國立臺灣大學理學院數學系

碩士論文

Department of Mathematics
College of Science
National Taiwan University

Master Thesis

考慮粒子大小與強交互作用之新泊松−玻爾茲曼方程

New Poisson-Boltzmann Models with Steric Effects and the Strongly Repulsive Interactions

蔡欣修

Hsin-Hsiu Tsai

指導教授：林太家 博士

Advisor: Tai-Chia Lin, Ph.D.

中華民國 107 年 6 月

June 2018

doi:10.6342/NTU201801038

國立臺灣大學碩士學位論文
口試委員會審定書

考慮粒子大小與強交互作用之新泊松-玻爾茲曼方程
New Poisson-Boltzmann Models with Steric Effects and the Strongly Repulsive Interactions

本論文係 蔡欣修 君 （R05221004） 在國立臺灣大學 數學 系完成之碩士學位論文，於民國 107 年 6 月 8 日承下列考試委員審查通過及口試及格，特此證明

口試委員：

林太家 （簽名）

（指導教授）

陳俊全

李俊璋

系主任、所長 （簽名）

（是否須簽章依各院系所規定）

doi:10.6342/NTU201801038

致謝

感謝林太家老師的細心指導，讓我對數學分析領域有更深刻的了解。除此之外，老師也教導我論文寫作技巧，讓我受益良多。感謝李俊璋老師的耐心教導，時常在我遇到瓶頸時提供我新的點子，也因為老師，我對 Poisson-Boltzmann 方程有更全面的體悟。感謝黃詠翔學長和呂治鴻學長與我一起討論偏微分方程相關內容，讓我有更多工具可以使用。因為有許多人的指導，這篇論文才得以產生，感謝所有指導我的老師與學長。

蔡欣修

2018.06.30

doi:10.6342/NTU201801038

摘要

研究離子擴散的行為在很多應用問題上扮演重要的角色，如生物離子通道等等，而泊松-玻爾茲曼方程便是描述此行為的模型且被廣泛應用。隨著奈米科技的發展，許多新的結果被發現。然而，這些結果卻無法用泊松-玻爾茲曼方程解釋，因此有了 Bo Li 的模型。本論文研究 Poisson-Nernst-Planck 方程 with steric effects 的穩定態，New Poisson-Boltzmann 方程 with steric effects，並且證明可以從此模型推得 Li 的模型。

關鍵字：泊松-玻爾茲曼方程、泊松-能斯特-普朗克方程、新泊松-玻爾茲曼方程、位阻效應、強交互作用。

doi:10.6342/NTU201801038

Abstract

Studying the transport of ions plays an important role in many problems, such as ion channels. Over the past decades, original Poisson-Boltzmann (PB) equation was widely used to describe the electrolyte solutions. However, due to the development of nanotechnology, some new experiment outcomes were found but could not be described. Therefore, Li's model was constructed. In this work, we further investigate a new Poisson-Boltzmann (PB) type equation called the PB_ns equation, which is derived from the steady-state of the Poisson-Nernst-Planck system with steric effects and shows that PB_ns equation can reduce to Li's model.

Keywords: Poisson-Boltzmann equations, Poisson-Nerst-Plank equations, New Poisson-Boltzmann equations, steric effects, strongly repulsive interactions.

doi:10.6342/NTU201801038

Contents

doi:10.6342/NTU201801038

1 Introduction

Studying the transport of ions plays an important role in many problems, such as semiconductors, electro-kinetic fluids, colloidal systems in physics and ion channels in biology [1,4,12–14,18]. Over the past decades, original Poisson-Boltzmann (PB) equation was widely used to describe the electrolyte solutions [6,7,16,17]. However, due to the development of nanotechnology, experts found that without considering the steric effects of ions, some experiment outcomes can not be described. The importance of steric effects raised up. Particularly, Bikerman's model [2], Andelman's model [3] and Li's model [11] are all well-known models. The first two models consider that all the species are of the same ion size and Li's model goes further to consider the different ion size.

In this work, we further investigate a new Poisson-Boltzmann (PB) type equation called the PB_ns equation, which is derived from the steady-state of the Poisson-Nernst-Planck system with steric effects [12] which is represented as

$$\log c_0 + g_{00}c_0 + g_{01}c_1 + g_{02}c_2 = \mu_0, \tag{1.1}$$

$$\log c_1 + g_{10}c_0 + g_{11}c_1 + g_{12}c_2 = q_1\phi + \mu_1, \tag{1.2}$$

$$\log c_2 + g_{20}c_0 + g_{21}c_1 + g_{22}c_2 = -q_2\phi + \mu_2, \tag{1.3}$$

$$\varepsilon^2\Delta\phi = q_1c_1 - q_2c_2 \text{ in } \Omega, \tag{1.4}$$

$$\phi + \eta_\varepsilon \frac{\partial\phi}{\partial\nu} = \phi_{bd} \text{ on } \partial\Omega. \tag{1.5}$$

$\Omega \subset \mathbb{R}^n$ is an open bounded smooth domain. ϕ is the electrostatic potential. c_0 is the concentration of water which is the solvent. c_1, c_2 are the concentration of the anion and cation respectively. q_i is the valence of the ith ion species and is positive for $i = 1,2$. μ_i is the chemical potential of the ith ion species for $i = 0,1,2$.

doi:10.6342/NTU201801038

$g_{ij} = g_{ji} \sim \varepsilon_{ij}(a_i + a_j)^{12}$ is a positive constant depending on ion radii a_i, a_j and the energy coupling constant ε_{ij} of the ith and jth species ions, respectively for $i, j = 0, 1, 2$. $\phi_{bd} := \phi_{bd}(x) \in C^2(\partial\Omega)$ is the extra electrostatic potential at the boundary. ε is the dielectric constant and η_ε is a nonnegative constant depending on ε. Since $0 < \varepsilon << 1$ is fixed in this work, without loss of generality, we may assume $\varepsilon = 1$. Hence, (1.4)-(1.5) becomes

$$\Delta\phi = q_1 c_1 - q_2 c_2 \text{ in } \Omega, \tag{1.6}$$

$$\phi + \eta \frac{\partial \phi}{\partial \nu} = \phi_{bd} \text{ on } \partial\Omega. \tag{1.7}$$

We will prove that if $G = (g_{ij})$ is nonnegative definite and

$$\det \begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21} \end{bmatrix} \geq 0,$$

then ϕ and c_i, for $i = 0, 1, 2$ exist and are unique (c.f. theorem 2.1), and the solution can be obtained by Newton's method (c.f. theorem 2.4). In particular, we consider g_{ij}, for $i, j = 0, 1, 2$, as a function of Λ. That is, given Λ, there exists one set of g_{ij} and hence we obtain the corresponding ϕ_Λ, $c_{i,\Lambda}$, for $i = 0, 1, 2$. Moreover, we assume:

$(A1)$ $\frac{g_{i0}}{g_{00}} = \frac{g_{i1}}{g_{01}} = \frac{g_{i2}}{g_{02}} = \lambda_i > 0, \quad i = 1, 2.$

$(A2)$ $g_{ij} = \tilde{g}_{ij}\Lambda > 0, \quad i, j = 0, 1, 2.$

$(A3)$ $\mu_i = \tilde{\mu}_i\Lambda + \hat{\mu}_i, \quad \tilde{\mu}_i > 0, \quad i = 0, 1, 2.$

$(A4)$ $\lambda_i\tilde{\mu}_0 - \tilde{\mu}_i = 0, \quad i = 1, 2.$

doi:10.6342/NTU201801038

where $\tilde{g}_{ij}$, $\tilde{\mu}_i$, $\hat{\mu}_i$ are positive constants. Under this assumption,

$$G = \vec{g}\vec{g}^T, \text{ where } \vec{g} = \begin{bmatrix} g_{00} \\ g_{01} \\ g_{02} \end{bmatrix},$$

and

$$\lambda_1 = \frac{\tilde{g}_{01}}{\tilde{g}_{00}}, \quad \lambda_2 = \frac{\tilde{g}_{02}}{\tilde{g}_{00}}.$$

Moreover, we can observe that μ_i, which represents the chemical potential, is positive as Λ large enough. Also, it is clear that G is nonnegative definite and

$$\det \begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21} \end{bmatrix} \geq 0.$$

If we multiply λ_1 to (1.1) and subtract it by (1.2),

$$\lambda_1 \log c_{0,\Lambda} - \log c_{1,\Lambda} = -q_1\phi + \overline{\mu}_1. \tag{1.8}$$

Multiplying λ_2 to (1.1) and subtracting it by (1.3),

$$\lambda_2 \log c_{0,\Lambda} - \log c_{2,\Lambda} = q_2\phi + \overline{\mu}_2. \tag{1.9}$$

doi:10.6342/NTU201801038

Hence, the PB_ns equations become

$$
\begin{aligned}
\log c_{0,\Lambda} + g_{00} c_{0,\Lambda} + g_{01} c_{1,\Lambda} + g_{02} c_{2,\Lambda} &= \mu_0, \\
\lambda_1 \log c_{0,\Lambda} - \log c_{1,\Lambda} &= -q_1 \phi_\Lambda + \overline{\mu}_1, \\
\lambda_2 \log c_{0,\Lambda} - \log c_{2,\Lambda} &= q_2 \phi_\Lambda + \overline{\mu}_2, \\
\Delta \phi_\Lambda &= q_1 c_{1,\Lambda} - q_2 c_{2,\Lambda} \text{ in } \Omega, \\
\phi_\Lambda + \eta \tfrac{\partial \phi_\Lambda}{\partial \nu} &= \phi_{bd} \text{ on } \partial\Omega.
\end{aligned}
\tag{1.10}
$$

Here, $\overline{\mu}_i = \hat{\mu}_0 \lambda_i - \hat{\mu}_i$, $i = 1, 2$. Passing $\Lambda \to \infty$, $(c_{i,\Lambda}, \phi_\Lambda)$ converge uniformly to (c_0^*, ϕ^*) for $i = 0, 1, 2$ and $\phi_\Lambda \to \phi^*$ in $C^{2,\alpha}(\overline{\Omega})$ (c.f. Theorem 3.1), where (c_0^*, ϕ^*) satisfies

$$
\begin{aligned}
\tilde{g}_{00} c_0^* + \tilde{g}_{01} c_1^* + \tilde{g}_{02} c_2^* &= \tilde{\mu}_0, \\
\lambda_1 \log c_0^* - \log c_1^* &= -q_1 \phi^* + \overline{\mu}_1, \\
\lambda_2 \log c_0^* - \log c_2^* &= q_2 \phi^* + \overline{\mu}_2, \\
\Delta \phi^* &= q_1 c_1^* - q_2 c_2^* \text{ in } \Omega, \\
\phi^* + \eta \tfrac{\partial \phi^*}{\partial \nu} &= \phi_{bd} \text{ on } \partial\Omega.
\end{aligned}
\tag{1.11}
$$

This implies

$$
\begin{aligned}
c_0^* &= \tfrac{1}{\tilde{g}_{00}} (\tilde{\mu}_0 - \tilde{g}_{01} c_1^* - \tilde{g}_{02} c_2^*), \\
\tfrac{\tilde{g}_{01}}{\tilde{g}_{00}} \log \tilde{g}_{00} c_0^* - \log \tilde{g}_{01} c_1^* &= -q_1 \phi^* + (\overline{\mu}_1 + \log \tilde{g}_{00} - \log \tilde{g}_{01}), \\
\tfrac{\tilde{g}_{02}}{\tilde{g}_{00}} \log \tilde{g}_{00} c_0^* - \log \tilde{g}_{02} c_2^* &= q_2 \phi^* + (\overline{\mu}_2 + \log \tilde{g}_{00} - \log \tilde{g}_{02}), \\
\Delta \phi^* &= q_1 c_1^* - q_2 c_2^* \text{ in } \Omega, \\
\phi^* + \eta \tfrac{\partial \phi^*}{\partial \nu} &= \phi_{bd} \text{ on } \partial\Omega.
\end{aligned}
$$

which is Li's model. This shows that the PB_ns model can reduce to Li's model by passing limit.

doi:10.6342/NTU201801038

There are two main difficulties when dealing with the limiting behavior of PB_ns equations. Firstly, the PBns model is an differential equation coupled with algebraic equations. Unfortunately, we can not solve them explicitly. Therefore, to deal with the differential equation, we have to consider the algebraic equations and vice versa. Secondly, there are too many unknown parameters such as c_0, c_1, c_2, and ϕ. To overcome this difficulty, we hope that we can transform c_1, c_2, and ϕ into functions of c_0, and this can be achieved by (1.8)-(1.9) plus maximal principle estimate (c.f. proposition 3.2).

The following are the main procedures when coping with limiting behavior.

1. The existence and uniqueness of ϕ and c_i, for $i = 0,1,2$ (c.f. section 2).

If $G = (g_{ij})$ is nonnegative definite and $g_{00}g_{12} \geq g_{01}g_{20}$, then the PB_ns equations have the unique solution. Moreover, the unique solution still can exists even though G is not nonnegative definite (c.f. section 4).

2. Maximal principle estimate (c.f. proposition 3.2).

With maximal principle estimate, we can transform ϕ into a function of c_0.

3. $c_{i,\Lambda}(\phi_\Lambda)$ and ϕ_Λ are uniformly bounded to Λ, for $i = 0,1,2$ (c.f. proposition 3.3).

The advantage of uniform boundedness is that a uniformly bounded term multiply a term which converges to 0 still converges to 0. Note that $c_{i,\Lambda}(\phi)$ is still uniformly bounded, for $i = 0,1,2$, provided $\phi(x)$ is bounded (c.f. proposition 3.4).

4. $(c_{i,\Lambda}, \phi_\Lambda)$ converge uniformly to (c_0^*, ϕ^*), for $i = 0,1,2$ (c.f. theorem 3.1).

Because $c_{i,\Lambda}(\phi_\Lambda)$ and ϕ_Λ are uniformly bounded to Λ, unformally, differentiating the first equation of (1.10) by Λ, then since $\frac{\log c_{0,\Lambda} - \hat{\mu}_0}{\Lambda} \to 0$ as $\Lambda \to \infty$, we can see the uniform convergence of (1.10) to (1.11).

