = \Gamma - fb^T$, where $\Gamma = \mathrm{diag}\,\{\alpha_1, \alpha_2, \ldots, \alpha_n\}$ and $b = (\alpha_1^2, \alpha_2^2, \ldots, \alpha_n^2)^T$, one has

   $$R = e^{\mathcal{V}D(f)}L$$

   where $L = (l_1, l_2, \ldots, l_n)^T$ and $R = (r_1, r_2, \ldots, r_n)^T$;

   (ii) for $C(\tau) = e^{\mathcal{V}D(f)\tau}L \in \mathbb{R}^n$, $\tau \in [0, 1]$, one has

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

   This reduction had been done in [31] for a general setup and is reviewed in Section 2 for the case with $Q = 0$ considered in this paper.

(2) The study of the reduced problem in (1) is naturally carried out in two steps. We first focus on the sub-problem (i). Making use of the special structure that $D(f)$ is a diagonal matrix minus a rank one matrix, we examine the relation between the vector $f$ and the eigenvalues of $D(f)$. This has been well studied in the standard pole placement problem (see, e.g. [37, 38] and references therein). The most relevant result is that the vector $f$ can be explicitly expressed in terms of the eigenvalues of $D(f)$ and a matrix $G$ that transforms $D(f)$ similarly to its Jordan form is also explicit in terms of the eigenvalues (Section 3.1). An important observation is that the eigenvalues of $D(f)$ so that $R = e^{\mathcal{V}D(f)}L$ are determined by zeros of a meromorphic function $g(z)$ defined in terms of $\mathcal{V}$, $\alpha_k$'s, $L$ and $R$ (Section 3.2). The function $g(z)$ is equivalent to the transcendental function appeared in [54]. In Section 3.3, by an application of Cauchy Argument Principle, we are able to determine the number and the location of zeros of $g(z)$ with sufficient information. It turns out that there are infinitely many choices for $f$ so that $R = e^{\mathcal{V}D(f)}L$.

   In Section 3.4, we show that, to meet also the requirement (ii) in (1), the vector $f$ is unique, which then provides a unique singular orbit.

Several properties of the singular solution are discussed in Section 3.5.

(3) In Section 4, we prove that, for $\varepsilon > 0$ small, there is a unique solution of the BVP (1.1) and (1.2) in the vicinity of the singular orbit constructed above. This is accomplished by establishing a transversal condition that depends on detailed information on the singular orbit.

# 2 The geometric singular perturbation framework for the BVP and a reduction.

## 2.1 Problem setup

A geometric singular perturbation framework was developed in [31] that applies to a general setting for a reduction of the BVP to a system of nonlinear algebraic equations. We will review the procedure for the present setting. As stated in the introduction, we will study the BVP of cPNP systems with $n$ ion species and zero permanent charge $Q = 0$. For simplicity, we also set $h(x) = 1$.

Denote the derivative with respect to $x$ by overdot. The BVP (1.1) and (1.2) becomes, for $k = 1, 2, \cdots, n$,

$$\varepsilon^2 \ddot{\phi} = -\sum_{s=1}^{n} \alpha_s c_s, \quad \dot{c}_k + \alpha_k c_k \dot{\phi} = -J_k, \quad \dot{J}_k = 0, \tag{2.1}$$

with the boundary conditions

$$\phi(0) = \mathcal{V},\ c_k(0) = l_k \geq 0; \quad \phi(1) = 0,\ c_k(1) = r_k \geq 0. \tag{2.2}$$

Denote $\mathbb{R}^n_+ = \{y \in \mathbb{R}^n : y_k \geq 0 \text{ for } k = 1, 2, \ldots, n\}$. A vector $y \in \mathbb{R}^n$ will be treated as a column vector and the corresponding row vector is denoted by $y^T$. We will use the notion

$$\begin{aligned} C(x) =&(c_1(x), c_2(x), \cdots, c_n(x))^T, \quad J = (J_1, J_2, \cdots, J_n)^T, \\ L =&(l_1, l_2, \cdots, l_n)^T, \quad R = (r_1, r_2, \cdots, r_n)^T. \end{aligned}$$

We will assume

$$\mathcal{V} \geq 0, \quad L \neq 0, \quad R \neq 0, \quad (l_k, r_k) \neq (0, 0) \text{ for } k = 1, 2, \cdots, n, \tag{2.3}$$

and the electroneutrality boundary condition

$$\sum_{s=1}^{n} \alpha_s l_s = \sum_{s=1}^{n} \alpha_s r_s = 0. \tag{2.4}$$

*Remark* 2.1. (i) If $(\phi(x), C(x), J)$ is a solution of (2.1) and (2.2), then

$$(\phi^*(x), C^*(x), J^*) = (\phi(1-x) - \mathcal{V}, C(1-x), -J)$$

is a solution of (2.1) with the boundary conditions

$$\phi^*(0) = -\mathcal{V},\ c_k^*(0) = r_k; \quad \phi^*(1) = 0,\ c_k^*(1) = l_k.$$

Thus, the assumption that $\mathcal{V} \geq 0$ in (2.3) does not lose any generality.

(ii) The assumption that $(l_k, r_k) \neq (0, 0)$ in (2.3) is made for simplicity since, if $l_k = r_k = 0$ for some $k$, then the BVP (2.1) and (2.2) can be reduced by removing the $k$th components of $C(x)$ and $J$. This assumption is only used in Theorem 3.8.

(iii) The case where $L = 0$ or $R = 0$ corresponds to a terminal turning point of the singularly perturbed BVP and it seems that the approach in this paper cannot handle this case directly. □

To continue, we will convert the BVP (2.1) and (2.2) to *a connecting problem* (see, e.g. [11, 31] for PNP systems and [24, 25, 29, 53] for general settings). Introduce $u = \varepsilon\dot{\phi}$ and $w = x$. System (2.1) becomes, for $k = 1, 2, \cdots, n$,

$$\begin{aligned} \varepsilon\dot{\phi} =& u, \quad \varepsilon\dot{u} = -\sum_{s=1}^{n} \alpha_s c_s, \\ \varepsilon\dot{c}_k =& -\alpha_k c_k u - \varepsilon J_k, \quad \dot{J} = 0, \quad \dot{w} = 1. \end{aligned} \tag{2.5}$$

As in [31], we will treat system (2.5) as a singularly perturbed dynamical system with the singular parameter $\varepsilon$. The phase space is $\mathbb{R}^{2n+3}$ with the state variable $(\phi, u, C, J, w)$.

Associated to the boundary value conditions (2.2), we introduce two subsets $B_0$ and $B_1$ of $\mathbb{R}^{2n+3}$ as

$$\begin{aligned} B_0 =& \{(\phi, u, C, J, w) : \phi = \mathcal{V},\ C = L,\ w = 0\}, \\ B_1 =& \{(\phi, u, C, J, w) : \phi = 0,\ C = R,\ w = 1\}. \end{aligned}$$

Then, the BVP (2.1) and (2.2) is equivalent to the following *connecting problem*: finding an orbit of (2.5) from $B_0$ to $B_1$. Such an orbit is called *a connecting orbit*.

By *a singular connecting orbit*, or simply, *a singular orbit*, we mean the zeroth order approximation in $\varepsilon$ of a connecting orbit. Therefore, a singular orbit consists of connected orbits of the limiting slow system of (2.5) and of its corresponding limiting fast system. Orbits of the limiting slow system of (2.5) are called *regular layer orbits* and those of the corresponding limiting fast system are called *singular layer orbits* such as boundary layers and/or internal layers.

We will apply the geometric singular perturbation framework to analyze our connecting problem. The general framework for connecting orbit problems consists of two main steps: (i) A construction of a singular connecting orbit; (ii) An application of Exchange Lemma (see, e.g., [24, 25, 29, 53]) to establish the existence and uniqueness of a connecting orbit near the singular connecting orbit.

## 2.2 The singular connecting orbit problem and a reduction.

In this part, based on special structures of (2.1), the singular connecting orbit problem will be reduced to an algebraic problem.

As shown in Section 3 in [31], with the electroneutrality boundary condition (2.4), there is no boundary layers. (With the assumption $Q = 0$, there is no internal layers either.) Therefore, a singular orbit is simply a connecting orbit of the limiting slow system (2.5) for the present problem.

Note that system (2.5) is degenerate at $\varepsilon = 0$ in the sense that all dynamical information on $(\phi, c_1, \cdots, c_n)$ would be lost when setting $\varepsilon = 0$. Following the treatment in [11, 31], we rescale the dependent variables by introducing

$$u = \varepsilon p, \quad \alpha_n c_n = -\sum_{s=1}^{n-1} \alpha_s c_s - \varepsilon q. \tag{2.6}$$

In replacing $(u, c_n)$ with $(p, q)$, system (2.5) becomes, for $k = 1, \cdots, n-1$,

$$\begin{aligned} \dot{\phi} =& p, \quad \varepsilon \dot{p} = q, \quad \varepsilon \dot{q} = \Big(\sum_{s=1}^{n-1} (\alpha_s - \alpha_n)\alpha_s c_s - \varepsilon \alpha_n q\Big)p + \mathcal{I}, \\ \dot{c}_k =& -\alpha_k c_k p - J_k, \quad \dot{J} = 0, \quad \dot{w} = 1, \end{aligned} \tag{2.7}$$

where $\mathcal{I} = \sum_{s=1}^{n} \alpha_s J_s$ is the current defined in (1.3). The sets $B_L$ and $B_R$ become

$$\begin{aligned} B_0^* =& \{(\phi, p, q, \hat{C}, J, w) : \phi = \mathcal{V}, \ q = 0, \ \hat{C} = \hat{L}, \ w = 0\}, \\ B_1^* =& \{(\phi, p, q, \hat{C}, J, w) : \phi = 0, \ q = 0, \ \hat{C} = \hat{R}, \ w = 1\}, \end{aligned} \tag{2.8}$$

where $\hat{L} = (l_1, l_2, \ldots, l_{n-1})^T$, $\hat{R} = (r_1, r_2, \ldots, r_{n-1})^T$, and $\hat{C} = (c_1, c_2, \ldots, c_{n-1})^T$. The condition that $q = 0$ at $w = x = 0$ and $w = x = 1$ follows from (2.4) and (2.6). The connecting problem becomes: finding an orbit of (2.7) to connect $B_0^*$ and $B_1^*$.

*Remark* 2.2. Under the electroneutrality condition (2.4) and $Q = 0$ considered in this work, one can rewrite (2.1) to (2.7) directly. System (2.5) was introduced in [11, 31] since its corresponding fast system is suitable for the study of singular layers problem. The latter would present in the case that either (2.4) is not assumed and/or $Q \neq 0$. In that case, both (2.5) and (2.7) are needed. □

When $\varepsilon = 0$, system (2.7) reduces to its limiting slow system, for $k = 1, \cdots, n-1$,

$$\begin{aligned} q =&0, \quad \Big(\sum_{s=1}^{n-1}(\alpha_s - \alpha_n)\alpha_s c_s\Big)p + \mathcal{I} = 0, \\ \dot{\phi} =&p, \quad \dot{c}_k = -\alpha_k p c_k - J_k, \quad \dot{J} = 0, \quad \dot{w} = 1. \end{aligned} \tag{2.9}$$

The algebraic equations define *the slow manifold* $\mathcal{S}$ (see, e.g. [24]),

$$\mathcal{S} = \left\{ p = -\frac{\mathcal{I}}{\sum_{s=1}^{n-1}(\alpha_s - \alpha_n)\alpha_s c_s}, \ q = 0 \right\}. \tag{2.10}$$

The corresponding fast system of (2.7) is, for $k = 1, \cdots, n-1$,

$$\begin{aligned} \phi' =&\varepsilon p, \quad p' = q, \quad q' = \Big(\sum_{s=1}^{n-1}(\alpha_s - \alpha_n)\alpha_s c_s - \varepsilon\alpha_n q\Big)p + \mathcal{I}, \\ c_k' =& -\varepsilon\alpha_k c_k p - \varepsilon J_k, \quad J' = 0, \quad w' = \varepsilon, \end{aligned}$$

and its limiting system at $\varepsilon = 0$ is, for $k = 1, \cdots, n-1$,

$$\begin{aligned} \phi' =&0, \quad p' = q, \quad q' = \Big(\sum_{s=1}^{n-1}(\alpha_s - \alpha_n)\alpha_s c_s\Big)p + \mathcal{I}, \\ c_k' =&0, \quad J' = 0, \quad w' = 0. \end{aligned} \tag{2.11}$$

The slow manifold $\mathcal{S}$ is the set of equilibria of (2.11) and the linearization at each point on $\mathcal{S}$ has $(2n+1)$ zero eigenvalues and the other two eigenvalues are $\pm\sqrt{\sum_{s=1}^{n-1}(\alpha_s - \alpha_n)\alpha_s c_s}$. The $(2n+1)$ zero eigenvalues reflect the fact that $\mathcal{S}$ is the set of equilibria of (2.11) and $\dim \mathcal{S} = 2n+1$. The other two eigenvalues are the so-called normal eigenvalues associated to the slow manifold $\mathcal{S}$.

An important observation is that, on the slow manifold $\mathcal{S}$ where $q = 0$, or equivalently, $\sum_{s=1}^{n} \alpha_s c_s = 0$ from (2.6), one has

$$\sum_{s=1}^{n-1} (\alpha_s - \alpha_n)\alpha_s c_s = \sum_{s=1}^{n-1} \alpha_s^2 c_s - \alpha_n \sum_{s=1}^{n-1} \alpha_s c_s = \sum_{s=1}^{n} \alpha_s^2 c_s. \tag{2.12}$$

Since $c_k$'s are concentrations of ion species, we will be interested in solutions with $c_k \geq 0$ for $k = 1, 2, \cdots, n$ and $\sum_{s=1}^{n} \alpha_s^2 c_s > 0$. Note that $\sum_{s=1}^{n} \alpha_s^2 c_s$ is positive at $x = 0$ and $x = 1$ due to $C(0) = L \neq 0$ and $C(1) = R \neq 0$ assumed in (2.3). Therefore, the slow manifold $\mathcal{S}$ is normally hyperbolic; in particular, it persists for $\varepsilon > 0$ small (see, e.g, [12, 16]).

