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帕松波兹曼類方程的邊界層解

Boundary Layer Solutions to PB Type Equations

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Boundary Layer Solutions to PB Type Equations

本論文係呂治鴻（D06221001）在國立臺灣大學數學系博士班完成之博士學位論文，於民國 114 年 06 月 06 日承下列考試委員審查通過及口試及格，特此證明。

The undersigned, appointed by the Department of Mathematics on 06 June 2025 have examined a Doctoral Dissertation entitled above presented by Jhih-Hong Lyu (D0622001) candidate and hereby certify that it is worthy of acceptance.

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光陰荏苒，轉眼間已過數十年頭。於民國九十八年透過指考進入國立臺灣大學後，我立刻申請了改分發進入數學系。原以爲大學的數學會像高中數學一樣有趣，不料又是原文書，又是抽象的證明。所幸到了二三年級後狀況逐漸改善，也因著外文系崔綺雲學姊的介紹，認識了朱樺老師與林太家老師。雖然我只有定期的參加基督教的小排聚會並沒有與老師們討論數學，但他們以善意與溫暖接納我。由於輔修哲學系的緣故，我並沒有在大三的時候修大三的必修課偏微分方程式導論，而是在四年級才修，而此時開課的教授是林紹雄老師。林紹雄老師素來以板書快速、難度深聞名。所幸的是當時我只有這門數學課，因此我全心全意地研讀偏微分方程式，也從中開啓了我對這門學科的興趣。

大學畢業後我順利考上數學碩班，但入學前我決定先保留學籍並且先回高中母校進行教師實習。在當中認識了許多很棒的夥伴，後來也有許多人日後也保持聯絡，這裡特別想感謝韓萱與莊慈。在跟著這群夥伴實習的過程中，無疑是最輕鬆自在而且可以保持著類似高中生活的感覺。在其中我也發現到或許比起教學，我可能更喜歡研究。進入研究所後，一方面修著比大學更難的課程，二方面開始找林太家老師從事研究。在這過程中不得不提及的人便是國立清華大學的李俊璋老師。在我碩士班初期主要的合作對象便是李俊璋老師，他帶領我認識 Poisson–Boltzmann (PB) 方程與非局部非線性的相關問題，而在這段期間尤其需要感謝同時期的同儕們，如耿弘、亦行、旻哲、欣修、秉軒、舜傑、簡鴻宇學長、陳世昕學長等人。在碩士班畢業後，我決定留在台大攻讀博士班。而在三年級時則遭逢太家老師罹患重大疾病，此時的學長們也基於年限與生涯的考量紛紛更換指導教授。我仍基於研究興趣，還是選擇繼續跟隨太家老師，而李俊璋老師則在其中先協助我從事一項先導的工作（第四章）。特別是在完成主要工作後，我們向身體已好轉的林太家老師報告這項工作時，他便提出一項極有意思的問題而使我發在某一部分的內容進行更深入的思考而得到突破性的分析結果。

此時我已經進入博士班的後半段，四年級下半時我與林太家老師開始進行 PB-steric 方程式的推導與建模（第二章）。在這項工作結束後，我們便針對所推導出的模型進行邊界層理論的分析。在太家老師的介紹與推薦下，我於六至七年級期間便前往美國伊利諾理工學院訪問 Chun Liu 教授，Chun Liu 教授的著作豐富，亦對 PB 方程理論結合相關物理律而進行模型推導有深入的看法。在這期間除了特別感謝 Chun Liu 教授外亦感謝陳祁安學弟在芝加哥生活上的各種協助。

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返臺後，我希望能在畢業後立刻就業，因此休學當兵並逐步修改論文投稿。在這期間我遇到相當棒的同袍柏鈞、政榕、育豪、冠鈞、佑嘉、昭維、志函、煒琪、庭維、奕信與濬智，而待在退除役官兵輔導委員會擔任替代役，我特別感謝退輔會的就學就業處所給予的環境，讓我在處理公務之餘能夠靜下心來修改論文從事研究。 在這樣的服役期間，我持續改進本博士論文第三章的內容，而在 2025 年初得到一項創新的成果。而這項突破性成果也特別需要感謝太家老師不斷地提出具有挑戰性的疑問，而在消化理解這些疑問時最終將謎題解開。

對於第三章中，我們爲了研究邊界層而需要使用到一些微分幾何學的技巧與概念，在此要特別感謝耿弘與退休教授黃武雄老師。他們不厭其煩且深入淺出的說明了許多微分幾何中的重要技巧，讓我能在第三章的研究中靈活的使用適當的坐標系處理問題，而讓文章更加簡潔而完整。後來黃武雄老師也邀請我協助編排他所著的《大域微分幾何》，在協助編排與出版的過程中也向黃武雄老師請教其中的內容使我獲益良多。

除了在研究過程中的夥伴們，我也有很多生命中需要值得感謝的人。首先是各路朋友，如經常與我討論複雜數學問題的林浩誼、從 Yahoo 奇摩知識 + 認識的王國鑫、一起討論怪人的涂景婷、分享各類生活駭客級知識的王冠倫、修課時認識的公務員蔡承珈、介紹多益檢定應用程式「刷刷庫」給我的丁婉茜。也要感謝每年固定聚會的高中同學們馮韋綸、楊自文、蔡雨恩、陳俊輔等人。感謝台大的社團如手搖飲料社張嘉家、蛋糕社社長籃予彤與賴芊予、研究生協會會長周芷萱與于閔如兩人則帶領我對校內政治與學術政治有了更多的認識。也要感謝台大交流版的眾管理員們莊孝穎、盧姳儒、黃政凱、黃冠霖等人。再者，我也要感謝我的家教學生們讓我的教學技巧更加純熟豐富並擴展了我的視野，特別感謝台大的林昀萱與許馨文、師大的曾子芸與陳律翰、國北教的王虹萱、陽明的郭子綾、淡江的謝欣妤與李瑜、巴黎索邦的游垚騰等人。也要感謝經常舉辦桌遊活動的唐啓荼、黃雅雅等人，讓我在煩悶的生活中可以轉換心情。

最後我最需要感謝的是我的父母與家人們，他們在我求學的過程中無條件的支持與付出讓我基本上無後顧之憂。特別是協助我在台北安家，免除長期的租房困擾。也要感謝一直走路陪伴我解決許多困難的靖雯，沒有她的幫忙，我幾乎絕大多數的問題都會懸而未決，感謝的心情實在無法窮盡。需要感謝的人還有很多，但空間總是有限，就讓這些感激之情帶在心中，繼續向未來努力，不愧對國家社會家庭與老師對我的期許。

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中文摘要 Abstract in Chinese

帕松波茲曼方程式可被用於描述電解質液的離子濃度分布情形，從而在生物化學與電化學領域中有諸多重要的應用，在細胞膜上的離子通道便是一重要例子。然而傳統的帕松波茲曼方程式視離子爲質點而不帶有體積，而離子通過狹窄的離子通道時便有不可忽略的體積效應。在既有的文獻中已經有許多將體積效應納入考量的模型，但這些模型均無法描述如密度泛函理論中所產生的非單調總電荷密度的現象，這就啓發我們去推導更一般的帕松波茲曼模型。這樣的模型不僅涵蓋傳統與修正後的帕松波茲曼模型，也能產生具非單調總電荷密度的方程式。

更進一步地，由於離子通道的複雜幾何結構，我們研究一般光滑區域上的帕松波茲曼類方程隨介電常數趨於零時所產生的邊界解。此處帕松波茲曼類方程包含了傳統、修正後與電中性條件下的電荷守恆帕松波茲曼模型。源於電荷守恆條件下的非局部非線性項使得離子守恆的帕松波茲曼模型的分析更加困難，其結果也有別於傳統與修正後的帕松波茲曼模型。透過主軸坐標系統、指數型估計與移動平面法，我們嚴格地證明了邊界層解的二階漸近展開式，其中包含了均曲率項。進一步地，我們也計算出許多關鍵的物理量的漸近展開式，這包括了電位、電場、總電荷密度與總電荷，而這些物理量也揭示了區域幾何的影響。

相較於前段所研究的電荷守恆帕松波茲曼模型爲電中性條件，其電位保持均勻有界性。而對於非電中性條件下，電位便會隨著介電常數趨於零時而產生爆破現象。對於最極端的非電中性條件，我們研究一維上帶單粒子的電荷守恆帕松波茲曼模型。透過適當的平移假設下，我們將問題轉爲邊界爆破問題。藉由解的表達式，我們研究了近場與遠場展開從而完整的刻畫了靠近邊界區域的解的所有漸近行爲，也證明了總電荷密度的邊界集中性。另一方面，我們研究了雙離子的電荷守恆帕松波茲曼模型的差異。形式上來看，當雙離子模型中的其中一粒子總濃度相當小時便會趨近單離子模型，而我們給出一充分條件去證明這樣的猜測成立。

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英文摘要 Abstract in English

The Poisson–Boltzmann (PB) equation serves as a fundamental model for describing ionic concentration distributions in electrolyte solutions, with significant applications in both biochemical and electrochemical fields. One prominent example arises in the study of ion channels on cellular membranes. However, the classical PB equation treats ions as point particles without volume, which becomes inadequate when ions pass through narrow channels so the steric effect should not be negligible. Although several modified models incorporating steric effects have been proposed in the literature, they cannot capture the non-monotonic behavior of total ionic charge density observed in density functional theory. This motivates us to derive a more general Poisson–Boltzmann framework that not only includes the classical and modified PB models, but also includes the model that has non-monotonic total ionic charge density.

Further, motivated by the complex geometry of ion channels, we investigate the boundary layer behavior of Poisson–Boltzmann type equations as the dielectric constant tends to zero in general smooth domains. Here the PB type equations include the classical PB, modified PB, and charge-conserving PB models with the electroneutrality condition. Due to the presence of nonlocal nonlinear terms arising from the charge conservation, the analysis of charge-conserving PB models presents the analytical challenges and leads to different behaviors compared to that of other models. By employing principal coordinate systems, exponential-type estimates, and the moving plane arguments, we rigorously derive second-order asymptotic expansions of boundary layer solutions, incorporating curvature-dependent terms. We also compute asymptotic expansions for several key physical quantities, including the electrostatic potential, electric field, total charge density, and total charge, thereby revealing the influence of domain geometry on the ionic distributions.

In contrast to the electroneutral regime, where the electrostatic potential remains uniformly bounded, the potential exhibits blow-up behavior under non-electroneutral conditions as the dielectric constant tends to zero. To explore this extreme case, we examine the one-dimensional charge-conserving PB model with a single species. Under an appropriate shift assumption, we reformulate the problem as a boundary

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blow-up problem. Thanks to the explicit solution representation, we can analyze both near-field and far-field expansions and hence provide a complete characterization of the asymptotic behavior near the boundary. In addition, we rigorously establish the boundary concentration phenomenon of the total ionic charge density. On the other hand, we also investigate the differences arising in charge-conserving PB models with two ionic species. Formally, such two-species model would approach to the single-species model when the total concentration of one ions species becomes sufficiently small. We provide a sufficient condition to justify this conjecture.

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1 Introduction

The Poisson–Boltzmann (PB) equation arises as a central model in electrostatics for describing ionic distributions in electrolytes, particularly in biophysics and materials science (cf. [6,23,29,99]). It plays a crucial role in the study of charged interfaces in electrodes, colloidal science, and biological membranes (cf. [3,17,22,24,27,62,114, 115]). In this thesis, we shall investigate various extensions and analytical aspects of the PB equation in the presence of steric effect and boundary layer structure.

In Chapter 2, we introduce the classical and several modified PB equations, which all can be represented as in the following form (cf. [9,11,12,33,43,69,80,82,88,90]):

$$-\nabla\cdot(\varepsilon\nabla\phi)=\rho_0+f(\phi):=\rho_0+\sum_{i=1}^{I}z_ic_i(\phi).$$

Here ϕ denotes the electrostatic potential, ρ_0 is the permanent charge, f is the total ionic charge density, and ε is the dielectric constant. In addition, I is the number of ion species, c_i is the ith concentration and z_i is its valence for $i=1,\ldots,I$. However, duo to simulations based on density functional theory (cf. [39,60,95,111]), the total ionic charge density f could be oscillatory while ionic charge density f of classical and modified PB equations must be strictly decreasing. This inspires us to derive a general PB model, called the PB-steric equations, which not only include classical and modified PB equations but also produce oscillatory charge density.

To obtain the PB-steric equations, we consider to empoly the Lennard-Jones (LJ) potential, which is a well-known model for the interaction between a pair of ions (and solvent molecules) and is usually used in the density functional theory and molecular dynamics simulation. Due to the strong singularity from the repulsive part of the LJ potential, we replace it by the approximated LJ potential to describe the steric repulsion of ions and solvent moleculus and get the following PB-steric equations:

$$\begin{aligned}&-\nabla\cdot(\varepsilon\nabla\phi_\Lambda)=\rho_0+\sum_{i=1}^{I}z_ic_{i,\Lambda},\\&\ln(c_{i,\Lambda})+z_i\phi_\Lambda+\Lambda\sum_{j=0}^{I}g_{ij}c_{j,\Lambda}=\mu_i:=\Lambda\tilde{\mu}_i+\hat{\mu}_i\quad\text{for } i=0,1,\ldots,I,\end{aligned}$$

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where $c_{0,\Lambda}$ is the concentration of solvent molecules, $c_{i,\Lambda}$ is the concentration of ith ion species, and $\Lambda g_{ij} \geq 0$ represents the strength of steric repulsion between the ith and jth ions (or solvent molecules). The parameter Λ comes from the approximated LJ potential. In [84], Lin and Eisenberg showed the approximated LJ potential tends to LJ potential in some sense when Λ goes to infinity. Hence it is natural to expect that the PB-steric equations will approach modified PB equations as Λ goes to infinity. Under suitable assumptions on g_{ij} and $\tilde{\mu}_i$, we prove that ϕ_Λ converges to the solution ϕ^* to the modified PB equations in $\mathcal{C}^m(\overline{\Omega})$ for $m \in \mathbb{N}$ (cf. Theorems 2.1 and 2.2). On the other hand, we also propose a concrete assumption on g_{ij} and $\tilde{\mu}_i$ to obtain oscillatory total ionic charge density (see Remark 2.4). Therefore, the PB-steric equations can be regarded as a general model of PB equations.

Under suitable assumptions on g_{ij} and $\tilde{\mu}_i$, we can obtain the concentration $c_{i,\Lambda}(\phi)$, which is determined by the Lambert type functions. Moreover, we study the properties of the total ionic charge density $f_\Lambda(\phi) = \sum_{i=1}^{I} z_i c_{i,\Lambda}(\phi)$. As Λ goes to infinity, it is not hard to show $c_{i,\Lambda}$ and f_Λ converge to c_i^* and f^* in $\mathcal{C}^m([a,b])$ for $m \in \mathbb{N}$ and $a < b$, respectively. Note that f_Λ is unbounded on $\mathbb{R}$ while f^* is bounded on $\mathbb{R}$ so we cannot obtain the uniform convergence of f_Λ on $\mathbb{R}$ as Λ goes to infinity. Hence it is crucial to establish the uniform boundedness of the solution ϕ_Λ with respect to Λ. Such uniform boundedness cannot simply be obtained by maximum principle under the Robin boundary condition, which leads to a difficutly in analysis.

In Chapter 3, we study the boundary layer solutions to PB type equations in general bounded smooth domains (including multiply connected domains). Here PB type equations include classical, modified and charge-conserving PB (CCPB) equations. The classical PB and modified PB equations can be represented by

$$-\varepsilon\Delta\phi_\varepsilon = f(\phi_\varepsilon) \quad \text{in } \Omega,$$

where the dielectric constant $\varepsilon > 0$ is assumed to be independent of spatial variable and ϕ_ε is the electric potential. Here f is a smooth function for the total ionic charge density which satisfies the following conditions

(F1) The function $f = f(\phi)$ is smooth, strictly decreasing in ϕ, and satisfies

$$m_f = m_f(\mathcal{K}) := \sqrt{-\max_{\phi\in\mathcal{K}} f'(\phi)} > 0 \quad \text{for any compact interval } \mathcal{K} \subseteq \mathbb{R}.$$

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(F2) The function f has a unique zero point ϕ^*, i.e., $f(\phi^*) = 0$, where ϕ^* is called as reference potential (cf. [4,41]).