5. $\phi_\Lambda \to \phi^*$ in $C^{2,\alpha}(\overline{\Omega})$ (c.f. theorem 3.1).

doi:10.6342/NTU201801038

By the standard elliptic theorem,

$$|\phi_\Lambda - \phi^*|_{2,\alpha;\Omega} \leq C(|\phi_\Lambda - \phi^*|_{0;\Omega} + |f_\Lambda(\phi_\Lambda) - f^*(\phi^*)|_{0,\alpha;\Omega}),$$

where $f_\Lambda = q_1 c_{1,\Lambda} - q_2 c_{2,\Lambda}$ and $f^* = q_1 c_1^* - q_2 c_2^*$, C is a constant. This result thus follows from the uniform convergence of $(c_{i,\Lambda}, \phi_\Lambda)$, for $i = 0, 1, 2$, and the convergence of $[f_\Lambda(\phi_\Lambda) - f^*(\phi^*)]_{\alpha;\Omega}$ to 0.

This paper is organized as follows: Firstly, we prove the existence and uniqueness of ϕ and c_i, for $i = 0, 1, 2$. Secondly, we discuss the limiting behavior. In the last of this work, we generalize the assumption that G is nonnegative definite.

2 Existence and Uniqueness

The PB free energy can be denoted as

$$E[\phi, c_0, c_1, c_2] = \int_\Omega \sum_{i=0}^2 (c_i \log c_i + \tfrac{g_{ii}}{2} c_i^2) + g_{01} c_0 c_1 + g_{02} c_0 c_2 + g_{12} c_1 c_2$$
$$-(\mu_0 + 1)c_0 - (q_1 \phi + \mu_1 + 1)c_1 - (-q_2 \phi + \mu_2 + 1)c_2 - \tfrac{1}{2}|\nabla \phi|^2 dx.$$

It is clear that $\delta_{c_i} E = 0$, for $i = 0, 1, 2$, and $\delta_\phi E = 0$ imply (1.1)-(1.3) and (1.6) respectively. The existence and uniqueness theorem is as follows:

Theorem 2.1. *Let Ω be a bounded smooth domain and $\phi_{bd} \in C^2(\partial\Omega)$. Suppose that G is nonnegative definite and*

$$\det \begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21} \end{bmatrix} \geq 0,$$

doi:10.6342/NTU201801038

then (1.6) *has a unique solution* $\phi_0 \in C^\infty(\Omega) \cap C^{2,\alpha}(\overline{\Omega})$ *for some* $\alpha > 0$ *with the boundary condition* (1.7).

To prove this theorem, we divide it into two parts, algebraic equations part and differential equation part.

2.1 Algebraic Equations

In the beginning, we prove the existence of c_i, for $i = 0,1,2$, by intermediate value theorem.

Theorem 2.2. *For any fixed* ϕ*, there exists* c_i*,* $i = 0,1,2$*, satisfying* (1.1)-(1.3).

Proof. For any fixed $\phi \in \mathbb{R}$, let $\mu_0 = \alpha$, $q_1\phi + \mu_1 = \beta$, $-q_2\phi + \mu_2 = \gamma$. Then (1.1)-(1.3) become

$$\log c_0 + g_{00}c_0 + g_{01}c_1 = \alpha - g_{02}c_2, \tag{2.1}$$

$$\log c_1 + g_{10}c_0 + g_{11}c_1 = \beta - g_{12}c_2, \tag{2.2}$$

$$\log c_2 + g_{20}c_0 + g_{21}c_1 + g_{22}c_2 = \gamma. \tag{2.3}$$

Given any c_2, by (2.1),

$$c_1 = \frac{1}{g_{01}}(\alpha - g_{02}c_2 - \log c_0 - g_{00}c_0),$$

and

$$\log c_0 + g_{00}c_0 \leq \alpha - g_{02}c_2.$$

Since $\log c_0 + g_{00}c_0$ is monotone increasing to c_0, we obtain that c_0 has an upper bound $M = M(c_2)$, where $\log M + g_{00}M = \alpha - g_{02}c_2$. Observe that $c_1 \to 0$ as $c_0 \to M$.

doi:10.6342/NTU201801038

Let

$$h_1(c_0) = \log(\frac{1}{g_{01}}(\alpha - g_{02}c_2 - \log c_0 - g_{00}c_0)) + g_{10}c_0 + \frac{g_{11}}{g_{01}}(\alpha - g_{02}c_2 - \log c_0 - g_{00}c_0)$$
$$-\beta + g_{12}c_2$$
$$= \log(\frac{1}{g_{01}}(-\log c_0 - g_{00}c_0 + \alpha - g_{02}c_2)) - \frac{g_{11}}{g_{01}}(\log c_0 + g_{00}c_0) + g_{10}c_0 + \frac{g_{11}}{g_{01}}(\alpha - g_{02}c_2)$$
$$-\beta + g_{12}c_2.$$

Then $h_1 \to \infty$ as $c_0 \to 0$ and $h_1 \to -\infty$ as $c_0 \to M$. By intermediate value theorem, there exists $c_0^s \in (0, M)$ such that $h_1(c_0^s) = 0$. Hence we have the result that for given c_2, there exists $c_0 = c_0(c_2)$, $c_1 = c_1(c_2)$ such that (2.1) and (2.2) hold.

The last step is to solve c_2 by (2.3). Observe first that c_0 and c_1 are bounded if c_2 is bounded by (2.2). Secondly, $c_0 \to 0$ and $c_1 \to 0$ as $c_2 \to \infty$ by (2.1) and (2.2) respectively. Let

$$h_2(c_2) = \log c_2 + g_{20}c_0 + g_{21}c_1 + g_{22}c_2 - \gamma.$$

Then $h_2 \to -\infty$ as $c_2 \to 0$ and $h_2 \to \infty$ as $c_2 \to \infty$. By intermediate value theorem, there exists c_2^s such that $h_2(c_2^s) = 0$ and we complete the proof. ■

Next, we prove the uniqueness of c_i for fixed $\phi \in \mathbb{R}$ by the nonnegative definiteness of $G = (g_{ij})$. This means c_i is a function of ϕ, for $i = 0, 1, 2$.

Theorem 2.3. *If $G = (g_{ij})$ is nonnegative definite, then c_i is a function of ϕ, for $i = 0, 1, 2$.*

doi:10.6342/NTU201801038

Proof. For any fixed ϕ, let

$$c^1 = \begin{bmatrix} c_0^1 \\ c_1^1 \\ c_2^1 \end{bmatrix}, c^2 = \begin{bmatrix} c_0^2 \\ c_1^2 \\ c_2^2 \end{bmatrix}$$

be two solutions of (1.1)-(1.3). Then

$$\begin{bmatrix} \log \frac{c_0^1}{c_0^2} \\ \log \frac{c_1^1}{c_1^2} \\ \log \frac{c_2^1}{c_2^2} \end{bmatrix} + G(c^1 - c^2) = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

Multiplying $(c^1 - c^2)^T$,

$$(c^1 - c^2)^T \begin{bmatrix} \log \frac{c_0^1}{c_0^2} \\ \log \frac{c_1^1}{c_1^2} \\ \log \frac{c_2^1}{c_2^2} \end{bmatrix} + (c^1 - c^2)^T G(c^1 - c^2) = 0.$$

Since G is nonnegative definite, $(c^1 - c^2)^T G(c^1 - c^2) \geq 0$. Also,

$$(c^1 - c^2)^T \begin{bmatrix} \log \frac{c_0^1}{c_0^2} \\ \log \frac{c_1^1}{c_1^2} \\ \log \frac{c_2^1}{c_2^2} \end{bmatrix} \geq 0.$$

This implies

$$(c^1 - c^2)^T \begin{bmatrix} \log \frac{c_0^1}{c_0^2} \\ \log \frac{c_1^1}{c_1^2} \\ \log \frac{c_2^1}{c_2^2} \end{bmatrix} = 0.$$

doi:10.6342/NTU201801038

Hence $c^1 = c^2$. ■

Remark 2.1. *We have known that c_i is a function of ϕ, for $i = 0,1,2$. In particular, if G is nonnegative definite and consider $\mathbf{f}(c_0,c_1,c_2,\phi) = (f_1,f_2,f_3)$, where*

$$f_1 = \log c_0 + g_{00}c_0 + g_{01}c_1 + g_{02}c_2 - \mu_0,$$

$$f_2 = \log c_1 + g_{10}c_0 + g_{11}c_1 + g_{12}c_2 - q_1\phi + \mu_1,$$

$$f_3 = \log c_2 + g_{20}c_0 + g_{21}c_1 + g_{22}c_2 + q_2\phi - \mu_2,$$

then $\det[\frac{\partial(f_1,f_2,f_3)}{\partial(c_0,c_1,c_2)}] = M > 0$ (c.f. proposition 2.5), where

$$M = \det\begin{bmatrix} \frac{1}{c_0} + g_{00} & g_{01} & g_{02} \\ g_{10} & \frac{1}{c_1} + g_{11} & g_{12} \\ g_{20} & g_{21} & \frac{1}{c_2} + g_{22} \end{bmatrix}.$$

Since $\mathbf{f}$ is a smooth function, by implicit function theorem, c_i is a smooth function to ϕ, for $i = 0,1,2$.

Numerically, we can use Newton's method to solve the algebraic equations.

Theorem 2.4. *If the initial guess is near the root of (1.1)-(1.3) enough, then the Newton's method converges to the root.*

Proof. Consider an arbitrary closed ball B of the root. Let

$$F(c_0,c_1,c_2) = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix} = \begin{bmatrix} \log c_0 + g_{00}c_0 + g_{01}c_1 + g_{02}c_2 - \mu_0 \\ \log c_1 + g_{10}c_0 + g_{11}c_1 + g_{12}c_2 - q_1\phi - \mu_1 \\ \log c_2 + g_{20}c_0 + g_{21}c_1 + g_{22}c_2 + q_2\phi - \mu_2 \end{bmatrix}.$$

doi:10.6342/NTU201801038

Applying Newton's method,

$$\begin{bmatrix} c_0^{(n+1)} \\ c_1^{(n+1)} \\ c_2^{(n+1)} \end{bmatrix} = \begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) F(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}),$$

where $A(c_0, c_1, c_2) = \begin{bmatrix} \frac{1}{c_0} + g_{00} & g_{01} & g_{02} \\ g_{10} & \frac{1}{c_1} + g_{11} & g_{12} \\ g_{20} & g_{21} & \frac{1}{c_2} + g_{22} \end{bmatrix}$.

Let $\begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix}$ be the root of $F = 0$. Then

$$\begin{bmatrix} c_0^{(n+1)} \\ c_1^{(n+1)} \\ c_2^{(n+1)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix}$$

$$= \begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} + A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)})(F(\hat{c}_0, \hat{c}_1, \hat{c}_2) - F(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}))$$

$$= \begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} + A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) \begin{bmatrix} \hat{f}_1(\hat{c}_0, \hat{c}_1, \hat{c}_2) - f_1(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) \\ \hat{f}_2(\hat{c}_0, \hat{c}_1, \hat{c}_2) - f_2(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) \\ \hat{f}_3(\hat{c}_0, \hat{c}_1, \hat{c}_2) - f_3(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) \end{bmatrix}.$$

Applying the mean value theorem component by component,

doi:10.6342/NTU201801038

$$\begin{bmatrix} c_0^{(n+1)} \\ c_1^{(n+1)} \\ c_2^{(n+1)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix}$$

$$= \begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} - A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) A(c_0^*, c_1^*, c_2^*) (\begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix})$$

$$= (I - A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) A(c_0^*, c_1^*, c_2^*)) (\begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix})$$

$$= A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)}) \begin{bmatrix} \frac{1}{c_0^{(n)}} - \frac{1}{c_0^*} & 0 & 0 \\ 0 & \frac{1}{c_1^{(n)}} - \frac{1}{c_1^*} & 0 \\ 0 & 0 & \frac{1}{c_2^{(n)}} - \frac{1}{c_2^*} \end{bmatrix} (\begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix}),$$

where $c_i^* \in (c_i^{(n)}, \hat{c}_i)$for $i = 0, 1, 2$. Therefore,

$$\| \begin{bmatrix} c_0^{(n+1)} \\ c_1^{(n+1)} \\ c_2^{(n+1)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} \|$$

$$\leq \|A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)})\| \| \begin{bmatrix} \frac{1}{c_0^{(n)}} - \frac{1}{c_0^*} & 0 & 0 \\ 0 & \frac{1}{c_1^{(n)}} - \frac{1}{c_1^*} & 0 \\ 0 & 0 & \frac{1}{c_2^{(n)}} - \frac{1}{c_2^*} \end{bmatrix} \| \| \begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} \|.$$

Since B is compact, there exists a constant M such that $\|A^{-1}(c_0^{(n)}, c_1^{(n)}, c_2^{(n)})\| \leq M$.

doi:10.6342/NTU201801038

Hence, if $\begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix}$ is closed enough to $\begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix}$, then

$$\| \begin{bmatrix} c_0^{(n+1)} \\ c_1^{(n+1)} \\ c_2^{(n+1)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} \| \leq \frac{1}{2} \| \begin{bmatrix} c_0^{(n)} \\ c_1^{(n)} \\ c_2^{(n)} \end{bmatrix} - \begin{bmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \hat{c}_2 \end{bmatrix} \|.$$

This implies $\begin{bmatrix} c_0^{(n+1)} \\ c_1^{(n+1)} \\ c_2^{(n+1)} \end{bmatrix}$ is also in B and we can repeat this process until it converges.