On the slow manifold $\mathcal{S}$, system (2.9) reads, for $k = 1, 2, \ldots, n-1$,

$$\begin{aligned} \dot{\phi} &= -\frac{\mathcal{I}}{\sum_{s=1}^{n-1} (\alpha_s - \alpha_n)\alpha_s c_s}, \\ \dot{c}_k &= \frac{\mathcal{I}}{\sum_{s=1}^{n-1} (\alpha_s - \alpha_n)\alpha_s c_s} \alpha_k c_k - J_k, \\ \dot{J} &= 0, \quad \dot{w} = 1. \end{aligned} \tag{2.13}$$

The next result follows easily from (2.13). The proof will be omitted.

**Proposition 2.1.** *Let $(\phi(x), \hat{C}(x), J, w(x))$ be a solution of (2.13) and let $\alpha_n c_n(x) = -\sum_{s=1}^{n-1} \alpha_s c_s(x)$. Suppose $(\phi(0), C(0), w(0)) = (\mathcal{V}, L, 0)$ and $(\phi(1), C(1), w(1)) = (0, R, 1)$. If $\sum_{s=1}^{n} \alpha_s^2 c_s(x) > 0$ for $x \in [0, 1]$, then, $\mathcal{I}$ and $\mathcal{V}$ have the same sign; in particular, $\mathcal{I} = 0$ if and only if $\mathcal{V} = 0$. If $\mathcal{V} = 0$, then the solution is given by, for $x \in [0, 1]$,*

$$\phi(x) = 0, \ C(x) = (1 - x)L + xR, \ J = L - R, \ w(x) = x.$$

In the sequel, due to (i) in Remark 2.1 and Proposition 2.1, we will consider the case where $\mathcal{V} > 0$, and hence, $\mathcal{I} > 0$.

Recall the relation (2.12). If we multiply $\mathcal{V}\mathcal{I}^{-1} \sum_{s=1}^{n-1} (\alpha_s - \alpha_n)\alpha_s c_s(x)$ on the right-hand-side of system (2.13), the phase portrait remains the same – this is equivalent to a solution-dependent change of the independent variable. In term of the new independent variable, say $\tau$, system (2.13) becomes, for $k = 1, 2, \ldots, n-1$,

$$\begin{aligned} &\frac{d}{d\tau}\phi = -\mathcal{V}, \quad \frac{d}{d\tau} c_k = \mathcal{V}\alpha_k c_k - \mathcal{V}\mathcal{I}^{-1} J_k \sum_{s=1}^{n-1} (\alpha_s - \alpha_n)\alpha_s c_s, \\ &\frac{d}{d\tau} J = 0, \quad \frac{d}{d\tau} w = \mathcal{V}\mathcal{I}^{-1} \sum_{s=1}^{n-1} (\alpha_s - \alpha_n)\alpha_s c_s. \end{aligned} \tag{2.14}$$

It should be emphasized that system (2.13) is equivalent to system (2.14) if and only if $\sum_{s=1}^{n} \alpha_s^2 c_s > 0$.

In [31], an analysis for the BVP was conducted directly on system (2.14). In this work, we reformulate (2.14) so that $c_n$ will be treated equally as $c_1, \ldots, c_{n-1}$. Use the identity (2.12) and system (2.14) to get

$$\frac{d}{d\tau} c_n = \mathcal{V} \alpha_n c_n - \mathcal{V} J_n \mathcal{I}^{-1} \sum_{s=1}^{n} \alpha_s^2 c_s(\tau).$$

Combining this equation with (2.14) one has

$$\begin{aligned} \frac{d}{d\tau}\phi &= -\mathcal{V}, \quad \frac{d}{d\tau} C = \mathcal{V} D C, \quad \sum_{s=1}^{n} \alpha_s c_s = 0, \\ \frac{d}{d\tau} J &= 0, \quad \frac{d}{d\tau} w = \mathcal{V} \mathcal{I}^{-1} b^T C, \end{aligned} \tag{2.15}$$

where the matrix $D$, depending on the unknown $J$, is given by

$$D = \Gamma - \mathcal{I}^{-1} J b^T$$

with $\Gamma = \operatorname{diag}\{\alpha_1, \alpha_2, \ldots, \alpha_n\}$ and $b = (\alpha_1^2, \alpha_2^2, \ldots, \alpha_n^2)^T$.

*Remark* 2.3. Given an orbit $(\phi, C, J, w)$ of (2.15), one can determine a singular orbit $(\phi, p, q, \hat{C}, J, w)$ of (2.7) with $(p, q)$ in (2.10). $\square$

Concerning the matrix $D$, we have

**Lemma 2.2.** *Denote* $e = (1, 1, \ldots, 1)^T$ *and set*

$$x_0 = \Gamma e = (\alpha_1, \alpha_2, \ldots, \alpha_n)^T \quad \textit{and} \quad y_0 = \Gamma^{-1} J = (J_1/\alpha_1, J_2/\alpha_2, \ldots, J_n/\alpha_n)^T.$$

*Then,* $x_0^T D = 0$, $D y_0 = 0$, $x_0^T y_0 = \mathcal{F}$, *and*

$$e^T D = x_0^T - \mathcal{F} \mathcal{I}^{-1} b^T,$$

*where* $\mathcal{F} = \sum_{s=1}^{n} J_s$ *is the flow rate of matter defined in (1.4).*

*In particular, zero is an eigenvalue of* $D$*, and it is a simple eigenvalue if and only if* $\mathcal{F} \neq 0$*. If* $\mathcal{F} = 0$*, then* $e^T$ *is the first left generalized vector of* $D$ *associated to the zero eigenvalue.*

*Proof.* It can be checked by a direct calculation. $\square$

If we multiply $x_0^T$ from left to the $C$-equation in (2.15), we get that $\sum_{s=1}^n \alpha_s c_s$ is a constant. This, together with $\sum_{s=1}^n \alpha_s c_s = 0$, shows that (2.14) and (2.15) are equivalent.

Once $J$ is known, so is $D$, and the solution of (2.15) with $(\phi, C, w) = (\mathcal{V}, L, 0)$ at $\tau = 0$ would be explicitly given by

$$\phi(\tau) = \mathcal{V} - \tau\mathcal{V}, \quad C(\tau) = e^{\mathcal{V}D\tau}L, \quad w(\tau) = \mathcal{V}\mathcal{I}^{-1}\int_0^\tau b^T C(z)\,dz. \tag{2.16}$$

To connect $B_0$ to $B_1$, it requires $(\phi(\tau_0), C(\tau_0), w(\tau_0)) = (0, R, 1)$ for some $\tau_0 > 0$; that is, from (2.16),

$$\tau_0 = 1, \quad R = e^{\mathcal{V}D}L, \quad \mathcal{I} = \mathcal{V}\int_0^1 b^T e^{\mathcal{V}Dz}L\,dz. \tag{2.17}$$

The singular connecting problem is reduced to problem $\mathrm{BVP}_0$: *for $L$ and $R$ satisfying (2.3) and (2.4) and $\mathcal{V} > 0$, find $f = \mathcal{I}^{-1}J \in \mathbb{R}^n$ so that*

*(i)* $D = D(f) = \Gamma - fb^T$ *solves*

$$R = e^{\mathcal{V}D}L; \tag{2.18}$$

*(ii) for $\tau \in (0,1)$, $C(\tau) = e^{\mathcal{V}D\tau}L$ has NO negative component.*

*Remark* 2.4. Once $f = \mathcal{I}^{-1}J$ is determined, a singular orbit $(\phi, C, J, w)$ of (2.15) and (2.8) can be uniquely determined from (2.16), (2.17) and the relation $J = \mathcal{I}f$. It remains to verify that $\sum_{s=1}^n \alpha_s J_s = \mathcal{I}$ for consistence. Indeed, from the last equation in (2.17) and $fb^T = \Gamma - D$, one has

$$\begin{aligned} J = &\mathcal{I}f = \mathcal{V}\int_0^1 fb^T e^{\mathcal{V}Dz}L\,dz = \mathcal{V}\int_0^1 \Gamma e^{\mathcal{V}Dz}L\,dz - \mathcal{V}\int_0^1 De^{\mathcal{V}Dz}L\,dz \\ = &\mathcal{V}\int_0^1 \Gamma e^{\mathcal{V}Dz}L\,dz - \int_0^1 \frac{d}{dz}e^{\mathcal{V}Dz}L\,dz = \mathcal{V}\int_0^1 \Gamma e^{\mathcal{V}Dz}L\,dz - R + L. \end{aligned}$$

It then follows from (2.4) that $\sum_{s=1}^n \alpha_s J_s = \mathcal{V}\int_0^1 b^T e^{\mathcal{V}Dz}L\,dz = \mathcal{I}$. $\square$

## 3 The reduced singular connecting problem $\mathrm{BVP}_0$.

In this section, we will provide a complete solution to the reduced singular connecting problem $\mathrm{BVP}_0$ in (2.18) in a slightly general setting; more precisely, we assume

(A1) $\alpha_1, \alpha_2, \ldots, \alpha_n$ are real and distinct, $\Gamma = \operatorname{diag}\{\alpha_1, \alpha_2, \cdots, \alpha_n\}$, and $b = (b_1, b_2, \ldots, b_n)^T \in \mathbb{R}^n$ with $b_k > 0$ for $k = 1, 2, \ldots, n$;

(A2) $L, R \in \mathbb{R}^n$ with $L \neq 0$ and $R \neq 0$, and $l_k, r_k \geq 0$ for any $k$; $\mathcal{V} > 0$.

Our main problem in this section is:

*Assume (A1) and (A2). Determine $f \in \mathbb{R}^n$ so that, if $C(\tau) = e^{\mathcal{V}D(f)\tau}L$ where $D(f) = \Gamma - fb^T$, then*

$$(P): \quad (i)\ R = e^{\mathcal{V}D(f)}L; \quad (ii)\ c_k(\tau) \geq 0 \ \text{ for } \ \tau \in (0,1). \tag{3.1}$$

Comparing to assumptions for $\mathrm{BVP}_0$, we comment that, for problem (P), $\alpha_k$'s are not assumed to be integers, $b_k = \alpha_k^2$ is not assumed, $L$ and $R$ are not assumed to satisfy (2.4).

Our analysis on problem (P) will be accomplished through several steps. In §3.1, we discuss relations between the vector $f$ and the set of eigenvalues of $D(f)$. In §3.2, the determination of $f$ satisfying only $R = e^{\mathcal{V}D(f)}L$ is reduced to that of zeros of a meromorphic function $g(z)$. The number and the location of zeros of $g(z)$ are examined by an application of Cauchy Argument Principle in §3.3. It turns out, there are *infinite choices* for $f$ so that $R = e^{\mathcal{V}D(f)}L$. However, with the extra requirement that, for $C(\tau) = e^{\mathcal{V}D(f)\tau}L$, $c_k(\tau) \geq 0$ for all $k$ and for $\tau \in (0,1)$, problem (P) has a unique solution. The latter is established in §3.4.

## 3.1 Relation between $f$ and eigenvalues of $D(f)$

For a given vector $f$, the set of eigenvalues (always counting multiplicities) of $D(f)$ is uniquely determined. We will find that a prescribed set of $n$ eigenvalues for $D(f)$ will determine a unique vector $f$ as well.

The matrix $D(f)$, more precisely $D^T(f)$, arises from the standard pole placement problem (see, e.g., [37, 38]). Suppose the eigenvalues of $D(f)$ are given. Then $f$ is unique and the closed-form formula for $f$ can be derived. The spectral decomposition of $D(f)$ can be explicitly formulated. The following results can be derived essentially from [37, 38].

**Theorem 3.1.** *Suppose $\lambda_1, \ldots, \lambda_p$ are distinct eigenvalues of $D(f)$ with algebraic multiplicities $s_1, \ldots, s_p$ (therefore, $s_1 + s_2 + \ldots + s_p = n$). Then*

$$f_j = \frac{1}{b_j} \frac{\prod_{k=1}^{p} (\alpha_j - \lambda_k)^{s_k}}{\prod_{1 \leq k \leq n, k \neq j} (\alpha_j - \alpha_k)} \quad \text{for } \ j = 1, 2, \ldots, n, \tag{3.2}$$

*and*

$$D(f) = G^{-1}\Lambda G, \tag{3.3}$$

*where*

$$\Lambda = \begin{bmatrix} \Lambda_1 & & \\ & \ddots & \\ & & \Lambda_p \end{bmatrix}, \quad \Lambda_j = \begin{bmatrix} \lambda_j & & & \\ 1 & \lambda_j & & \\ & \ddots & \ddots & \\ & & 1 & \lambda_j \end{bmatrix}_{s_j \times s_j}, \tag{3.4}$$

$$G = \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_p \end{bmatrix} B =: VB, \tag{3.5}$$

*with* $B = \mathrm{diag}\,\{b_1, \dots, b_n\}$*, and, if* $\lambda_j \notin \{\alpha_1, \alpha_2, \dots, \alpha_n\}$*, then*

$$V_j = \begin{bmatrix} \frac{1}{\alpha_1-\lambda_j} & \frac{1}{\alpha_2-\lambda_j} & \cdots & \frac{1}{\alpha_n-\lambda_j} \\ \frac{1}{(\alpha_1-\lambda_j)^2} & \frac{1}{(\alpha_2-\lambda_j)^2} & \cdots & \frac{1}{(\alpha_n-\lambda_j)^2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{(\alpha_1-\lambda_j)^{s_j}} & \frac{1}{(\alpha_2-\lambda_j)^{s_j}} & \cdots & \frac{1}{(\alpha_n-\lambda_j)^{s_j}} \end{bmatrix} \tag{3.6}$$

*and, if* $\lambda_j = \alpha_k$ *for some* $k$*, then*

$$V_j = \begin{bmatrix} 0 & \cdots & 0 & -1 & 0 & \cdots & 0 \\ \frac{1}{\alpha_1-\alpha_k} & \cdots & \frac{1}{\alpha_{k-1}-\alpha_k} & 0 & \frac{1}{\alpha_{k+1}-\alpha_k} & \cdots & \frac{1}{\alpha_n-\alpha_k} \\ \frac{1}{(\alpha_1-\alpha_k)^2} & \cdots & \frac{1}{(\alpha_{k-1}-\alpha_k)^2} & 0 & \frac{1}{(\alpha_{k+1}-\alpha_k)^2} & \cdots & \frac{1}{(\alpha_n-\alpha_k)^2} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{1}{(\alpha_1-\alpha_k)^{s_j-1}} & \cdots & \frac{1}{(\alpha_{k-1}-\alpha_k)^{s_j-1}} & 0 & \frac{1}{(\alpha_{k+1}-\alpha_k)^{s_j-1}} & \cdots & \frac{1}{(\alpha_n-\alpha_k)^{s_j-1}} \end{bmatrix}. \tag{3.7}$$

*Proof.* The formula (3.2) can be found from the proof of [38, Theorem 2.1] with the assumptions $b_j = 1$ and $\lambda_j \notin \{\alpha_1, \dots, \alpha_m\}$ for $j = 1, \dots, n$. Here we provide a different proof with the condition $b_j \neq 0$ ($j = 1, \dots, n$) only.