For instance, function $f(\phi) = \sum_{i=1}^{I} z_i c_i^{\mathrm{b}} \exp(-z_i\phi)$ describes the total ionic charge density of the classical PB equation, and satisfies (F1)–(F2), where I is the number of ion species, $z_i \neq 0$ is the valence and c_i^{b} is the concentration of the ith species in the bulk (cf. [33,69]). On the other hand, the CCPB equation can be denoted as

$$-\varepsilon\Delta\phi_\varepsilon = \sum_{i=1}^{I} \frac{m_i z_i \exp(-z_i\phi_\varepsilon)}{\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y} \quad \text{in } \Omega,$$

where $m_i > 0$ and z_i are the total concentration and the valence of ith ion species (cf. [34,70,73,105,112]) for $i = 1, \ldots, I$. For the CCPB equation, we assume the electroneualtiry condition holds, i.e.,

$$\sum_{i=1}^{I} m_i z_i = 0.$$

Due to the integral term $\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y$, the CCPB equation has nonlocal nonlinearity, which makes it more difficult than classical and modified PB equations. Note that the CCPB equation can be written as $-\varepsilon\Delta\phi_\varepsilon = f_\varepsilon(\phi_\varepsilon) := \sum_{i=1}^{I} z_i c_{i,\varepsilon}^{\mathrm{b}} \exp(-z_i\phi_\varepsilon)$ in Ω, which has the same form as the classical PB equation. Here $f_\varepsilon(\phi) = \sum_{i=1}^{I} z_i c_{i,\varepsilon}^{\mathrm{b}} \exp(-z_i\phi)$ presents the total ionic charge density and $c_{i,\varepsilon}^{\mathrm{b}} = m_i / \left(\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y\right)$ is the concentration of the ith ion species in the bulk.

For the general bounded smooth domain $\Omega \subseteq \mathbb{R}^d$ ($d \geq 2$), we consider the following assumption.

(D) $\Omega = \Omega_0 - \bigcup_{k=1}^{K} \Omega_k$, $K \in \mathbb{N} \cup \{0\}$ (the number of holes) and Ω_k are bounded, smooth, simply connected domains with $\Omega_k \subset\subset \Omega_0$ for $k \in \{1, \ldots, K\}$ and $\mathrm{dist}(\Omega_i, \Omega_j) > 0$ for $i, j \in \{1, \ldots, K\}$ and $i \neq j$. Here dist denotes the distance.

The boundary condition of PB type equations is the Robin boundary condition given by

$$\phi_\varepsilon + \gamma_k\sqrt{\varepsilon}\partial_\nu\phi_\varepsilon = \phi_{bd,k} \quad \text{on } \partial\Omega_k \text{ for } k = 0, 1, \ldots, K,$$

where $\phi_{bd,k}$ is a constant for the given external electric potential, and $\gamma_k > 0$ is the ratio of Stern-layer width to the Debye screening length (cf. [8,18,96,100]).

To study the singularly perturbation problems of PB type equations with the Robin boundary condition, we assume $\varepsilon > 0$ (related to the Debye length) as a small

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parameter tending to zero (cf. [7, 31, 37, 61, 94]). We characterize the asymptotic expansions of solution ϕ_ε across three distinct regions based on their distance from the boundary (cf. Theorems 3.1 and 3.2):

- Region I, where the distance from the boundary is at most $T\sqrt{\varepsilon}$,
- Region II, where the distance ranges between $T\sqrt{\varepsilon}$ and ε^β,
- Region III, where the distance is at least ε^β,

for given parameters $T > 0$ and $0 < \beta < 1/2$. In region I, we derive second-order asymptotic formulas explicitly incorporating the effect of boundary mean curvature while expoential decay estimate are established for Regions II and III. Furthermore, we obtain the asymptotic expnasions for several crucial physical quantites, including the electric potential, electric field, total ionic charge density and total ionic charge, revealing how domain geometry regulates electrostatic interactions. Based on the total ionic charge across three distinct regions, we find that the marjority of charged particles concentrate within the region I whose volume is smaller than Region II as ε goes to zero. In addition, the toal ionic charge in Region III decays exponentially as ε tends to zero, which demostrates the emergence of electroneutrality in the bulk region.

To rigorously prove the asymptotic expansions of PB type equations, we establish the uniform boundedness of the solution ϕ_ε and then employ the principal coordinate system to get the local convergence in $\mathbb{R}^d_+$. Using the expoential-type estimate and the moving plane arguments, we derive the second-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$. However, unlike the case of classical and modified PB equations, the unique zero ϕ_ε^* of total ionic charge density f_ε may depend on the parameter ε, which presents particular analytical challenges from its nonlocal nonlinearity term. We use the electroneutrality condition to prove, by contradiction, the uniform boundedness of $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon}$, where ϕ_0^* is the limit of ϕ_ε^* as ε goes to zero. Based on the uniform boundedness of $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon}$, we are able to derive the second order term of $\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y$, f_ε, and ϕ_ε, which shows the nonlocal effect appears in the second-order asymptotic expansion of the solution to the CCPB equation.

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In Chapter 4, we pay a particular attention on the one-dimensional CCPB equation with single species, which can be represented as

$$-u_\lambda''(r) = \rho_\lambda(r) := \frac{\lambda e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} \quad \text{for } r \in (0,1).$$

Clearly, the electroneutrality condition cannot not hold on the interval $(0,1)$. To understand the non-electroneutral phenomenon near the charged surface, $\lambda(= 1/\varepsilon)$ is assumed a large positive parameter corresponding to the number of ions occupying an electrolytic region. Due to the shift invariance of the CCPB equation with single species, we impose the following condition at $r = 0$:

$$u_\lambda(0) = u_\lambda'(0) = 0,$$

which immediately implies

$$u_\lambda'(1) = -\lambda \to -\infty.$$

Then by mean value theorem, there exists an interior point $r_{\text{int}}^\lambda \in (0,1)$ depending on λ such that when $\lambda \to \infty$, the net charge density $\rho_\lambda(r_{\text{int}}^\lambda) = \lambda$ asymptotically blows up. Such a phenomenon occurs only when the interior point r_{int}^λ is sufficiently close to the boundary point $r = 1$ as λ tends to infinity.

To clarify the boundary structure of the CCPB equation with single species, we study the near- and far-field expansions. The near-field expansion focuses on the refined asymptotics of $u_\lambda(r_{p,\alpha}^\lambda)$ and $u_\lambda'(r_{p,\alpha}^\lambda)$, where α and p are positive constants independent of λ and

$$r_{p,\alpha}^\lambda = 1 - \frac{p}{\lambda^\alpha} \in (0,1) \qquad (\lambda \gg 1)$$

is sufficiently close to the boundary point $r = 1$. The far-field expansion focuses on the refined asymptotics for u_λ in $\mathcal{C}^1(K)$ as $\lambda \to \infty$, where K (independent of λ) is a compact subset of $[0,1)$ (cf. [44, 45]). We prove that the solution asymptotically blows up in a thin region attached to the boundary and establishes the refined near- and far-field expansions in Theorems 4.2 and 4.3. Moreover, we obtain the boundary concentration phenomenon of the net charge density, which mathematically confirms the physical description that the non-neutral phenomenon occurs near the charge surface Corollary 4.1.

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Moreover, we develope a novel comparison with the CCPB equation for monovalent binary ions, which is represented as

$$v''_{\mu,\lambda}(r) = \frac{\mu e^{v_{\mu,\lambda}(r)}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\,\mathrm{d}s} - \frac{\lambda e^{-v_{\mu,\lambda}(r)}}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\,\mathrm{d}s} \quad \text{for } r \in (0,1),$$

with the same boundary condition of u_λ:

$$v_{\mu,\lambda}(0) = v'_{\mu,\lambda}(0) = 0.$$

Here μ and λ are positive parameters related to the total number of anions and cations, respectively. When $\mu = \lambda$, the electroneutrality condition holds and $v_{\mu,\lambda} \equiv 0$, which is a trivial solution. For the case that $0 < \mu \ll \lambda$, i.e., the total number of cations is great larger than that of anions, it seems that $v_{\mu,\lambda}$ approaches u_λ. However, the asymptotic beahvior of those nonlocal terms are unknown, it is not clear that $0 < \mu \ll \lambda$ implies $\frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\,\mathrm{d}s} \ll \frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\,\mathrm{d}s}$. Hence a question is naturally raised: What does the relation between μ and λ make

$$\lim_{\lambda\to\infty} \|v_{\mu,\lambda} - u_\lambda\|_{\mathcal{C}^1([0,1])} = 0$$

holds? Here $\|\cdot\|_{\mathcal{C}^1([0,1])}$ is the standard $\mathcal{C}^1$-norm over the interval $[0,1]$. We prove the $\mathcal{C}^1$-convergence under the assumption $\lim\limits_{\lambda\to\infty} \mu\lambda = 0$ (cf. Theorem 4.1) and show the relation between $v_{\mu,\lambda}$ and u_λ as below.

$$v_{\mu,\lambda} \xrightarrow[\lambda \text{ fixed and } \mu\to 0]{\text{(uniformly)}} u_\lambda \xrightarrow[\lambda\to\infty]{\text{(pointwise)}} U := \lim_{\lambda\to\infty} u_\lambda$$

$$v_{\mu,\lambda} - u_\lambda \xrightarrow[\lambda\to\infty \text{ and } \mu\lambda\to 0]{\text{(uniformly)}} 0$$

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2 PB-steric equations: A general model of Poisson–Boltzmann equations[1]

2.1 Introduction

Understanding the distribution of ions in the electrolyte is one of the most crucial problems in many physical and electrochemical fields. As a well-known mathematical model, the Poisson–Boltzmann (PB) equations play a central role in the study of ionic distribution. The classical PB equations [69, 87] treat ions as point particles without size and can be denoted as

$$-\nabla \cdot (\varepsilon \nabla \phi) = 4\pi\rho_0 + 4\pi \sum_{i=1}^{I} z_i e_0 c_i(\phi), \tag{2.1}$$

$$k_B T \ln(c_i) + z_i e_0 \phi = \mu_i \quad \text{for } i = 1, \dots, I, \tag{2.2}$$

where ϕ is the electrostatic potential, ε is the dilelectric function, and ρ_0 is the permanent charge density function. In addition, I is the number of ion species, c_i is the concentration of ith ion species with the valence $z_i \neq 0$ for $i = 1, \dots, I$. Moreover, $c_i = c_i^{\mathrm{b}} \exp(-z_i e_0 \phi / k_B T)$, where c_i^{b} is the concentration of the ith ion species in the bulk, k_B is the Boltzmann constant, T is the absolute temperature, e_0 is the elementary charge, and $\mu_i = k_B T \ln(c_i^{\mathrm{b}})$ is the chemical potential. However, when ions are crowded, steric repulsions may appear due to ion sizes, so the classical PB equations should be modified [25, 26, 65, 66].

Under the hypothesis of volume exclusion, one may study the case of two-species ions with the same radius and obtain the following modified PB equations (cf. [9, 10, 12, 58]):

$$-\nabla \cdot (\varepsilon \nabla \phi) = 4\pi(z_1 e_0 c_1 + z_2 e_0 c_2), \tag{2.3}$$

$$c_i = c_i^{\mathrm{b}} \frac{e^{-z_i e_0 \phi / k_B T}}{1 - \gamma + \frac{\gamma}{z_1 - z_2}\left(c_1^{\mathrm{b}} e^{-z_1 e_0 \phi / k_B T} + c_2^{\mathrm{b}} e^{-z_2 e_0 \phi / k_B T}\right)}, \tag{2.4}$$

[1]This chapter is adapted from an article co-authored with my advisor, Professor Tai-Chia Lin, and published in [90]. In this work, my main contributions include providing the rigorous mathematical proofs, producing the numerical figures, and constructing the oscillatory total ionic charge density.

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for $i = 1, 2$, where γ is the total bulk volume fraction of ions, and $z_1 > 0$ and $z_2 < 0$ are the valence of cations and anions, respectively. Moreover, the concentrations of ion species in bulk are given by $c_1^{\mathrm{b}} = -z_2$ and $c_2^{\mathrm{b}} = z_1$. For the background and development of (2.3)–(2.4), we refer the interested reader to [43, 67]. Furthermore, when ions and solvent molecules may have different sizes, the associated PB equations become

$$-\nabla \cdot (\varepsilon \nabla \phi) = 4\pi \rho_0 + 4\pi \sum_{i=1}^{I} z_i e_0 c_i(\phi), \tag{2.5}$$

$$k_B T \ln(c_i) - k_B T \frac{v_i}{v_0} \ln(c_0) + z_i e_0 \phi = \bar{\mu}_i \quad \text{for } i = 1, \ldots, I, \tag{2.6}$$

$$\sum_{i=0}^{I} v_i c_i = 1, \tag{2.7}$$

where $c_0 = \frac{1}{v_0}\left(1 - \sum_{i=1}^{I} v_i c_i\right)$ is the concentration of solvent molecules with the volume v_0 and the valence $z_0 = 0$, v_i is the volume of ith ion species, and $\bar{\mu}_i$ is the associated chemical potential for $i = 1, \ldots, I$ (cf. [80–82, 88]). Equations (2.1)–(2.7) can be denoted as

$$-\nabla \cdot (\varepsilon \nabla \phi) = 4\pi \rho_0 + 4\pi \sum_{i=1}^{I} z_i e_0 c_i, \tag{2.8}$$

$$\mu_i = k_B T \ln(c_i) + z_i e_0 \phi + \mu_i^{\mathrm{ex}} + U_i^{\mathrm{wall}} \quad \text{for } i = 0, 1, \ldots, I, \tag{2.9}$$

with different μ_i and μ_i^{ex}, where μ_i is the chemical potential, μ_i^{ex} is the excess chemical potential which describes the interaction potential of ions and solvent molecules. Besides, U_i^{wall} is the potential which comes from the interactions of ions and solvent molecules with the wall. Under $U_i^{\mathrm{wall}} = 0$ and conditions of μ_i and μ_i^{ex}, equations (2.8)–(2.9) become the following equations.

- (2.1)–(2.2) if $\mu_i = k_B T \ln(c_i^{\mathrm{b}})$ and $\mu_i^{\mathrm{ex}} = 0$ for $i = 1, \ldots, I$.
- (2.3)–(2.4) if $\mu_i = k_B T \ln(c_i^{\mathrm{b}})$ and

  $$\mu_i^{\mathrm{ex}} = k_B T \ln\left(1 - \gamma + \frac{\gamma}{z_1 - z_2}(c_1^{\mathrm{b}} e^{-z_1 e_0 \phi / k_B T} + c_2^{\mathrm{b}} e^{-z_2 e_0 \phi / k_B T})\right)$$

  for $i = 1, 2$.
- (2.5)–(2.7) if $\mu_i = \bar{\mu}_i$ and $\mu_i^{\mathrm{ex}} = -k_B T \frac{v_i}{v_0} \ln(c_0)$ for $i = 1, \ldots, I$, where $c_0 = \frac{1}{v_0}\left(1 - \sum_{i=1}^{I} v_i c_i\right)$.

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The steric interactions of ions can produce oscillations in concentration (density) profiles but such oscillations cannot be obtained by equations (2.1)–(2.4) (cf. [39, 60, 95, 111]). In [117], the oscillatory concentrations can be found in equations (2.5)–(2.7) so it is natural to ask if there exists oscillatory total ionic charge density. However, the total ionic charge density $\sum_{i=1}^{I} z_i c_i(\phi)$ of equations (2.1)–(2.7) is decreasing to ϕ (see [82] and Propositions 2.6 and 2.10 below). This motivates us to derive a general model of PB equations, called the Poisson–Boltzmann equations with steric effects (PB-steric equations), which not only include equations (2.1)–(2.7) but also have oscillatory total ionic charge density $\sum_{i=1}^{I} z_i c_i(\phi)$ under different assumptions of steric effects and chemical potentials.

To get the PB-steric equations, we consider to use the Lennard-Jones (LJ) potential which is a well-known model for the interaction between a pair of ions (and solvent molecules) and is important in the density functional theory and molecular dynamics simulation (cf. [5, 64, 72, 79, 101]). We set the energy functional $\iint_{\mathbb{R}^d} \psi(x-y) c_i(x) c_j(y)\,\mathrm{d}x\,\mathrm{d}y$ to describe the energy of steric repulsion of c_i and c_j for $i, j = 0, 1, \ldots, I$. Here $\psi(z) = |z|^{-12}$ comes from the repulsive part of LJ potential with strong singularity at the origin which makes the energy functional $\iint_{\mathbb{R}^d} \psi(x-y) c_i(x) c_j(y)\,\mathrm{d}x\,\mathrm{d}y$ hard to study. Hence we replace the LJ potential by the approximate LJ potentials (cf. [50, 84]) to describe the steric repulsion of ions and solvent molecules and we obtain the following PB-steric equations:

$$-\nabla \cdot (\varepsilon \nabla \phi) = 4\pi \rho_0 + 4\pi \sum_{i=1}^{I} z_i e_0 c_i, \tag{2.10}$$

$$k_B T \ln(c_i) + z_i e_0 \phi + \Lambda \sum_{j=0}^{I} g_{ij} c_j = \Lambda \tilde{\mu}_i + \hat{\mu}_i \quad \text{for } i = 0, 1, \ldots, I, \tag{2.11}$$

where c_0 is the concentration of solvent molecules, c_i is the concentration of ith ion species, and $\Lambda g_{ij} \geq 0$ represents the strength of steric repulsion between the ith and jth ions (or solvent molecules). One may see Appendix 2A for the derivation of (2.10)–(2.11) when matrix (g_{ij}) is symmetric.