■

2.2 Differential Equation

Consider the functional

$$E_\eta[\phi] = \frac{1}{2}\int_\Omega |\nabla\phi|^2 dx + \int_\Omega F(e^{q_1\phi}, e^{-q_2\phi})dx + B_\eta[\phi],$$

where $\frac{dF}{d\phi} = q_1c_1 - q_2c_2$ and $F(\phi)$ is strictly convex to ϕ which will be defined in proposition 2.6.

$$B_\eta[\phi] = \begin{cases} \frac{1}{2\eta}\int_{\partial\Omega}(\phi - \phi_{bd})^2 dS & \text{if } \eta > 0. \\ 0 & \text{if } \eta = 0. \end{cases}$$

Hence, (1.6)-(1.7) can be regarded as the Euler-Lagrange equation of E_η. To prove the existence and uniqueness of ϕ, we need the monotonicity of c_1 and c_2 to ϕ.

doi:10.6342/NTU201801038

Proposition 2.5. *If G is nonnegative definite and*

$$\det\begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21} \end{bmatrix} \geq 0,$$

then $\frac{dc_1}{d\phi} = \frac{M_1}{M} > 0$, $\frac{dc_2}{d\phi} = \frac{M_2}{M} < 0$, *where*

$$M = \det\begin{bmatrix} \frac{1}{c_0}+g_{00} & g_{01} & g_{02} \\ g_{10} & \frac{1}{c_1}+g_{11} & g_{12} \\ g_{20} & g_{21} & \frac{1}{c_2}+g_{22} \end{bmatrix},$$

$$M_1 = \det\begin{bmatrix} \frac{1}{c_0}+g_{00} & 0 & g_{02} \\ g_{10} & q_1 & g_{12} \\ g_{20} & -q_2 & \frac{1}{c_2}+g_{22} \end{bmatrix},$$

$$M_2 = \det\begin{bmatrix} \frac{1}{c_0}+g_{00} & g_{01} & 0 \\ g_{10} & \frac{1}{c_1}+g_{11} & q_1 \\ g_{20} & g_{21} & -q_2 \end{bmatrix}.$$

Proof. Differentiating the system (1.1)-(1.3) with respect to ϕ, then

$$\begin{bmatrix} \frac{1}{c_0}+g_{00} & g_{01} & g_{02} \\ g_{10} & \frac{1}{c_1}+g_{11} & g_{12} \\ g_{20} & g_{21} & \frac{1}{c_2}+g_{22} \end{bmatrix} \begin{bmatrix} \frac{dc_0}{d\phi} \\ \frac{dc_1}{d\phi} \\ \frac{dc_2}{d\phi} \end{bmatrix} = \begin{bmatrix} 0 \\ q_1 \\ -q_2 \end{bmatrix}.$$

By Cramer's rule,

$$\frac{dc_1}{d\phi} = \frac{M_1}{M}, \quad \frac{dc_2}{d\phi} = \frac{M_2}{M}.$$

doi:10.6342/NTU201801038

If G is nonnegative definite, then

$$\det\begin{bmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{bmatrix}, \det\begin{bmatrix} g_{00} & g_{02} \\ g_{20} & g_{22} \end{bmatrix}, \det\begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \geq 0.$$

This implies that

$$\begin{aligned} M = & \frac{1}{c_0c_1c_2} + \frac{g_{00}}{c_1c_2} + \frac{g_{11}}{c_0c_2} + \frac{g_{22}}{c_0c_1} + \frac{g_{00}g_{11} - g_{01}g_{10}}{c_2} \\ & + \frac{g_{00}g_{22} - g_{02}g_{20}}{c_1} + \frac{g_{11}g_{22} - g_{12}g_{21}}{c_0} + \det G > 0 \end{aligned},$$

$$M_1 = \frac{q_1}{c_0c_2} + \frac{q_1g_{22} + q_2g_{12}}{c_0} + \frac{q_1g_{00}}{c_2} + q_1(g_{00}g_{22} - g_{02}g_{20}) + q_2(g_{00}g_{12} - g_{02}g_{10}) > 0 \ ,$$

$$M_2 = -\frac{q_2}{c_0c_1} - \frac{q_1g_{21} + q_2g_{11}}{c_0} - \frac{q_2g_{00}}{c_1} - q_2(g_{00}g_{11} - g_{01}g_{10}) - q_1(g_{00}g_{21} - g_{01}g_{20}) < 0 \ \cdot$$

Hence,

$$\frac{dc_1}{d\phi} = \frac{M_1}{M} > 0, \quad \frac{dc_2}{d\phi} = \frac{M_2}{M} < 0.$$

■

Secondly, we need to define $F(e^{q_1\phi}, e^{-q_2\phi})$ in the functional.

Proposition 2.6. *Let* $(X_1, X_2) = (e^{q_1\phi}, e^{-q_2\phi})$*. Let* G *be nonnegative definite and*

$$\det\begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21} \end{bmatrix} \geq 0.$$

Then there exists a differentiable function $F(\phi) = F(X_1, X_2)$ *such that*

$$\frac{dF}{d\phi} = q_1c_1 - q_2c_2.$$

doi:10.6342/NTU201801038

Moreover, $F(\phi)$ is a strictly convex function to ϕ.

Proof. Let $(c_1, c_2) = (\theta_1 X_1, \theta_2 X_2)$ for some $\theta_1 = \theta_1(\phi)$ and $\theta_2 = \theta_2(\phi)$. Then (1.1)-(1.3) becomes to

$$\begin{aligned} &\log c_0 + g_{00}c_0 + g_{01}\theta_1 X_1 + g_{02}\theta_2 X_2 = \mu_0, \\ &\log \theta_1 + g_{01}c_0 + g_{11}\theta_1 X_1 + g_{12}\theta_2 X_2 = \mu_1, \\ &\log \theta_2 + g_{02}c_0 + g_{21}\theta_1 X_1 + g_{22}\theta_2 X_2 = \mu_2. \end{aligned} \tag{2.4}$$

Differentiating (2.4) with respect to X_1 and X_2, we obtain

$$\begin{bmatrix} \frac{1}{c_0} + g_{00} & g_{01}X_1 & g_{02}X_2 \\ g_{01} & \frac{1}{\theta} + g_{11}X_1 & g_{12}X_2 \\ g_{02} & g_{21}X_1 & \frac{1}{\theta_2} + g_{22}X_2 \end{bmatrix} \begin{bmatrix} \frac{\partial c_0}{\partial X_1} \\ \frac{\partial \theta_1}{\partial X_1} \\ \frac{\partial \theta_2}{\partial X_1} \end{bmatrix} = - \begin{bmatrix} g_{01}\theta_1 \\ g_{11}\theta_1 \\ g_{21}\theta_1 \end{bmatrix},$$

and

$$\begin{bmatrix} \frac{1}{c_0} + g_{00} & g_{01}X_1 & g_{02}X_2 \\ g_{01} & \frac{1}{\theta} + g_{11}X_1 & g_{12}X_2 \\ g_{02} & g_{21}X_1 & \frac{1}{\theta_2} + g_{22}X_2 \end{bmatrix} \begin{bmatrix} \frac{\partial c_0}{\partial X_2} \\ \frac{\partial \theta_1}{\partial X_2} \\ \frac{\partial \theta_2}{\partial X_2} \end{bmatrix} = - \begin{bmatrix} g_{02}\theta_2 \\ g_{12}\theta_2 \\ g_{22}\theta_2 \end{bmatrix}.$$

Applying Cramer's rule,

$$\frac{\partial \theta_2}{\partial X_1} = \frac{\partial \theta_1}{\partial X_2} = \frac{-1}{A}(c_0^{-1}g_{12} + g_{00}g_{12} - g_{01}g_{02}),$$

where

$$A = \det \begin{bmatrix} \frac{1}{c_0} + g_{00} & g_{01}X_1 & g_{02}X_2 \\ g_{01} & \frac{1}{\theta_1} + g_{11}X_1 & g_{12}X_2 \\ g_{02} & g_{12}X_1 & \frac{1}{\theta_2} + g_{22}X_2 \end{bmatrix}$$

doi:10.6342/NTU201801038

$$= X_1 X_2 \det \begin{bmatrix} \frac{1}{c_0} + g_{00} & g_{01} & g_{02} \\ g_{01} & \frac{1}{\theta_1 X_1} + g_{11} & g_{12} \\ g_{02} & g_{12} & \frac{1}{\theta_2 X_2} + g_{22} \end{bmatrix} > 0.$$

Let $f(X_1, X_2) = (\theta_1(X_1, X_2), \theta_2(X_1, X_2))$. Then

$$\nabla \times f = \frac{\partial \theta_2}{\partial X_1} - \frac{\partial \theta_1}{\partial X_2} = 0.$$

By the curl-divergence theorem, f is a gradient of some $F : \mathbb{R}^2 \to \mathbb{R}$. That is,

$$\nabla F(X_1, X_2) = f(X_1, X_2) = (\theta_1(X_1, X_2), \theta_2(X_1, X_2)).$$

Therefore,

$$\frac{dF}{d\phi} = \frac{dF}{dX_1}\frac{dX_1}{d\phi} + \frac{dF}{dX_2}\frac{dX_2}{\phi} = \theta_1 q_1 X_1 - \theta_2 q_2 X_2 = q_1 c_1 - q_2 c_2.$$

Moreover, proposition 2.5 implies

$$\frac{d^2F}{d\phi^2} = q_1 \frac{dc_1}{d\phi} - q_2 \frac{dc_2}{d\phi} > 0.$$

Hence F is strictly convex to ϕ. ■

To prove the existence of ϕ, we apply the standard direct method to find the minimizer ϕ_0 in $\mathbb{H}_\eta(\Omega)$, where

$$\mathbb{H}_\eta = \begin{cases} H^1(\Omega) & \text{if } \eta > 0. \\ \{u \in H^1(\Omega) : u - \phi_{bd} \in H_0^1(\Omega)\} & \text{if } \eta = 0. \end{cases}$$

doi:10.6342/NTU201801038

Hence ϕ_0 satisfies

$$\int_\Omega [\nabla\phi_0 \nabla v + (q_1 c_1(\phi_0) - q_2 c_2(\phi_0))v] dx + \hat{B}_\eta[\phi_0; v] = 0, \tag{2.5}$$

for any $v \in H^1(\Omega)$ if $\eta > 0$ and $v \in H_0^1(\Omega)$ if $\eta = 0$ where

$$\hat{B}_\eta[\phi_0; v] = \begin{cases} \frac{1}{\eta}\int_{\partial\Omega}(\phi_0 - \phi_{bd}) v dS & \text{if } \eta > 0. \\ 0 & \text{if } \eta = 0. \end{cases}$$

The theorem is as follows:

Theorem 2.7. *Let G be nonnegative definite and*

$$\det \begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21} \end{bmatrix} \geq 0.$$

Then E_η has a minimizer $\phi_0 \in \mathbb{H}_\eta$.

Proof. If $\eta > 0$, then

$$E_\eta[\phi] = \frac{1}{2}\int_\Omega |\nabla\phi|^2 dx + \int_\Omega F(e^{q_1\phi}, e^{-q_2\phi}) dx + \frac{1}{2\eta}\int_{\partial\Omega}(\phi - \phi_{bd})^2 dS.$$

for $\phi \in H^1(\Omega)$.

Claim: $E_\eta[\phi]$ is coercive on $H^1(\Omega)$.

Since F is strictly convex to ϕ and $q_1 c_1 > q_2 c_2$ for some large ϕ, there exists a constant $m \in \mathbb{R}$ such that

$$\int_\Omega F(e^{q_1\phi}, e^{-q_2\phi}) dx \geq m. \tag{2.6}$$

doi:10.6342/NTU201801038

On the other hand, by Young's inequality,

$$\begin{aligned}&\tfrac{1}{2}\int_\Omega |\nabla\phi|^2dx+\tfrac{1}{2\eta}\int_{\partial\Omega}(\phi-\phi_{bd})^2dS\\&\geq C_\eta\left(\int_\Omega|\nabla\phi|^2dx+\int_{\partial\Omega}|\phi|^2dS\right)-\tfrac{7}{2\eta}\int_{\partial\Omega}|\phi_{bd}|^2dS,\end{aligned} \tag{2.7}$$

where $C_\eta=\min\{\frac{1}{2},\frac{1}{4\eta}\}$. By (2.6)-(2.7),

$$E_\eta[\phi]\geq C_\eta\left(\int_\Omega|\nabla\phi|^2dx+\int_{\partial\Omega}|\phi|^2dS\right)-\frac{7}{2\eta}\int_{\partial\Omega}|\phi_{bd}|^2dS+m. \tag{2.8}$$

Note that $\phi_{bd}\in L^2(\partial\Omega)$. To complete the claim, we also need Friedrichs' inequality.

$$\int_\Omega|\phi|^2dx\leq C^2\left(\int_\Omega|\nabla\phi|^2dx+\int_{\partial\Omega}|\phi|^2dS\right),\quad \forall\phi\in H^1(\Omega), \tag{2.9}$$

where C is a positive constant depending only on the space dimension n and the measures of Ω and $\partial\Omega$.

Let $M>0$ and $\phi\in H^1(\Omega)$ satisfying $|E_\eta[\phi]|<M$. Then (2.8)-(2.9) immediately give

$$\|\phi\|_{H^1(\Omega)}:=\left(\int_\Omega|\phi|^2+|\nabla\phi|^2dx\right)^{\frac{1}{2}}\leq C(M),$$

for some constant $C(M)$. This prove the claim.