Note that the characteristic polynomial of $D(f)$ is

$$\begin{aligned}
\prod_{k=1}^{p}(\lambda-\lambda_k)^{s_k} &= \det(\lambda I-\Gamma+fb^T)=\det(\lambda I-\Gamma)\Big(1+\sum_{s=1}^{n}\frac{b_sf_s}{\lambda-\alpha_s}\Big)\\
&= \prod_{k=1}^{n}(\lambda-\alpha_k)\Big(1+\sum_{s=1}^{n}\frac{b_sf_s}{\lambda-\alpha_s}\Big) \qquad (3.8)\\
&= \prod_{k=1}^{n}(\lambda-\alpha_k)+\sum_{s=1}^{n}b_sf_s\prod_{k=1,k\neq s}^{n}(\lambda-\alpha_k).
\end{aligned}$$

For each $j$, evaluate (3.8) at $\lambda=\alpha_j$ to get

$$b_jf_j=\frac{\prod_{k=1}^{p}(\alpha_j-\lambda_k)^{s_k}}{\prod_{1\le k\le n,k\neq j}(\alpha_j-\alpha_k)},$$

which gives formula (3.2) for $f_j$.

The formula (3.6) for $V_j$ in (3.5) can be derived from the general formula given in [37, Theorem 2.3] for $D^T(f)$ with $A=\Gamma$.

In case that $\lambda_j=\alpha_k$ for some $k$, let $\lambda_j(\delta)=\alpha_k+\delta$ be an eigenvalue of $D(f(\delta))$ with algebraic multiplicity $s_j$ where $f(\delta)$ is determined by (3.2) with only $\lambda_j$ replaced by $\lambda_j(\delta)$. For sufficiently small $\delta\neq 0$, $\lambda_j(\delta)\notin\{\alpha_1,\dots,\alpha_n\}$. Thus,

$$\Lambda_j(\delta)V_j(\delta)B=V_j(\delta)B(\Gamma-f(\delta)b^T), \qquad (3.9)$$

where $\Lambda_j(\delta)$ and $V_j(\delta)$ are obtained from $\Lambda_j$ and $V_j$ with $\lambda_j$ replaced with $\lambda_j(\delta)$. Define

$$\widetilde{V}_j(\delta)=(\Lambda_j(\delta)-\alpha_kI)V_j(\delta).$$

Then

$$\widetilde{V}_j(\delta)=\begin{bmatrix}\delta & & & \\ 1 & \delta & & \\ & \ddots & \ddots & \\ & & 1 & \delta\end{bmatrix}\begin{bmatrix}\frac{1}{\alpha_1-\alpha_k-\delta} & \cdots & \frac{1}{-\delta} & \cdots & \frac{1}{\alpha_n-\alpha_k-\delta}\\ \frac{1}{(\alpha_1-\alpha_k-\delta)^2} & \cdots & \frac{1}{(-\delta)^2} & \cdots & \frac{1}{(\alpha_n-\alpha_k-\delta)^2}\\ \vdots & & \vdots & \ddots & \vdots\\ \frac{1}{(\alpha_1-\alpha_k-\delta)^{s_j}} & \cdots & \frac{1}{(-\delta)^{s_j}} & \cdots & \frac{1}{(\alpha_n-\alpha_k-\delta)^{s_j}}\end{bmatrix},$$

and one can show

$$\lim_{\delta\to 0}\widetilde{V}_j(\delta)=V_j,$$

where $V_j$ is defined in (3.7).

Since $\Lambda_j(\delta)$ and $\Lambda_j(\delta)-\alpha_kI$ commute, by multiplying $\Lambda_j(\delta)-\alpha_kI$ to (3.9) from left, one has

$$\Lambda_j(\delta)\widetilde{V}_j(\delta)B=\widetilde{V}_j(\delta)B(\Gamma-f(\delta)b^T).$$

By taking $\delta \to 0$ and using the fact that $f(\delta)$ is a continuous function, we finally have

$$\Lambda_j V_j B = V_j B(\Gamma - fb^T).$$

The matrix $G$ defined in (3.5) is invertible if all $\lambda_j \notin \{\alpha_1, \dots, \alpha_n\}$ ([37]). It can be proved that $G$ is still invertible when some eigenvalues are equal to some $\alpha_k$, since after deleting the rows and columns in $G$ on which the entry $-1$ in $V_j$ defined in (3.7) locates, the resulting matrix has the same structure as the former case. $\square$

*Remark* 3.1. (i) If $D(f) = \Gamma - fb^T$ has $n$ distinct eigenvalues, then the matrix $V$ is the Cauchy matrix associated to $\alpha_j$'s and $\lambda_j$'s.

(ii) If $\lambda_j$ is an eigenvalue of $D(f)$ with algebraic multiplicity $s_j$, then $D(f)$ has a single $s_j \times s_j$ Jordan block associated to $\lambda_j$.

(iii) It is obvious that if $\lambda_j = \alpha_k$ for some $k$, then $f_k = 0$.

(iv) The formula (3.1) gives an explicit dependence of $f$ on eigenvalues of $D(f)$. Based on (3.8), if $f_j \neq 0$ for all $j$, then the eigenvalues of $D(f)$ are the zeros of the secular equation

$$1 + \sum_{s=1}^{n} \frac{b_s f_s}{\lambda - \alpha_s} = 0.$$

Thus, in general, the dependence of eigenvalues on $f$ is implicit. This is the reason that, in the sequel, the problem will be examined in terms of eigenvalues of $D(f)$ as in [54] instead of $f$ as in [31]. $\square$

## 3.2 A meromorphic function and its relation to $R = e^{\mathcal{V}D(f)}L$.

We now incorporate the condition (i) $R = e^{\mathcal{V}D(f)}L$ of problem (P) posted in the beginning of this section.

For the given $L$, $R$, $\alpha_k$'s, $b$ and $\mathcal{V}$ in (A1) and (A2), let $g: \mathbb{C} \to \mathbb{C}$ be the meromorphic function defined as

$$g(z) = \sum_{k=1}^{n} \frac{b_k r_k}{\alpha_k - z} - e^{\mathcal{V}z} \sum_{k=1}^{n} \frac{b_k l_k}{\alpha_k - z}. \tag{3.10}$$

Set

$$\begin{aligned} \mathcal{P}_1 &= \left\{k \in \{1, \dots, n\} : r_k \neq e^{\mathcal{V}\alpha_k} l_k\right\}, \\ \mathcal{P}_2 &= \left\{k \in \{1, \dots, n\} : r_k = e^{\mathcal{V}\alpha_k} l_k\right\}. \end{aligned} \tag{3.11}$$

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

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

**Lemma 3.2.** *The function $g(z)$ can be expressed as*

$$g(z) = g_1(z) + g_2(z)$$

*where*

$$g_1(z) = \sum_{k\in\mathcal{P}_1} \frac{b_k(r_k - e^{\mathcal{V}z}l_k)}{\alpha_k - z} \quad \text{and} \quad g_2(z) = \sum_{k\in\mathcal{P}_2} \frac{b_k(r_k - e^{\mathcal{V}z}l_k)}{\alpha_k - z}.$$

*For $k \in \mathcal{P}_1$, $z = \alpha_k$ is a simple pole of $g(z)$, and, for $k \in \mathcal{P}_2$, $z = \alpha_k$ is a removable pole of $g(z)$. In fact,*

$$g_2(z) = \sum_{k\in\mathcal{P}_2} \sum_{s=0}^{\infty} \frac{\mathcal{V}^{s+1} b_k r_k (z-\alpha_k)^s}{(s+1)!}$$

*is analytic.*

*Proof.* The formula for $g_2(z)$ can be simply obtained by

$$\begin{aligned} g_2(z) &= \sum_{k\in\mathcal{P}_2} \frac{b_k(r_k - e^{\mathcal{V}z}l_k)}{\alpha_k - z} = \sum_{k\in\mathcal{P}_2} \frac{b_k r_k (e^{\mathcal{V}(z-\alpha_k)} - 1)}{z - \alpha_k} \\ &= \sum_{k\in\mathcal{P}_2} \sum_{s=0}^{\infty} \frac{\mathcal{V}^{s+1} b_k r_k (z-\alpha_k)^s}{(s+1)!}. \end{aligned}$$

The rest statements are clear. □

Recall that $z = \lambda \in \mathbb{C}$ is a root of $g(z) = 0$ with multiplicity $s \geq 1$ if

$$g(\lambda) = g'(\lambda) = \ldots = g^{(s-1)}(\lambda) = 0 \ \text{ and } \ g^{(s)}(\lambda) \neq 0.$$

Our next result establishes a direct relation between the eigenvalues of $D(f)$ with the zeros of $g(z)$ in order to satisfy $R = e^{\mathcal{V}D(f)}L$.

**Theorem 3.3.** *Let $\lambda_1, \lambda_2, \ldots, \lambda_p$ be distinct eigenvalues of $D(f)$ with algebraic multiplicities $s_1, s_2, \ldots, s_p$, respectively. (So $f$ is defined by (3.2).) Then the matrix $D(f) = \Gamma - fb^T$ satisfies $R = e^{\mathcal{V}D(f)}L$ if and only if, for each $j = 1, 2, \ldots, p$,*

- *(a) if $\lambda_j \notin \{\alpha_1, \ldots, \alpha_n\}$, then $\lambda_j$ is a root of $g(z) = 0$ with multiplicity at least $s_j$;*
- *(b) if $\lambda_j = \alpha_k$ for some $k$, then $r_k = e^{\mathcal{V}\alpha_k} l_k$, and hence, $k \in \mathcal{P}_2$; furthermore, if $s_j > 1$, then $z = \alpha_k$ is a root of $g(z) = 0$ with multiplicity at least $s_j - 1$.*

*Proof.* It follows from (3.3) that

$$GR = e^{\mathcal{V}\Lambda} GL.$$

and hence, for each $j = 1, 2, \dots, p$,

$$V_j BR = e^{\mathcal{V}\Lambda_j} V_j BL. \tag{3.12}$$

From (3.4), it is easy to compute that

$$e^{\mathcal{V}\Lambda_j} = e^{\mathcal{V}\lambda_j} \begin{bmatrix} 1 & & & \\ \mathcal{V} & 1 & & \\ \vdots & \ddots & \ddots & \\ \frac{\mathcal{V}^{s_j-1}}{(s_j-1)!} & \dots & \mathcal{V} & 1 \end{bmatrix}.$$

If $\lambda_j \notin \{\alpha_1, \dots, \alpha_n\}$, then, by comparing the components on both sides of (3.12), one has

$$\begin{aligned} \sum_{k=1}^{n} \frac{b_k r_k}{\alpha_k - \lambda_j} &= e^{\mathcal{V}\lambda_j} \sum_{k=1}^{n} \frac{b_k l_k}{\alpha_k - \lambda_j}, \\ \sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - \lambda_j)^2} &= e^{\mathcal{V}\lambda_j} \left( \mathcal{V} \sum_{k=1}^{n} \frac{b_k l_k}{\alpha_k - \lambda_j} + \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - \lambda_j)^2} \right), \\ &\vdots \\ \sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - \lambda_j)^s} &= e^{\mathcal{V}\lambda_j} \sum_{q=1}^{s} \frac{\mathcal{V}^{s-q}}{(s-q)!} \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - \lambda_j)^q}, \\ &\vdots \\ \sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - \lambda_j)^{s_j}} &= e^{\mathcal{V}\lambda_j} \sum_{q=1}^{s_j} \frac{\mathcal{V}^{s_j-q}}{(s_j-q)!} \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - \lambda_j)^q}. \end{aligned} \tag{3.13}$$

For the function $g(z)$ defined in (3.10), the display (3.13) implies that

$$g(\lambda_j) = g'(\lambda_j) = \dots = g^{(s_j-1)}(\lambda_j) = 0;$$

that is, $\lambda_j$ is a root of $g(z) = 0$ with multiplicity at least $s_j$.

If $\lambda_j = \alpha_k$ for some $k$, then $V_k$ is given by (3.7). The relation $r_k = e^{\mathcal{V}\alpha_k} l_k$ follows from the first component on both sides of (3.12). If $s_j > 1$, then, by comparing the rest of components of (3.12), we have

$$g(\alpha_k) = g'(\alpha_k) = \dots = g^{s_j-2}(\alpha_k) = 0.$$

Hence, beside the relation $r_k = e^{\mathcal{V}\alpha_k} l_k$, $z = \alpha_k$ is a root of $g(z) = 0$ with multiplicity at least $s_j - 1$. $\square$

*Remark* 3.2. (i) Even if $r_k = e^{\mathcal{V}\alpha_k} l_k$ for some $k$, as we will see in §3.3 that the number $\alpha_k$ needs NOT to be an eigenvalue of $D(f)$ to have $R = e^{\mathcal{V}D(f)}L$. If $\alpha_k$ is a simple eigenvalue of $D(f)$, then $r_k = e^{\mathcal{V}\alpha_k} l_k$ but $\alpha_k$ may or may not be a root of $g(z) = 0$.