In this chapter, we generalize (2.10)–(2.11) to all matrices (g_{ij}) (which may include nonsymmetric matrices) such that (2.11) has a unique solution $c_i = c_i(\phi)$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$. The nonsymmetry of matrix (g_{ij}) may come from the potential U_i^{wall} which describes how the ions and solvent molecules interact with

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the wall. Note that (2.10)–(2.11) can be expressed by (2.8)–(2.9) with the chemical potential $\mu_i = \Lambda\tilde{\mu}_i + \hat{\mu}_i$ and the excess chemical potential μ_i^{ex} and the potential U_i^{wall} satisfying $\mu_i^{\text{ex}} + U_i^{\text{wall}} = \Lambda \sum_{j=0}^{I} g_{ij} c_j$ for $i = 0, 1, \ldots, I$. For the sake of simplify, we set $k_B T = e_0 = 1$ and write $4\pi\varepsilon$ instead of ε so (2.10)–(2.11) become

$$-\nabla \cdot (\varepsilon \nabla \phi) = \rho_0 + \sum_{i=1}^{I} z_i c_i \quad \text{in } \Omega, \tag{2.12}$$

$$\ln(c_i) + z_i \phi + \Lambda \sum_{j=0}^{I} g_{ij} c_j = \Lambda\tilde{\mu}_i + \hat{\mu}_i \quad \text{for } i = 0, 1, \ldots, I, \tag{2.13}$$

where Ω is a bounded smooth domain in $\mathbb{R}^d$ $(d \geq 2)$. Under suitable conditions of g_{ij} such that system (2.13) has a unique solution $c_i = c_i(\phi)$ (which may depend on parameter Λ) for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$, equation (2.12) becomes a nonlinear elliptic equation

$$-\nabla \cdot (\varepsilon \nabla \phi) = \rho_0 + \sum_{i=1}^{I} z_i c_i(\phi) \quad \text{in } \Omega. \tag{2.14}$$

Then for all possible $g_{ij} \geq 0$, equation (2.14) and its limiting equation (as $\Lambda \to \infty$) are called as the PB-steric equations. Hereafter, the boundary condition of (2.14) is considered as the Robin boundary condition

$$\phi + \eta \frac{\partial \phi}{\partial \nu} = \phi_{bd} \quad \text{on } \partial\Omega, \tag{2.15}$$

where $\phi_{bd} \in \mathcal{C}^\infty(\partial\Omega)$ is the extra electrostatic potential and $\eta \geq 0$ is a constant related to the surface dielectric constant (cf. [8, 94, 116]).

The strength of steric effect is determined by Λg_{ij}'s in the PB-steric equations (2.13)–(2.14). As $\Lambda = 0$ (or $g_{ij} = 0$), (2.13) has the same form as (2.2) and the PB-steric equations (2.13)–(2.14) become the classical PB equations (2.1)–(2.2). On the other hand, when g_{ij}'s are positive constants, a larger Λ produces stronger steric repulsion. This motivates us to expect that as Λ tends to infinity, the steric repulsion becomes extremely strong so that volume exclusion holds true and ions can be described by the lattice gas model as for the mean-field approximation of the modified PB equations (2.3)–(2.4) (cf. [12, 43]). To justify this, we prove that as $\Lambda \to \infty$, the PB-steric equations (2.13)–(2.14) may approach to the modified PB equations (2.3)–(2.4) (see Theorem 2.1 and Remark 2.1). Moreover, we prove that as $\Lambda \to \infty$, the PB-steric equations (2.13)–(2.14) may approach to the modified PB equations (2.5)–(2.7) (see Theorem 2.2 and Remark 2.5).

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In order to obtain equations (2.3)–(2.4), we need the assumptions of steric effects (g_{ij}) and chemical potentials ($\tilde{\mu}_i$) given by

(A1) $g_{i0} = g_{00} = 1 - \gamma$ and $g_{ij} = g_{0j} = \gamma/Z$ for $i, j = 1, \ldots, I$,

(A2) $\tilde{\mu}_i = \tilde{\mu}_0$ for $i = 1, \ldots, I$,

where $0 \le \gamma \le 1$, $\tilde{\mu}_0 > 0$, $\hat{\mu}_0$ (in (2.13)) and $Z = \sum_{i=1}^{I} |z_i|$ are constants independent of Λ. Then by (A1) and (A2), system (2.13) has a unique solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$, which satisfies

$$c_{i,\Lambda} = c_{0,\Lambda} e^{\bar{\mu}_i - z_i \phi} \quad \text{for } \phi \in \mathbb{R} \text{ and } i = 1, \ldots, I, \tag{2.16}$$

$$\ln(c_{0,\Lambda}) + \Lambda H(\gamma, z_1, \ldots, z_I, \phi) c_{0,\Lambda} = \Lambda \tilde{\mu}_0 + \hat{\mu}_0 \quad \text{for } \phi \in \mathbb{R}, \tag{2.17}$$

$$H(\gamma, z_1, \ldots, z_I, \phi) = 1 - \gamma + \frac{\gamma}{Z} \sum_{j=1}^{I} e^{\bar{\mu}_j - z_j \phi}, \tag{2.18}$$

where $\bar{\mu}_i = \hat{\mu}_i - \hat{\mu}_0$ is a constant independent of Λ for $i = 1, \ldots, I$. Note that (2.17) can be solved in terms of the principal branch of Lambert W function (cf. [93]), which implies that $c_{i,\Lambda}$ are positive smooth functions for $i = 0, 1, \ldots, I$ (see Proposition 2.1). Recall that the Lambert W function $W_0(x)$ can be defined by $W_0(x) e^{W_0(x)} = x$ for all $x \ge e^{-1}$, and the range of $W_0(x)$ is $[-1, \infty)$. Hence the PB-steric equation (2.14) can be expressed as

$$-\nabla \cdot (\varepsilon \nabla \phi_\Lambda) = \rho_0 + f_\Lambda(\phi_\Lambda) \quad \text{in } \Omega, \tag{2.19}$$

where function $f_\Lambda = f_\Lambda(\phi)$ is denoted as

$$f_\Lambda(\phi) = \sum_{i=1}^{I} z_i c_{i,\Lambda}(\phi) \quad \text{for } \phi \in \mathbb{R}. \tag{2.20}$$

By the standard method of a nonlinear elliptic equation, we may obtain the existence and uniqueness of (2.19) with the Robin boundary condition (2.15).

Using the implicit function theorem on Banach spaces (cf. [21, Theorem 15.1]), we prove that $c_{i,\Lambda}$ converges to c_i^* in space $\mathcal{C}^m[a,b]$ as Λ tends to infinity for $m \in \mathbb{N}$ and $a < b$, where c_i^* satisfies

$$c_i^*(\phi) = \frac{\tilde{\mu}_0 e^{\bar{\mu}_i - z_i \phi}}{H(\gamma, z_1, \ldots, z_I, \phi)} \quad \text{for } \phi \in \mathbb{R} \text{ and } i = 0, 1, \ldots, I. \tag{2.21}$$

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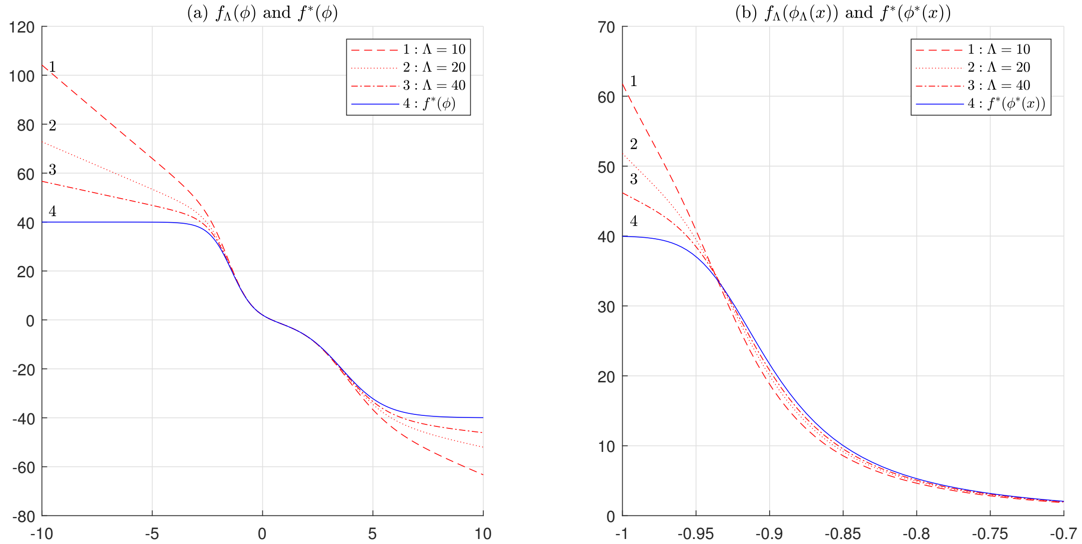

Figure 2.1: The profiles of $f_\Lambda(\phi)$ and $f_\Lambda(\phi_\Lambda(x))$ and their limiting functions under assumptions (A1)–(A2). In (a), curves 1–3 are profiles of function f_Λ (defined in (2.20)) with $\Lambda = 10,\ 20,\ 40$, and curve 4 is the profile of function f^* (defined in (2.22)). In (b), curves 1–3 are the profiles of function $f_\Lambda \circ \phi_\Lambda$ with $\Lambda = 10,\ 20,\ 40$, and curve 4 is the profile of function $f^* \circ \phi^*$.

Thus function f_Λ also converges to f^* in space $\mathcal{C}^m[a, b]$ as Λ goes to infinity for $m \in \mathbb{N}$ and $a < b$, where

$$f^*(\phi) = \sum_{i=1}^{I} z_i c_i^*(\phi) \quad \text{for } \phi \in \mathbb{R} \tag{2.22}$$

(see Corollary 2.5 and Figure 2.1). Moreover, for the asymptotic limit of (2.19), we obtain the following theorem.

Theorem 2.1. *Let $\Omega \subsetneq \mathbb{R}^d$ be a bounded smooth domain, $\varepsilon \in \mathcal{C}^\infty(\overline{\Omega})$ be a positive function, $\rho_0 \in \mathcal{C}^\infty(\overline{\Omega})$, $\phi_{bd} \in \mathcal{C}^\infty(\partial\Omega)$, $z_0 = 0$, and $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$. Assume that (A1) and (A2) hold true. Then the solution ϕ_Λ to PB-steric equation (2.19) with the Robin boundary condition (2.15) satisfies*

$$\lim_{\Lambda\to\infty} \|\phi_\Lambda - \phi^*\|_{\mathcal{C}^m(\overline{\Omega})} = 0 \quad \textit{for } m \in \mathbb{N},$$

where ϕ^* is the solution to

$$-\nabla \cdot (\varepsilon \nabla \phi^*) = \rho_0 + f^*(\phi^*) \quad \textit{in } \Omega \tag{2.23}$$

with the Robin boundary condition (2.15).

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Remark 2.1. *When $I = 2$, (2.21)–(2.23) become (2.3)–(2.4). Besides, (2.23) is the limiting equation of (2.19) as $\Lambda \to \infty$. This shows the PB-steric equations include the modified PB equations (2.3)–(2.4).*

Remark 2.2. *When $I = 2$, we replace the assumption (A1) by*

(A1)′ $g_{i0} = g_{00} = 1 - \gamma$, $g_{ij} = g_{0j} = \gamma_j$ *for* $i, j = 0, 1, 2$, *and* $\gamma = \gamma_1 + \gamma_2$.

Then by (A1)′ and (A2), system (2.13) has a unique solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ *for* $\phi \in \mathbb{R}$ *and* $i = 0, 1, 2$. *Due to* $z_1 z_2 < 0$, *we can calculate directly to get*

$$\frac{\mathrm{d}f_\Lambda}{\mathrm{d}\phi} = \frac{(\gamma z_1 z_2 - z_1^2\gamma_1 - z_2^2\gamma_2)e^{\bar{\mu}_1+\bar{\mu}_2-(z_1+z_2)\phi} - (z_1^2 e^{\bar{\mu}_1 - z_1\phi} + z_2^2 e^{\bar{\mu}_2 - z_2\phi})((\Lambda c_{0,\Lambda})^{-1} + 1 - \gamma)}{(\Lambda c_{0,\Lambda})^{-1} + 1 - \gamma + \gamma_1 e^{\bar{\mu}_1 - z_1\phi} + \gamma_2 e^{\bar{\mu}_2 - z_2\phi}} c_{0,\Lambda} < 0,$$

which implies function f_Λ *is decreasing to* ϕ. *Hence one can follow the similar argument in Sections 2.2 and 2.3 to obtain the same conclusion of Theorem 2.1.*

Remark 2.3. *When $I \geq 2$, we replace the assumption (A1) by*

(A1)″ $g_{i0} = g_{00} = 1 - \gamma$, *and* $g_{ij} = g_{0j} = \gamma|z_j|/Z$ *for* $i, j = 1, \ldots, N$.

Then by (A1)″ and (A2), system (2.13) has a unique solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ *for* $\phi \in \mathbb{R}$ *and* $i = 0, 1, \ldots, I$. *Since* $z_i z_j < 0$ *for some* $i, j \in \{1, \ldots, I\}$, *we can calculate directly to get* $\mathrm{d}f_\Lambda/\mathrm{d}\phi < 0$, *which implies function* f_Λ *is decreasing to* ϕ. *Hence one can follow the similar argument in Sections 2.2 and 2.3 to obtain the same conclusion of Theorem 2.1.*

Remark 2.4. *As $I = 3$, we replace the assumption (A1) by*

(A1)‴ $g_{i0} = g_{00} = 1 - \gamma$, $g_{ij} = g_{0j} = \gamma_j$ *for* $i, j = 0, 1, 2, 3$ *and* $\gamma = \gamma_1 + \gamma_2 + \gamma_3$.

Then by (A1)‴ and (A2), system (2.13) has a unique solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ *for* $\phi \in \mathbb{R}$ *and* $i = 0, 1, 2, 3$. *But for some* Λ, *function* f_Λ *and* $f_\Lambda \circ \phi_\Lambda$ *(total ionic charge density) may become oscillatory (see Figure 2.2). One can see the proof in Appendix 2C and numerical methods in Section 2.4. Such oscillatory total ionic charge density* $f_\Lambda = f_\Lambda(\phi)$ *cannot be obtained in the classical and modified PB equations (2.1)–(2.7).*

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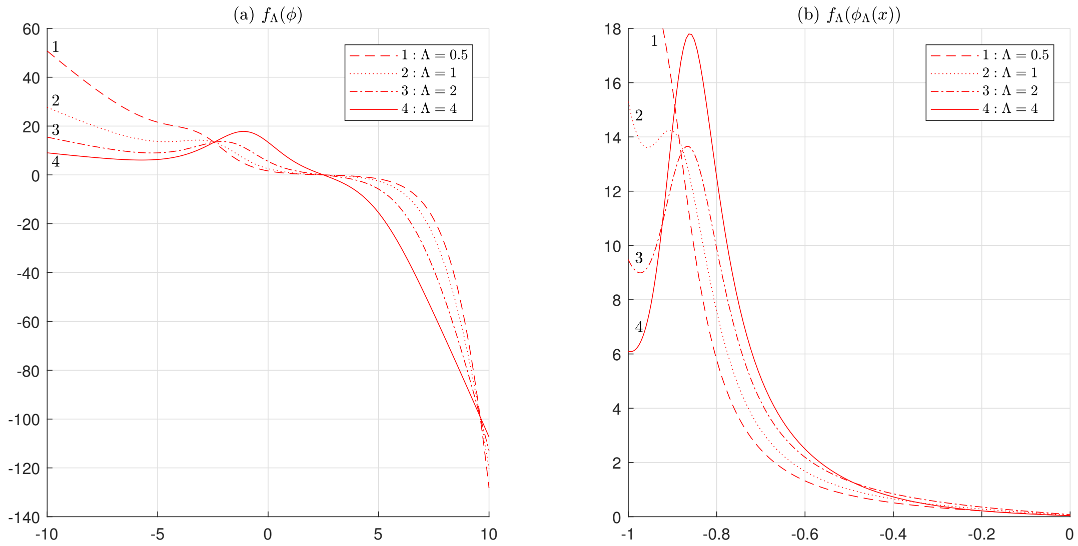

Figure 2.2: The profiles of $f_\Lambda(\phi)$ and $f_\Lambda(\phi_\Lambda(x))$ under assumptions (A1)$'''$ and (A2). In (a), curves 1–4 are profiles of function $f_\Lambda = \sum_{i=1}^{3} z_i c_{i,\Lambda}$ with $\Lambda = 0.5,\ 1,\ 2,\ 4$. In (b), curves 1–4 are the profiles of function $f_\Lambda \circ \phi_\Lambda$ with $\Lambda = 0.5,\ 1,\ 2,\ 4$.