In accordance with the definition of an infimum, there exists a minimizing sequence $\{\phi_n\}_{n=1}^\infty\subset H^1(\Omega)$ such that

$$\lim_{n\to\infty}E_\eta[\phi_n]=d:=\inf_{\phi\in H^1(\Omega)}E_\eta[\phi]. \tag{2.10}$$

By (2.10) and coerciveness of E_η, we get $\sup_{n\in\mathbb{N}}\|\phi_n\|_{H^1(\Omega)}<\infty$. Along with (2.8), we may obtain $\sup_{n\in\mathbb{N}}\int_{\partial\Omega}|\phi_n|^2dS<\infty$. Consequently, there exists a subsequence of $\{\phi_n\}$(for

doi:10.6342/NTU201801038

notation convenience, we still denote it by $\{\phi_n\}$) such that $\phi_n \rightharpoonup \phi_0$ weakly in $H^1(\Omega)$ and $\phi_n \rightharpoonup \Gamma\phi_0$ weakly in $L^2(\partial\Omega)$ as $n \to \infty$, where $\Gamma\phi_0$ is the trace of ϕ_0 on $\partial\Omega$. Note that $\phi_n \rightharpoonup \phi_0$ weakly in $H^1(\Omega)$ implies $\nabla\phi_n \rightharpoonup \nabla\phi_0$ weakly in $L^2(\Omega)$. Then by the standard theorem, we have

$$\liminf_{n\to\infty} \int_\Omega |\nabla\phi_n|^2 dx \geq \int_\Omega |\nabla\phi_0|^2 dx, \tag{2.11}$$

$$\liminf_{n\to\infty} \int_{\partial\Omega} |\phi_n - \phi_{bd}|^2 dS \geq \int_{\partial\Omega} |\Gamma\phi_0 - \phi_{bd}|^2 dS, \tag{2.12}$$

and

$$\lim_{n\to\infty} \phi_n = \phi_0 \text{ a.e. in } \Omega. \tag{2.13}$$

On the other hand, the Fatou's lemma and (2.13) give

$$\liminf_{n\to\infty} \int_\Omega F(\phi_n) dx \geq \int_\Omega F(\phi_0) dx. \tag{2.14}$$

Combining (2.10)-(2.12) and (2.14), we get

$$d = \lim_{n\to\infty} E_\eta[\phi_n] \geq E_\eta[\phi_0] \geq d.$$

Therefore, the minimum d is achieved at $\phi_0 \in H^1(\Omega)$.

If $\eta = 0$, then it becomes a Dirichlet problem. Thus by theorem 2 of [5], we get the minimizer $\phi_0 \in \{u \in H^1(\Omega) : u - \phi_{bd} \in H_0^1(\Omega)\}$. ■

To deal with the regularity of ϕ_0, firstly, we let

$$f(\phi) = q_1 c_1(\phi) - q_2 c_2(\phi).$$

doi:10.6342/NTU201801038

Since f is monotone increasing from $-\infty$ to ∞ which we can see from (1.1)-(1.3) and proposition 2.5, there exists a unique s such that $f(s) = 0$. Hence

$$\Delta\phi = f(\phi) = f(\phi) - f(s) = \begin{cases} \frac{f(\phi)-f(s)}{\phi-s}(\phi - s) & \text{if } \phi \neq s, \\ \frac{df(\phi)}{d\phi}(\phi - s) & \text{if } \phi = s, \end{cases}$$

This implies that ϕ_0 is a weak solution of the equation

$$\Delta\phi = \begin{cases} \frac{f(\phi_0)-f(s)}{\phi_0-s}(\phi - s) & \text{if } \phi_0 \neq s, \\ \frac{df(\phi_0)}{d\phi}(\phi - s) & \text{if } \phi_0 = s, \end{cases}$$

Here, we need some information to $\frac{f(\phi_0)-f(s)}{\phi_0-s}$.

Proposition 2.8. *There exists $M > 0$ such that $|\frac{df(\phi)}{d\phi}| < M$ for all $\phi \in \mathbb{R}$. In particular, $|\frac{f(\phi_1)-f(\phi_2)}{\phi_1-\phi_2}| < M$ for all $\phi_1, \phi_2 \in \mathbb{R}$.*

Proof.

$$\frac{df(\phi)}{d\phi} = q_1\frac{dc_1}{d\phi} - q_2\frac{dc_2}{d\phi}$$

Using the same notation as proposition 2.5,

$$\begin{aligned}\frac{dc_1}{d\phi} &= \frac{M_1}{M} \\ &= \frac{\frac{q_1}{c_0c_2} + \frac{q_1g_{22}+q_2g_{12}}{c_0} + \frac{q_1g_{00}}{c_2} + q_1(g_{00}g_{22}-g_{02}g_{20}) + q_2(g_{00}g_{12}-g_{02}g_{10})}{\frac{1}{c_0c_1c_2} + \frac{g_{00}}{c_1c_2} + \frac{g_{11}}{c_0c_2} + \frac{g_{22}}{c_0c_1} + \frac{g_{00}g_{11}-g_{01}g_{10}}{c_2} + \frac{g_{00}g_{22}-g_{02}g_{20}}{c_1} + \frac{g_{11}g_{22}-g_{12}g_{21}}{c_0} + \det G},\end{aligned}$$

$$\begin{aligned}\frac{dc_2}{d\phi} &= \frac{M_2}{M} \\ &= \frac{-\frac{q_2}{c_0c_1} - \frac{q_1g_{21}+q_2g_{11}}{c_0} - \frac{q_2g_{00}}{c_1} - q_2(g_{00}g_{11}-g_{01}g_{10}) - q_1(g_{00}g_{21}-g_{01}g_{20})}{\frac{1}{c_0c_1c_2} + \frac{g_{00}}{c_1c_2} + \frac{g_{11}}{c_0c_2} + \frac{g_{22}}{c_0c_1} + \frac{g_{00}g_{11}-g_{01}g_{10}}{c_2} + \frac{g_{00}g_{22}-g_{02}g_{20}}{c_1} + \frac{g_{11}g_{22}-g_{12}g_{21}}{c_0} + \det G}.\end{aligned}$$

doi:10.6342/NTU201801038

By (1.1)-(1.3), if $\phi \to \infty$, then c_0, $c_2 \to 0$ and $c_1 \to \infty$. This implies that

$$\frac{dc_1}{d\phi} \to \frac{q_1}{g_{11}} \text{ as } \phi \to \infty,$$
$$\frac{dc_2}{d\phi} \to 0 \text{ as } \phi \to \infty.$$

Similarly,

$$\frac{dc_1}{d\phi} \to 0 \text{ as } \phi \to -\infty,$$
$$\frac{dc_2}{d\phi} \to \frac{-q_2}{g_{22}} \text{ as } \phi \to -\infty.$$

Since $\frac{df(\phi)}{d\phi}$ is continuous to ϕ, there exists $M > 0$ such that $|\frac{df(\phi)}{d\phi}| < M$ for all $\phi \in \mathbb{R}$. By mean value theorem, $|\frac{f(\phi_1)-f(\phi_2)}{\phi_1-\phi_2}| < M$ for all $\phi \in \mathbb{R}$. ■

By proposition 2.8, $\frac{f(\phi_0)-f(s)}{\phi_0-s}$ is bounded. Applying theorem 3.14 of [15], we obtain $\phi_0 \in C^{0,\alpha}(\overline{\Omega})$ for some $\alpha > 0$.

Consider $\Delta\phi = f(\phi_0)$ again. If $\eta > 0$, then by proposition 2.8, for any $x, y \in \Omega$,

$$|f(\phi_0(x)) - f(\phi_0(y))| = |\frac{f(\phi_0(x)) - f(\phi_0(y))}{\phi_0(x) - \phi_0(y)}(\phi_0(x) - \phi_0(y))| < M|\phi_0(x) - \phi_0(y)|.$$

Hence $\phi_0 \in C^{0,\alpha}(\overline{\Omega})$ implies $f \in C^{0,\alpha}(\overline{\Omega})$. By the standard elliptic theorem (c.f. Theorem 6.31 of [8]), there exists a unique solution $\Phi \in C^{2,\alpha}(\overline{\Omega})$. In particular,

$$\int_\Omega [\nabla\Phi\nabla v + (q_1c_1(\phi_0) - q_2c_2(\phi_0))v]dx + \frac{1}{\eta}\int_{\partial\Omega}(\Phi - \phi_{bd})vdS = 0 \tag{2.15}$$

for any $v \in H^1(\Omega)$. If we subtract (2.5) by (2.15) and let $v = \phi_0 - \Phi$, then

$$\int_\Omega |\nabla(\phi_0 - \Phi)|^2 dx + \frac{1}{\eta}\int_{\partial\Omega}(\phi_0 - \Phi)^2 dS = 0$$

This implies $\nabla(\phi_0 - \Phi) = 0$ in Ω and $\phi_0 = \Phi$ in trace sense on $\partial\Omega$ almost everywhere.

doi:10.6342/NTU201801038

Hence $\phi_0 = \Phi$ almost everywhere in Ω. Since $\phi_0 \in C^{0,\alpha}(\overline{\Omega})$ and $\Phi \in C^{2,\alpha}(\overline{\Omega})$, $\phi_0 = \Phi$ on $\overline{\Omega}$. This shows that $\phi_0 \in C^{2,\alpha}(\overline{\Omega})$. Applying the standard elliptic regularity theorem (c.f. Theorem 6.17 of [8]), $\phi_0 \in C^{\infty}(\Omega) \cap C^{2,\alpha}(\overline{\Omega})$. Similar argument can be applied for $\eta = 0$ (c.f. Theorem 6.14 of [8]).

At last, we prove the uniqueness of the solution. Suppose $\phi_1, \phi_2 \in C^{\infty}(\Omega) \cap C^{2,\alpha}(\overline{\Omega})$ are two distinct solutions of (1.6)-(1.7). Subtracting (1.6) for $\phi = \phi_2$ by (1.6) for $\phi = \phi_1$, multiplying $\phi_1 - \phi_2$ and then integrating it over Ω with integration by parts and the fact $(\phi_1 - \phi_2) + \eta \frac{\partial}{\partial \nu}(\phi_1 - \phi_2) = 0$ on $\partial\Omega$,

$$\begin{aligned}
&\textstyle\int_{\Omega} |\nabla(\phi_1 - \phi_2)|^2 dx + \frac{1}{\eta} \int_{\partial\Omega} (\phi_1 - \phi_2)^2 dS \\
&+ q_1 \textstyle\int_{\Omega} (c_1(\phi_1) - c_1(\phi_2))(\phi_1 - \phi_2) dx \\
&- q_1 \textstyle\int_{\Omega} (c_2(\phi_1) - c_2(\phi_2))(\phi_1 - \phi_2) dx = 0.
\end{aligned}$$

By proposition 2.5,

$$q_1 \int_{\Omega} (c_1(\phi_1) - c_1(\phi_2))(\phi_1 - \phi_2) dx - q_2 \int_{\Omega} (c_2(\phi_1) - c_2(\phi_2))(\phi_1 - \phi_2) dx \geq 0.$$

Therefore,

$$\int_{\Omega} |\nabla(\phi_1 - \phi_2)|^2 dx + \frac{1}{\eta} \int_{\partial\Omega} (\phi_1 - \phi_2)^2 dS \leq 0,$$

which implies $\phi_1 = \phi_2$ in $\overline{\Omega}$.

doi:10.6342/NTU201801038

3 Limiting Behavior of ϕ and c_i

In this section, we assume:

$(A1)$ $\frac{g_{i0}}{g_{00}} = \frac{g_{i1}}{g_{01}} = \frac{g_{i2}}{g_{02}} = \lambda_i > 0, \quad i = 1,2.$

$(A2)$ $g_{ij} = \tilde{g}_{ij}\Lambda > 0, \quad i,j = 0,1,2.$

$(A3)$ $\mu_i = \tilde{\mu}_i\Lambda + \hat{\mu}_i, \quad \tilde{\mu}_i > 0, \quad i = 0,1,2.$

$(A4)$ $\lambda_i\tilde{\mu}_0 - \tilde{\mu}_i = 0, \quad i = 1,2.$

where $\tilde{g}_{ij}$,, $\tilde{\mu}_i$, $\hat{\mu}_i$ are positive constants. Under this assumption,

$$G = \vec{g}\vec{g}^T, \text{ where } \vec{g} = \begin{bmatrix} g_{00} \\ g_{01} \\ g_{02} \end{bmatrix}.$$

Since, it is clear that G is nonnegative definite and

$$\det \begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21} \end{bmatrix} \geq 0,$$

the existence and uniqueness of ϕ and c_i, for $i = 0,1,2$, can be asserted. As a result, we can further consider the limiting behavior. The theorem is as follows:

Theorem 3.1. *Let Ω be a bounded open smooth domain in $\mathbb{R}^n$ and suppose that $(A1)-(A4)$ hold. Then*

(i) $(c_{i,\Lambda}, \phi_\Lambda) \to (c_i^*, \phi^*)$ uniformly, for $i = 0,1,2$.

(ii) $\phi_\Lambda \to \phi^*$ in $C^{2,\alpha}(\overline{\Omega})$.

where (c_i^*, ϕ^*) satisfies

$$\tilde{g}_{00}c_0^* + \tilde{g}_{01}c_1^* + \tilde{g}_{02}c_2^* = \tilde{\mu}_0, \tag{3.1}$$

$$\lambda_1 \log c_0^* - \log c_1^* = -q_1\phi^* + \overline{\mu}_1, \tag{3.2}$$

$$\lambda_2 \log c_0^* - \log c_2^* = q_2\phi^* + \overline{\mu}_2, \tag{3.3}$$

doi:10.6342/NTU201801038

$$\Delta\phi^* = q_1 c_1^* - q_2 c_2^* \text{ in } \Omega, \tag{3.4}$$

$$\phi^* + \eta \frac{\partial \phi^*}{\partial \nu} = \phi_{bd} \text{ on } \partial\Omega. \tag{3.5}$$

In particular, $\phi_\Lambda - \phi^* = O(\frac{1}{\Lambda})$ *as* $\Lambda \to \infty$.

3.1 Uniform Boundness of ϕ and c_i

To deal with the limiting behavior, we should understand the order of ϕ and c_i, for $i = 0,1,2$ with respect to Λ first. For any fixed Λ, according to (1.8), (1.9), we can write

$$\begin{aligned} c_1 &= e^{-\overline{\mu}_1} e^{q_1\phi} (c_0)^{\lambda_1}, \\ c_2 &= e^{-\overline{\mu}_2} e^{-q_2\phi} (c_0)^{\lambda_2}. \end{aligned} \tag{3.6}$$

Hence (1.6) becomes

$$\Delta\phi = q_1 e^{-\overline{\mu}_1} e^{q_1\phi} (c_0)^{\lambda_1} - q_2 e^{-\overline{\mu}_2} e^{-q_2\phi} (c_0)^{\lambda_2} \tag{3.7}$$

with the boundary condition (1.7).