(ii) Concerning the statement on the multiplicity in (a) of Theorem 3.3, it is possible that $\lambda_j$ is an eigenvalue of $D(f)$ of multiplicity $s_j$ while it is a root of $g(z) = 0$ of multiplicity strictly greater than $s_j$. Similar remark applies to that in the statement (b). These observations are based on results of locations of roots of $g(z)$ in §3.3. $\square$

### 3.3 Cauchy Argument Principle and zeros of $g(z)$

We will apply Cauchy Argument Principle to identify the number and the location of zeros of the function $g(z)$ defined in (3.10). Recall,

**Cauchy Argument Principle:** *Let $h(z)$ be a meromorphic function in $\Omega \subset \mathbb{C}$ with the zeros $z_j$ and the poles $p_k$. Then,*

$$\frac{1}{2\pi i}\int_\gamma \frac{h'(z)}{h(z)} dz = \sum_j n(\gamma, z_j) - \sum_k n(\gamma, p_k)$$

*for every cycle $\gamma$ which is homologous to zero in $\Omega$ and does not pass through any of the zeros or poles. Here $n(\gamma, a)$ is the winding number of $\gamma$ about $a$.*

For the meromorphic function $g(z)$ defined in (3.10), we have

**Lemma 3.4.** *For each integer $p$, there is no zero $z_0$ of $g(z)$ with $Im(z_0) = (2p+1)\pi/\mathcal{V}$.*

*Proof.* We write $g(z) = R(z) + iI(z)$ where $R(z)$ and $I(z)$ are real-valued. It follows from the definition of $g(z)$ in (3.10) that

$$\begin{aligned} R(z) =& \sum_{k=1}^n \frac{b_k r_k(\alpha_k - x)}{(\alpha_k - x)^2 + y^2} \\ &- e^{\mathcal{V}x}\Big(\cos(\mathcal{V}y)\sum_{k=1}^n \frac{b_k l_k(\alpha_k - x)}{(\alpha_k - x)^2 + y^2} - y\sin(\mathcal{V}y)\sum_{k-1}^n \frac{b_k l_k}{(\alpha_k - x)^2 + y^2}\Big), \\ I(z) =& y\sum_{k=1}^n \frac{b_k r_k}{(\alpha_k - x)^2 + y^2} \\ &- e^{\mathcal{V}x}\Big(\sin(\mathcal{V}y)\sum_{k=1}^n \frac{b_k l_k(\alpha_k - x)}{(\alpha_k - x)^2 + y^2} + y\cos(\mathcal{V}y)\sum_{k=1}^n \frac{b_k l_k}{(\alpha_k - x)^2 + y^2}\Big). \end{aligned}$$

For any integer $p$, let $z = x + iy_p$ with $y_p = (2p+1)\pi/\mathcal{V}$. Then, $y_p \neq 0$, $\sin(\mathcal{V}y_p) = 0$ and $\cos(\mathcal{V}y_p) = -1$, and hence,

$$I(z) = y_p\Big(\sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - x)^2 + y_p^2} + e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - x)^2 + y_p^2}\Big) \neq 0.$$

Therefore, $g(z) \neq 0$ if $Im(z) = y_p = (2p+1)\pi/\mathcal{V}$. □

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

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

Recall the definitions of $\mathcal{P}_1$ and $\mathcal{P}_2$ in (3.11). Let $m$ be the number of elements in $\mathcal{P}_1$. Then $(n-m)$ is the number of elements in $\mathcal{P}_2$. It follows from Lemma 3.2 that $g(z)$ has $m$ simple poles at $\alpha_k$'s for $k \in \mathcal{P}_1$.

**Theorem 3.5.** *The meromorphic function $g(z)$ has infinitely 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 $S_p \backslash S_{p-1}$, one in each connected component.*

*Proof.* Note that $g(\bar{z}) = \overline{g(z)}$. Thus, complex zeros of $g(z)$ must be in conjugate pairs.

We now consider zeros of $g(z)$ in each stripe $S_p$ for any integer $p \geq 0$. Let $z = x + iy$. For $a > 0$, consider the rectangle $B_{a,p}$ bounded by lines $x = \pm a$ and $y = \pm(2p+1)\pi/\mathcal{V}$. We will take $a > \max\{|\alpha_j| : j = 1, 2, \ldots, n\}$ so that the $m$ poles $\alpha_k$'s for $k \in \mathcal{P}_1$ of $g(z)$ are always contained in $B_{a,p}$.

By the Cauchy Argument Principle, the number of zeros of $g(z)$ in the rectangle $B_{a,p}$ is

$$N_{a,p} = \frac{1}{2\pi i}\int_{\Gamma} \frac{g'(z)}{g(z)} dz + m, \tag{3.14}$$

where $\Gamma$ is the boundary of the rectangle $B_{a,p}$ oriented counter-clockwise.

We now fix an integer $p \geq 0$ and denote $y_p = (2p+1)\pi/\mathcal{V}$.

Write $N_{a,p} = N^v_{a,p} + N^h_{a,p} + m$ where $N^v_{a,p}$ is the sum of integrals in (3.14) over the two vertical segments of $\Gamma$ and $N^h_{a,p}$ is that over the two horizontal segments; that is,

$$\begin{aligned} N^v_{a,p} =& \frac{1}{2\pi}\int_{-y_p}^{y_p} \left(\frac{g'(a+iy)}{g(a+iy)} - \frac{g'(-a+iy)}{g(-a+iy)}\right) dy, \\ N^h_{a,p} =& \frac{1}{2\pi i}\int_{-a}^{a} \left(\frac{g'(x-iy_p)}{g(x-iy_p)} - \frac{g'(x+iy_p)}{g(x+iy_p)}\right) dx. \end{aligned}$$

We will estimate the term $N^v_{a,p}$ first. Note that

$$g'(z) = \sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - z)^2} - e^{\mathcal{V}z} \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - z)^2} - \mathcal{V} e^{\mathcal{V}z} \sum_{k=1}^{n} \frac{b_k l_k}{\alpha_k - z}.$$

For the fixed $p \geq 0$ and for $y \in [-(2p+1)\pi/\mathcal{V}, (2p+1)\pi/\mathcal{V}]$, one has, as $x = -a \to -\infty$, $e^{\mathcal{V}z} \to 0$ since $\mathcal{V} > 0$, and hence,

$$\frac{g'(z)}{g(z)} = O\left( \frac{\sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - z)^2}}{\sum_{k=1}^{n} \frac{b_k r_k}{\alpha_k - z}} \right) \to 0.$$

On the other hand, as $x = a \to \infty$, one has $|e^{\mathcal{V}z}| = e^{\mathcal{V}a} \to \infty$, and hence,

$$\frac{g'(z)}{g(z)} \to \mathcal{V}.$$

We thus conclude that

$$\lim_{a \to \infty} N^v_{a,p} = \frac{1}{2\pi} \int_{-y_p}^{y_p} \mathcal{V} dy = 2p + 1. \tag{3.15}$$

We now work on the other term $N^h_{a,p}$. It follows from $y_p = (2p+1)\pi/\mathcal{V}$ that $e^{\mathcal{V}(x \pm y_p)} = -e^{\mathcal{V}x}$. Thus

$$\begin{aligned} g(x \pm iy_p) =& \sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - x) \mp iy_p} + e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - x) \mp iy_p}, \\ g'(x \pm iy_p) =& \sum_{k=1}^{n} \frac{b_k r_k}{[(\alpha_k - x) \mp iy_p]^2} \\ & + e^{\mathcal{V}x} \Big( \sum_{k=1}^{n} \frac{b_k l_k}{[(\alpha_k - x) \mp iy_p]^2} + \mathcal{V} \sum_{k=1}^{m} \frac{b_k l_k}{(\alpha_k - x) \mp iy_p} \Big), \end{aligned}$$

and hence, from $g(z) = R(z) + iI(z)$,

$$\begin{aligned} R_\pm(x) :=& R(x \pm iy_p) = \sum_{k=1}^{n} \frac{b_k r_k (\alpha_k - x)}{(\alpha_k - x)^2 + y_p^2} + e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k (\alpha_k - x)}{(\alpha_k - x)^2 + y_p^2}, \\ I_\pm(x) :=& I(x \pm iy_p) = \pm y_p \Big( \sum_{k=1}^{n} \frac{b_k r_k}{(\alpha_k - x)^2 + y_p^2} + e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - x)^2 + y_p^2} \Big). \end{aligned}$$

Let $g'(z) = R'(z) + iI'(z)$. A direct calculation yields

$$\begin{aligned}
R'_{\pm}(x) :=& R'(x \pm iy_p) = \sum_{k=1}^{n} \frac{b_k r_k [(\alpha_k - x)^2 - y_p^2]}{[(\alpha_k - x)^2 + y_p^2]^2} \\
&+ e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k [(\alpha_k - x)^2 - y_p^2]}{[(\alpha_k - x)^2 + y_p^2]^2} + \mathcal{V} e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k (\alpha_k - x)}{(\alpha_k - x)^2 + y_p^2}, \\
I'_{\pm}(x) :=& I'(x \pm iy_p) = \pm 2y_p \sum_{k=1}^{n} \frac{b_k r_k (\alpha_k - x)}{[(\alpha_k - x)^2 + y_p^2]^2} \\
&\pm 2y_p e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k (\alpha_k - x)}{[(\alpha_k - x)^2 + y_p^2]^2} \pm \mathcal{V} y_p e^{\mathcal{V}x} \sum_{k=1}^{n} \frac{b_k l_k}{(\alpha_k - x)^2 + y_p^2}.
\end{aligned}$$

Since

$$\frac{g'(x \pm iy_p)}{g(x \pm iy_p)} = \frac{R'_{\pm}(x) R_{\pm}(x) + I'_{\pm}(x) I_{\pm}(x)}{R_{\pm}(x)^2 + I_{\pm}(x)^2} + i \frac{I'_{\pm}(x) R_{\pm}(x) - R'_{\pm}(x) I_{\pm}(x)}{R_{\pm}(x)^2 + I_{\pm}(x)^2},$$

and $N_{a,p}$ and $N^h_{a,p}$ have to be real, the real part in the above expression will not contribute to $N^h_{a,p}$. By using the additional fact that

$$R_+(x) = R_-(x),\ R'_+(x) = R'_-(x),\ I_+(x) = -I_-(x),\ I'_+(x) = -I'_-(x),$$

we have

$$\begin{aligned}
N^h_{a,p} =& \frac{1}{2\pi} \int_{-a}^{a} \Big( \frac{I'_-(x) R_-(x) - R'_-(x) I_-(x)}{R_-(x)^2 + I_-(x)^2} - \frac{I'_+(x) R_+(x) - R'_+(x) I_+(x)}{R_+(x)^2 + I_+(x)^2} \Big) dx \\
=& \frac{1}{\pi} \int_{-a}^{a} \frac{I_+(x) R'_+(x) - R_+(x) I'_+(x)}{R_+(x)^2 + I_+(x)^2} dx.
\end{aligned}$$

Note that $R'_+(x)$ and $I'_+(x)$ are indeed the derivatives of $R_+(x)$ and $I_+(x)$ with respect to $x$. Note also that $I_+(x) = I(x + iy_p) \neq 0$. Therefore,

$$\begin{aligned}
\frac{I_+(x) R'_+(x) - R_+(x) I'_+(x)}{R_+(x)^2 + I_+(x)^2} =& \frac{I_+(x) R'_+(x) - R_+(x) I'_+(x)}{I_+(x)^2} \frac{I_+(x)^2}{R_+(x)^2 + I_+(x)^2} \\
=& \frac{\left(\frac{R_+(x)}{I_+(x)}\right)'}{1 + \left(\frac{R_+(x)}{I_+(x)}\right)^2} = \left( \arctan \frac{R_+(x)}{I_+(x)} \right)'.
\end{aligned}$$

Hence,

$$N^h_{a,p} = \frac{1}{\pi} \left( \arctan \frac{R_+(a)}{I_+(a)} - \arctan \frac{R_+(-a)}{I_+(-a)} \right).$$

Based on simple observations, one has

$$\lim_{a\to\infty} \frac{R_+(a)}{I_+(a)} = -\infty \quad \text{and} \quad \lim_{a\to\infty} \frac{R_+(-a)}{I_+(-a)} = \infty.$$

Therefore,

$$\lim_{a\to\infty} N^h_{a,p} = -1. \tag{3.16}$$

Finally, combining (3.15) and (3.16), one has

$$\lim_{a\to\infty} N_{a,p} = \lim_{a\to\infty} N^v_{a,p} + \lim_{a\to\infty} N^h_{a,p} + m = (2p+1) - 1 + m = 2p + m.$$

We conclude that, for each integer $p \geq 0$, $g(z)$ has exactly $m + 2p$ zeros in the stripe $S_p$. The other statements then follow directly. □

### 3.4 Solutions of problem (P) in (3.1).

First of all, as a direct consequence of Theorems 3.3 and 3.5, we have

**Theorem 3.6.** *There are infinitely many ways to choose the eigenvalues of $D(f)$ to satisfy $R = e^{\mathcal{V}D(f)}L$.*

*Furthermore, if the eigenvalues of $D(f)$ are restricted in the stripe $S_0$, then the choice is unique. They are all the $m$ zeros of $g(z)$ in $S_0$ together with all the $(n-m)$ removable poles $\alpha_k$'s for $k \in \mathcal{P}_2$.*

We now impose the condition that, for $C(\tau) = e^{\mathcal{V}D(f)\tau}L$,

$$c_k(\tau) \geq 0, \quad \forall \tau \in (0,1) \text{ and } k = 1, 2, \ldots, n. \tag{3.17}$$

We will establish the uniqueness result for problem (P) first.