To obtain (2.5)–(2.7), we need the assumptions of g_{ij} and $\tilde{\mu}_i$ given by

(A3) $g_{ij} = \lambda_i \lambda_j$ for $i, j = 0, 1, \ldots, I$,

(A4) $\tilde{\mu}_i = \lambda_i \tilde{\mu}_0$ for $i = 0, 1, \ldots, I$,

where $\lambda_i > 0$, $\tilde{\mu}_0 > 0$ and $\hat{\mu}_i$ (in (2.13)) are constants independent of Λ. Here $\tilde{\mu}_0$ is replaced by $\lambda_0 \tilde{\mu}_0$ and λ_0 might not be 1. By (A3)–(A4), system (2.13) has a unique solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$, which satisfies

$$c_{i,\Lambda} = (c_{0,\Lambda})^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i \phi} \quad \text{for } \phi \in \mathbb{R} \text{ and } i = 1, \ldots, I, \tag{2.24}$$

$$\ln(c_{0,\Lambda}) + \Lambda \sum_{j=0}^{I} \lambda_0 \lambda_j (c_{0,\Lambda})^{\lambda_j/\lambda_0} e^{\bar{\mu}_j - z_j \phi} = \Lambda \lambda_0 \tilde{\mu}_0 + \hat{\mu}_0 \quad \text{for } \phi \in \mathbb{R}, \tag{2.25}$$

where $\bar{\mu}_i = \hat{\mu}_i - \frac{\lambda_i}{\lambda_0} \hat{\mu}_0$ is a constant independent of Λ for $i = 0, 1, \ldots, I$. Note that as $\lambda_j/\lambda_0 = 1$ for $j = 1, \ldots, I$, (2.25) can be solved by the Lambert W function, but here some λ_j/λ_0 may not be equal to one so we may call $c_{0,\Lambda}$ as a Lambert-type function. Then we apply the implicit function theorem on (2.25) and obtain that $c_{0,\Lambda}(\phi)$ is a positive smooth function (see Proposition 2.7). Hence the PB-steric equation (2.14) can be expressed as

$$-\nabla \cdot (\varepsilon \nabla \phi_\Lambda) = \rho_0 + \tilde{f}_\Lambda(\phi_\Lambda) \quad \text{in } \Omega, \tag{2.26}$$

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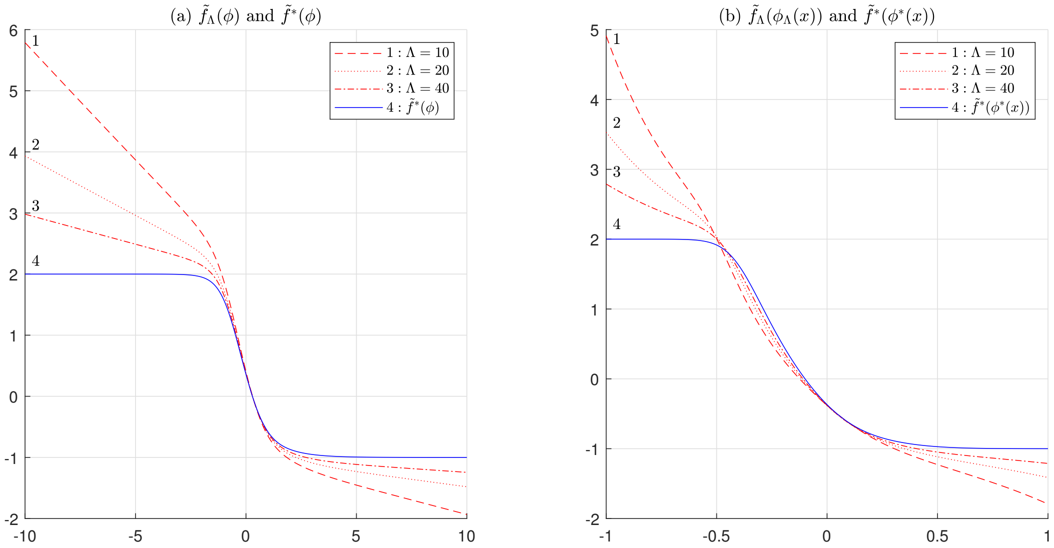

Figure 2.3: The profiles of $\tilde{f}_\Lambda(\phi)$ and $\tilde{f}_\Lambda(\phi_\Lambda(x))$ and their limiting functions under assumptions (A3)–(A4). In (a), curves 1–3 are profiles of function $\tilde{f}_\Lambda$ (defined in (2.27)) with $\Lambda = 10, 20, 40$, and curve 4 is the profile of function $\tilde{f}^*$ (defined in (2.30)). In (b), curves 1–3 are the profiles of function $\tilde{f}_\Lambda \circ \phi_\Lambda$ with $\Lambda = 10, 20, 40$, and curve 4 is the profile of function $\tilde{f}^* \circ \phi^*$.

where function $\tilde{f}_\Lambda = \tilde{f}_\Lambda(\phi)$ is denoted as

$$\tilde{f}_\Lambda(\phi) = \sum_{i=1}^{I} z_i c_{i,\Lambda}(\phi) \quad \text{for } \phi \in \mathbb{R}. \tag{2.27}$$

Note that the existence and uniqueness of (2.26) with the Robin boundary condition (2.15) can be obtain by the standard method of the nonlinear elliptic equation, but (2.19) and (2.26) are different because they have different nonlinear terms f_Λ and $\tilde{f}_\Lambda$.

By the implicit function theorem on Banach spaces (cf. [21, Theorem 15.1]), we prove that $c_{i,\Lambda}$ converges to c_i^* in space $\mathcal{C}^m[a,b]$ as Λ tends to infinity for $m \in \mathbb{N}$ and $a < b$ (See Proposition 2.8). Here function c_i^* satisfies

$$c_i^*(\phi) = (c_0^*(\phi))^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\phi} > 0 \quad \text{for } \phi \in \mathbb{R} \text{ and } i = 1, \dots, I, \tag{2.28}$$

$$\sum_{i=0}^{I} \lambda_i c_i^*(\phi) = \sum_{i=0}^{I} \lambda_i (c_0^*(\phi))^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\phi} = \tilde{\mu}_0 \quad \text{for } \phi \in \mathbb{R}, \tag{2.29}$$

where $\bar{\mu}_i = \hat{\mu}_i - \frac{\lambda_i}{\lambda_0}\hat{\mu}_0$ for $i = 0, 1, \dots, I$. Thus function $\tilde{f}_\Lambda$ also converges to $\tilde{f}^*$ in

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space $\mathcal{C}^m[a,b]$ as Λ goes to infinity for $m \in \mathbb{N}$ and $a < b$, where

$$\tilde{f}^*(\phi) = \sum_{i=1}^{I} z_i c_i^*(\phi) \tag{2.30}$$

(see Corollary 2.9 and Figure 2.3). Moreover, for the asymptotic limit of (2.26), we have the following theorem.

Theorem 2.2. *Let $\Omega \subsetneq \mathbb{R}^d$ be a bounded smooth domain, $\varepsilon \in \mathcal{C}^\infty(\overline{\Omega})$ be a positive function, $\rho_0 \in \mathcal{C}^\infty(\overline{\Omega})$, $\phi_{bd} \in \mathcal{C}^\infty(\partial\Omega)$, $z_0 = 0$, and $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$. Assume that (A3)–(A4) hold true. Then the solution ϕ_Λ to PB-steric equation (2.26) with the Robin boundary condition (2.15) satisfies*

$$\lim_{\Lambda\to\infty} \|\phi_\Lambda - \phi^*\|_{\mathcal{C}^m(\overline{\Omega})} = 0 \quad \textit{for } m \in \mathbb{N},$$

where ϕ^* is the solution to

$$-\nabla \cdot (\varepsilon \nabla \phi^*) = \rho_0 + \tilde{f}^*(\phi^*) \quad \textit{in } \Omega \tag{2.31}$$

with the Robin boundary condition (2.15).

Remark 2.5. *As $\lambda_i = v_i/v_0$, $\tilde{\mu}_0 = 1/v_0$, $c_i^* = c_i$ and $\phi^* = \phi$, (2.28)–(2.31) become (2.5)–(2.7) (up to scalar multiples). Besides, (2.31) is the limiting equation of (2.26) as $\Lambda \to \infty$. This shows the PB-steric equations include the modified PB equations (2.5)–(2.7).*

Before proving Theorems 2.1 and 2.2, we note that f_Λ and $\tilde{f}_\Lambda$ are strictly decreasing and unbounded on $\mathbb{R}$ (see Propositions 2.1 and 2.7) but f^* and $\tilde{f}^*$ are strictly decreasing and bonunded on $\mathbb{R}$ (see Propositions 2.6 and 2.10) so we cannot obtain the uniform convergence of f_Λ on $\mathbb{R}$ as Λ goes to infinity. Since we only have the uniform boundedness of f_Λ and $\tilde{f}_\Lambda$ on any bounded interval $[a,b]$ but not the entire space $\mathbb{R}$, we first have to prove the uniform boundedness of ϕ_Λ (the solution to (2.19) and (2.26)) with respect to Λ (see Lemmas 2.11 and 2.13) in order to use the convergence of f_Λ and $\tilde{f}_\Lambda$ in space $\mathcal{C}^m[a,b]$ for $m \in \mathbb{N}$ and $a < b$. Here (2.16) and (2.28) are crucial for the proofs of Lemmas 2.11 and 2.13, respectively. Notice that $\rho_0 = \rho_0(x)$ may be any nonzero smooth function and the boundary condition may be the Robin boundary condition but not Dirichlet boundary condition so one cannot simply use the maximum principle on (2.19) and (2.26) to prove Lemmas 2.11

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and 2.13. Then we can apply $W^{2,p}$ estimate (cf. [2, Theorem 15.2]), the Schauder's estimate (cf. [38, Theorem 6.30]) and the uniqueness of solution to prove that ϕ_Λ converges to ϕ^* in space $\mathcal{C}^m(\overline{\Omega})$ as Λ tends to infinity for $m \in \mathbb{N}$ and obtain the proofs of Theorems 2.1 and 2.2.

In Section 2.4, we provide numerical simulation on nonlinear elliptic equations (2.19), (2.23), (2.26) and (2.31) with the Robin boundary condition (2.15). The one-dimensional domain $\Omega = (-1, 1)$ is discretized by the Legendre–Gauss–Lobatto (LGL) points (cf. [28]). Then we use the LGL points to discretize equations (2.19), (2.23), (2.26), (2.31) and the Robin boundary condition (2.15), and then solve them numerically with the command `fsolve` in Matlab. Under assumptions (A1)–(A2) and (A3)–(A4), we show the profiles of numerical solutions ϕ_Λ and ϕ^* to support Theorems 2.1 and 2.2, respectively. In addition, under assumption (A1)$'''$ and (A2), we present the profiles of numerical solution ϕ_Λ whose total ionic charge density is oscillatory in Figure 2.2(b).

Organization. The rest of the chapter is organized as follows. In Section 2.2, we analyze of functions f_Λ, f^*, $\tilde{f}_\Lambda$ and $\tilde{f}^*$ under the assumptions (A1)–(A2) and (A3)–(A4), respectively. The proof of Theorems 2.1 and 2.2 are stated in Section 2.3. Numerical schemes are shown in Section 2.4.

2.2 Analysis of nonlinear terms under (A1)–(A2) and (A3)–(A4)

2.2.1 Analysis of $c_{i,\Lambda}$ and f_Λ under (A1)–(A2)

In this section, we first show how to use assumptions (A1) and (A2) to apply Gaussian elimination to solve system (2.13) and obtain a unique positive smooth solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$. Then we establish the asymptotic behavior of $c_{i,\lambda}$ (as ϕ tends to infinity) and the strict decrease and unboundedness of $f_\Lambda = \sum_{i=1}^{I} z_i c_{i,\Lambda}$ (see Proposition 2.1).

For functions $c_{i,\Lambda}$ and f_Λ under the assumptions (A1) and (A2), we have the following.

Proposition 2.1. *Assume that $z_0 = 0$, (A1) and (A2) hold true. Suppose $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$.*

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(a) *System* (2.13) *can be solved uniquely by*

$$c_{i,\Lambda}(\phi) = \frac{W_0\left(\Lambda H(\gamma, z_1, \ldots, z_I, \phi)e^{\Lambda\tilde{\mu}_0+\hat{\mu}_0}\right)}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} e^{\bar{\mu}_i - z_i\phi} \tag{2.32}$$

for $\phi \in \mathbb{R}$ *and* $i = 0, 1, \ldots, I$, *where* W_0 *denotes the principal branch of Lambert W function (cf.* [93]*).*

(b) *Function* $f_\Lambda = \sum_{i=1}^{I} z_i c_{i,\Lambda}$ *is strictly decreasing on* $\mathbb{R}$.

(c) *Let* $\mathcal{J}_1 = \{j : z_j = \max_{0\le k\le I} z_k\}$ *and* $\mathcal{J}_2 = \{j : z_j = \min_{0\le k\le I} z_k\}$. *Then*

(i) $\lim_{\phi\to-\infty} c_{j_0,\Lambda}(\phi) = \infty$ *for* $j_0 \in \mathcal{J}_1$, *and* $\lim_{\phi\to-\infty} c_{k,\Lambda}(\phi) = 0$ *for* $k \notin \mathcal{J}_1$;

(ii) $\lim_{\phi\to\infty} c_{j_0,\Lambda}(\phi) = \infty$ *for* $j_0 \in \mathcal{J}_2$, *and* $\lim_{\phi\to\infty} c_{k,\Lambda}(\phi) = 0$ *for* $k \notin \mathcal{J}_2$.

(d) *For each* $\Lambda > 0$, *the range of* f_Λ *is entire space* $\mathbb{R}$, *and* $\lim_{\phi\to\pm\infty} f_\Lambda(\phi) = \mp\infty$.

Proof. By (A1)–(A2), system (2.13) can be expressed as

$$\ln(c_{i,\Lambda}) + z_i\phi + \Lambda\left((1-\gamma)c_{0,\Lambda} + \frac{\gamma}{Z}\sum_{j=1}^{I} c_{j,\Lambda}\right) = \Lambda\tilde{\mu}_0 + \hat{\mu}_i \quad \text{for } i = 0, 1, \ldots, I. \tag{2.33}$$

Subtracting (2.33) for $i \neq 0$ from that for $i = 0$, we get

$$\ln(c_{i,\Lambda}/c_{0,\Lambda}) + z_i\phi = \hat{\mu}_i - \hat{\mu}_0 := \bar{\mu}_i,$$

which implies (2.16) under the assumption $z_0 = 0$. Then we plug (2.16) into (2.33) for $i = 0$ to get (2.17), which implies

$$[\Lambda H(\gamma, z_1, \ldots, z_I, \phi)c_{0,\Lambda}]\, e^{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)c_{0,\Lambda}} = \Lambda H(\gamma, z_1, \ldots, z_I, \phi)e^{\Lambda\tilde{\mu}_0+\hat{\mu}_0} \tag{2.34}$$

for $\phi \in \mathbb{R}$. From theorems of Lambert W function in [93], (2.34) has a unique smooth positive solution $c_{0,\Lambda}$ denoted by

$$c_{0,\Lambda}(\phi) = \frac{W_0\left(\Lambda H(\gamma, z_1, \ldots, z_I, \phi)e^{\Lambda\tilde{\mu}_0+\hat{\mu}_0}\right)}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} \quad \text{for } \phi \in \mathbb{R}. \tag{2.35}$$

By (2.16) and (2.35), we arrive at (2.32) and complete the proof of (a).