Since ϕ is continuous on $\overline{\Omega}$ which is compact, the maximum and minimum exist. To obtain the upper bound and the lower bound of ϕ, we have two cases. One case is that the extrema of ϕ happens in Ω. In this case, we deal with it by (3.7). The other case is that the extrema of ϕ happens on $\partial\Omega$. In this case, we deal with it by the boundary condition. The following is the proposition.

Proposition 3.2. *Let* ϕ_0 *be the solution of* (1.6) *with boundary condition* (1.7)*. Then* $m^* \le \phi_0 \le M^*$*, where*

$$m^* = \min\left\{ \min_{\partial\Omega} \phi_{bd}, \min_{\overline{\Omega}} \frac{1}{q_1 + q_2} \log \frac{q_2 c_0^{\lambda_2} e^{-\overline{\mu}_2}}{q_1 c_0^{\lambda_1} e^{-\overline{\mu}_1}} \right\},$$

doi:10.6342/NTU201801038

$$M^* = \max\left\{\max_{\partial\Omega}\phi_{bd}, \max_{\overline{\Omega}}\frac{1}{q_1+q_2}\log\frac{q_2(c_0)^{\lambda_2}e^{-\overline{\mu}_2}}{q_1(c_0)^{\lambda_1}e^{-\overline{\mu}_1}}\right\}.$$

Proof. We only prove the lower bound part. The other part is similar. Since ϕ_0 is continuous in a compact set $\overline{\Omega}$, there exists $x_0 \in \overline{\Omega}$ such that $\phi_0(x) \geq \phi_0(x_0)$ for all $x \in \overline{\Omega}$. If $x_0 \in \Omega$, then

$$0 \leq \Delta\phi_0(x_0) = q_1 e^{-\overline{\mu}_1} e^{q_1\phi_0(x_0)}[c_0(\phi_0(x_0))]^{\lambda_1} - q_2 e^{-\overline{\mu}_2} e^{-q_2\phi_0(x_0)}[c_0(\phi_0(x_0))]^{\lambda_2}.$$

This implies

$$q_2 e^{-\overline{\mu}_2} e^{-q_2\phi_0(x_0)}[c_0(\phi_0(x_0))]^{\lambda_2} \leq q_1 e^{-\overline{\mu}_1} e^{q_1\phi_0(x_0)}[c_0(\phi_0(x_0))]^{\lambda_1}.$$

Hence,

$$\phi_0(x) \geq \phi_0(x_0) \geq \frac{1}{q_1+q_2}\log\frac{q_2[c_0(\phi_0(x_0))]^{\lambda_2}e^{-\overline{\mu}_2}}{q_1[c_0(\phi_0(x_0))]^{\lambda_1}e^{-\overline{\mu}_1}}.$$

If $x_0 \in \partial\Omega$, then $\eta\frac{\partial\phi_0}{\partial\nu}(x_0) \leq 0$. By (1.7), $\phi_0(x) \geq \phi_0(x_0) \geq \phi_{bd}$. Combining these two results, we complete the proof. ■

Applying proposition 3.2, we can show that ϕ_Λ, $c_{i,\Lambda}(\phi_\Lambda)$ are uniformly bounded. To prove this proposition, Observe that if $c_{0,\Lambda}(\phi_\Lambda)$ is uniformly bounded, then so are $c_{1,\Lambda}(\phi_\Lambda)$, $c_{2,\Lambda}(\phi_\Lambda)$ and ϕ_Λ by (3.6) and proposition 3.2. Hence, to obtain the estimate, we consider (1.2) and replace $c_{1,\Lambda}$, $c_{2,\Lambda}$ and ϕ_Λ by $c_{0,\Lambda}$.

Proposition 3.3. *Suppose that (A1)-(A4) holds, then ϕ_Λ, $c_{i,\Lambda}(\phi_\Lambda)$ are uniformly bounded in Λ. Moreover, $c_{i,\Lambda}(\phi_\Lambda)$ is uniformly bounded and away from 0 to Λ for $i = 0, 1, 2$.*

Proof. According to proposition 3.2, there are four cases:

doi:10.6342/NTU201801038

(i) $\min_{\partial\Omega}\phi_{bd} \le \phi_\Lambda \le \max_{\partial\Omega}\phi_{bd}$.

(ii) $\min_{\partial\Omega}\phi_{bd} \le \phi_\Lambda \le \max_{\overline{\Omega}} \frac{1}{q_1+q_2}\log\frac{q_2(c_{0,\Lambda})^{\lambda_2}e^{-\overline{\mu}_2}}{q_1(c_{0,\Lambda})^{\lambda_1}e^{-\overline{\mu}_1}}$.

(iii) $\min_{\overline{\Omega}} \frac{1}{q_1+q_2}\log\frac{q_2(c_{0,\Lambda})^{\lambda_2}e^{-\overline{\mu}_2}}{q_1(c_{0,\Lambda})^{\lambda_1}e^{-\overline{\mu}_1}} \le \phi_\Lambda \le \max_{\partial\Omega}\phi_{bd}$.

(iv) $\min_{\overline{\Omega}} \frac{1}{q_1+q_2}\log\frac{q_2(c_{0,\Lambda})^{\lambda_2}e^{-\overline{\mu}_2}}{q_1(c_{0,\Lambda})^{\lambda_1}e^{-\overline{\mu}_1}} \le \phi_\Lambda \le \max_{\overline{\Omega}} \frac{1}{q_1+q_2}\log\frac{q_2(c_{0,\Lambda})^{\lambda_2}e^{-\overline{\mu}_2}}{q_1(c_{0,\Lambda})^{\lambda_1}e^{-\overline{\mu}_1}}$.

Claim: $c_{0,\Lambda}$ has a uniform upper bound.

If $c_{0,\Lambda} \ge 1$, then $\log c_{0,\Lambda} \ge 0$, and hence by (1.1), $g_{00}c_{0,\Lambda} \le \mu_0$. This implies $c_{0,\Lambda} \le \max\{1, \frac{\tilde{\mu}_0\Lambda+\hat{\mu}_0}{\tilde{g}_{00}\Lambda}\}$ which is uniformly bounded to Λ. Hence there exists c_M such that $c_{0,\Lambda} \le c_M$ for all Λ sufficient large.

Claim: $c_{0,\Lambda}$ has a uniform lower bound which is larger than 0.

By (1.2) and (3.6),

$$\lambda_1 \log c_{0,\Lambda} - \lambda_1\hat{\mu}_0 + \Lambda(\tilde{g}_{10}c_{0,\Lambda} + \tilde{g}_{11}(c_{0,\Lambda})^{\lambda_1}e^{-\overline{\mu}_1}e^{q_1\phi_\Lambda} + \tilde{g}_{12}(c_{0,\Lambda})^{\lambda_2}e^{-\overline{\mu}_2}e^{-q_2\phi_\Lambda} - \tilde{\mu}_1) = 0.$$

Using the inequality $x \ge \log(1+x)$ for $x > -1$, then

$$\lambda_1(c_{0,\Lambda}-1) - \lambda_1\hat{\mu}_0 + \Lambda[\tilde{g}_{10}c_{0,\Lambda} + \tilde{g}_{11}(c_{0,\Lambda})^{\lambda_1}e^{-\overline{\mu}_1}e^{q_1M^*} + \tilde{g}_{12}(c_{0,\Lambda})^{\lambda_2}e^{-\overline{\mu}_2}e^{-q_2m^*} - \tilde{\mu}_1] \ge 0. \tag{3.8}$$

For case(i), since (3.8) holds for any point in $\overline{\Omega}$, if $\min_{\overline{\Omega}} c_{0,\Lambda} < 1$, then

$$\begin{aligned}&\lambda_1((\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_m} - 1) - \lambda_1\hat{\mu}_0\\ &+\Lambda[\tilde{g}_{10}(\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_m} + \tilde{g}_{11}(\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_m}e^{-\overline{\mu}_1}e^{q_1M^*} + \tilde{g}_{12}(\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_m}e^{-\overline{\mu}_2}e^{-q_2m^*} - \tilde{\mu}_1] \ge 0,\end{aligned}$$

doi:10.6342/NTU201801038

where $\lambda_m = \min\{1, \lambda_1, \lambda_2\}$. Hence $c_{0,\Lambda} \geq (\frac{\tilde{\mu}_1\Lambda + \hat{\mu}_0\lambda_1 + \lambda_1}{A\Lambda + \lambda_1})^{\frac{1}{\lambda_m}}$, where

$$A = \tilde{g}_{10} + \tilde{g}_{11}e^{-\overline{\mu}_1}e^{q_1 M^*} + \tilde{g}_{12}e^{-\overline{\mu}_2}e^{-q_2 m^*}.$$

This implies $c_{0,\Lambda} \geq \min\{1, (\frac{\tilde{\mu}_1\Lambda + \hat{\mu}_0\lambda_1 + \lambda_1}{A\Lambda + \lambda_1})^{\frac{1}{\lambda_m}}\}$ which is uniformly bounded to Λ. As a result, there exists $c_m > 0$ which is independent of Λ such that $c_{0,\Lambda} \geq c_m$.

For case (iv), without loss of generality, we may assume $\lambda_2 \geq \lambda_1$. Since

$$m^* = \min_{\overline{\Omega}} \frac{1}{q_1 + q_2} \log \frac{q_2 (c_{0,\Lambda})^{\lambda_2} e^{-\overline{\mu}_2}}{q_1 (c_{0,\Lambda})^{\lambda_1} e^{-\overline{\mu}_1}} = \frac{1}{q_1 + q_2} \log \frac{q_2 (\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_2 - \lambda_1} e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}},$$

and

$$M^* = \max_{\overline{\Omega}} \frac{1}{q_1 + q_2} \log \frac{q_2 (c_{0,\Lambda})^{\lambda_2} e^{-\overline{\mu}_2}}{q_1 (c_{0,\Lambda})^{\lambda_1} e^{-\overline{\mu}_1}} \leq \frac{1}{q_1 + q_2} \log \frac{q_2 (c_M)^{\lambda_2 - \lambda_1} e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}},$$

we have by (3.8),

$$\lambda_1 c_{0,\Lambda} + \Lambda[\tilde{g}_{10} c_{0,\Lambda} + \tilde{g}_{11} (c_{0,\Lambda})^{\lambda_1} e^{-\overline{\mu}_1} (\tfrac{q_2 e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}})^{\frac{q_1}{q_1+q_2}} (c_M)^{\frac{q_1}{q_1+q_2}(\lambda_2 - \lambda_1)}$$
$$+ \tilde{g}_{12} (c_{0,\Lambda})^{\lambda_2} e^{-\overline{\mu}_2} (\tfrac{q_2 e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}})^{\frac{-q_2}{q_1+q_2}} (\min_{\overline{\Omega}} c_{0,\Lambda})^{\frac{-q_2}{q_1+q_2}(\lambda_2 - \lambda_1)}] \geq \tilde{\mu}_1 \Lambda + \hat{\mu}_0 \lambda_1 + \lambda_1.$$

If $\min_{\overline{\Omega}} c_{0,\Lambda} < 1$, then

$$\lambda_1 (\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_n} + \Lambda(\tilde{g}_{10} (\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_n} + \tilde{g}_{11} (\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_n} e^{-\overline{\mu}_1} (\tfrac{q_2 e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}})^{\frac{q_1}{q_1+q_2}} (c_M)^{\frac{-q_2}{q_1+q_2}(\lambda_2 - \lambda_1)}$$
$$+ \tilde{g}_{12} (\min_{\overline{\Omega}} c_{0,\Lambda})^{\lambda_n} e^{-\overline{\mu}_2} (\tfrac{q_2 e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}})^{\frac{-q_2}{q_1+q_2}}) \geq \tilde{\mu}_1 \Lambda + \hat{\mu}_0 \lambda_1 + \lambda_1,$$

where $\lambda_n = \min\{1, \lambda_1, \frac{q_1\lambda_2 + q_2\lambda_1}{q_1+q_2}\}$ Hence $c_{0,\Lambda} \geq \min\{1, (\frac{\tilde{\mu}_1\Lambda + \hat{\mu}_0\lambda_1 + \lambda_1}{B\Lambda + \lambda_1})^{\frac{1}{\lambda_n}}\}$, where

$$B = \tilde{g}_{10} + \tilde{g}_{11} e^{-\overline{\mu}_1} (\frac{q_2 e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}})^{\frac{q_1}{q_1+q_2}} (c_M)^{\frac{-q_2}{q_1+q_2}(\lambda_2 - \lambda_1)} + \tilde{g}_{12} e^{-\overline{\mu}_2} (\frac{q_2 e^{-\overline{\mu}_2}}{q_1 e^{-\overline{\mu}_1}})^{\frac{-q_2}{q_1+q_2}}.$$

doi:10.6342/NTU201801038

This implies that there exists c_m such that $c_{0,\Lambda} \geq c_m$.

The arguments are similar for case (ii) and (iii) and we complete the claim.

Since $c_{0,\Lambda}$ is uniformly bounded, then so are $c_{1,\Lambda}$, $c_{2,\Lambda}$ and ϕ_Λ by (3.6) and proposition 3.2.

■

Since what we are interested are not only $c_{i,\Lambda}(\phi_\Lambda)$ but also $c_{i,\Lambda}(\phi^*)$, we need the following proposition.