**Theorem 3.7.** *Assume (A1) and (A2). If $C(\tau) = e^{\mathcal{V}D(f)\tau}L$ satisfies $C(1) = R$ and (3.17), then all the $n$ eigenvalues $\lambda_j$'s of $D(f)$ must be in the stripe $S_0$. Hence, problem (P) has at most one solution.*

*Proof.* If all the $n$ eigenvalues $\lambda_j$'s of $D(f)$ are in the stripe $S_0$ and $R = e^{\mathcal{V}D(f)}L$, then, from Theorem 3.6, the choice is unique. Suppose, on the contrary, that $\lambda_j \notin S_0$ for some eigenvalue $\lambda_j$ of $D(f)$ so that $|\mathrm{Im}(\lambda_j)| > \pi/\mathcal{V}$. From Theorems 3.3 and 3.5, $\lambda_j$ must be a simple zero of $g(z)$. Using (3.3), one has, for $\tau \in (0,1)$,

$$\sum_{k=1}^{n} \frac{b_k c_k(\tau)}{\alpha_k - \lambda_j} - e^{\mathcal{V}\lambda_j \tau} \sum_{k=1}^{n} \frac{b_k l_k}{\alpha_k - \lambda_j} = 0. \tag{3.18}$$

Since $|\mathrm{Im}(\lambda_j)| > \pi/\mathcal{V}$, there exists $\tau_j \in (0,1)$ so that $|\mathrm{Im}(\tau_j\lambda_j)| = \pi/\mathcal{V}$. If we set $\tilde{\lambda} = \tau_j\lambda_j$, then $|\mathrm{Im}(\tilde{\lambda})| = \pi/\mathcal{V}$ and, from (3.18), $\tilde{\lambda}$ is a root of

$$\sum_{k=1}^{n} \frac{b_k c_k(\tau_j)}{\tau_j\alpha_k - z} - e^{\mathcal{V}z} \sum_{k=1}^{n} \frac{b_k l_k}{\tau_j \alpha_k - z} = 0.$$

This contradicts to Lemma 3.4 with $p = 0$ since $c_k(\tau_j) \geq 0$. □

We now show that $C(\tau) = e^{\mathcal{V}D(f)\tau}L$ determined by the unique choice of eigenvalues in Theorem 3.7 does satisfy (3.17).

**Theorem 3.8.** *Assume (A1), (A2) and $(l_k, r_k) \neq (0,0)$ for $k = 1, 2, \ldots, n$. Suppose the eigenvalues of $D(f)$ so that $R = e^{\mathcal{V}D(f)}L$ are chosen in the stripe $S_0$. Then $C(\tau) = e^{\mathcal{V}D(f)\tau}L$ satisfies (3.17). Furthermore, for $k = 1, 2, \ldots, n$, $c_k(\tau) > 0$ for $\tau \in (0,1)$.*

*Proof.* We denote the $n$ eigenvalues of $D(f)$ from the stripe $S_0$ as $\beta_1, \beta_2, \ldots, \beta_n$ where $\beta_1, \beta_2, \ldots, \beta_m$ are the $m$ zeros (possibly repeated) of $g(z)$ in $S_0$ and, for $m+1 \leq k \leq n$, $\beta_k = \alpha_j$ for some $j \in \mathcal{P}_2$. It is possible that, for some $1 \leq k \leq m$, $\beta_k \in \{\alpha_j : j \in \mathcal{P}_2\}$.

For $C(\tau) = e^{\mathcal{V}D(f)\tau}L$, we set

$$A = \{\tau \in (0,1) : \ c_j(s) > 0 \ \text{ for } \ j = 1, 2, \ldots, n \ \text{ and for } \ 0 < s \leq \tau\}.$$

We will show that $A = (0,1)$ in three steps.

Step 1. First of all, it is clear that $A$ is open and connected.

Step 2. Next, we show that $A \neq \emptyset$. If $c_j(0) = l_j > 0$ for every $j$, then, by continuity, we have, for $\tau > 0$ small, $\tau \in A$. Suppose $l_j = 0$ for some $j$, say, $l_n = 0$. If $n \in \mathcal{P}_2$, that is, $r_n = e^{\mathcal{V}\alpha_n} l_n$, then $r_n = 0$. This contradicts to the assumption that $(l_n, r_n) \neq (0,0)$. Therefore, $n \in \mathcal{P}_1$. To complete this step, we will show that $dc_n/d\tau > 0$ at $\tau = 0$.

It follows from $C(\tau) = e^{\mathcal{V}D(f)\tau}L$ that

$$\frac{dc_n}{d\tau}(\tau) = \mathcal{V}\alpha_n c_n(\tau) - \mathcal{V} f_n b^T C(\tau).$$

Thus,

$$\frac{dc_n}{d\tau}(0) = \mathcal{V}\alpha_n c_n(0) - \mathcal{V} f_n b^T C(0) = -\mathcal{V} f_n \sum_{s=1}^{n} b_s l_s.$$

Since $\mathcal{V}\sum_{s=1}^{n} b_s l_s > 0$, to conclude that $(dc_n/d\tau)(0) > 0$, it suffices to show

$$f_n < 0. \tag{3.19}$$

Note that, from (3.2),

$$f_n = \frac{\prod_{k=1}^{m}(\alpha_n - \beta_k)\prod_{k\in\mathcal{P}_2}(\alpha_n - \alpha_k)}{b_n\prod_{k=1}^{n-1}(\alpha_n - \alpha_k)} = \frac{\prod_{k=1}^{m}(\alpha_n - \beta_k)}{b_n\prod_{k\in\mathcal{P}_1, k\neq n}(\alpha_n - \alpha_k)}. \tag{3.20}$$

The sign of the denominator in the last expression of (3.20) is $(-1)^p$ where $p$ is the number of $\alpha_k$'s with $k \in \mathcal{P}_1$ that are larger than $\alpha_n$. Without loss of generality, we may assume that $\mathcal{P}_1 = \{1, 2, \ldots, m-1, n\}$ and

$$\alpha_1 > \alpha_2 > \cdots > \alpha_p > \alpha_n > \alpha_{p+1} \cdots > \alpha_{m-1}.$$

For the sign of the numerator in the last expression of (3.20), we need to determine the number of $\beta_k$'s for $k = 1, 2, \ldots, m$ that are *real* and in $(\alpha_n, \infty)$ since any pair of complex conjugate $\beta_k$'s provides a positive factor for the numerator. Note that all the real $\beta_k$'s are the real zeros of $g(z)$. So we only need to consider $g(z)$ for real $z$. For a real zero $\beta_k$ of $g(z)$, if $\beta_k < \alpha_n$, then the factor $\alpha_n - \beta_k$ in the numerator is positive; if $\beta_k > \alpha_n$ and $\beta_k$ has an even multiplicity, then the factors associated to $\beta_k$ provide an overall positive factor for the numerator; if $\beta_k > \alpha_n$ and $\beta_k$ has an odd multiplicity, then the factors associated to $\beta_k$ provide an overall negative factor for the numerator. Thus the number of negative factors in the numerator equals the number of zeros of $g(z)$ in $(\alpha_n, \infty)$ with odd multiplicities.

Let $T$ be the total number of sign changes of $g(z)$ for $z \in (\alpha_n, \infty)$, let $T_0$ be the number of zeros with odd multiplicities of $g(z)$ for $z \in (\alpha_n, \infty)$, and let $T_1$ be the number of sign changes of $g(z)$ as $z$ crosses the poles $\alpha_j \in (\alpha_n, \infty)$ for $j = 1, 2, \ldots, p$. It is clear that $T = T_0 + T_1$.

Since $l_n = 0$ and $n \in \mathcal{P}_1$, we have $r_n \neq 0$, and hence, $r_n > 0$. We can write $g(z)$ in (3.10) as

$$\begin{aligned} g(z) &= \sum_{k=1}^{n} \frac{b_k r_k}{\alpha_k - z} - e^{\mathcal{V}z}\sum_{k=1}^{n}\frac{b_k l_k}{\alpha_k - z} \\ &= \frac{b_n r_n}{\alpha_n - z} + \sum_{k=1}^{n-1}\frac{b_k r_k}{\alpha_k - z} - e^{\mathcal{V}z}\sum_{k=1}^{n-1}\frac{b_k l_k}{\alpha_k - z}. \end{aligned}$$

It is clear that $g(z) \to \infty$ as $z \to \infty$. Note also that, as $z \to \alpha_n^+$, $\frac{b_n r_n}{\alpha_n - z} \to -\infty$ and all other terms in $g(z)$ stay bounded. Thus, $g(z) \to -\infty$ as $z \to \alpha_n^+$. In particular, $T$ is odd. Now, near each pole $\alpha_j \in (\alpha_n, \infty)$ for $j = 1, 2, \ldots, p$, it follows from $r_j - e^{\mathcal{V}\alpha_j} l_j \neq 0$ that, if $g(z) \to -\infty$ as $z \to \alpha_j^+$, then $g(z) \to \infty$ as $z \to \alpha_j^-$, and vise versa. Thus, near each such a pole $\alpha_j$, $g(z)$ changes sign exactly once, and hence, $T_1 = p$. Thus, $T_0 = T - p$.

We emphasize that $\beta_1, \beta_2, \cdots, \beta_m$ contain all zeros of $g(z)$ in the stripe $S_0$, particularly, ALL *real* zeros (counting multiplicity) of $g(z)$. Since $T$ is odd, we conclude that the sign of the numerator in the last expression of $f_n$ in (3.20) is $(-1)^{T_0} = (-1)^{p+1}$; that is, it is opposite to that of the denominator of $f_n$, and hence, $f_n < 0$. Therefore, $A \neq \emptyset$.

Step 3. Since $A \neq \emptyset$, we can set $\tau_0 = \sup A$. Then, $\tau_0 \in (0, 1]$. If $\tau_0 = 1$, then $A = (0, 1)$ and the theorem is proved. Suppose $\tau_0 < 1$. Then

$$\begin{aligned} c_k(\tau) >& 0 \;\text{ for all }\; k \;\text{ and for }\; \tau \in (0, \tau_0), \\ c_j(\tau_0) =& 0 \;\text{ and }\; c_j'(\tau_0) \leq 0 \;\text{ for some }\; j, \;\text{ and} \\ c_k(\tau_0) \geq& 0 \;\text{ for }\; k \neq j \;\text{ and, for at least one } k,\; c_k(\tau_0) > 0. \end{aligned} \tag{3.21}$$

We may again assume $j = n$. We will follow more or less the same argument as in Step 2 to show that $c_n'(\tau_0) > 0$ to get a contradiction.

If $n \in \mathcal{P}_2$, then $\alpha_n$ is an eigenvalue of $D(f)$ so that $f_n = 0$ from (3.2). It then follows from

$$\frac{dc_n}{d\tau}(\tau) = \mathcal{V}\alpha_n c_n(\tau) - \mathcal{V} f_n b^T C(\tau) = \mathcal{V}\alpha_n c_n(\tau)$$

that $c_n(\tau) = e^{\mathcal{V}\alpha_n(\tau - \tau_0)} c_n(\tau_0) = 0$ for all $\tau \in [0, 1]$. This contradicts to $(l_n, r_n) \neq (0, 0)$ in (2.3). Therefore, $n \in \mathcal{P}_1$. It follows from (3.21) that

$$\frac{dc_n}{d\tau}(\tau_0) = \mathcal{V}\alpha_n c_n(\tau_0) - \mathcal{V} f_n b^T C(\tau_0) = -\mathcal{V} f_n \sum_{s=1}^{n} b_s c_s(\tau_0) \leq 0,$$

and hence, $f_n \geq 0$. It is also clear that $f_n \neq 0$ since $n \in \mathcal{P}_1$.

Next, we will apply the same argument as for (3.19) in Step 2 to show $f_n < 0$ for a contradiction. In the argument in Step 2, $l_n = 0$ is critical for the sign changing behavior of $g(z)$ for $z \in (\alpha_n, \infty)$. Here we need to replace $l_n = 0$ with $c_n(\tau_0) = 0$ as follows.

It follows from $C(\tau_0) = e^{\mathcal{V}D(f)\tau_0} L$ and $R = e^{\mathcal{V}D(f)} L$ that

$$R = e^{\mathcal{V}(1-\tau_0)D(f)} C(\tau_0). \tag{3.22}$$

In the definition of $g(z)$ in (3.10), if we replace $L$ with $C(\tau_0)$ and $\mathcal{V}$ with $\mathcal{V}(1 - \tau_0)$, we get

$$h(z; \tau_0) = \sum_{k=1}^{n} \frac{b_k r_k}{\alpha_k - z} - e^{\mathcal{V}(1-\tau_0)z} \sum_{k=1}^{n} \frac{b_k c_k(\tau_0)}{\alpha_k - z}. \tag{3.23}$$

Recall that, for $k = 1, 2, \ldots, n$, $\beta_k$ is an eigenvalue of $D(f)$ as defined in the beginning of the proof. In Theorem 3.3, if we replace the condition $R = e^{\mathcal{V}D(f)}L$ with (3.22) and $g(z)$ with $h(z;\tau_0)$, then we conclude that, for $k = 1, 2, \ldots, n$, $\beta_k$ is either a zero or a removable pole of $h(z;\tau_0)$. Note that, if $\alpha_k$ is a removable pole of $g(z)$, that is, $r_k = e^{\mathcal{V}\alpha_k}l_k$, then $f_k = 0$, and hence, $c_k(\tau) = e^{\mathcal{V}\alpha_k\tau}l_k$. In particular, $r_k = e^{\mathcal{V}(1-\tau_0)\alpha_k}c_k(\tau_0)$, that is, $\alpha_k$ is also a removable pole of $h(z;\tau_0)$. It is easy to see that the converse is also true. Hence, $\beta_{m+1}, \beta_{m+2}, \ldots, \beta_n$ are precisely all the removable poles of $h(z;\tau_0)$, and $\beta_1, \beta_2, \ldots, \beta_m$ are necessarily zeros of $h(z;\tau_0)$.