Next we state the proof of (b). We differentiate (2.17) with respect to ϕ and get

$$\frac{1}{c_{0,\Lambda}}\frac{\mathrm{d}c_{0,\Lambda}}{\mathrm{d}\phi} + \Lambda H(\gamma, z_1, \ldots, z_I, \phi)\frac{\mathrm{d}c_{0,\Lambda}}{\mathrm{d}\phi} - \Lambda c_{0,\Lambda}\frac{\gamma}{Z}\sum_{j=1}^{I} z_j e^{\bar{\mu}_j - z_j\phi} = 0,$$

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which gives

$$\frac{\mathrm{d}c_{0,\Lambda}}{\mathrm{d}\phi} = \frac{\frac{\gamma}{Z}\sum_{j=1}^{I} z_j e^{\bar{\mu}_j - z_j\phi}}{(\Lambda c_{0,\Lambda})^{-1} + H(\gamma, z_1, \dots, z_I, \phi)} c_{0,\Lambda}. \tag{2.36}$$

On the other hand, by (2.16), we write f_Λ as $f_\Lambda(\phi) = \sum_{i=1}^{I} z_i c_{0,\Lambda} e^{\bar{\mu}_i - z_i\phi}$ for $\phi \in \mathbb{R}$. Then differentiating f_Λ with respect to ϕ and using (2.36), we get

$$\begin{aligned}\frac{\mathrm{d}f_\Lambda}{\mathrm{d}\phi} &= \sum_{i=1}^{I} z_i \frac{\mathrm{d}c_{i,\Lambda}}{\mathrm{d}\phi} = \frac{\mathrm{d}c_{0,\Lambda}}{\mathrm{d}\phi}\sum_{i=1}^{I} z_i e^{\bar{\mu}_i - z_i\phi} - c_{0,\Lambda}\sum_{i=1}^{I} z^2 e^{\bar{\mu}_i - z_i\phi} \\ &= \left(\frac{\frac{\gamma}{Z}\left(\sum_{i=1}^{I} z_i e^{\bar{\mu}_i - z_i\phi}\right)\left(\sum_{i=1}^{I} z_i e^{\bar{\mu}_i - z_i\phi}\right)}{(\Lambda c_{0,\Lambda})^{-1} + H(\gamma, z_1, \dots, z_I, \phi)} - \sum_{i=1}^{I} z_i^2 e^{\bar{\mu}_i - z_i\phi}) \right) c_{0,\Lambda}.\end{aligned} \tag{2.37}$$

Note the inequality

$$\begin{aligned}&\left(\sum_{i=1}^{I} z_i^2 e^{\bar{\mu}_i - z_i\phi}\right)\left[(\Lambda c_{0,\Lambda})^{-1} + H(\gamma, z_1, \dots, z_I, \phi)\right] \\ &> \frac{\gamma}{Z}\left(\sum_{i=1}^{I} z_i^2 e^{\bar{\mu}_i - z_i\phi}\right)\left(\sum_{i=1}^{I} e^{\bar{\mu}_i - z_i\phi}\right) > \frac{\gamma}{Z}\left(\sum_{i=1}^{I} z_i e^{\bar{\mu}_i - z_i\phi}\right)^2,\end{aligned} \tag{2.38}$$

where we have used the fact that $z_i z_j < 0$ for some $i, j \in \{1, \dots, I\}$. Therefore, by (2.37)–(2.38), we have $\mathrm{d}f_\Lambda/\mathrm{d}\phi < 0$ on $\mathbb{R}$ and the proof of (b) is complete.

To prove (c), we need the following claim.

Claim 2.2. *There holds that*

$$\lim_{\phi\to\pm\infty} \frac{W_0(\Lambda H(\gamma, z_1, \dots, z_I, \phi) e^{\Lambda\tilde{\mu}_0 + \hat{\mu}_0})}{\ln\Lambda + \ln(H(\gamma, z_1, \dots, z_I, \phi)) + \Lambda\tilde{\mu}_0 + \hat{\mu}_0} = 1. \tag{2.39}$$

Proof of Claim 2.2. Recall the asymptotic behavior of Lambert W function in [49, 93]

$$\ln x - \ln\ln x + \frac{\ln\ln x}{2\ln x} \le W_0(x) \le \ln x - \ln\ln x + \frac{e}{e-1}\frac{\ln\ln x}{\ln x} \quad \text{for } x \ge e. \tag{2.40}$$

Since $z_i z_j < 0$ for some $i, j \in \{1, \dots, I\}$, it is clear that $\lim_{\phi\to\pm\infty} \sum_{i=1}^{I} e^{\bar{\mu}_i - z_i\phi} = \infty$, which implies that

$$\lim_{\phi\to\pm\infty} \Lambda H(\gamma, z_1, \dots, z_I, \phi) e^{\Lambda\tilde{\mu}_0 + \hat{\mu}_0} = \infty.$$

Then by (2.40), we obtain (2.39) and complete the proof of Claim 2.2. □

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Now we state the proof of (c). Since $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$, we know $z_{i_0} > 0$ for $i_0 \in \mathcal{J}_1$ and $z_{j_0} < 0$ for $j_0 \in \mathcal{J}_2$. Then for $i_0 \in \mathcal{J}_1$, we may use (2.16), (2.35) and Claim 2.2 to get

$$\begin{aligned}
\lim_{\phi \to -\infty} c_{i_0,\Lambda}(\phi) &= \lim_{\phi \to -\infty} c_{0,\Lambda}(\phi) e^{\bar{\mu}_{i_0} - z_{i_0}\phi} \\
&= \lim_{\phi \to -\infty} \frac{e^{\bar{\mu}_{i_0} - z_{i_0}\phi}}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} W_0(\Lambda H(\gamma, z_1, \ldots, z_I, \phi) e^{\Lambda \tilde{\mu}_0 + \hat{\mu}_0}) \\
&= \frac{Z}{\Lambda \gamma \sum\limits_{i \in \mathcal{J}_1} e^{\bar{\mu}_i - \bar{\mu}_{i_0}}} \lim_{\phi \to -\infty} W_0(\Lambda H(\gamma, z_1, \ldots, z_I, \phi) e^{\Lambda \tilde{\mu}_0 + \hat{\mu}_0}) = \infty.
\end{aligned}$$

On the other hand, for $k \notin \mathcal{J}_1$, we have

$$\begin{aligned}
\lim_{\phi \to -\infty} c_{k,\Lambda}(\phi) &= \lim_{\phi \to -\infty} \frac{e^{\bar{\mu}_k - z_k \phi}}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} W_0(\Lambda H(\gamma, z_1, \ldots, z_I, \phi) e^{\Lambda \tilde{\mu}_0 + \hat{\mu}_0}) \\
&= \lim_{\phi \to -\infty} \frac{e^{\bar{\mu}_k - z_k \phi}}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} (\ln \Lambda + \ln(H(\gamma, z_1, \ldots, z_I, \phi)) + \Lambda \tilde{\mu}_0 + \hat{\mu}_0) = 0.
\end{aligned}$$

Thus the proof of (c)(i) is complete. Similarly, for $j_0 \in \mathcal{J}_2$, we combine (2.16), (2.17), and Claim 2.2 to get

$$\begin{aligned}
\lim_{\phi \to \infty} c_{j_0,\Lambda}(\phi) &= \lim_{\phi \to \infty} c_{0,\Lambda}(\phi) e^{\bar{\mu}_{j_0} - z_{j_0}\phi} \\
&= \lim_{\phi \to \infty} \frac{e^{\bar{\mu}_{j_0} - z_{j_0}\phi}}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} W_0(\Lambda H(\gamma, z_1, \ldots, z_I, \phi) e^{\Lambda \tilde{\mu}_0 + \hat{\mu}_0}) \\
&= \frac{Z}{\Lambda \gamma \sum\limits_{j \in \mathcal{J}_2} e^{\bar{\mu}_j - \bar{\mu}_{j_0}}} \lim_{\phi \to \infty} W_0(\Lambda H(\gamma, z_1, \ldots, z_I, \phi) e^{\Lambda \tilde{\mu}_0 + \hat{\mu}_0}) = \infty.
\end{aligned}$$

On the other hand, for $k \notin \mathcal{J}_2$, we have

$$\begin{aligned}
\lim_{\phi \to \infty} c_{k,\Lambda}(\phi) &= \lim_{\phi \to \infty} \frac{e^{\bar{\mu}_k - z_k \phi}}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} W_0(\Lambda H(\gamma, z_1, \ldots, z_I, \phi) e^{\Lambda \tilde{\mu}_0 + \hat{\mu}_0}) \\
&= \lim_{\phi \to \infty} \frac{e^{\bar{\mu}_k - z_k \phi}}{\Lambda H(\gamma, z_1, \ldots, z_I, \phi)} (\ln \Lambda + \ln(H(\gamma, z_1, \ldots, z_I, \phi)) + \Lambda \tilde{\mu}_0 + \hat{\mu}_0) = 0.
\end{aligned}$$

Therefore, we complete the proof of (c).

Finally, we give the proof of (d). From (2.20), function f_Λ can be denoted as $f_\Lambda(\phi) = \sum\limits_{i \in \mathcal{J}_1} z_i c_{i,\Lambda}(\phi) + \sum\limits_{i \notin \mathcal{J}_1} z_i c_{i,\Lambda}(\phi)$ for $\phi \in \mathbb{R}$, where $\mathcal{J}_1$ is defined in (c)(i). Then by (c)(i), we have $\lim\limits_{\phi \to -\infty} f_\Lambda(\phi) = \infty$. Similarly, by (c)(ii), we have $\lim\limits_{\phi \to \infty} f_\Lambda(\phi) = -\infty$. Therefore, we conclude (d) and complete the proof of Proposition 2.1. $\square$

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2.2.2 Analysis of c_i^* and f^* under (A1)–(A2)

Function c_0^* is the limit $\lim_{\Lambda\to\infty} c_{0,\Lambda}$, where function $c_{0,\Lambda}$ is the solution to (2.17) for $\Lambda > 0$. Let $\delta = \Lambda^{-1}$ and $\tilde{c}_{0,\delta} = c_{0,\Lambda}$. Then by (2.17), $\tilde{c}_{0,\delta}$ satisfies

$$\delta \ln(\tilde{c}_{0,\delta}(\phi)) + H(\gamma, z_1, \dots, z_I, \phi)\tilde{c}_{0,\delta} = \tilde{\mu}_0 + \delta\hat{\mu}_0 \quad \text{for } \phi \in \mathbb{R}. \tag{2.41}$$

Notice that $\Lambda \to \infty$ is equivalent to $\delta \to 0^+$ so c_0^* also equals the limit $\lim_{\delta\to 0^+} \tilde{c}_{0,\delta}$. Moreover c_0^* is defined by (2.21) wtih $i = 0$, which is (2.41) with $\delta = 0$. The convergence of $\tilde{c}_{0,\delta}$ as $\delta \to 0^+$, i.e. the convergence of $c_{0,\Lambda}$ as $\Lambda \to \infty$ is proved in Proposition 2.3, so by (2.16), we obtain the convergence of $c_{i,\Lambda}$ as $\Lambda \to \infty$.

Proposition 2.3. *Let $c_{i,\Lambda}$ and c_i^* be defined in (2.32) and (2.21), respectively.*

(a) For $\phi \in \mathbb{R}$, $\lim_{\Lambda\to\infty} c_{i,\Lambda}(\phi) = c_i^*(\phi)$ for $i = 0, 1, \dots, I$.

(b) $\lim_{\Lambda\to\infty} \|c_{i,\Lambda} - c_i^*\|_{\mathcal{C}^m[a,b]} = 0$ for $i = 0, 1, \dots, I$, $m \in \mathbb{N}$, and $a < b$, where $\|h\|_{\mathcal{C}^m[a,b]} := \sum_{k=0}^{m} \|h^{(k)}\|_\infty$ for $h \in \mathcal{C}^m[a, b]$.

Proof. To prove (a), we need the following claim.

Claim 2.4. *Assume that (A1)–(A2) hold ture. Then there holds that*

$$\lim_{\Lambda\to\infty} \frac{W_0(\Lambda H(\gamma, z_1, \dots, z_N, \phi)e^{\Lambda\tilde{\mu}_0+\hat{\mu}_0})}{\Lambda\tilde{\mu}_0} = 1 \quad \textit{for } \phi \in \mathbb{R}.$$

Note that $H(\gamma, z_1, \dots, z_I, \phi)$ is independent of Λ so the proof of Claim 2.4 follows directly from (2.40) and we omit it here.

By Proposition 2.1(a) and Claim 2.4, it follows that

$$\lim_{\Lambda\to\infty} c_{i,\Lambda}(\phi) = e^{\bar{\mu}_i - z_i\phi} \lim_{\Lambda\to\infty} \frac{\Lambda\tilde{\mu}_0}{\Lambda H(\gamma, z_1, \dots, z_I, \phi)} = \frac{\tilde{\mu}_0 e^{\bar{\mu}_i - z_i\phi}}{H(\gamma, z_1, \dots, z_I, \phi)} = c_i^*(\phi)$$

for $i = 0, 1 \dots, I$, which implies (a).

To prove (b), we fix $m \in \mathbb{N}$, $a, b \in \mathbb{R}$ and $a < b$ arbitrarily. Let $\|\cdot\|_{\mathcal{C}^m} := \|\cdot\|_{\mathcal{C}^m[a,b]}$ for notational convenience. For $\Lambda > 0$, let $\delta = \Lambda^{-1}$, $\tilde{c}_{0,\delta} = c_{0,\Lambda}$, $w_\delta = \ln(\tilde{c}_{0,\delta})$, and $w^* = \ln(c_0^*)$. Obviously, $\delta \to 0^+$ is equivalent to $\Lambda \to \infty$. Hence by (2.16), it suffices to show that $\lim_{\delta\to 0^+} \|e^{w_\delta} - e^{w^*}\|_{\mathcal{C}^m} = 0$. Because $w_\delta = \ln(\tilde{c}_{0,\delta})$ and $\tilde{c}_{0,\delta} = c_{0,\Lambda}$, equation (2.41) can be denoted as $K_1(w_\delta(\phi), \delta) = 0$ for $\delta > 0$ and $\phi \in [a, b]$, where K_1 is a $\mathcal{C}^1$-function on $\mathcal{C}^m[a, b] \times \mathbb{R}$ defined by

$$K_1(w(\phi), \delta) = \delta w(\phi) + H(\gamma, z_1, \dots, z_I, \phi)e^{w(\phi)} - \tilde{\mu}_0 - \delta\hat{\mu}_0 \tag{2.42}$$

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for all $w \in \mathcal{C}^m[a,b]$ and $\phi \in [a,b]$. Note that $K_1(w^*, 0) = 0$ by (a). A direct calculation for Fréchet derivative of (2.42) gives

$$D_w K_1(w(\phi), \delta) = \delta + H(\gamma, z_1, \dots, z_N, \phi) e^{w(\phi)}$$

for all $w \in \mathcal{C}^m[a,b]$ and $\phi \in [a,b]$. Then by (a), we get $D_w K_1(w^*(\phi), 0) = \tilde{\mu}_0 > 0$ for all $\phi \in [a,b]$. This implies that $D_w K_1(w^*, 0) I$ is a bounded and invertible linear map on the Banach space $\mathcal{C}^m[a,b]$, where I is an identity map. Hence by the implicit function theorem on Banach spaces (cf. [21, Corollary 15.1]), there exists an open subset $B_{\delta_0}(w^*) \times (-\delta_0, \delta_0) \subsetneq \mathcal{C}^m[a,b] \times \mathbb{R}$ and a unique $\mathcal{C}^1$-function $\tilde{w}(\cdot, \delta)$ of $\delta \in (-\delta_0, \delta_0)$ with $\tilde{w}(\cdot, \delta) \in B_{\delta_0}(w^*) \subset \mathcal{C}^m[a,b]$ for $\delta \in (-\delta_0, \delta_0)$ such that $K_1(\tilde{w}(\cdot, \delta), \delta) = 0$ for all $\delta \in (-\delta_0, \delta_0)$, which gives $\lim\limits_{\delta \to 0^+} \|\tilde{w}(\cdot, \delta) - w^*\|_{\mathcal{C}^m} = 0$. By Proposition 2.1(a), equation $K_1(w, \delta) = 0$ has a unique solution $w = w_\delta$, which implies $\tilde{w}(\cdot, \delta) = w_\delta(\cdot)$ for $\delta \in (-\delta_0, \delta_0)$. Therefore, we obtain $\lim\limits_{\delta \to 0^+} \|w_\delta - w^*\|_{\mathcal{C}^m} = 0$, i.e., $\lim\limits_{\delta \to 0^+} \|e^{w_\delta} - e^{w^*}\|_{\mathcal{C}^m} = 0$, and complete the proof of Proposition 2.3(ii). □

Corollary 2.5. $\lim\limits_{\Lambda \to \infty} \|f_\Lambda - f^*\|_{\mathcal{C}^m[a,b]} = 0$ *for* $m \in \mathbb{N}$ *and* $a < b$.

Proof. It follows from Proposition 2.3(b) and the fact that $f_\Lambda(\phi) = \sum\limits_{i=1}^{I} z_i c_{i,\Lambda}(\phi)$ and $f^*(\phi) = \sum\limits_{i=1}^{I} z_i c_i^*(\phi)$ for $\phi \in \mathbb{R}$. □

For function f^*, we have the following proposition.