Proposition 3.4. *Suppose that $(A1)$-$(A4)$ holds, then $c_{i,\Lambda}(\phi)$ is uniformly bounded and away from 0 to Λ for $i = 0,1,2$, provided $\phi(x)$ is bounded.*

Proof. The proof is the same as proposition 3.3 case (i). ■

Remark 3.1. *Since $c_{i,\Lambda}(\phi)$ is uniformly bounded and away from 0, for $i = 0,1,2$, provided $\phi(x)$ is bounded. By proposition 2.5 and $(A1)-(A2)$,*

$$\frac{dc_{1,\Lambda}}{d\phi} = \frac{M_1}{M} = \frac{\frac{1}{c_{0,\Lambda}c_{2,\Lambda}} + \frac{q_1 g_{22}}{c_{0,\Lambda}} + \frac{q_1 g_{00}}{c_{2,\Lambda}}}{\frac{1}{c_{0,\Lambda}c_{1,\Lambda}c_{2,\Lambda}} + \frac{g_{00}}{c_{1,\Lambda}c_{2,\Lambda}} + \frac{g_{11}}{c_{0,\Lambda}c_{2,\Lambda}} + \frac{g_{22}}{c_{0,\Lambda}c_{1,\Lambda}}}$$

$$= \frac{c_{1,\Lambda} + q_1 g_{22} c_{1,\Lambda} c_{2,\Lambda} + q_1 g_{00} c_{0,\Lambda} c_{1,\Lambda}}{1 + g_{00} c_{0,\Lambda} + g_{11} c_{1,\Lambda} + g_{22} c_{1,\Lambda}}$$

$$= \frac{\frac{c_{1,\Lambda}}{\Lambda} + q_1 \tilde{g}_{22} c_{1,\Lambda} c_{2,\Lambda} + q_1 \tilde{g}_{00} c_{0,\Lambda} c_{1,\Lambda}}{\frac{1}{\Lambda} + \tilde{g}_{00} c_{0,\Lambda} + \tilde{g}_{11} c_{1,\Lambda} + \tilde{g}_{22} c_{1,\Lambda}},$$

which is uniformly bounded and away from 0. The same argument can be applied to $\frac{dc_{2,\Lambda}}{d\phi}$.

Now, we can start to prove theorem 3.1. In the beginning, we use (1.6)-(1.7) and (3.4)-(3.5) to prove that $\phi_\Lambda \to \phi^*$ uniformly as $\Lambda \to \infty$. Next, we can divide (1.1) by Λ and subtract it by (3.1). Consequently, applying (3.6), we can show $c_{0,\Lambda} \to c_0^*$

doi:10.6342/NTU201801038

uniformly provided $\phi_\Lambda \to \phi^*$ uniformly as $\Lambda \to \infty$. This implies $c_{i,\Lambda} \to c_i^*$ uniformly also, for $i = 1,2$. Finally, we show

$$[f_\Lambda(\phi_\Lambda) - f^*(\phi^*)]_{\alpha;\Omega} \to 0 \text{ as } \Lambda \to \infty,$$

where $f_\Lambda = q_1 c_{1,\Lambda} - q_2 c_{2,\Lambda}$ and $f^* = q_1 c_1^* - q_2 c_2^*$. Therefore, by the standard elliptic theorem and the uniform convergence results, $\phi_\Lambda \to \phi^*$ in $C^{2,\alpha}(\overline{\Omega})$.

3.2 Proof of Theorem 3.1

Proof. **Claim:** $\phi_\Lambda \to \phi^*$ uniformly.

Subtracting (1.6) by (3.4),

$$\Delta(\phi_\Lambda - \phi^*) = q_1(c_{1,\Lambda}(\phi_\Lambda) - c_1^*(\phi^*)) - q_2(c_{2,\Lambda}(\phi_\Lambda) - c_2^*(\phi^*))$$

Let

$$A_1 = c_{1,\Lambda}(\phi_\Lambda) - c_{1,\Lambda}(\phi^*), \quad A_2 = c_{1,\Lambda}(\phi^*) - c_1^*(\phi^*),$$

$$B_1 = c_{2,\Lambda}(\phi_\Lambda) - c_{2,\Lambda}(\phi^*), \quad B_2 = c_{2,\Lambda}(\phi^*) - c_2^*(\phi^*).$$

Then

$$\Delta(\phi_\Lambda - \phi^*) = q_1(A_1 + A_2) - q_2(B_1 + B_2).$$

For A_1, applying mean value theorem,

$$A_1 = \frac{dc_{1,\Lambda}}{d\phi}(\phi_{s_1})(\phi_\Lambda - \phi^*),$$

where $\phi_{s_1} \in (\phi_\Lambda, \phi^*)$. By remark 3.1, $\frac{dc_{1,\Lambda}}{d\phi}$ is positive and uniformly bounded away from 0.

doi:10.6342/NTU201801038

For A_2, dividing (1.1) by Λ and subtracting it by (3.1),

$$\tilde{g}_{00}(c_{0,\Lambda}(\phi^*)-c_0^*(\phi^*))+\tilde{g}_{01}(c_{1,\Lambda}(\phi^*)-c_1^*(\phi^*))+\tilde{g}_{02}(c_{2,\Lambda}(\phi^*)-c_2^*(\phi^*))=\frac{\hat{\mu}_0-\log c_{0,\Lambda}(\phi^*)}{\Lambda}.$$

By (3.6),

$$\tilde{g}_{00}(c_{0,\Lambda}(\phi^*)-c_0^*(\phi^*))+\tilde{g}_{01}e^{-\overline{\mu}_1}e^{q_1\phi^*}((c_{0,\Lambda}(\phi^*))^{\lambda_1}-(c_0^*(\phi^*))^{\lambda_1})$$
$$+\tilde{g}_{02}e^{-\overline{\mu}_2}e^{-q_2\phi^*}((c_{0,\Lambda}(\phi^*))^{\lambda_2}-(c_0^*(\phi^*))^{\lambda_2})=\frac{\hat{\mu}_0-\log c_{0,\Lambda}(\phi^*)}{\Lambda}.$$

This implies that

$$A(c_{0,\Lambda}(\phi^*)-c_0^*(\phi^*))=\frac{\hat{\mu}_0-\log c_{0,\Lambda}(\phi^*)}{\Lambda},$$

where

$$A=\tilde{g}_{00}+\tilde{g}_{01}e^{-\overline{\mu}_1}e^{q_1\phi^*}\frac{(c_{0,\Lambda}(\phi^*))^{\lambda_1}-(c_0^*(\phi^*))^{\lambda_1}}{c_{0,\Lambda}(\phi^*)-c_0^*(\phi^*)}+\tilde{g}_{02}e^{-\overline{\mu}_2}e^{-q_2\phi^*}\frac{(c_{0,\Lambda}(\phi^*))^{\lambda_2}-(c_0^*(\phi^*))^{\lambda_2}}{c_{0,\Lambda}(\phi^*)-c_0^*(\phi^*)}.$$

Since the right hand side tends to 0 uniformly as Λ tends to infinity by proposition 3.4 and $A\geq\tilde{g}_{00}$, $A_2\to 0$ as $\Lambda\to\infty$. Moreover, since the right hand side is of $O(\frac{1}{\Lambda})$ as $\Lambda\to\infty$, A_2 is of $O(\frac{1}{\Lambda})$ as $\Lambda\to\infty$.

The same argument can be applied to B_1 ,B_2. That is,

$$B_1=\frac{dc_{2,\Lambda}}{d\phi}(\phi_{s_2})(\phi_\Lambda-\phi^*),$$

where $\frac{dc_{2,\Lambda}}{d\phi}(\phi_{s_2})$ is negative and bounded away from 0, $\phi_{s_2}\in(\phi_\Lambda,\phi^*)$. B_2 is of $O(\frac{1}{\Lambda})$ as $\Lambda\to\infty$.

doi:10.6342/NTU201801038

If $\max_{\overline{\Omega}}(\phi_\Lambda - \phi^*)^2 = (\phi_\Lambda - \phi^*)^2(x_\Lambda)$, where $x_\Lambda \in \partial\Omega$, then we have $\frac{\partial(\phi_\Lambda - \phi^*)^2}{\partial\nu}(x_\Lambda) \geq 0$. Since $(\phi_\Lambda - \phi^*)(x_\Lambda) + \eta\frac{\partial(\phi_\Lambda - \phi^*)}{\partial\nu}(x_\Lambda) = 0$, $(\phi_\Lambda - \phi^*)^2(x_\Lambda) + \frac{\eta}{2}\frac{\partial(\phi_\Lambda - \phi^*)^2}{\partial\nu}(x_\Lambda) = 0$. This implies $\phi_\Lambda = \phi^*$.

If $\max_{\overline{\Omega}}(\phi_\Lambda - \phi^*)^2 = (\phi_\Lambda - \phi^*)^2(x_\Lambda)$, where $x_\Lambda \in \Omega$, then

$$
\begin{aligned}
0 &\geq \Delta(\phi_\Lambda - \phi^*)^2(x_\Lambda) \geq 2\Delta(\phi_\Lambda - \phi^*)(x_\Lambda)(\phi_\Lambda - \phi^*)(x_\Lambda) \\
&= 2(q_1(A_1 + A_2) - q_2(B_1 + B_2))(\phi_\Lambda - \phi^*)(x_\Lambda).
\end{aligned}
$$

This implies that

$$
\begin{aligned}
&(q_1\frac{dc_{1,\Lambda}}{d\phi}(\phi_{s_1}) - q_2\frac{dc_{2,\Lambda}}{d\phi}(\phi_{s_2}))\max_{\overline{\Omega}}(\phi_\Lambda - \phi^*)^2 = (q_1\frac{dc_{1,\Lambda}}{d\phi}(\phi_{s_1}) - q_2\frac{dc_{2,\Lambda}}{d\phi}(\phi_{s_2}))(\phi_\Lambda - \phi^*)^2(x_\Lambda) \\
&= (q_1A_1 - q_2B_1)(\phi_\Lambda - \phi^*)(x_\Lambda) \leq (-q_1A_2 + q_2B_2)(\phi_\Lambda - \phi^*)(x_\Lambda) \\
&\leq (-q_1A_2 + q_2B_2)(\sup_{\overline{\Omega}}|\phi_\Lambda| + \sup_{\overline{\Omega}}|\phi^*|) = O(\tfrac{1}{\Lambda}) \text{ as } \Lambda \to \infty.
\end{aligned}
$$

Since $q_1\frac{dc_{1,\Lambda}}{d\phi}(\phi_{s_1}) - q_2\frac{dc_{2,\Lambda}}{d\phi}(\phi_{s_2})$ is positive and bounded away from 0, we complete the proof.

Claim: $c_{i,\Lambda}(\phi_\Lambda) \to c_i^*(\phi^*)$ uniformly, for $i = 0, 1, 2$.

Dividing (1.1) by Λ and subtracting it by (3.1),

$$
\begin{aligned}
&\tilde{g}_{00}(c_{0,\Lambda}(\phi_\Lambda) - c_0^*(\phi^*)) + \tilde{g}_{01}e^{-\overline{\mu}_1}((c_{0,\Lambda}(\phi_\Lambda))^{\lambda_1}e^{q_1\phi_\Lambda} - (c_0^*(\phi^*))^{\lambda_1}e^{q_1\phi^*}) \\
&+\tilde{g}_{02}e^{-\overline{\mu}_2}((c_{0,\Lambda}(\phi_\Lambda))^{\lambda_2}e^{-q_2\phi_\Lambda} - (c_0^*(\phi^*))^{\lambda_2}e^{-q_2\phi^*}) = \frac{\hat{\mu}_0 - \log c_{0,\Lambda}(\phi_\Lambda)}{\Lambda}.
\end{aligned}
$$

doi:10.6342/NTU201801038

This implies that

$$\tilde{g}_{00}(c_{0,\Lambda}(\phi_\Lambda)-c_0^*(\phi^*))+\tilde{g}_{01}e^{-\overline{\mu}_1}e^{q_1\phi^*}((c_{0,\Lambda}(\phi_\Lambda))^{\lambda_1}-(c_0^*(\phi^*))^{\lambda_1})$$
$$+\tilde{g}_{02}e^{-\overline{\mu}_2}e^{-q_2\phi^*}((c_{0,\Lambda}(\phi_\Lambda))^{\lambda_2}-(c_0^*(\phi^*))^{\lambda_2})$$
$$=\frac{\hat{\mu}_0-\log c_{0,\Lambda}(\phi_\Lambda)}{\Lambda}+\tilde{g}_{01}e^{-\overline{\mu}_1}(c_{0,\Lambda}(\phi_\Lambda))^{\lambda_1}(e^{q_1\phi^*}-e^{q_1\phi_\Lambda})+\tilde{g}_{02}e^{-\overline{\mu}_2}(c_{0,\Lambda}(\phi_\Lambda))^{\lambda_2}(e^{-q_2\phi^*}-e^{-q_2\phi_\Lambda}).$$

Hence,

$$C(c_{0,\Lambda}(\phi_\Lambda)-c_0^*(\phi^*))=\frac{\hat{\mu}_0-\log c_{0,\Lambda}(\phi_\Lambda)}{\Lambda}+\tilde{g}_{01}e^{-\overline{\mu}_1}(c_{0,\Lambda}(\phi_\Lambda))^{\lambda_1}(e^{q_1\phi^*}-e^{q_1\phi_\Lambda})$$
$$+\tilde{g}_{02}e^{-\overline{\mu}_2}(c_{0,\Lambda}(\phi_\Lambda))^{\lambda_2}(e^{-q_2\phi^*}-e^{-q_2\phi_\Lambda}),$$

where

$$C=\tilde{g}_{00}+\tilde{g}_{01}e^{-\overline{\mu}_1}e^{q_1\phi^*}\frac{(c_{0,\Lambda}(\phi_\Lambda))^{\lambda_1}-(c_0^*(\phi^*))^{\lambda_1}}{c_{0,\Lambda}(\phi_\Lambda)-c_0^*(\phi^*)}+\tilde{g}_{02}e^{-\overline{\mu}_2}e^{-q_2\phi^*}\frac{(c_{0,\Lambda}(\phi_\Lambda))^{\lambda_2}-(c_0^*(\phi^*))^{\lambda_2}}{c_{0,\Lambda}(\phi_\Lambda)-c_0^*(\phi^*)}.$$

Since $\phi_\Lambda\to\phi^*$ uniformly, the right hand side of the equation tends to 0 as Λ tends to infinity. Observe that $C\geq\tilde{g}_{00}$, and hence $c_{0,\Lambda}(\phi_\Lambda)\to c_0^*(\phi^*)$ uniformly as $\Lambda\to\infty$. Note that if $c_{0,\Lambda}(\phi_\Lambda)=c_0^*(\phi^*)$, then it is nothing to prove.