Note that, for $k = 1, 2, \ldots, n$, $\beta_k \in S_0$ where

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

is the stripe associated to $g(z)$. Associated to $h(z;\tau_0)$, the corresponding stripe is

$$S_0(h) = \big\{z = x + iy :\ y \in \big(-\pi/\mathcal{V}(1-\tau_0), \pi/\mathcal{V}(1-\tau_0)\big)\big\}\,.$$

Since $0 < \tau_0 < 1$, $S_0(g) \subset S_0(h)$, and hence, $\beta_k \in S_0(h)$ for all $k = 1, 2, \ldots, n$. As established above, $h(z;\tau_0)$ has $(n-m)$ poles. An application of Theorem 3.5 then concludes that $h(z;\tau_0)$ has exactly $m$ zeros in $S_0(h)$; most importantly, just as emphasized in the last paragraph in Step 2, $\beta_1, \beta_2, \ldots, \beta_m$ (counting multiplicity) are precisely all zeros of $h(z;\tau_0)$ in $S_0(h)$, particularly, they include ALL *real* zeros of $h(z;\tau_0)$.

It is clear that $r_n \neq 0$ since, otherwise, $\alpha_n$ would be a removable pole of $h(z;\tau_0)$ due to $c_n(\tau_0) = 0$, and hence, it contradicts to $n \in \mathcal{P}_1$. With $r_n > 0$ and $c_n(\tau_0) = 0$, one can apply exactly the same argument for (3.19) in Step 2 to conclude that $f_n < 0$. The contradiction then completes the proof. $\square$

*Remark* 3.3. (i) It is extremely important to note that the zeros $\beta_1, \beta_2, \ldots, \beta_m$ of $h(z;\tau_0)$ in (3.23) are all zeros of $g(z)$ in the stripe $S_0$. But all other zeros of $h(z;\tau_0)$ may not be zeros of $g(z)$, and vise verse.

(ii) It seems that the proof in Step 3 only involves real zeros of $g(z)$ among $\beta_1, \beta_2, \ldots, \beta_m$. It is actually not the case. It is worthwhile to explain this in a detail for a better understanding of the proof. Suppose $\{\beta_1, \beta_2\}$ is a pair of complex conjugate zeros of $g(z)$ in $S_0(g)$. If one replaces this pair by a pair $\{\hat{\beta}_1, \hat{\beta}_2\}$ outside $S_0(g)$, then there is the corresponding solution $C(\tau)$. Assume $\tau_0 \in (0, 1)$ is the corresponding value in (3.21) in Step 3 for this solution $C(\tau)$. Then, for $\tau \in [0, \tau_0]$, one can define $h(z;\tau)$ as in (3.23) with $\tau_0$ being replaced by $\tau$. It is clear that $h(z;0) = g(z)$ and $\hat{\beta}_1, \hat{\beta}_2, \beta_3, \ldots, \beta_m$ are zeros of $h(z;\tau)$ for $\tau \in [0, \tau_0]$. By continuity and

Lemma 3.4, $\beta_3, \dots, \beta_m \in S_0(h(z;\tau_0))$ and $\hat{\beta}_1, \hat{\beta}_2$ are still outside $S_0(h(z;\tau_0))$. An application of Theorem 3.5 to $h(z;\tau_0)$ gives that there are two additional zeros of $h(z;\tau_0)$ in $S_0(h(z;\tau_0))$. If these two zeros are real, then their locations may affect the counting of sign changes and the proof may not go through in this case. In fact, this must be the case due to the uniqueness result in Theorem 3.7. $\square$

### 3.5 The unique solution of problem BVP$_0$ and properties.

In this part, we consider the reduced problem BVP$_0$; in particular, we recall $b = (\alpha_1^2, \alpha_2^2, \dots, \alpha_n^2)^T$. We first summarize the result concerning the existence and uniqueness of solutions to problem BVP$_0$ in (2.18).

**Theorem 3.9.** *Assume (2.3), (2.4) and $\mathcal{V} > 0$. Problem $BVP_0$ in (2.18) has a unique solution with a stronger property that for all $k = 1, 2, \dots, n$, $c_k(\tau) > 0$ for $\tau \in (0, 1)$. The unique solution is attained when all the eigenvalues of $D(f)$ are chosen in $S_0$. In addition, zero must be an eigenvalue of $D(f)$.*

*In particular, a unique singular orbit $(\phi, C, J, w)$ for the connecting problem (2.15) and (2.8) is obtained with $c_k(\tau) > 0$ for $\tau \in (0, 1)$ and for all $k = 1, 2, \dots, n$.*

*Proof.* The existence and uniqueness for problem BVP$_0$ in (2.18) follows directly from Theorems 3.7 and 3.8. The fact that zero must be an eigenvalue of $D(f)$ follows from $b = (\alpha_1^2, \alpha_2^2, \dots, \alpha_n^2)^T$ and the condition (2.4), given in Lemma 2.2. One then obtains a unique singular orbit for the connecting problem (2.15) and (2.8) from Remark 2.4. $\square$

We now discuss several properties of the unique solution.

**Proposition 3.10.** *Under the assumption that $\mathcal{V} > 0$, for each $1 \le k \le n$, the quantities $J_k$ and $e^{\alpha_k \mathcal{V}} l_k - r_k$ have the same sign, i.e., they are either both positive, negative, or zero.*

*Furthermore, if $\alpha_k J_k \le 0$ (equivalently, $\alpha_k e^{\alpha_k \mathcal{V}} l_k \le \alpha_k r_k$), then $c_k(\tau)$ is monotone; more precisely, if $J_k \ge 0$ (equivalently, $e^{\alpha_k \mathcal{V}} l_k \ge r_k$) and $\alpha_k < 0$, then $c_k(\tau)$ is decreasing, and, if $J_k \le 0$ (equivalently, $e^{\alpha_k \mathcal{V}} l_k \le r_k$) and $\alpha_k > 0$, then $c_k(\tau)$ is increasing.*

*Proof.* The $C$-equation in (2.15) gives, for $k = 1, 2, \dots, n$,

$$\frac{d}{d\tau} c_k = \mathcal{V} \alpha_k c_k - \mathcal{V} \mathcal{I}^{-1} J_k \sum_{s=1}^{n} \alpha_s^2 c_s(\tau). \tag{3.24}$$

Thus, from the variation of parameters, for $0 \le \tau \le 1$,

$$c_k(\tau) = e^{\alpha_k \mathcal{V}\tau}\rho(\tau),$$

where

$$\rho(\tau) = l_k - \mathcal{V}\mathcal{I}^{-1}J_k \int_0^\tau e^{-\alpha_k \mathcal{V}t} \sum_{s=1}^n \alpha_s^2 c_s(t)\, dt.$$

Note that

$$\rho'(\tau) = -\mathcal{V}\mathcal{I}^{-1}J_k e^{-\alpha_k \mathcal{V}\tau} \sum_{s=1}^n \alpha_s^2 c_s(\tau).$$

Since $\sum_{s=1}^n \alpha_s^2 c_s(\tau) > 0$ for $\tau \in (0,1)$, $\rho'(\tau)$ and $J_k$ have opposite signs. So $(\rho(0) - \rho(1))J_k > 0$ when $J_k \neq 0$ and $\rho(0) - \rho(1) = 0$ when $J_k = 0$. The conclusion follows from $\rho(0)) = l_k$ and $\rho(1) = e^{-\alpha_k \mathcal{V}} r_k$.

The monotonicity property of $c_k(\tau)$ follows directly from (3.24) since $\mathcal{V} > 0$ and $\mathcal{I} > 0$. $\square$

**Example 3.11.** In this numerical example, we show that, if $\alpha_k J_k > 0$, then $c_k(\tau)$ may NOT be monotone. In this sense, the conclusion on monotonicity of $c_k(\tau)$ in Proposition 3.10 is sharp.

We choose $(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (-3, -1, 4, 1)$ with $n = 4$. For the boundary condition (2.2), we take $\mathcal{V} = 1$,

$$L = C(0) = \begin{bmatrix} 1 \\ 12 \\ 3 \\ 3 \end{bmatrix} \quad \text{and} \quad R = C(1) \approx \begin{bmatrix} 2.207276647028657 \\ 8.829106588114627 \\ 0.367879441171448 \\ 13.979418764514806 \end{bmatrix}.$$

Figure 1 shows the solution curves of $C(x) = [c_1(x), c_2(x), c_3(x), c_4(x)]^T$ for $0 \le x \le 1$.

$$J = \mathcal{I}f \approx \mathcal{I} \begin{bmatrix} -0.102889 \\ -0.098838 \\ 0.159516 \\ -0.045568 \end{bmatrix}.$$

The eigenvalues of $\mathcal{V}D(f) = D(f)$ (due to $\mathcal{V} = 1$) are all in the stripe $S_0$ and are given by

$$\lambda_1 \approx -1.697052, \quad \lambda_{2,3} \approx 0.607600 \pm 0.501512i, \quad \lambda_4 = 0.$$

Note that $\alpha_k J_k > 0$ for $k = 1, 2, 3$ so that the monotonicity condition in Proposition 3.10 is not satisfied. The plots in Figure 1 show that $c_1$

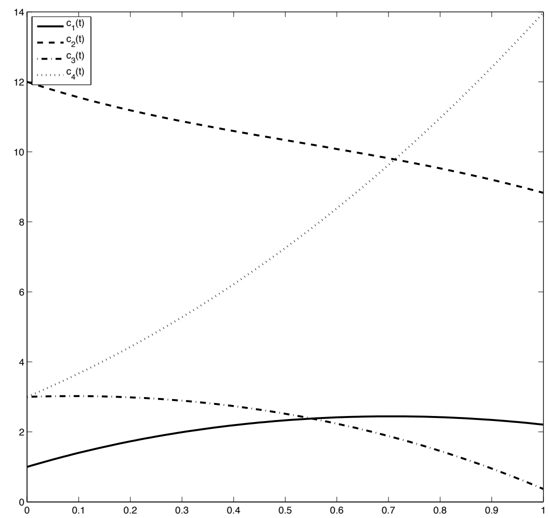


Figure 1: *$c_1$ (solid curve) is NOT monotone; $c_2$ (dashed curve) and $c_3$ (dashed-point curve) are decreasing; $c_4$ (point curve) is increasing.*

(solid curve) is NOT monotone but both $c_2$ (dashed curve) with $\alpha_2 < 0$ and $c_3$ (dashed-point curve) with $\alpha_3 > 0$ are decreasing. The curve $c_4$ (point curve) is increasing that agrees with the implication of Proposition 3.10 since $\alpha_4 J_4 < 0$ and $\alpha_4 > 0$. $\square$

**Proposition 3.12.** *The flow rate of matter $\mathcal{F}$ is simply determined by*

$$\mathcal{F} = \sum_{s=1}^{n} l_s - \sum_{s=1}^{n} r_s. \tag{3.25}$$

*Proof.* From $dC/d\tau = \mathcal{V}DC$ and $\sum_{s=1}^{n} \alpha_s c_s = 0$ in (2.15), one has

$$\frac{d}{d\tau} \sum_{s=1}^{n} c_s = \mathcal{V} \sum_{s=1}^{n} \alpha_s c_s - \mathcal{V}\mathcal{I}^{-1}\mathcal{F}b^T C = -\mathcal{V}\mathcal{I}^{-1}\mathcal{F}b^T C. \tag{3.26}$$

Integrate above from $\tau = 0$ to $\tau = 1$ and apply (2.17) to get

$$\sum_{s=1}^{n} c_s(1) - \sum_{s=1}^{n} c_s(0) = -\mathcal{F}\mathcal{V}\mathcal{I}^{-1} \int_0^1 b^T C(z)\, dz = -\mathcal{F}.$$

This completes the proof. $\square$

We remark that the identity (3.25) holds as long as (2.15) with (2.2) has a solution with $\sum_{s=1}^{n}\alpha_s^2 c_s > 0$. It does not rely on any particular results in previous parts of Section 3.

For the remaining part of this subsection, we derive a number of formulas related to the important quantities $J_k$'s, $\mathcal{I}$ and $\mathcal{F}$ in terms of the eigenvalues of $D(f)$.

Let $\lambda_1, \lambda_2, \ldots, , \lambda_p$ be the distinct eigenvalues of $D(f)$ with algebraic multiplicities $s_1, s_2, \ldots, s_p$, respectively, that are determined in Theorem 3.7. Recall that zero is always an eigenvalue of $D(f)$. Without loss of generality, we assume $\lambda_p = 0$. Then, for $j = 1, 2, \ldots, n$ with $b_j = \alpha_j^2$, the identity (3.2) becomes

$$f_j = \frac{\prod_{k=1}^{p-1}(\alpha_j - \lambda_k)^{s_k}}{\alpha_j^{2-s_p}\prod_{1\le k\le n, k\ne j}(\alpha_j - \alpha_k)}. \tag{3.27}$$

Let

$$Z(s_p) = \{q \in \mathbb{Z} : 2 - s_p \le q \le 0\}$$

be the set of nonpositive integers associated to $s_p \ge 1$. Note that $Z(s_p) = \emptyset$ if $s_p = 1$ and $Z(s_p) = \{0\}$ if $s_p = 2$.

**Proposition 3.13.** *Under the above setup, we have*

(i) $\displaystyle\sum_{k=1}^{n}\alpha_k^q J_k = 0$ *for* $q \in Z(s_p)$;

(ii) $\displaystyle\sum_{k=1}^{n}\alpha_k^{1-s_p}J_k = \sum_{k=1}^{n}\alpha_k^{1-s_p}l_k - \sum_{k=1}^{n}\alpha_k^{1-s_p}r_k + \sum_{j=1}^{s_p}\frac{\mathcal{V}^{s_p-j+1}}{(s_p-j+1)!}\sum_{k=1}^{n}\alpha_k^{2-j}l_k \ne 0;$

(iii) $\displaystyle\mathcal{I} = (-1)^{s_p-1}\frac{\prod_{k=1}^{n}\alpha_k}{\prod_{k=1}^{p-1}\lambda_k^{s_k}}\sum_{k=1}^{n}\alpha_k^{1-s_p}J_k;$

(iv) $\displaystyle\sum_{k=1}^{n}\alpha_k^{2-s}c_k(\tau) = \sum_{j=1}^{s}\frac{(\mathcal{V}\tau)^{s-j}}{(s-j)!}\sum_{k=1}^{n}\alpha_k^{2-j}l_k$ *for* $s = 1, \ldots, s_p$.