Proposition 2.6. *Let* f^* *be the function defined in* (2.22).

(a) Function f^* *is strictly decreasing on* $\mathbb{R}$.

(b) Function f^* *satisfies* $m^* < f^*(\phi) < M^*$ *for all* $\phi \in \mathbb{R}$, *where*

$$m^* = \lim_{\phi \to \infty} f^*(\phi) < 0 \quad \textit{and} \quad M^* = \lim_{\phi \to -\infty} f^*(\phi) > 0.$$

Proof. By (2.21)–(2.22), f^* can be expressed as

$$f^*(\phi) = \frac{\tilde{\mu}_0}{H(\gamma, z_1, \dots, z_I, \phi)} \sum_{i=1}^{I} z_i e^{\bar{\mu}_i - z_i \phi} \quad \text{for } \phi \in \mathbb{R}. \tag{2.43}$$

Then differentiating (2.43) with respect to ϕ gives

$$\frac{\mathrm{d}f^*}{\mathrm{d}\phi} = \tilde{\mu}_0 \left(\frac{\frac{\gamma}{Z}\left(\sum\limits_{i=1}^{I} z_i e^{\bar{\mu}_i - z_i \phi}\right)^2}{\left(H(\gamma, z_1, \dots, z_I, \phi)\right)^2} - \frac{\sum\limits_{i=1}^{I} z_i^2 e^{\bar{\mu}_i - z_i \phi}}{H(\gamma, z_1, \dots, z_I, \phi)} \right.$$

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$$\leq \frac{\tilde{\mu}_0 \gamma}{Z} \frac{\left(\sum_{i=1}^{I} z_i e^{\bar{\mu}_i - z_i \phi}\right)^2 - \sum_{i=1}^{I} e^{\bar{\mu}_i - z_i \phi} \sum_{i=1}^{I} z_i^2 e^{\bar{\mu}_i - z_i \phi}}{\left(H(\gamma, z_1, \ldots, z_I, \phi)\right)^2} < 0 \quad \text{for } \phi \in \mathbb{R}.$$

Here the last inequality comes from the Cauchy–Schwarz inequality and the fact that $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$. Therefore, we complete the proof of (a).

To prove (b), we note that

$$m^* := \tilde{\mu}_0 \lim_{\phi \to \infty} \frac{\left(\sum_{j \in \mathcal{J}_2} + \sum_{j \notin \mathcal{J}_2}\right) z_j e^{\bar{\mu}_j - z_j \phi}}{1 - \gamma + \frac{\gamma}{Z}\left(\sum_{j \in \mathcal{J}_2} + \sum_{j \notin \mathcal{J}_2}\right) e^{\bar{\mu}_j - z_j \phi}} = \frac{\tilde{\mu}_0 Z}{\gamma} \frac{\sum_{j \in \mathcal{J}_2} z_j e^{\bar{\mu}_j}}{\sum_{j \in \mathcal{J}_2} e^{\bar{\mu}_j}} < 0$$

and

$$M^* := \tilde{\mu}_0 \lim_{\phi \to -\infty} \frac{\left(\sum_{i \in \mathcal{J}_1} + \sum_{i \notin \mathcal{J}_1}\right) z_i e^{\bar{\mu}_i - z_i \phi}}{1 - \gamma + \frac{\gamma}{Z}\left(\sum_{i \in \mathcal{J}_1} + \sum_{i \notin \mathcal{J}_1}\right) e^{\bar{\mu}_i - z_i \phi}} = \frac{\tilde{\mu}_0 Z}{\gamma} \frac{\sum_{i \in \mathcal{J}_1} z_i e^{\bar{\mu}_i}}{\sum_{i \in \mathcal{J}_1} e^{\bar{\mu}_i}} > 0,$$

where $\mathcal{J}_1$ and $\mathcal{J}_2$ are defined in Proposition 2.1(c). By (a), f^* is strictly decreasing, so we have $m^* < f^*(\phi) < M^*$ for all $\phi \in \mathbb{R}$ and complete the proof of Proposition 2.6.

□

2.2.3 Analysis of $c_{i,\Lambda}$ and $\tilde{f}_\Lambda$ under (A3)–(A4)

In this section, we use assumptions (A3)–(A4) and apply Gaussian elimination to solve system (2.13) and obtain a unique positive smooth solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$. Then we establish the asymptotic behavior of $c_{i,\Lambda}$ (as ϕ tends to infinity), and the strict decrease and unboundedness of $\tilde{f}_\Lambda = \sum_{i=1}^{I} z_i c_{i,\Lambda}$ (see Proposition 2.7).

For functions $c_{i,\Lambda}$ and $\tilde{f}_\Lambda$, we have the following proposition.

Proposition 2.7. *Assume that $z_0 = 0$, (A3)–(A4) hold true. Suppose $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$.*

(a) System (2.13) has a unique, smooth, and positive solution $c_{i,\Lambda} = c_{i,\Lambda}(\phi)$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$.

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(b) Function $\tilde{f}_\Lambda = \sum_{i=1}^{I} z_i c_{i,\Lambda}$ *is strictly decreasing on* $\mathbb{R}$*.*

(c) (i) If $z_k \geq 0$ $(z_k \leq 0)$*, then* $\sup_{\phi\geq 0} c_{k,\Lambda}(\phi) \leq e^{\Lambda\lambda_k\tilde{\mu}_0+\hat{\mu}_k}$ $(\sup_{\phi\leq 0} c_{k,\Lambda}(\phi) \leq e^{\Lambda\lambda_k\tilde{\mu}_0+\hat{\mu}_k})$*.*

(ii) There exist $i_0, j_0 \in \{1, \ldots, I\}$*,* $z_{i_0} > 0$ *and* $z_{j_0} < 0$ *such that* $\limsup_{\phi\to-\infty} c_{i_0,\Lambda}(\phi) = \infty$ *and* $\limsup_{\phi\to\infty} c_{j_0,\Lambda}(\phi) = \infty$*.*

(d) For each $\Lambda > 0$*, the range of* $\tilde{f}_\Lambda$ *is entire space* $\mathbb{R}$*, and* $\lim_{\phi\to\pm\infty} \tilde{f}_\Lambda(\phi) = \mp\infty$*.*

Proof. By (A3)–(A4), system (2.13) can be expressed as

$$\ln(c_{i,\Lambda}) + z_i\phi + \Lambda\sum_{j=0}^{I}\lambda_i\lambda_j c_{j,\Lambda} = \Lambda\lambda_i\tilde{\mu}_0 + \hat{\mu}_i \quad \text{for } \phi\in\mathbb{R} \text{ and } i = 0, 1, \ldots, I. \tag{2.44}$$

Multiplying (2.44) for $i = 0$ by λ_i/λ_0, we obtain

$$\frac{\lambda_i}{\lambda_0}\ln c_{0,\Lambda} + \Lambda\sum_{j=0}^{I}\lambda_i\lambda_j c_{j,\Lambda} = \Lambda\lambda_i\tilde{\mu}_0 + \frac{\lambda_i}{\lambda_0}\hat{\mu}_0. \tag{2.45}$$

Then we subtract (2.44) from (2.45) to get

$$\ln c_{i,\Lambda} - \frac{\lambda_i}{\lambda_0}\ln c_{0,\Lambda} + z_i\phi = \hat{\mu}_i - \frac{\lambda_i}{\lambda_0}\hat{\mu}_0 := \bar{\mu}_i,$$

which implies (2.24). Plugging (2.24) into (2.44) for $i = 0$, we get (2.25). Then we denote (2.25) as $g_1(c_{0,\Lambda}, \phi) = 0$, where g_1 is defined by

$$g_1(t,\phi) = \ln t + \Lambda\sum_{j=0}^{I}\lambda_0\lambda_j t^{\lambda_j/\lambda_0} e^{\bar{\mu}_j - z_j\phi} - \Lambda\lambda_0\tilde{\mu}_0 - \hat{\mu}_0 \quad \text{for } t > 0 \text{ and } \phi\in\mathbb{R}.$$

Notice that, for any $\phi\in\mathbb{R}$, function g_1 is strictly increasing for $t > 0$, and the range of g_1 is entire space $\mathbb{R}$. Then there exists a unique positive number $c_{0,\Lambda}(\phi)$ such that $g_1(c_{0,\Lambda}(\phi), \phi) = 0$ for $\phi\in\mathbb{R}$. Moreover, since g_1 is smooth for $t > 0$, $\phi\in\mathbb{R}$, and

$$\frac{\partial g_1}{\partial t}(t,\phi) = \frac{1}{t} + \Lambda\sum_{j=0}^{I}\lambda_j^2 t^{(\lambda_j-\lambda_0)/\lambda_0} e^{\bar{\mu}_j - z_j\phi} > 0 \quad \text{for } t > 0 \text{ and } \phi\in\mathbb{R},$$

then by the implicit function theorem (cf. [68, Theorem 3.3.1]), $c_{0,\Lambda} = c_{0,\Lambda}(\phi)$ is a smooth and positive function on $\mathbb{R}$. Therefore, by (2.24), each $c_{i,\Lambda}$ is smooth and positive on $\mathbb{R}$ and we complete the proof of (a).

To prove (b), we differentiate (2.44) with respect to ϕ and obtain

$$(D_\Lambda + \Lambda G)\frac{\mathrm{d}\mathbf{c}_\Lambda}{\mathrm{d}\phi} = -\mathbf{z} \quad \text{for } \phi\in\mathbb{R}, \tag{2.46}$$

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where $D_\Lambda = \operatorname{diag}((c_{0,\Lambda})^{-1}, \cdots, (c_{I,\Lambda})^{-1})$ is positive definite, $G = [\lambda_0 \ \cdots \ \lambda_I]^\mathsf{T}[\lambda_0 \ \cdots \ \lambda_I]$, $\mathbf{c}_\Lambda = [c_{0,\Lambda} \ \cdots \ c_{I,\Lambda}]^\mathsf{T}$, and $\mathbf{z} = [z_0 \ \cdots \ z_I]^\mathsf{T}$. It is obvious that $D_\Lambda + \Lambda G$ is positive definite and invertible with inverse matrix $(D_\Lambda + \Lambda G)^{-1}$ which is also positive definite. Then (2.46) gives $\mathrm{d}\mathbf{c}_\Lambda/\mathrm{d}\phi = -(D_\Lambda + \Lambda G)^{-1}\mathbf{z}$, and $\mathrm{d}\tilde{f}_\Lambda/\mathrm{d}\phi$ becomes

$$\frac{\mathrm{d}\tilde{f}_\Lambda}{\mathrm{d}\phi} = \sum_{i=1}^{I} z_i \frac{\mathrm{d}c_{i,\Lambda}}{\mathrm{d}\phi} = \mathbf{z}^\mathsf{T} \frac{\mathrm{d}\mathbf{c}_\Lambda}{\mathrm{d}\phi} = -\mathbf{z}^\mathsf{T} \left(D_\Lambda + \Lambda G\right)^{-1} \mathbf{z} < 0 \quad \text{for } \phi \in \mathbb{R}.$$

Here we have used the fact that $\mathbf{z} \neq 0$ and we complete the proof of (b).

To prove (c), we first suppose that $z_k \geq 0$ for some $k \in \{0, \dots, I\}$. Then (2.44) implies

$$\sup_{\phi \geq 0} \ln c_{k,\Lambda}(\phi) = \sup_{\phi \geq 0} \left(\Lambda\lambda_k\tilde{\mu}_0 + \hat{\mu}_k - z_k\phi - \Lambda \sum_{j=0}^{I} \lambda_i\lambda_j c_{j,\Lambda}(\phi) \right) \leq \Lambda\lambda_k\tilde{\mu}_0 + \hat{\mu}_k < \infty,$$

and $\sup_{\phi \geq 0} c_{k,\Lambda}(\phi) \leq e^{\Lambda\lambda_k\tilde{\mu}_0 + \hat{\mu}_k}$. Here we have used the fact that $c_{i,\Lambda}(\phi) > 0$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \cdots, I$. Similarly, if $z_k \leq 0$ and $k \in \{0, 1, \dots, I\}$, then (2.44) implies

$$\sup_{\phi \leq 0} \ln c_{k,\Lambda}(\phi) = \sup_{\phi \leq 0} \left(\Lambda\lambda_k\tilde{\mu}_0 + \hat{\mu}_k - z_k\phi - \Lambda \sum_{j=0}^{I} \lambda_i\lambda_j c_{j,\Lambda}(\phi) \right) \leq \Lambda\lambda_k\tilde{\mu}_0 + \hat{\mu}_k < \infty,$$

and $\sup_{\phi \leq 0} c_{k,\Lambda}(\phi) \leq e^{\Lambda\lambda_k\tilde{\mu}_0 + \hat{\mu}_k}$. Hence the proof of (c)(i) is complete. To see (c)(ii), since $z_i z_j < 0$ for some $i, j \in \{1, \dots, I\}$, then both index sets $\mathcal{J}_1' = \{i : z_i > 0\}$ and $\mathcal{J}_2' = \{j : z_j < 0\}$ are nonempty. Now we claim that there exists $j_1 \in \mathcal{J}_1'$ such that $\limsup_{\phi \to -\infty} c_{j_1,\Lambda}(\phi) = \infty$. We prove this by contradiction. Suppose $\sup_{\phi \leq 0} c_{j,\Lambda}(\phi) < \infty$ for all $j \in \mathcal{J}_1'$. Then there exists $K_1 > 0$ such that $0 < c_{j,\Lambda}(\phi) < K_1$ for $\phi \leq 0$ and $j \in \mathcal{J}_1'$. By equation (2.44) and (c)(i), we have

$$\begin{aligned}
z_j\phi &= \Lambda\lambda_j\tilde{\mu}_0 + \hat{\mu}_j - \ln(c_{j,\Lambda}(\phi)) - \Lambda\lambda_j \sum_{k=0}^{I} \lambda_k c_{k,\Lambda}(\phi) \\
&\geq \Lambda\lambda_j\tilde{\mu}_0 + \hat{\mu}_j - \ln(K_1) - \Lambda\lambda_j \left(\sum_{k \in \mathcal{J}_1'} \lambda_k K_1 + \sum_{k \notin \mathcal{J}_1'} \lambda_k e^{\Lambda\lambda_k\tilde{\mu}_0 + \hat{\mu}_k} \right)
\end{aligned}$$

for $j \in \mathcal{J}_1'$ and $\phi \leq 0$, which leads a contradiction by letting $\phi \to -\infty$. Hence there exists $j_1 \in \mathcal{J}_1'$ such that $\limsup_{\phi \to -\infty} c_{j_1,\Lambda}(\phi) = \infty$. We also prove this by contradiction. Suppose $\sup_{\phi \geq 0} c_{j,\Lambda}(\phi) < \infty$ for all $j \in \mathcal{J}_2'$. Then there exists $K_2 > 0$ such that $0 < c_{j,\Lambda}(\phi) \leq K_2$ for $\phi \geq 0$ and $j \in \mathcal{J}_2'$. By equation (2.44) and (c)(i), we have

$$z_j\phi = \Lambda\lambda_j\tilde{\mu}_0 + \hat{\mu}_j - \ln(c_{j,\Lambda}(\phi)) - \Lambda\lambda_j \sum_{k=0}^{I} \lambda_k c_{k,\Lambda}(\phi)$$

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$$\geq \Lambda\lambda_j\tilde{\mu}_0 + \hat{\mu}_j - \ln(K_2) - \Lambda\lambda_j \left(\sum_{k\in\mathcal{J}_2'} \lambda_k K_2 + \sum_{k\notin\mathcal{J}_2'} \lambda_k e^{\Lambda\lambda_k\tilde{\mu}_0+\hat{\mu}_k} \right)$$

for $j \in \mathcal{J}_2'$ and $\phi \leq 0$, which leads a contradiction by letting $\phi \to \infty$. Hence there exists $j_2 \in \mathcal{J}_2'$ such that $\limsup_{\phi\to\infty} c_{j_2,\Lambda}(\phi) = \infty$. Therefore, the proof of (c)(ii) is complete.