By (3.6) and mean value theorem,

$$|c_{1,\Lambda}(\phi_\Lambda)-c_1^*(\phi^*)|=|e^{\overline{\mu}_1-q_1\phi_\Lambda}[c_{0,\Lambda}(\phi_\Lambda)]^{\lambda_1}-e^{\overline{\mu}_1-q_1\phi^*}[c_0^*(\phi^*)]^{\lambda_1}|$$
$$\leq|e^{\overline{\mu}_1-q_1\phi_\Lambda}[c_{0,\Lambda}(\phi_\Lambda)]^{\lambda_1}-e^{\overline{\mu}_1-q_1\phi_\Lambda}[c_0^*(\phi^*)]^{\lambda_1}|+|e^{\overline{\mu}_1-q_1\phi_\Lambda}[c_0^*(\phi^*)]^{\lambda_1}-e^{\overline{\mu}_1-q_1\phi^*}[c_0^*(\phi^*)]^{\lambda_1}|$$
$$\leq C(|c_{0,\Lambda}(\phi_\Lambda)-c_0^*(\phi^*)|+|\phi_\Lambda-\phi^*|)$$

which tends to 0 as $\Lambda\to\infty$, for some constant C. The same argument can be applied to $c_{2,\Lambda}(\phi_\Lambda)$. Therefore, $c_{i,\Lambda}(\phi_\Lambda)\to c_i^*(\phi^*)$ uniformly as $\Lambda\to\infty$.

Claim: $\frac{dc_{1,\Lambda}}{d\phi}(\phi)\to\frac{dc_1^*}{d\phi}(\phi)$ uniformly provided $\phi(x)$ is bounded.

doi:10.6342/NTU201801038

Differentiating the first three equations of (1.10) and (1.11) with respect to ϕ, then by Cramer's rule,

$$\frac{dc_{1,\Lambda}}{d\phi} = \frac{N_{1,\Lambda}}{N_\Lambda}, \quad \frac{dc_1^*}{d\phi} = \frac{N_1^*}{N^*},$$

where

$$N_\Lambda = \Lambda \det \begin{bmatrix} \frac{1}{c_{0,\Lambda}\Lambda} + \tilde{g}_{00} & \tilde{g}_{01} & \tilde{g}_{02} \\ \frac{\lambda_1}{c_{0,\Lambda}} & \frac{-1}{c_{1,\Lambda}} & 0 \\ \frac{\lambda_2}{c_{0,\Lambda}} & 0 & \frac{-1}{c_{2,\Lambda}} \end{bmatrix},$$

$$N_{1,\Lambda} = \Lambda \det \begin{bmatrix} \frac{1}{c_{0,\Lambda}\Lambda} + \tilde{g}_{00} & 0 & \tilde{g}_{02} \\ \frac{\lambda_1}{c_{0,\Lambda}} & -q_1 & 0 \\ \frac{\lambda_2}{c_{0,\Lambda}} & q_2 & \frac{-1}{c_{2,\Lambda}} \end{bmatrix},$$

$$N^* = \det \begin{bmatrix} \tilde{g}_{00} & \tilde{g}_{01} & \tilde{g}_{02} \\ \frac{\lambda_1}{c_0^*} & \frac{-1}{c_1^*} & 0 \\ \frac{\lambda_2}{c_0^*} & 0 & \frac{-1}{c_2^*} \end{bmatrix},$$

$$N_1^* = \det \begin{bmatrix} \tilde{g}_{00} & 0 & \tilde{g}_{02} \\ \frac{\lambda_1}{c_0^*} & -q_1 & 0 \\ \frac{\lambda_2}{c_0^*} & q_2 & \frac{-1}{c_2^*} \end{bmatrix}.$$

By proposition 3.4, N_Λ is bounded and away from 0. In particular, since $c_{0,\Lambda}$ is uniformly bounded and away from 0, $\frac{1}{c_{0,\Lambda}\Lambda} \to 0$ as $\Lambda \to \infty$. Moreover, by the same argument as the previous claim, $c_{i,\Lambda}(\phi) \to c_i^*(\phi)$ uniformly as $\Lambda \to \infty$. Hence, $(N_\Lambda, N_{1,\Lambda}) \to (N^*, N_1^*)$ uniformly as $\Lambda \to \infty$. This implies the claim. The same argument can be used to prove $\frac{dc_{2,\Lambda}}{d\phi}(\phi) \to \frac{dc_2^*}{d\phi}(\phi)$ uniformly as $\Lambda \to \infty$.

Claim: $\phi_\Lambda \to \phi^*$ in $C^{2,\alpha}(\overline{\Omega})$.

doi:10.6342/NTU201801038

Let $f_\Lambda = q_1 c_{1,\Lambda} - q_2 c_{2,\Lambda}$ and $f^* = q_1 c_1^* - q_2 c_2^*$. Then

$$\begin{cases} \Delta(\phi_\Lambda - \phi^*) = f_\Lambda(\phi_\Lambda) - f^*(\phi^*) & \text{in } \Omega, \\ (\phi_\Lambda - \phi^*) + \frac{\partial(\phi_\Lambda - \phi^*)}{\partial \nu} = 0 & \text{on } \partial\Omega. \end{cases}$$

By the standard elliptic theorem (c.f. Theorem 6.30 of [8]),

$$|\phi_\Lambda - \phi^*|_{2,\alpha;\Omega} \le C(|\phi_\Lambda - \phi^*|_{0;\Omega} + |f_\Lambda(\phi_\Lambda) - f^*(\phi^*)|_{0,\alpha;\Omega}).$$

Since $\phi_\Lambda \to \phi^*$ and $f_\Lambda \to f^*$ uniformly as $\Lambda \to \infty$, it suffices to show

$$[f_\Lambda(\phi_\Lambda) - f^*(\phi^*)]_{\alpha;\Omega} \to 0 \text{ as } \Lambda \to \infty.$$

Since $\frac{df^*}{d\phi}(\phi)$ is continuous on a compact set which contains the image of $\phi_\Lambda(x)$ and $\phi^*(x)$ (c.f. Proposition 3.4), given $\varepsilon > 0$, there exists $\delta > 0$ such that if $|\phi_1 - \phi_2| < \delta$, then $|\frac{df^*}{d\phi}(\phi_1) - \frac{df^*}{d\phi}(\phi_2)| < \varepsilon$.

For $|\phi^*(x) - \phi^*(y)| \ge \frac{\delta}{2}$ and given $x, y \in \Omega$,

$$\begin{aligned} &|f_\Lambda(\phi_\Lambda(x)) - f^*(\phi^*(x)) - [f_\Lambda(\phi_\Lambda(y)) - f^*(\phi^*(y))]| \\ &\le \tfrac{2}{\delta}|f_\Lambda(\phi_\Lambda(x)) - f^*(\phi^*(x)) - [f_\Lambda(\phi_\Lambda(y)) - f^*(\phi^*(y))]||\phi^*(x) - \phi^*(y)| \\ &\le \tfrac{2}{\delta}|f_\Lambda(\phi_\Lambda(x)) - f^*(\phi^*(x)) - [f_\Lambda(\phi_\Lambda(y)) - f^*(\phi^*(y))]|[\phi^*]_{\alpha;\Omega}|x-y|^\alpha. \end{aligned}$$

This implies that

$$\begin{aligned} &\sup_{x \ne y} \tfrac{1}{|x-y|^\alpha}|f_\Lambda(\phi_\Lambda(x)) - f^*(\phi^*(x)) - [f_\Lambda(\phi_\Lambda(y)) - f^*(\phi^*(y))]| \\ &\le \sup_{x \ne y} \tfrac{2}{\delta}|f_\Lambda(\phi_\Lambda(x)) - f^*(\phi^*(x)) - [f_\Lambda(\phi_\Lambda(y)) - f^*(\phi^*(y))]|[\phi^*]_{\alpha;\Omega}. \end{aligned}$$

doi:10.6342/NTU201801038

Since the right hand side is a continuous function on $\overline{\Omega}\times\overline{\Omega}$, it attains its maximum at (x_Λ, y_Λ). Hence,

$$\begin{aligned}&\sup_{x\neq y}\tfrac{1}{|x-y|^\alpha}|f_\Lambda(\phi_\Lambda(x))-f^*(\phi^*(x))-[f_\Lambda(\phi_\Lambda(y))-f^*(\phi^*(y))]|\\&\leq \tfrac{2}{\delta}|f_\Lambda(\phi_\Lambda(x_\Lambda))-f^*(\phi^*(x_\Lambda))-[f_\Lambda(\phi_\Lambda(y_\Lambda))-f^*(\phi^*(y_\Lambda))]|[\phi^*]_{\alpha;\Omega}.\end{aligned}$$

Since $f_\Lambda(\phi_\Lambda)\to f^*(\phi^*)$ uniformly as $\Lambda\to\infty$, the right hand side tends to 0 as $\Lambda\to\infty$.

For $|\phi^*(x)-\phi^*(y)|<\frac{\delta}{2}$ and given $x,y\in\Omega$, by mean value theorem,

$$\begin{aligned}&|f_\Lambda(\phi_\Lambda(x))-f^*(\phi^*(x))-(f_\Lambda(\phi_\Lambda(y))-f^*(\phi^*(y)))|\\&=|\tfrac{df_\Lambda}{d\phi}(\phi_{s,\Lambda})(\phi_\Lambda(x)-\phi_\Lambda(y))-\tfrac{df^*}{d\phi}(\phi_s^*)(\phi^*(x)-\phi^*(y))|\end{aligned}$$

where $\phi_{s,\Lambda}\in(\phi_\Lambda(x),\phi_\Lambda(y))$ and $\phi_s^*\in(\phi^*(x),\phi^*(y))$. Let

$$\begin{aligned}A&=\tfrac{df_\Lambda}{d\phi}(\phi_{s,\Lambda})(\phi_\Lambda(x)-\phi_\Lambda(y)-\phi^*(x)+\phi^*(y)),\\B&=(\tfrac{df_\Lambda}{d\phi}(\phi_{s,\Lambda})-\tfrac{df^*}{d\phi}(\phi_s^*))(\phi^*(x)-\phi^*(y)).\end{aligned}$$

Then

$$|f_\Lambda(\phi_\Lambda(x))-f^*(\phi^*(x))-(f_\Lambda(\phi_\Lambda(y))-f^*(\phi^*(y)))|\leq|A|+|B|.$$

For A, since $\frac{df_\Lambda}{d\phi}(\phi_{s,\Lambda})$ is uniformly bounded (c.f. Remark 3.1), there exists a constant $C>0$ such that

$$|A|\leq C[\phi_\Lambda-\phi^*]_{\alpha;\Omega}|x-y|^\alpha.$$

which tends to 0 as $\Lambda\to\infty$ by theorem 3.14 of [15].

For B, since $\frac{df_\Lambda}{d\phi}(\phi_{s,\Lambda})\to\frac{df^*}{d\phi}(\phi_{s,\Lambda})$ uniformly as $\Lambda\to\infty$ by the previous claim, for

doi:10.6342/NTU201801038

Λ large enough,

$$\begin{aligned}|B| &\leq (|\tfrac{df^*}{d\phi}(\phi_{s,\Lambda}) - \tfrac{df_\Lambda}{d\phi}(\phi_{s,\Lambda})| + |\tfrac{df^*}{d\phi}(\phi_{s,\Lambda}) - \tfrac{df^*}{d\phi}(\phi_s^*)|)|\phi^*(x) - \phi^*(y)| \\ &\leq (\varepsilon + |\tfrac{df^*}{d\phi}(\phi_{s,\Lambda}) - \tfrac{df^*}{d\phi}(\phi_s^*)|[\phi^*]_{\alpha;\Omega}|x-y|^\alpha.\end{aligned}$$

Since $\phi_\Lambda \to \phi^*$ uniformly as $\Lambda \to \infty$ and $|\phi^*(x) - \phi^*(y)| < \frac{\delta}{2}$, for Λ large enough, $|\phi_{s,\Lambda} - \phi_s^*| < \delta$. Hence,

$$|B| \leq 2\varepsilon[\phi^*]_{\alpha;\Omega}|x-y|^\alpha.$$

Letting $\varepsilon \to 0$, we get $\sup\limits_{x\neq y} \frac{|B|}{|x-y|^\alpha} \to 0$. This complete the claim. ■

4 Generalization of G

In this section, we generalize the condition that G is nonnegative definite. The main difference is from theorem 2.3 and proposition 2.5 which can be replaced by the following proposition and theorem. The rest of the proofs are all the same as before.

For the proposition, we consider c_0, c_1, and c_2 as three variables and apply Lagrange multiplier to find the condition such that $M > 0$ (c.f. proposition 2.5).