*Proof.* To prove (i), from (3.3), (3.4) and (3.5), one has

$$V_p B D(f) = \Lambda_p V_p B. \tag{3.28}$$

From $\lambda_p = 0 \notin \{\alpha_1, \alpha_2, \ldots, \alpha_n\}$, $b_j = \alpha_j^2$ for $1 \le j \le n$, and (3.6), one has

$$V_p B = \begin{bmatrix} \alpha_1 & \alpha_2 & \ldots & \alpha_n \\ 1 & 1 & \ldots & 1 \\ \alpha_1^{-1} & \alpha_2^{-1} & \ldots & \alpha_n^{-1} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_1^{2-s_p} & \alpha_2^{2-s_p} & \ldots & \alpha_n^{2-s_p} \end{bmatrix}_{s_p \times n},$$

whose $j$th row is $(\alpha_1^{2-j}, \alpha_2^{2-j}, \ldots, \alpha_n^{2-j})$.

Recall that $D(f) = \Gamma - \mathcal{I}^{-1} J b^T$. The first row in (3.28) gives

$$b^T - \mathcal{I}^{-1}\Big(\sum_{k=1}^n \alpha_k J_k\Big) b^T = 0,$$

which is automatic since $\sum_{k=1}^n \alpha_k J_k = \mathcal{I}$. If $s_p \ge 2$, then, for $q \in Z(s_p)$, the $(2-q)$th row in (3.28) gives

$$(\alpha_1^{q+1}, \alpha_2^{q+1}, \ldots, \alpha_n^{q+1}) = \mathcal{I}^{-1}\Big(\sum_{k=1}^n \alpha_k^q J_k\Big) b^T + (\alpha_1^{q+1}, \alpha_2^{q+1}, \ldots, \alpha_n^{q+1}).$$

This establishes the statement (i). The above relation allows one to conclude that $\sum_{k=1}^n \alpha_k^{1-s_p} J_k \neq 0$ holds because, otherwise, the algebraic multiplicity of $\lambda_p = 0$ would be strictly greater than $s_p$. An alternative argument for this will be given below after formulas in (ii) and (iii) are established.

We will derive the formulas in (ii) and (iv). We first apply Theorem 3.3 by replacing $R = e^{\mathcal{V}D(f)} L$ there with $C(\tau) = e^{\mathcal{V}D(f)\tau} L$ to conclude that $\lambda_p = 0$ is a zero of

$$g(z;\tau) = \sum_{k=1}^n \frac{\alpha_k^2 c_k(\tau)}{\alpha_k - z} - e^{\mathcal{V}\tau z} \sum_{k=1}^n \frac{\alpha_k^2 l_k}{\alpha_k - z}$$

of multiplicity $s_p$. Thus, similar to the formulas in (3.13), for $s = 1, \ldots, s_p$,

$$\sum_{k=1}^n \alpha_k^{2-s} c_k(\tau) = \sum_{j=1}^s \frac{(\mathcal{V}\tau)^{s-j}}{(s-j)!} \sum_{k=1}^n \alpha_k^{2-j} l_k,$$

which is precisely the formula in (iv). In particular,

$$\sum_{k=1}^n \alpha_k^{2-s_p} c_k(\tau) = \sum_{j=1}^{s_p} \frac{(\mathcal{V}\tau)^{s_p-j}}{(s_p-j)!} \sum_{k=1}^n \alpha_k^{2-j} l_k.$$

By taking integrations from $\tau = 0$ to $\tau = 1$, one has

$$\int_0^1 \sum_{k=1}^{n} \alpha_k^{2-s_p} c_k(\tau) d\tau = \sum_{j=1}^{s_p} \frac{\mathcal{V}^{s_p - j}}{(s_p - j + 1)!} \sum_{k=1}^{n} \alpha_k^{2-j} l_k. \tag{3.29}$$

It follows from $\frac{d}{d\tau} C = \mathcal{V} D C$ and $D = \Gamma - \mathcal{I}^{-1} J b^T$ that

$$\frac{d}{d\tau} \sum_{k=1}^{n} \alpha_k^{1-s_p} c_k(\tau) = \mathcal{V} \left( \sum_{k=1}^{n} \alpha_k^{2-s_p} c_k(\tau) - \mathcal{I}^{-1} \Big( \sum_{k=1}^{n} \alpha_k^{1-s_p} J_k \Big) b^T C(\tau) \right).$$

By taking integrations from $\tau = 0$ to $\tau = 1$ and using (3.29) and (2.17), one has

$$\sum_{k=1}^{n} \alpha_k^{1-s_p} r_k - \sum_{k=1}^{n} \alpha_k^{1-s_p} l_k = \sum_{j=1}^{s_p} \frac{\mathcal{V}^{s_p - j + 1}}{(s_p - j + 1)!} \sum_{k=1}^{n} \alpha_k^{2-j} l_k - \sum_{k=1}^{n} \alpha_k^{1-s_p} J_k.$$

This provides the formula in (ii).

We now establish the formula in (iii). Using (3.27) and the relation $J = \mathcal{I} f$, one has

$$\sum_{k=1}^{n} \alpha_k^{1-s_p} J_k = \mathcal{I} \sum_{k=1}^{n} \alpha_k^{1-s_p} f_k = \mathcal{I} \sum_{j=1}^{n} \frac{\mu(\alpha_j)}{\alpha_j \prod_{k=1, k\neq j}^{n} (\alpha_j - \alpha_k)},$$

where

$$\mu(t) = \prod_{k=1}^{p-1} (t - \lambda_k)^{s_k}$$

is a polynomial of degree $(n - s_p)$ that is strictly less than $n$. Interpolating the polynomial $\mu(t)$ at the nodes $0, \alpha_1, \ldots, \alpha_n$, one has

$$\mu(t) = \mu(0) \frac{\prod_{k=1}^{n} (t - \alpha_k)}{\prod_{k=1}^{n} (0 - \alpha_k)} + \sum_{j=1}^{n} \mu(\alpha_j) \frac{t \prod_{k=1, k\neq j}^{n} (t - \alpha_k)}{\alpha_j \prod_{k=1, k\neq j}^{n} (\alpha_j - \alpha_k)}.$$

The coefficients of $t^n$ on both sides give

$$0 = \frac{\mu(0)}{\prod_{k=1}^{n} (0 - \alpha_k)} + \sum_{j=1}^{n} \frac{\mu(\alpha_j)}{\alpha_j \prod_{k=1, k\neq j}^{n} (\alpha_j - \alpha_k)}.$$

Thus,

$$\sum_{j=1}^{n} \alpha_k^{1-s_p} f_k = -\frac{\mu(0)}{\prod_{k=1}^{n} (0 - \alpha_k)} = (-1)^{s_p - 1} \frac{\prod_{k=1}^{p-1} \lambda_k^{s_k}}{\prod_{k=1}^{n} \alpha_k} \neq 0.$$

The formula for $\mathcal{I}$ in (iii) then follows. Since $\mathcal{I} \neq 0$ and $\sum_{j=1}^{n} \alpha_k^{1-s_p} f_k \neq 0$, we have $\sum_{j=1}^{n} \alpha_k^{1-s_p} J_k \neq 0$. $\square$

**Corollary 3.14.** *The following statements are equivalent*

*(a) As an eigenvalue of $D(f)$, $\lambda_p = 0$ has multiplicity $s_p \geq 2$;*

*(b) The flow rate of matter $\mathcal{F} = 0$;*

*(c) $\sum_{k=1}^{n} l_k = \sum_{k=1}^{n} r_k$;*

*(d) $\sum_{k=1}^{n} c_k(\tau) = \sum_{k=1}^{n} l_k$ for all $\tau$.*

*Proof.* The equivalence between (a) and (b) is a consequence of (i) of Proposition 3.13 with $q = 0$. This has been also shown in Lemma 2.2. The equivalence between (b) and (c) follows from $\mathcal{F} = \sum_{k=1}^{n} l_k - \sum_{k=1}^{n} r_k$ in (3.25). The equivalence between (b) and (d) follows from (3.26). $\square$

# 4 Existence and uniqueness of solutions of BVP (2.1) and (2.2) for $\varepsilon > 0$ small.

In this section, we will establish that, for $\varepsilon > 0$ small, the BVP (2.1) and (2.2) has a unique solution in the vicinity of the singular orbit constructed in the previous section. We will work on the equivalent connecting problem (2.7) and (2.8).

Let $(\phi(\tau; J^0), C(\tau; J^0), J^0, w(\tau; J^0))$ be the unique singular connecting orbit of (2.15) and (2.8) which is established in Theorem 3.9. Note that

$$\begin{aligned}(\phi(0; J^0), C(0; J^0), J^0, w(0; J^0)) =& (\mathcal{V}, L, J^0, 0),\\ (\phi(1; J^0), C(1; J^0), J^0, w(1; J^0)) =& (0, R, J^0, 1).\end{aligned}$$

From Remark 2.3, this provides a unique singular connecting orbit for (2.7) and (2.8). We will then also refer to $(\phi(\tau; J^0), C(\tau; J^0), J^0, w(\tau; J^0))$ as the singular connecting orbit of (2.7) and (2.8).

We are ready to show

**Theorem 4.1.** *For $\varepsilon > 0$ small, the connecting problem (2.7) and (2.8) has a unique solution near the singular orbit $(\phi(\tau; J^0), C(\tau; J^0), J^0, w(\tau; J^0))$.*

*Proof.* For $\varepsilon > 0$, let $M_0^\varepsilon$ be the collection of the forward orbits of (2.7) starting from $B_0^*$ defined in (2.8). Let $M_0^0$ be the limiting object of $M_0^\varepsilon$ as $\varepsilon \to 0$. Since the vector field of (2.7) is not tangent to $B_0^*$ (due to $\dot{w} = 1 \neq 0$), we have $\dim M_0^\varepsilon = \dim B_0^* + 1 = n+2$. By continuity, $\dim M_0^0 = n+2$. The uniqueness of the singular orbit $(\phi(\tau;J^0), C(\tau;J^0), J^0, w(\tau;J^0))$ implies that $M_0^0 \cap B_1^*$ contains one point where $B_1^*$ is defined in (2.8). Note that $\dim B_1^* = n+1$, and hence,

$$\dim M_0^0 + \dim B_1^* - \dim \mathbb{R}^{2n+3} = (n+2) + (n+1) - (2n+3) = 0.$$

This implies that, if $M_0^0$ and $B_1^*$ intersect transversally, then, for $\varepsilon > 0$ small, $M_0^\varepsilon$ and $B_1^*$ intersect transversally too; in particular, the connecting problem (2.7) and (2.8) has a unique solution near the singular orbit.

Since the slow manifold $\mathcal{S}$ is normally hyperbolic as established in §2.2, it persists for $\varepsilon > 0$ small ([12, 16]). Note that the singular connecting orbit belongs to the slow manifold $\mathcal{S}$. It thus suffices to check the transversal intersection condition of $M_0^0$ and $B_1^*$ on the slow manifold $\mathcal{S}$. It follows again from $\dot{w} = 1$ that it suffices to check the transversal intersection condition of $M_0^0$ and $B_1^*$ on the slow manifold $\mathcal{S} \cap \{w = 1\}$.

In view of (2.10), the slow manifold $\mathcal{S}$ can be parameterized by $(\phi, C, J, w)$ with $\sum_{s=1} \alpha_s c_s = 0$.

Note that, near the unique intersection point $(\phi, C, J, w) = (0, R, J^0, 1)$ of $M_0^0$ and $B_1^*$, the set $M_0^0 \cap \mathcal{S} \cap \{w = 1\}$ is given by the set

$$\Big\{ (\phi(\tau(J); J), C(\tau(J); J), J, 1) : \; J \Big\}$$

where, recalling from (2.16),

$$1 = w(\tau(J)) = \mathcal{V}\mathcal{I}^{-1} b^T \int_0^{\tau(J)} C(z; J)\, dz \tag{4.1}$$

and

$$\phi(\tau(J); J) = \mathcal{V} - \mathcal{V}\tau(J), \quad C(\tau(J); J) = e^{\mathcal{V} D(\mathcal{I}^{-1} J)\tau(J)} L.$$

The set $B_1^* \cap \mathcal{S} \cap \{w = 1\}$ is parameterized as $\{(0, R, J, 1) : \; J\}$.

Since $\dim(\mathcal{S} \cap \{w = 1\}) = 2n$, to show the transversal intersection of $M_0^0$ and $B_1^*$ in $\mathcal{S} \cap \{w = 1\}$, one needs to find $2n$ linearly independent vectors that each is tangent either to $M_0^0 \cap \mathcal{S} \cap \{w = 1\}$ or to $B_1^* \cap \mathcal{S} \cap \{w = 1\}$.

There are $n$ linear independent vectors in the directions of $J$ that are tangent to $B_1^* \cap \mathcal{S} \cap \{w = 1\}$. We thus need to find $n$ linear independent vectors that are tangent to $M_0^0 \cap \mathcal{S} \cap \{w = 1\}$ but not to $B_1^* \cap \mathcal{S} \cap \{w = 1\}$.