Finally, we give the proof of (d). From (2.27), function $\tilde{f}_\Lambda$ can be denoted as

$$\tilde{f}_\Lambda(\phi) = \sum_{i\in\mathcal{J}_1'} z_i c_{i,\Lambda}(\phi) + \sum_{i\in\mathcal{J}_2'} z_i c_{i,\Lambda}(\phi) \quad \text{for } \phi \in \mathbb{R}. \tag{2.47}$$

Then by (c)(i), we note that

$$\sum_{i\in\mathcal{J}_1'} z_i c_{i,\Lambda}(\phi) \leq \sum_{i\in\mathcal{J}_1'} z_i e^{\Lambda\lambda_i\tilde{\mu}_0+\hat{\mu}_i} \quad \text{for } \phi \geq 0. \tag{2.48}$$

Moreover, by (c)(ii), there exists $i_2 \in \mathcal{J}_2'$ and a sequence $\{\phi_n\}_{n=1}^\infty$ with $\lim_{n\to\infty} \phi_n = \infty$ such that $\lim_{n\to\infty} z_{i_2} c_{i_2,\Lambda}(\phi_n) = -\infty$. Thus, by (2.47)–(2.48), we get

$$\tilde{f}_\Lambda(\phi_n) \leq \sum_{i\in\mathcal{J}_1'} z_i e^{\Lambda\lambda_i\tilde{\mu}_0+\hat{\mu}_i} + z_{i_2} c_{i_2,\Lambda}(\phi_n) \to -\infty \quad \text{as } n \to \infty,$$

which implies that $\lim_{\phi\to\infty} \tilde{f}_\Lambda(\phi) = -\infty$ because of the strict decrease of $\tilde{f}_\Lambda$ (see (b)). On the other hand, by (c)(i), we also note that

$$\sum_{i\in\mathcal{J}_2'} z_i c_{i,\Lambda}(\phi) \geq \sum_{i\in\mathcal{J}_2'} z_i e^{\Lambda\lambda_i\tilde{\mu}_0+\hat{\mu}_i} \quad \text{for } \phi \leq 0. \tag{2.49}$$

Moreover, by (c)(ii), there exists $i_1 \in \mathcal{J}_1'$ and a sequence $\{\phi_n\}_{n=1}^\infty$ with $\lim_{n\to\infty} \phi_n = -\infty$ such that $\lim_{n\to\infty} z_{i_1} c_{i_1,\Lambda}(\phi_n) = \infty$. Thus, by (2.47) and (2.49), we obtain

$$\tilde{f}_\Lambda(\phi_n) \geq z_{i_1} c_{i_1,\Lambda}(\phi_n) + \sum_{i\in\mathcal{J}_2'} z_i e^{\Lambda\lambda_i\tilde{\mu}_0+\hat{\mu}_i} \to \infty \quad \text{as } n \to \infty,$$

which implies that $\lim_{\phi\to-\infty} \tilde{f}_\Lambda(\phi) = \infty$ because of (b). Therefore, we conclude (d) and complete the proof of Proposition 2.7. □

2.2.4 Analysis of c_i^* and $\tilde{f}^*$ under (A3)–(A4)

In this section, we apply the implicit function theorem to show the existence of c_i^* and use the implicit function theorem on Banach space to show the convergence of

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$c_{0,\Lambda}$ as $\Lambda \to \infty$ (see Proposition 2.8). More precisely, we let $\delta = \Lambda^{-1}$ and $\tilde{c}_{0,\delta} = c_{0,\Lambda}$. Then by (2.25), function $\tilde{c}_{0,\delta}$ satisifes

$$\delta \ln(\tilde{c}_{0,\delta}(\phi)) + \lambda_0 \sum_{i=0}^{I} \lambda_i (\tilde{c}_{0,\delta}(\phi))^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\phi} = \lambda_0\tilde{\mu}_0 + \delta\hat{\mu}_0 \quad \text{for } \phi \in \mathbb{R}. \tag{2.50}$$

Notice that $\Lambda \to \infty$ is equivalent to $\delta \to 0^+$ so c_0^* also equals the limit $\lim\limits_{\delta\to 0^+} \tilde{c}_{0,\delta}$. Moreover, c_0^* satisfies (2.29) which is equation (2.50) with $\delta = 0$. Besides, by (2.24), functions c_i^* satisfy the equation (2.28) for $i = 1, \ldots, I$. The existence and uniqueness of equations (2.28)–(2.29) and the convergence of $\tilde{c}_{0,\delta}$ as $\delta \to 0^+$, i.e., the convergence of $c_{0,\Lambda}$ as $\Lambda \to \infty$, are proved in Proposition 2.8. Then by (2.24) and (2.27), we can obtain the convergence of $c_{i,\Lambda}$ and $\tilde{f}_\Lambda$ as $\Lambda \to \infty$.

Now we state Proposition 2.8 as follows.

Proposition 2.8. *Let $c_{i,\Lambda}$ be defined in (2.24)–(2.25) for $i = 0, 1, \ldots, I$ and $\Lambda > 0$ (cf. Proposition 2.7(a)).*

(a) Equations (2.28)–(2.29) have a unique solution $(c_0^*, \ldots, c_N^*)$ and each function $c_i^* = c_i^*(\phi)$ is a smooth and positive function for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$.

(b) $\lim\limits_{\Lambda\to\infty} \|c_{i,\Lambda} - c_i^*\|_{\mathcal{C}^m[a,b]} = 0$ for $i = 0, 1, \ldots, I$, $m \in \mathbb{N}$ and $a < b$.

Proof. We first observe that equations (2.28)–(2.29) can be solved by the following problem.

$$\sum_{j=0}^{I} \lambda_j (c_0^*(\phi))^{\lambda_j/\lambda_0} e^{\bar{\mu}_j - z_j\phi} - \tilde{\mu}_0 = 0 \quad \text{for } \phi \in \mathbb{R},$$

which can be represented by $g_2(c_0^*(\phi), \phi) = 0$ for $\phi \in \mathbb{R}$. Here the function g_2 is defined by

$$g_2(t, \phi) = \sum_{j=0}^{I} \lambda_j t^{\lambda_j/\lambda_0} e^{\bar{\mu}_j - z_j\phi} - \tilde{\mu}_0 \quad \text{for } t > 0 \text{ and } \phi \in \mathbb{R}.$$

Notice that, for any $\phi \in \mathbb{R}$, function g_2 is strictly increasing for $t > 0$, and the range of g_2 is entire space $\mathbb{R}$. Then there exists a unique positivie number $c_0^*(\phi)$ such that $g_2(c_0^*(\phi), \phi) = 0$ for $\phi \in \mathbb{R}$. Moreover, since g_2 is smooth for $t > 0$, $\phi \in \mathbb{R}$, and

$$\frac{\partial g_2}{\partial t}(t, \phi) = \frac{1}{\lambda_0} \sum_{j=0}^{I} \lambda_j^2 t^{(\lambda_j - \lambda_0)/\lambda_0} e^{\bar{\mu}_j - z_j\phi} > 0 \quad \text{for } t > 0 \text{ and } \phi \in \mathbb{R},$$

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then by the implicit function theorem (cf. [68, Theorem 3.3.1]), $c_0^*(\phi)$ is a smooth and positive function on $\mathbb{R}$. Therefore, by (2.28), we obtain the smooth and positive functions c_i^* for $i = 1, \ldots, I$, and complete the proof of (a).

To prove (b), we fix $m \in \mathbb{N}$, $a, b \in \mathbb{R}$ and $a < b$ arbitrarily. Let $\|\cdot\|_{\mathcal{C}^m} := \|\cdot\|_{\mathcal{C}^m[a,b]}$ for notational convenience. For $\Lambda > 0$, let $\delta = \Lambda^{-1}$, $\tilde{c}_{0,\delta} = c_{0,\Lambda}$, $w_\delta = \ln(\tilde{c}_{0,\delta})$, and $w^* = \ln(c_0^*)$. Obviously, $\delta \to 0^+$ is equivalent to $\Lambda \to \infty$. Hence by (2.24), it suffices to show that $\lim\limits_{\delta\to 0^+} \|e^{w_\delta} - e^{w^*}\|_{\mathcal{C}^m} = 0$. Because $w_\delta = \ln(\tilde{c}_{0,\delta})$ and $\tilde{c}_{0,\delta} = c_{0,\Lambda}$, equation (2.50) can be denoted as $K_2(w_\delta(\phi), \delta) = 0$ for $\delta > 0$ and $\phi \in [a, b]$, where K_2 is a $\mathcal{C}^1$-function on $\mathcal{C}^m[a, b] \times \mathbb{R}$ defined by

$$K_2(w(\phi), \delta) = \delta w(\phi) + \lambda_0 \sum_{i=0}^{I} \lambda_i \exp\left(\frac{\lambda_i}{\lambda_0} w(\phi) + \bar{\mu}_i - z_i\phi\right) - \lambda_0\tilde{\mu}_0 - \delta\hat{\mu}_0 \qquad (2.51)$$

for all $w \in \mathcal{C}^m[a, b]$ and $\phi \in [a, b]$. Note that $K_2(w^*, 0) = 0$ by (a). A direct calculation for Fréchet derivative of (2.51) gives

$$D_w K_2(w(\phi), \delta) = \delta + \sum_{i=0}^{I} \lambda_i^2 \exp\left(\frac{\lambda_i}{\lambda_0} w(\phi) + \bar{\mu}_i - z_i\phi\right)$$

for all $w \in \mathcal{C}^m[a, b]$ and $\phi \in [a, b]$. By (a), we get

$$D_w K_2(w^*(\phi), 0) = \sum_{i=0}^{I} \lambda_i^2 (c_0^*(\phi))^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\phi} > 0 \quad \text{for } \phi \in [a, b].$$

Here we have used the fact that $w^* = \ln(c_0^*)$. This implies that $D_w K_2(w^*, 0)I$ is a bounded and invertible limear map on the Banach space $\mathcal{C}^m[a, b]$, where I is an identity map. Hence by the implicit function theorem on Banach space (cf. [21, Corollary 15.1]), there exists an open subset $B_{\delta_0}(w^*) \times (-\delta_0, \delta_0) \subsetneq \mathcal{C}^m[a, b] \times \mathbb{R}$ and a unique $\mathcal{C}^1$-function $\tilde{w}(\cdot, \delta)$ of $\delta \in (-\delta_0, \delta_0)$ with $\tilde{w}(\cdot, \delta) \in B_{\delta_0}(w^*) \subset \mathcal{C}^m[a, b]$ for $\delta \in (-\delta_0, \delta_0)$ such that $K_2(\tilde{w}(\cdot, \delta), \delta) = 0$ for all $\delta \in (-\delta_0, \delta_0)$, which gives $\lim\limits_{\delta\to 0^+} \|\tilde{w}(\cdot, \delta) - w^*\|_{\mathcal{C}^m} = 0$. By Proposition 2.7(a), equation $K_2(w, \delta) = 0$ has a unique solution $w = w_\delta$, which implies $\tilde{w}(\cdot, \delta) = w_\delta(\cdot)$ for $\delta \in (-\delta_0, \delta_0)$. Therefore, we obtain $\lim\limits_{\delta\to 0^+} \|w_\delta - w^*\|_{\mathcal{C}^m} = 0$, i.e., $\lim\limits_{\delta\to 0^+} \|e^{w_\delta} - e^{w^*}\|_{\mathcal{C}^m} = 0$, and complete the proof of Proposition 2.8(b). □

Corollary 2.9. $\lim\limits_{\Lambda\to\infty} \|\tilde{f}_\Lambda - \tilde{f}^*\|_{\mathcal{C}^m[a,b]} = 0$ *for* $m \in \mathbb{N}$ *and* $a < b$.

Proof. It follows from Proposition 2.8(b) and the fact that $\tilde{f}_\Lambda(\phi) = \sum\limits_{i=1}^{I} z_i c_{i,\Lambda}(\phi)$ and $\tilde{f}^*(\phi) = \sum\limits_{i=1}^{I} z_i c_i^*(\phi)$ for $\phi \in \mathbb{R}$. □

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For function $\tilde{f}^*$, we have the following propositions.

Proposition 2.10. *Let $\tilde{f}^*$ be defined in (2.30).*

(a) Function $\tilde{f}^*$ is strictly decreasing on $\mathbb{R}$.

(b) Function $\tilde{f}^*$ satisfies $m^* < \tilde{f}^*(\phi) < M^*$ for all $\phi \in \mathbb{R}$, where

$$m^* = \lim_{\phi\to\infty} \tilde{f}^*(\phi) < 0 \text{ and } M^* = \lim_{\phi\to-\infty} \tilde{f}^*(\phi) > 0.$$

Proof. Differentiating (2.28)–(2.29) with respect to ϕ gives

$$\sum_{j=0}^{I} \lambda_j \frac{\mathrm{d}c_j^*}{\mathrm{d}\phi} = 0, \quad \frac{\mathrm{d}c_i^*}{\mathrm{d}\phi} = \frac{\lambda_i}{\lambda_0}\frac{c_i^*}{c_0^*}\frac{\mathrm{d}c_0^*}{\mathrm{d}\phi} - z_i c_i^*, \quad \text{for } \phi \in \mathbb{R} \text{ and } i = 1, \ldots, I,$$

which implies $\dfrac{\mathrm{d}c_0^*}{\mathrm{d}\phi} = \lambda_0 c_0^* \dfrac{\sum_{i=1}^{I} z_i \lambda_i c_i^*}{\sum_{i=0}^{I} \lambda_i^2 c_i^*}$ for $\phi \in \mathbb{R}$. Consequently, we have

$$\frac{\mathrm{d}\tilde{f}^*}{\mathrm{d}\phi} = \sum_{i=1}^{I} z_i \frac{\mathrm{d}c_i^*}{\mathrm{d}\phi} = \frac{1}{\lambda_0 c_0^*}\frac{\mathrm{d}c_0^*}{\mathrm{d}\phi}\sum_{i=1}^{I} z_i\lambda_i c_i^* - \sum_{i=1}^{I} z_i^2 c_i^* = \frac{\left(\sum_{i=1}^{I} z_i \lambda_i c_i^*\right)^2}{\sum_{i=0}^{I} \lambda_i^2 c_i^*} - \sum_{i=1}^{I} z_i^2 c_i^* < 0$$

for $\phi \in \mathbb{R}$. Here the last inequality comes from the Cauchy–Schwarz inequality and the fact that $\lambda_i > 0$, $c_i^* > 0$ for $i \in \{0, 1, \ldots, I\}$, and $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$. Therefore, we complete the proof of (a).

To prove boundedness of $\tilde{f}^*$, we note that (2.28)–(2.29) imply $0 < c_i^*(\phi) < \tilde{\mu}_0/\lambda_i$ for $\phi \in \mathbb{R}$ and $i = 0, 1, \ldots, I$, and

$$|\tilde{f}^*(\phi)| \le \sum_{i=1}^{I} |z_i| c_i^*(\phi) \le \tilde{\mu}_0 \sum_{i=1}^{I} \frac{|z_i|}{\lambda_i} \le \tilde{\mu}_0 I \max_{0\le i\le I} \frac{|z_i|}{\lambda_i} \quad \text{for } \phi \in \mathbb{R}. \tag{2.52}$$

On the other hand, by (2.29) and (2.30), function $\tilde{f}^*$ can be represented as

$$\tilde{f}^*(\phi) = \sum_{i=1}^{I} z_i (c_0^*(\phi))^{\lambda_i/\lambda_0} \exp(\bar{\mu}_i - z_i\phi) \quad \text{for } \phi \in \mathbb{R}. \tag{2.53}$$

By (a) and (2.52), function $\tilde{f}^*$ is strictly decreasing and bounded on $\mathbb{R}$ so the limit $\lim_{\phi\to\infty} \tilde{f}^*(\phi)$, denoted by m^*, exists and is finite. Since $c_i^* < \tilde{\mu}_0/\lambda_i$ for $i = 0, 1 \ldots, I$, (2.28) implies

$$\lim_{\phi\to\infty} c_0^*(\phi) = \lim_{\phi\to\infty} [c_i^*(\phi)\exp(-\bar{\mu}_i + z_i\phi)]^{\lambda_0/\lambda_i} = 0 \quad \text{for } z_i < 0. \tag{2.54}$$

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Moreover, we use (2.28) and (2.54) to get

$$\lim_{\phi\to\infty} c_i^*(\phi) = \lim_{\phi\to\infty} \left[(c_0^*(\phi))^{\lambda_i/\lambda_0}\exp(\bar{\mu}_i - z_i\phi)\right] = 0 \quad \text{for } z_i > 0, \tag{2.55}$$

and hence (2.53) and (2.55) imply $m^* = \lim_{\phi\to\infty} \tilde{f}^*(\phi) \leq 0$. Now, we prove $m^* < 0$ by contradiction. Suppose $m^* = 0$. Then (2.55) gives $\lim_{\phi\to\infty} c_i^*(\phi) = 0$ for $i = 0, 1, \ldots, I$, which contradicts with (2.29) (by letting $\phi \to \infty$) and $\tilde{\mu}_0 > 0$. Similarly, we may prove $\lim_{\phi\to-\infty} \tilde{f}^*(\phi) = M^* > 0$ and complete the proof of Proposition 2.10. □

2.3 Proof of Theorems 2.1 and 2.2

Since f_Λ and $\tilde{f}_\Lambda$ are unbounded on $\mathbb{R}$ but f^* and $\tilde{f}^*$ are bounded on $\mathbb{R}$ so we cannot obtain the uniform convergence of f_Λ and $\tilde{f}_\Lambda$ on $\mathbb{R}$ as Λ goes to infinity (see Propositions 2.1, 2.6, 2.7 and 2.10). In order to use the convergence of f_Λ and $\tilde{f}_\Lambda$ in space $\mathcal{C}^m[a,b]$ for $m \in \mathbb{N}$ and $a < b$, we first have to prove the uniform boundedness of ϕ_Λ (the solution to (2.21) and (2.26)) with respect to Λ (see Lemmas 2.11 and 2.13). Here we notice that ρ_0 may be any nonzero smooth function and the boundary condition may be the Robin boundary condition but not Dirichlet boundary condition so one cannot simply use the maximum principle on (2.19) and (2.20) to obtain the uniform boundedness of ϕ_Λ.