Proposition 4.1. *Given $G = (g_{ij})$ and μ_i, for $i = 0,1,2$, suppose that*

$$(B1)\quad \det\begin{bmatrix} g_{00} & g_{01} \\ g_{10} & g_{11}\end{bmatrix}, \det\begin{bmatrix} g_{00} & g_{02} \\ g_{20} & g_{22}\end{bmatrix}, \det\begin{bmatrix} g_{00} & g_{01} \\ g_{20} & g_{21}\end{bmatrix} \geq 0,$$

$(B2)\quad \frac{E}{c_1^0 c_2^0} + \frac{F}{c_1^0} + \frac{H}{c_2^0} + J > 0,$

then we have $\frac{dc_1}{d\phi} > 0$ and $\frac{dc_2}{d\phi} < 0$, where

$$c_1^0 = \frac{-(AE+q_2H) + \sqrt{(AE+q_2H)^2 + 4q_2AH(a_0 - q_2E)}}{2q_2AH},$$
$$c_2^0 = \frac{-(BE+q_1F) + \sqrt{(BE+q_1F)^2 + 4q_1BF(a_0 - q_1E)}}{2q_1BF}.$$

doi:10.6342/NTU201801038

for some a_0 *satisfying*

$$\log c_1^0 + \log c_2^0 + Ac_1^0 + Bc_2^0 = C.$$

Here,

$$A = q_2 g_{11} + q_1 g_{21} - \tfrac{(q_2 g_{10} + q_1 g_{20}) g_{01}}{g_{00}+1},$$

$$B = q_2 g_{12} + q_1 g_{22} - \tfrac{(q_2 g_{10} + q_1 g_{20}) g_{02}}{g_{00}+1},$$

$$C = q_2 \mu_1 + q_1 \mu_2 - (q_2 g_{10} + q_1 g_{20})(\mu_0 + 1),$$

$$E = \tfrac{1}{c_0^M} + g_{00},$$

$$F = \tfrac{g_{22}}{c_0^M} + g_{00} g_{22} - g_{02} g_{20},$$

$$H = \tfrac{g_{11}}{c_0^M} + g_{00} g_{11} - g_{01} g_{10},$$

$$J = \tfrac{g_{11} g_{22} - g_{12} g_{21}}{c_0^M} + \det G,$$

where c_0^M *is the upper bound of* c_0*.*

Proof. The same as proposition 2.5, by $(B1)$, $M_1 > 0$ and $M_2 < 0$. Hence we only have to show $M > 0$. Firstly, by (1.1),

$$\log c_0 + g_{00} c_0 \le \mu_0.$$

Since $\log c_0 + g_{00} c_0$ is monotone increasing to c_0, there exists $c_0^M > 0$ such that $c_0 \le c_0^M$, where

$$\log c_0^M + g_{00} c_0^M = \mu_0.$$

Hence by $(B1)$,

$$M = \frac{1}{c_0 c_1 c_2} + \frac{g_{00}}{c_1 c_2} + \frac{g_{11}}{c_0 c_2} + \frac{g_{22}}{c_0 c_1} + \frac{g_{00} g_{11} - g_{01} g_{10}}{c_2}$$
$$\ge \tfrac{E}{c_1 c_2} + \tfrac{F}{c_1} + \tfrac{H}{c_2} + J.$$

doi:10.6342/NTU201801038

Note that under the assumption $(B1)$, E, F, H are all nonnegative.

On the other hand, using the fact that $\log(1+x) \leq x$ for $x > -1$ and by (1.1), then

$$c_0 - 1 + g_{00}c_0 + g_{01}c_1 + g_{02}c_2 \geq \mu_0.$$

Hence

$$c_0 \geq \frac{\mu_0 + 1 - g_{01}c_1 - g_{02}c_2}{g_{00}+1}. \tag{4.1}$$

Multiplying (1.2) by q_2 and (1.3) by q_1 and adding them together, then

$$\begin{aligned} &q_2 \log c_1 + q_1 \log c_2 + (q_2 g_{10} + q_1 g_{20})c_0 + (q_2 g_{11} + q_1 g_{21})c_1 + (q_2 g_{12} + q_1 g_{22})c_2 \\ &= q_2\mu_1 + q_1\mu_2. \end{aligned} \tag{4.2}$$

Substituting (4.1) into (4.2), then one may check

$$q_2 \log c_1 + q_1 \log c_2 + Ac_1 + Bc_2 \leq C.$$

Note that A, B are nonnegative under the assumption $(B1)$. Hence

$$M \geq \min_{(c_1,c_2)\in\Gamma_1} \frac{E}{c_1c_2} + \frac{F}{c_1} + \frac{H}{c_2} + J \geq \min_{(c_1,c_2)\in\Gamma_2} \frac{E}{c_1c_2} + \frac{F}{c_1} + \frac{H}{c_2} + J,$$

where

$$\begin{aligned} \Gamma_1 &= \{(y,z) : (x,y,z) \text{ satisfies (1.1) and (4.2) for some } x > 0\} \\ &\subseteq \{(y,z) : q_2 \log y + q_1 \log z + Ay + Bz \leq C\}, \\ \Gamma_2 &= \{(y,z) : q_2 \log y + q_1 \log z + Ay + Bz = C.\} \end{aligned}$$

Observe that the minimum must be attained in a bounded domain since if $c_1 \to \infty$,

doi:10.6342/NTU201801038

then $c_2 \to 0$ and vice versa. This makes $\frac{E}{c_1c_2}+\frac{F}{c_1}+\frac{H}{c_2}+J$ goes to infinity. Applying Lagrange multiplier, then

$$\begin{aligned}\frac{E}{c_1^2c_2}+\frac{F}{c_1^2}&=\lambda(\frac{q_2}{c_1}+A),\\ \frac{E}{c_1c_2^2}+\frac{H}{c_2^2}&=\lambda(\frac{q_1}{c_2}+B).\end{aligned}$$

This implies

$$(E+Fc_2)(q_1+Bc_2)=(E+Hc_1)(q_2+Ac_1).$$

Let $a=(E+Fc_2)(q_1+Bc_2)=(E+Hc_1)(q_2+Ac_1)$. Then

$$\begin{aligned}c_1&=\frac{-(AE+q_2H)+\sqrt{(AE+q_2H)^2+4q_2AH(a-q_2E)}}{2q_2AH},\\ c_2&=\frac{-(BE+q_1F)+\sqrt{(BE+q_1F)^2+4q_1BF(a-q_1E)}}{2q_1BF}.\end{aligned}$$

Denote $c_1=c_1(a)$ and $c_2=c_2(a)$. Then

$$q_2\log c_1(a)+q_1\log c_2(a)+Ac_1(a)+Bc_2(a)=C.$$

One may check that $q_2\log c_1(a)+q_1\log c_2(a)+Ac_1(a)+Bc_2(a)$ is monotone increasing to a. Hence, there exists a unique a_0 such that

$$q_2\log c_1^0+q_1\log c_2^0+Ac_1^0+Bc_2^0=C.$$

This implies

$$M\geq\min_{c_1,c_2\in\Gamma_2}\frac{E}{c_1c_2}+\frac{F}{c_1}+\frac{H}{c_2}+J=\frac{E}{c_1^0c_2^0}+\frac{F}{c_1^0}+\frac{H}{c_2^0}+J>0,$$

since the minimum must be attained in a bounded domain and this is the unique

doi:10.6342/NTU201801038

solution of Lagrange multiplier. ■

The proof of the next theorem is almost the same as the existence part of algebraic equations. The main difference is that we have more information to the monotonicity. Therefore, we can make sure the solution is unique when applying intermediate value theorem.

Theorem 4.2. *Under the hypothesis of proposition* 4.1*, and if*

$$\det \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \geq 0,$$

then c_i *is unique for given* ϕ*. That is,* c_i *is a function of* ϕ*, for* $i = 0, 1, 2$.

Proof. For any fixed ϕ, by (1.2),

$$c_2 = \frac{1}{g_{12}}(q_1\phi + \mu_1 - \log c_1 - g_{10}c_0 - g_{11}c_1).$$

Substituting it into (1.3),

$$\begin{aligned} &\log(\tfrac{1}{g_{12}}(q_1\phi + \mu_1 - \log c_1 - g_{10}c_0 - g_{11}c_1)) + g_{20}c_0 + g_{21}c_1 \\ &+ \tfrac{g_{22}}{g_{12}}(q_1\phi + \mu_1 - \log c_1 - g_{10}c_0 - g_{11}c_1) = -q_2\phi + \mu_2. \end{aligned}$$

Since $g_{11}g_{22} - g_{12}g_{21}$ is nonnegative, the left hand side is monotone decreasing to c_1. Hence for given c_0, there exists a unique c_1^s such that

$$\begin{aligned} &\log(\tfrac{1}{g_{12}}(q_1\phi + \mu_1 - \log c_1^s - g_{10}c_0 - g_{11}c_1^s)) + g_{20}c_0 + g_{21}c_1^s \\ &+ \tfrac{g_{22}}{g_{12}}(q_1\phi + \mu_1 - \log c_1^s - g_{10}c_0 - g_{11}c_1^s) = -q_2\phi + \mu_2. \end{aligned}$$

That is, c_1 is a function of c_0, and hence so is c_2. Note that the existence of c_1^s

doi:10.6342/NTU201801038

follows from theorem 2.2. Differentiating the system (1.1)-(1.3) with respect to c_0,

$$\frac{1}{c_0} + g_{00} + g_{01}c_1' + g_{02}c_2' = 0, \tag{4.3}$$

$$\frac{c_1'}{c_1} + g_{10} + g_{11}c_1' + g_{12}c_2' = 0, \tag{4.4}$$

$$\frac{c_2'}{c_2} + g_{20} + g_{21}c_1' + g_{22}c_2' = 0. \tag{4.5}$$

Applying Cramer's rule to (4.4) and (4.5),

$$c_1' = \frac{D_1}{D}, \quad c_2' = \frac{D_2}{D},$$

where

$$D = \det \begin{bmatrix} \frac{1}{c_1} + g_{11} & g_{12} \\ g_{21} & \frac{1}{c_2} + g_{22} \end{bmatrix},$$

$$D_1 = \det \begin{bmatrix} -g_{10} & g_{12} \\ -g_{20} & \frac{1}{c_2} + g_{22} \end{bmatrix},$$

$$D_2 = \det \begin{bmatrix} \frac{1}{c_1} + g_{11} & -g_{10} \\ g_{21} & -g_{20} \end{bmatrix}.$$

Substituting c_1' and c_2' into (4.3),

$$\frac{1}{D}(D(\frac{1}{c_0} + g_{00}) + g_{01}D_1 + g_{02}D_2) = \frac{M}{D} > 0.$$

Here, M is the same as the one in proposition 3.3. This implies that $\log c_0 + g_{00}c_0 + g_{01}c_1(c_0) + g_{02}c_2(c_0)$ is monotone increasing to c_0. Hence there exists a unique c_0^s

doi:10.6342/NTU201801038

such that

$$\log c_0^s + g_{00}c_0^s + g_{01}c_1(c_0^s) + g_{02}c_2(c_0^s) = \mu_0$$

and we complete the proof. Note that the existence of c_0^s follows from theorem 2.2. ■

We have known that $G = (g_{ij})$ is nonnegative definite if and only if $g_{ii} \geq 0$ for $i = 0, 1, 2$, $\det G \geq 0$ and

$$\det \begin{bmatrix} g_{00} & g_{01} \\ g_{10} & g_{11} \end{bmatrix}, \det \begin{bmatrix} g_{00} & g_{02} \\ g_{20} & g_{22} \end{bmatrix}, \det \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix} \geq 0.$$

In our generalized condition, we do not ask $\det G \geq 0$. For example, consider

$$G = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 2 \\ 2 & 2 & 3 \end{bmatrix}.$$

If $\mu_0 \to -\infty$, then $C_0^M \to 0$. This implies $J \to \infty$ and hence $(B2)$ holds for μ_0 small enough. Thus, c_i, for $i = 0, 1, 2$, can be written as a function of ϕ in this G.

5 Conclusion Remark

Li's model is a well-known model for electrolyte solutions. In this work, we introduce the PB_ns model which is derived from the steady-state of the Poisson-Nernst-Planck system with steric effects. Under the assumption $(A1) - (A4)$, PB_ns model can be reduced to Li's model by passing Λ to infinity. This shows that PB_ns equations is a more general model.

doi:10.6342/NTU201801038

References

[1] M.Z. Bazant, K. Thornton, A. Ajdari, Diffuse-charge dynamics in electrochemical systems, Phys. Rev. E 70, 021506 (2004).

[2] J. Bikerman, Structure and capacity of the electrical double layer, Phil. Mag. 33, 384-397 (1942).

[3] I. Borukhov, D. Andelman, H. Orland, Steric effects in electrolytes: a modified Poisson–Boltzmann equation, Phys. Rev. Lett. 79, 435 (1997).

[4] B. Eisenberg, Y. Hyon, C. Liu, Energy variational analysis of ions in water and channels: field theory for primitive models of complex ionic fluids, J. Chem. Phys. 133, 104104 (2010).

[5] Lawrence. C. Evans, Partial Differential Equations, American Mathematical Society (1998).

[6] M Fixman, The Poisson–Boltzmann equation and its application to polyelectrolytes, J. Chem. Phys. 70, 4995 (1979).

[7] F. Fogolari, A. Brigo, H. Molinari, The Poisson – Boltzmann equation for biomolecular electrostatics: a tool for structural biology, J. Mol. Recognit. 15, 377-392 (2002).

[8] David Gilbarg and Neil. s. Trudinger, Elliptic Partial Differential Equations of Second Order, Springer (2001).

[9] Chiun-Chang Lee, Hijin Lee, YunKyong Hyon, Tai-Chia Lin and Chun Liu, New Poisson–Boltzmann type equations: one-dimensional solutions, Nonlinearity 24, 431–458 (2011).

doi:10.6342/NTU201801038

[10] Qing Han and Fanghua Lin, Elliptic Partial Differential Equations, American Mathematical Society (2000).

[11] Bo Li, Pei Liu, Zhenli Xu and Shenggao Zhuo, Ionic size effects: generalized Boltzmann distributions, counterion stratification and modified Debye length, Nonlinearity 26, 2899-2922 (2013).

[12] Tai-Chia Lin and Eisenberg. B, Multiple solutions of steady-state Poisson-Nernst-Plank equations with steric effects, Nonlinearity 28, 2053-2080 (2015).

[13] W. Liu, Geometric singular perturbation approach to strady-state Poisson-Nernst-Planck systems, SIAM J. Appl. Math., 65(3), 754–766 (2005).

[14] P.A. Marcowich, The Stantionary Semiconductor Device Equations, Springer-Verlag (1986).

[15] Robin Nittka, Regularity of solitions of linear second order elliptic and parabolic boundary value problems on Lipschitz domains, J. Differential Equations 251, 860-880 (2011).

[16] W. Rocchia, E. Alexov, and B. Honig, Extending the Applicability of the Nonlinear Poisson−Boltzmann Equation: Multiple Dielectric Constants and Multivalent Ions, J. Phys. Chem. B, 105 (28), 6507–6514 (2001).

[17] Kim A. Sharp and Barry Honig, Calculating Total Electrostatic Energies with the Nonlinear Poisson-Boltzmann Equation, J. Phys. Chem. 94, 7684-7692 (1990).

[18] J. Zhang, X. Gong, C. Liu, W. Wen and P. Sheng, Electrorheological Fluid Dynamics, Phys. Rev. Lett. 101(19), 194503 (2008).

doi:10.6342/NTU201801038