If we denote $F(J) = (\mathcal{V} - \mathcal{V}\tau(J), C(\tau(J); J))$, then the desired transversality is equivalent to that $\mathbb{D}_J F(J^0)$ is of full rank, where $\mathbb{D}_J$ is the differential operator with respect to $J$; that is,

$$\operatorname{rank} \begin{bmatrix} -\mathcal{V}\nabla_J \tau(J^0) \\ \mathbb{D}_J C(1; J^0) \end{bmatrix} = \operatorname{rank} \begin{bmatrix} \nabla_J \tau(J^0) \\ \mathbb{D}_J C(1; J^0) \end{bmatrix} = n, \tag{4.2}$$

where

$$
\begin{aligned}
\nabla_J \tau(J^0) =& \big(\partial_{J_1}\tau(J^0), \partial_{J_2}\tau(J^0), \dots, \partial_{J_n}\tau(J^0)\big),\\
\mathbb{D}_J C(1; J^0) =& \partial_\tau C(1; J^0)\nabla_J \tau(J^0) + \partial_J C(1, J^0),
\end{aligned}
$$

and

$$
\partial_J C(1, J^0) = \left(\partial_{J_1} C(1, J^0), \partial_{J_2} C(1, J^0), \dots, \partial_{J_n} C(1, J^0)\right).
$$

In Lemma 4.2 to be proved below, we will show that (4.2) is true if and only if

$$
\det \int_0^1 b^T C(s; J^0) e^{-\mathcal{V} D s}\, ds \neq 0.
$$

We will assume Lemma 4.2 for the moment and complete the proof.

Denote the eigenvalues of $D(f)$ by $\lambda_1, \lambda_2, \dots, \lambda_n$, which are in conjugate pairs and $-\pi/\mathcal{V} < \mathrm{Im}\ \lambda_k < \pi/\mathcal{V}$ for $1 \leq k \leq n$ (see, e.g. Theorem 3.7). One has,

$$
\det \int_0^1 b^T C(s; J^0) e^{-\mathcal{V} D s}\, ds = \prod_{k=1}^{n} \int_0^1 b^T C(s; J^0) e^{-\mathcal{V} \lambda_k s}\, ds.
$$

Recall $b^T C(s; J^0) > 0$ for $s \in [0, 1]$. If $\lambda_k$ is real, then

$$
\int_0^1 b^T C(s; J^0) e^{-\mathcal{V} \lambda_k s}\, ds > 0.
$$

If $\lambda_k = x_k + y_k i$ with $y_k \neq 0$, then $0 < |y_k| < \pi/\mathcal{V}$ and $\overline{\lambda_k} = x_k - y_k i$ is another eigenvalue of $D(f)$. Note that $\sin(\mathcal{V} y_k s) \neq 0$ for $s \in (0, 1)$. Hence,

$$
\begin{aligned}
&\int_0^1 b^T C(s; J^0) e^{-\mathcal{V} \lambda_k s}\, ds \int_0^1 b^T C(s; J^0) e^{-\overline{\mathcal{V} \lambda_k} s}\, ds\\
&= \left(\int_0^1 b^T C(s; J^0) e^{-\mathcal{V} x_k s} \cos(\mathcal{V} y_k s)\, ds\right)^2 + \left(\int_0^1 b^T C(s; J^0) e^{-\mathcal{V} x_k s} \sin(\mathcal{V} y_k s)\, ds\right)^2\\
&\geq \left(\int_0^1 b^T C(s; J^0) e^{-\mathcal{V} x_k s} \sin(\mathcal{V} y_k s)\, ds\right)^2 > 0.
\end{aligned}
$$

The latter inequality holds true since $b^T C(s; J^0) = \sum_{s=1}^{n} \alpha_s^2 c_k(s) > 0$ and $\sin(\mathcal{V} y_k s) \neq 0$ for $s \in (0, 1)$. Consequently,

$$
\det \int_0^1 b^T C(s; J^0) e^{-\mathcal{V} D s}\, ds > 0.
$$

This completes the proof. $\square$

It remains to prove

**Lemma 4.2.** *The rank condition (4.2) holds if and only if*

$$\det \int_0^1 b^T C(s; J^0) e^{-\mathcal{V}Ds}\, ds \neq 0.$$

*Proof.* We multiply (4.1) by $\mathcal{V}^{-1}\mathcal{I} = \mathcal{V}^{-1} \sum_{s=1}^n \alpha_s J_s$ to get

$$\mathcal{V}^{-1} \sum_{s=1}^n \alpha_s J_s = b^T \int_0^{\tau(J)} C(z; J) dz.$$

Differentiating the above identity with respect to $J_k$ and evaluating at $J^0$, one has

$$\begin{aligned}\mathcal{V}^{-1}\alpha_k =& b^T C(1; J^0)\partial_{J_k}\tau(J^0) + b^T \int_0^1 \partial_{J_k} C(z; J^0)\, dz \\ =& (b^T R)\partial_{J_k}\tau(J^0) + b^T \int_0^1 \partial_{J_k} C(z; J^0)\, dz.\end{aligned}$$

Thus

$$\partial_{J_k}\tau(J^0) = \frac{\alpha_k}{\mathcal{V} b^T R} - \frac{1}{b^T R} b^T \int_0^1 \partial_{J_k} C(z; J^0)\, dz,$$

or

$$\nabla_J \tau(J^0) = \frac{1}{\mathcal{V} b^T R}\alpha^T - \frac{1}{b^T R} b^T \int_0^1 \partial_J C(z; J^0)\, dz, \tag{4.3}$$

where $\alpha^T = (\alpha_1, \ldots, \alpha_n)$. Note also,

$$\begin{aligned}\mathbb{D}_J C(1; J^0) =& \partial_\tau C(1; J^0)\nabla_J \tau(J^0) + \partial_J C(1; J^0) \\ =& \mathcal{V}DR\nabla_J\tau(J^0) + \partial_J C(1; J^0).\end{aligned} \tag{4.4}$$

From (4.3) and (4.4), one has

$$\begin{aligned}\begin{bmatrix} 1 & 0 \\ -\mathcal{V}DR & I \end{bmatrix} \begin{bmatrix} \nabla_J\tau(J^0) \\ \mathbb{D}_J C(1; J^0) \end{bmatrix} &= \begin{bmatrix} \nabla_J\tau(J^0) \\ -\mathcal{V}DR\nabla_J\tau(J^0) + \mathbb{D}_J C(1; J^0) \end{bmatrix} \\ &= \begin{bmatrix} \nabla_J\tau(J^0) \\ \partial_J C(1; J^0) \end{bmatrix},\end{aligned}$$

and hence,

$$\text{rank} \begin{bmatrix} \nabla_J\tau(J^0) \\ \mathbb{D}_J C(1; J^0) \end{bmatrix} = \text{rank} \begin{bmatrix} \nabla_J\tau(J^0) \\ \partial_J C(1; J^0) \end{bmatrix}.$$

Recall that $D = \Gamma - \mathcal{I}^{-1}Jb^T$ and $\mathcal{I} = \sum_{s=1}^n \alpha_s J_s$. Differentiate

$$\frac{d}{d\tau}C(\tau; J) = \mathcal{V}DC(\tau; J)$$

with respect to $J_k$ to get

$$\frac{d}{d\tau}\partial_{J_k}C(\tau; J) = \mathcal{V}D\partial_{J_k}C(\tau; J) + \alpha_k\mathcal{V}\mathcal{I}^{-2}Jb^TC(\tau; J) - \mathcal{V}\mathcal{I}^{-1}e_kb^TC(\tau; J),$$

where $e_k$ is the $k$th unit (column) vector. From $C(0; J) = L$, one has $\partial_{J_k}C(0; J) = 0$. An application of the variation of parameters gives

$$\begin{aligned}\partial_{J_k}C(z; J^0) =& \alpha_k\mathcal{V}\mathcal{I}^{-2}\int_0^z e^{\mathcal{V}D(z-s)}J^0b^TC(s; J^0)\,ds \\ & - \mathcal{V}\mathcal{I}^{-1}\int_0^z e^{\mathcal{V}D(z-s)}e_kb^TC(s; J^0)\,ds \\ =& \mathcal{V}\mathcal{I}^{-2}\left(\int_0^z b^TC(s; J^0)e^{\mathcal{V}D(z-s)}\,ds\right)(\alpha_kJ^0 - \mathcal{I}e_k).\end{aligned}$$

Hence, using the fact that $D = (I - \mathcal{I}^{-1}J^0\alpha^T)\Gamma$,

$$\begin{aligned}\partial_JC(z; J^0) =& \mathcal{V}\mathcal{I}^{-2}\left(\int_0^z b^TC(s; J^0)e^{\mathcal{V}D(z-s)}\,ds\right)(J^0\alpha^T - \mathcal{I}I) \\ =& -\mathcal{V}\mathcal{I}^{-1}\left(\int_0^z b^TC(s; J^0)De^{\mathcal{V}D(z-s)}\,ds\right)\Gamma^{-1}.\end{aligned} \tag{4.5}$$

It follows, with the change of the integration order, that

$$\begin{aligned}\int_0^1 \partial_JC(z; J^0)\,dz =& -\mathcal{I}^{-1}\left(\int_0^1\int_0^z b^TC(s; J^0)\mathcal{V}De^{\mathcal{V}D(z-s)}\,ds\,dz\right)\Gamma^{-1} \\ =& -\mathcal{I}^{-1}\left(\int_0^1 b^TC(s; J^0)\int_s^1 \mathcal{V}De^{\mathcal{V}D(z-s)}\,dz\,ds\right)\Gamma^{-1} \\ =& \mathcal{I}^{-1}\left(\int_0^1 b^TC(s; J^0)(I - e^{\mathcal{V}D(1-s)})\,ds\right)\Gamma^{-1}.\end{aligned}$$

From (4.1) with $J = J^0$ and $\tau(J^0) = 1$,

$$\int_0^1 b^TC(s; J^0)\,ds = \mathcal{V}^{-1}\mathcal{I}.$$

Therefore,

$$\int_0^1 \partial_JC(z; J^0)\,dz = \mathcal{V}^{-1}\Gamma^{-1} - \mathcal{I}^{-1}\left(\int_0^1 b^TC(s; J^0)e^{\mathcal{V}D(1-s)})\,ds\right)\Gamma^{-1}. \tag{4.6}$$

We also have, from (4.5) and (4.6), that

$$\begin{aligned}
\partial_J C(1; J^0) = & -\mathcal{I}^{-1}\left(\int_0^1 b^T C(s; J^0)\mathcal{V}De^{\mathcal{V}D(1-s)}\, ds\right)\Gamma^{-1} \\
= & \mathcal{V}D\int_0^1 \partial_J C(z; J^0)\, dz - D\Gamma^{-1} \\
= & \mathcal{V}D\int_0^1 \partial_J C(z; J^0)\, dz + (\mathcal{I}^{-1}J^0\alpha^T - I).
\end{aligned}$$

This, together with (4.3), gives

$$\begin{aligned}
\text{rank}\begin{bmatrix} \nabla_J\tau(J^0) \\ \mathbb{D}_J C(1; J^0) \end{bmatrix} = & \text{rank}\begin{bmatrix} \nabla_J\tau(J^0) \\ \partial_J C(1; J^0) \end{bmatrix} \\
= & \text{rank}\begin{bmatrix} \mathcal{V}^{-1}\alpha^T - b^T\int_0^1 \partial_J C(z; J^0)\, dz \\ \mathcal{I}^{-1}J^0\alpha^T - I + \mathcal{V}D\int_0^1 \partial_J C(z; J^0)\, dz \end{bmatrix}.
\end{aligned}$$

It is easily verified that, using $\alpha^T = b^T\Gamma^{-1}$,

$$\begin{aligned}
& \begin{bmatrix} 1 & \mathcal{V}^{-1}\alpha^T \\ 0 & I \end{bmatrix}\begin{bmatrix} 1 & 0 \\ -\mathcal{V}\mathcal{I}^{-1}J^0 & I \end{bmatrix}\begin{bmatrix} \mathcal{V}^{-1}\alpha^T - b^T\int_0^1 \partial_J C(z; J^0)\, dz \\ \mathcal{I}^{-1}J^0\alpha^T - I + \mathcal{V}D\int_0^1 \partial_J C(z; J^0)\, dz \end{bmatrix} \\
= & \begin{bmatrix} 1 & \mathcal{V}^{-1}b^T\Gamma^{-1} \\ 0 & I \end{bmatrix}\begin{bmatrix} \mathcal{V}^{-1}\alpha^T - b^T\int_0^1 \partial_J C(z; J^0)\, dz \\ -I + \mathcal{V}\Gamma\int_0^1 \partial_J C(z; J^0)\, dz \end{bmatrix} \\
= & \begin{bmatrix} 0 \\ -I + \mathcal{V}\Gamma\int_0^1 \partial_J C(z; J^0)\, dz \end{bmatrix}.
\end{aligned}$$

Thus, the rank condition (4.2) is equivalent to $\det M \neq 0$, where

$$M = -I + \mathcal{V}\Gamma\int_0^1 \partial_J C(z; J^0)\, dz.$$

Using (4.6),

$$M = -\mathcal{V}\mathcal{I}^{-1}\Gamma\left(\int_0^1 b^T C(s; J^0)e^{-\mathcal{V}Ds}\, ds\right)e^{\mathcal{V}D}\Gamma^{-1}.$$

Therefore, the rank condition (4.2) holds if and only if

$$\det\int_0^1 b^T C(s; J^0)e^{-\mathcal{V}Ds}\, ds \neq 0.$$

This completes the proof. □

## 5 Conclusion

In this paper, we apply the geometric singular perturbation framework to a study of the BVP of the one-dimensional cPNP systems for ion flow. For zero permanent charge, the existence and uniqueness of the relevant BVP is completely analyzed. It is interesting to note that it requires a number of ingredients to answer this basic question for such a seemly simple problem.

We point out that the cPNP system, studied in this paper as a model for ionic flow through membrane channels, is oversimplified in a number of ways: all PNP systems are primitive models in the sense that they simplify the medium effect by modeling it with dielectric coefficients, cPNP systems assume near infinite dilute conditions so that ion size effects can be ignored, the real model for the channel is of three-dimensional, and, the permanent charge $Q$ is a critically important quantity for individual ion channels.

Having said these, understanding this simplified problem, by no means simple as shown in this paper, is fundamental for analyzing any more sophisticated PNP models.

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