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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.

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

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

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

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

where the unknown variables are the electric potential ϕ, the concentration (number density) c_k and the flux density J_k of the kth 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-sectional area of the ion channel over x, $Q(x)$ is the permanent charge, and, for the kth 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 (ϕ, 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 [1–4,7–11,13–15,17–21,23,26–28,