2.3.1 Uniform boundedness of ϕ_Λ and $c_{0,\Lambda}(\phi_\Lambda)$ under (A1)—(A2)

Lemma 2.11. *There exist positive constants $M_1 \geq 1$, M_2, and M_3 independent of Λ such that*

(a) $\max_{x\in\overline{\Omega}} c_{0,\Lambda}(\phi_\Lambda(x)) \leq M_1$ *for* $\Lambda \geq 1$.

(b) $\|\phi_\Lambda\|_{L^\infty(\Omega)} \leq M_2$ *for* $\Lambda \geq 1$.

(c) $\min_{x\in\overline{\Omega}} c_{0,\Lambda}(\phi_\Lambda(x)) \geq M_3$ *for* $\Lambda \geq 1$.

Proof. Since $z_i z_j < 0$ for some $i, j \in \{1, \ldots, I\}$, then $\lim_{\phi\to\pm\infty} \sum_{i=1}^{I} e^{\bar{\mu}_i - z_i\phi} = \infty$, and

$$K := (\tilde{\mu}_0 + \hat{\mu}_0) \Big/ \left(1 - \gamma + \frac{\gamma}{Z}\min_{\phi\in\mathbb{R}} \sum_{i=1}^{I} \exp(\bar{\mu}_i - z_i\phi)\right) < \infty.$$

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Let $M_1 = \max\{K, 1\}$ and $\Lambda \geq 1$. We claim that $c_{0,\Lambda}(\phi_\Lambda(x)) \leq M_1$. Suppose that $\Omega_1 = \{x \in \overline{\Omega} : c_{0,\Lambda}(\phi_\Lambda(x)) > 1\}$ is nonempty. Otherwise, due to $M_1 \geq 1$, $c_{0,\Lambda}(\phi_\Lambda(x)) \leq 1 \leq M_1$ for $x \in \overline{\Omega}$, which is trivial. By (2.17), we have

$$c_{0,\Lambda}(\phi_\Lambda(x)) \leq \frac{\tilde{\mu}_0 + \Lambda^{-1}\hat{\mu}_0}{H(\gamma, z_1, \ldots, z_I, \phi_\Lambda(x))} \leq K \leq M_1 \quad \text{for } x \in \Omega_1.$$

Here we have used the fact that $\ln(c_{0,\Lambda}(\phi_\Lambda(x))) > 0$ for $x \in \Omega_1$ and $\Lambda \geq 1$. Therefore, we complete the proof of (a).

To prove (b), let ψ be the solution to equation $-\nabla \cdot (\varepsilon \nabla \psi) = \rho_0$ in Ω with the Robin boundary condition $\psi + \eta \frac{\partial \psi}{\partial \nu} = 0$ on $\partial\Omega$, and let $\bar{\phi}_\Lambda = \phi_\Lambda - \psi$. Then function $\bar{\phi}_\Lambda$ satisfies

$$-\nabla \cdot (\varepsilon \nabla \bar{\phi}_\Lambda) = f_\Lambda(\phi_\Lambda) \quad \text{in } \Omega. \tag{2.56}$$

Since ψ is independent of Λ and is continuous on $\overline{\Omega}$, then $\bar{\phi}_\Lambda$ is uniformly bounded if and only if ϕ_Λ is uniformly bounded, it suffices to show that $\max\limits_{\overline{\Omega}} \bar{\phi}_\Lambda \leq M_2$ and $\min\limits_{\overline{\Omega}} \bar{\phi}_\Lambda \geq -M_2$ for $\Lambda \geq 1$, where M_2 is a positive constant independent of Λ.

Now we prove that $\max\limits_{\overline{\Omega}} \bar{\phi}_\Lambda \leq M_2$ for $\Lambda \geq 1$, where M_2 is a positive constant independent of Λ. Suppose by contradiction that there exists a sequence Λ_k with $\lim\limits_{k\to\infty} \Lambda_k = \infty$ such that $\max\limits_{\overline{\Omega}} \bar{\phi}_{\Lambda_k} \geq k$ for $k \in \mathbb{N}$. Then there exists $x_k \in \Omega$ such that $\bar{\phi}_{\Lambda_k}(x_k) = \max\limits_{\overline{\Omega}} \bar{\phi}_{\Lambda_k}$, which implies $\nabla \bar{\phi}_{\Lambda_k}(x_k) = 0$ and $\Delta \bar{\phi}_{\Lambda_k}(x_k) \leq 0$. Note that because of the Robin boundary condition of $\bar{\phi}_{\Lambda_k}$, maximum point x_k cannot be located on the boundary $\partial\Omega$ as k sufficiently large. Hence without loss of generality, we assume each $x_k \in \Omega$ for $k \in \mathbb{N}$. For the sake of simplicity, in this proof, we set $c_{i,k} := c_{i,\Lambda_k}$, $\phi_k := \phi_{\Lambda_k}$, $f_k := f_{\Lambda_k}$, and $\bar{\phi}_k := \bar{\phi}_{\Lambda_k}$. By (2.56) with $\nabla \bar{\phi}_k(x_k) = 0$, $\Delta \bar{\phi}_k(x_k) \leq 0$ and function ε is positive, we have

$$0 \leq -\nabla \varepsilon(x_k) \cdot \nabla \bar{\phi}_k(x_k) - \varepsilon(x_k) \Delta \bar{\phi}_k(x_k) = f_k(\phi_k(x_k)). \tag{2.57}$$

Since $f_k(\phi_k) = \sum\limits_{i=1}^{I} z_i c_{i,k}(\phi_k)$, we can use (2.57) to get

$$0 < \sum_{z_i<0} (-z_i) c_{i,k}(\psi(x_k) + \bar{\phi}_k(x_k)) \leq \sum_{z_i>0} z_i c_{i,k}(\psi(x_k) + \bar{\phi}_k(x_k)). \tag{2.58}$$

By Proposition 2.1(c)(ii) and (2.58), $\lim\limits_{k\to\infty} \sum\limits_{z_i<0} (-z_i) c_{i,k}(\psi(x_k) + \bar{\phi}_k(x_k)) = 0$. This leads a contradiction with Proposition 2.1(c)(ii). Hence we complete the proof to show that $\max\limits_{\overline{\Omega}} \bar{\phi}_\Lambda \leq M_2$ for $\Lambda \geq 1$, where M_2 is a positive constant independent of Λ.

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On the other hand, we prove $\min_{\overline{\Omega}} \bar{\phi}_\Lambda \geq -M_2$ for $\Lambda \geq 1$. Suppose by contradiction that there exists a sequence Λ_k with $\lim_{k\to\infty} = \infty$ such that $\min_{\overline{\Omega}} \bar{\phi}_k \leq -k$ for $k \in \mathbb{N}$. Then there exists $x_k \in \Omega$ such that $\bar{\phi}_{\Lambda_k}(x_k) = \min_{\overline{\Omega}} \bar{\phi}_k$, which implies $\nabla\bar{\phi}_k(x_k) = 0$ and $\Delta\bar{\phi}_k(x_k) \geq 0$. Note that because of the Robin boundary condition of $\bar{\phi}_k$, minimum point x_k cannot be located on the boundary $\partial\Omega$ as k sufficiently large. Hence without loss of generality, we assume each $x_k \in \Omega$ for $k \in \mathbb{N}$. As in (2.58), we have

$$0 < \sum_{z_i>0} z_i c_{i,k}(\psi(x_k) + \bar{\phi}_k(x_k)) \leq \sum_{z_i<0} (-z_i) c_{i,k}(\psi(x_k) + \bar{\phi}_k(x_k)). \tag{2.59}$$

By Proposition 2.1(c)(i) and (2.59), $\lim_{k\to\infty} \sum_{z_i>0} z_i c_{i,k}(\psi(x_k)+\bar{\phi}_k(x_k)) = 0$. This leads a contradiction with Proposition 2.1(c)(i). Hence we complete the proof to show that $\min_{\overline{\Omega}} \bar{\phi}_\Lambda \geq -M_2$ for $\Lambda \geq 1$, where M_2 is a positive constant independent of Λ. Thus, the proof of (b) is complete.

Finally, we state the proof of (c). Suppose to the contrary that there exists Λ_k with $\lim_{k\to\infty} \Lambda_k = \infty$, and $x_k \in \overline{\Omega}$ is the minimum point of $c_{0,\Lambda_k}(\phi_{\Lambda_k}(x))$ such that $\lim_{k\to\infty} c_{0,\Lambda_k}(\phi_{\Lambda_k}(x_k)) = 0$. Notice that by (2.17), $c_{0,\Lambda}(\phi_\Lambda) > 0$ for $\Lambda \geq 1$ and $x \in \overline{\Omega}$. Then there exists $N_1 \in \mathbb{N}$ such that $\ln(c_{0,\Lambda_k}(\phi_{\Lambda_k}(x_k))) < 0$ for $k > N_1$. By (2.17) with $\phi = \phi_{\Lambda_k}(x_k)$, we get

$$H(\gamma, z_1, \ldots, z_I, \phi_{\Lambda_k}(x_k)) c_{0,\Lambda_k}(\phi_{\Lambda_k}(x_k)) > \tilde{\mu}_0 + \frac{\hat{\mu}_0}{\Lambda_k} \quad \text{for } k > N_1. \tag{2.60}$$

Taking $k \to \infty$, (2.60) and (b) imply $0 \geq \tilde{\mu}_0$, which contradicts assumption (A2). Therefore, we complete the proof of (c). The proof of Lemma 2.11 is complete. □

Remark 2.6. *By Lemma 2.11 and (2.16), we have $M_4 \leq c_{i,\Lambda}(\phi_\Lambda(x)) \leq M_5$ for $x \in \overline{\Omega}$, $\Lambda \geq 1$ and $i = 0, 1, \ldots, I$, where M_4 and M_5 are positive constants independent of Λ. Moreover, due to $f_\Lambda(\phi_\Lambda) = \sum_{i=1}^{I} z_i c_{i,\Lambda}(\phi_\Lambda)$, there exists a positive constant M_6 independent of Λ such that $\|f_\Lambda(\phi_\Lambda)\|_{L^\infty(\overline{\Omega})} \leq M_6$ for $\Lambda \geq 1$.*

2.3.2 Convergence of ϕ_Λ under (A1)–(A2)

Since ϕ_Λ is the solution to equation $-\nabla \cdot (\varepsilon\nabla\phi_\Lambda) = \rho_0 + f_\Lambda(\phi_\Lambda)$ in Ω with the Robin boundary condition $\phi_\Lambda + \eta\frac{\partial\phi_\Lambda}{\partial\nu} = \phi_{bd}$ on $\partial\Omega$, we use the $W^{2,p}$ estimate (cf. [2, Theorem 15.2]) to get $\|\phi_\Lambda\|_{W^{2,p}(\Omega)} \leq C(\|\rho_0 + f_\Lambda(\phi_\Lambda)\|_{L^p(\Omega)} + \|\phi_{bd}\|_{W^{1,p}(\Omega)})$ for all $p > 1$, where C is a positive constant independent of Λ. Hence by Remark 2.6, we

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have the uniform bound estimate of ϕ_Λ in $W^{2,p}$ norm. This implies that there exists a sequence of functions $\{\phi_{\Lambda_k}\}_{k=1}^{\infty}$, with $\lim_{k\to\infty}\Lambda_k=\infty$, such that ϕ_{Λ_k} converges to ϕ^* weakly in $W^{2,p}(\Omega)$. By Corollary 2.5, we have the convergence of function f_{Λ_k} to f^* in $\mathcal{C}^m[-M_2,M_2]$ for $m\in\mathbb{N}$, so ϕ^* satisfies (2.20) in a weak sense, where the positive constant M_2 comes from Lemma 2.11(b). Let $w_k=\phi_{\Lambda_k}-\phi^*$, $c_{i,k}:=c_{i,\Lambda_k}$, and $f_k:=f_{\Lambda_k}$. Then by Sobolev embedding, $w_k\in\mathcal{C}^{1,\alpha}(\overline{\Omega})$ for $\alpha\in(0,1)$, and $\lim_{k\to\infty}\|w_k\|_{\mathcal{C}^{1,\alpha}(\overline{\Omega})}=0$. Moreover, w_k satisfies $-\nabla\cdot(\varepsilon\nabla w_k)=f_k(w_k+\phi^*)-f^*(\phi^*)$ in Ω with the boundary condition $w_k+\eta\frac{\partial w_k}{\partial\nu}=0$ on $\partial\Omega$. Using the Schauder's estimate (cf. [38, Theorem 6.30]) with the mathematical induction, we get

$$\begin{aligned}&\|w_k\|_{\mathcal{C}^{m+2,\alpha}(\overline{\Omega})}\leq C\|f_k(w_k+\phi^*)-f^*(\phi^*)\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}\\ &\leq C'\sum_{i=1}^{I}\left(\|c_{i,k}(w_k+\phi^*)-c_i^*(w_k+\phi^*)\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}+\|c_i^*(w_k+\phi^*)-c_i^*(\phi^*)\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}\right),\end{aligned} \tag{2.61}$$

for all $m\in\mathbb{N}$ and $\alpha\in(0,1)$, where C and C' are positive constants independent of k. By Proposition 2.6(a) and induction hypothesis $\lim_{k\to\infty}\|w_k\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}=0$, we may use (2.61) to get $\lim_{k\to\infty}\|w_k\|_{\mathcal{C}^{m+2,\alpha}(\overline{\Omega})}=0$, i.e. $\lim_{k\to\infty}\|\phi_{\Lambda_k}-\phi^*\|_{\mathcal{C}^{m+2,\alpha}(\overline{\Omega})}=0$ for $m\in\mathbb{N}$ and $\alpha\in(0,1)$. Therefore, ϕ^* is the solution to (2.23) with the Robin boundary condition (2.15). To complete the proof of Theorem 2.1, we need to prove the following claim.

Claim 2.12. *For any $m\in\mathbb{N}$, we have $\lim_{\Lambda\to\infty}\|\phi_\Lambda-\phi^*\|_{\mathcal{C}^m(\overline{\Omega})}=0$.*

Proof. Suppose that there exist the sequences $\{\Lambda_k\}$ and $\{\tilde{\Lambda}_k\}$ tending to infinity such that sequences $\{\phi_{\Lambda_k}\}$ and $\{\phi_{\tilde{\Lambda}_k}\}$ have limits ϕ_1^* and ϕ_2^*, respectively. It is clear that ϕ_1^* and ϕ_2^* satisfy (2.23) with the Robin boundary condition (2.15). Now we want to prove that $\phi_1^*\equiv\phi_2^*$. Let $u=\phi_1^*-\phi_2^*$. Subtracting (2.23) with $\phi^*=\phi_2^*$ from that with $\phi^*=\phi_1^*$, we obtain $-\nabla\cdot(\varepsilon\nabla u)=c_1(x)u$ in Ω, where

$$c_1(x)=\begin{cases}\dfrac{f^*(\phi_1^*(x))-f^*(\phi_2^*(x))}{\phi_1^*(x)-\phi_2^*(x)} & \text{if } \phi_1^*(x)\neq\phi_2^*(x);\\ \dfrac{\mathrm{d}f^*}{\mathrm{d}\phi}(\phi_1^*(x)) & \text{if } \phi_1^*(x)=\phi_2^*(x).\end{cases}$$

By Proposition 2.6, we have $c_1<0$ in Ω which comes from the fact that if f is a strictly decreasing function on $\mathbb{R}$, then $\frac{f(\alpha)-f(\beta)}{\alpha-\beta}<0$ for $\alpha\neq\beta$. Since $\nabla\cdot(\varepsilon\nabla u)+c_1(x)u=0$ with $c_1<0$ in Ω, it is obvious that u cannot be a nonzero constant. Then by the strong maximum principle, we have that u attains its nonnegative maximum value and nonpositive minimum value at the boundary point. Suppose

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u has nonnegative maximum value and attains its maximum value at $x^* \in \partial\Omega$. Then by the boundary condition of u which is $u + \eta\frac{\partial u}{\partial \nu} = 0$ on $\partial\Omega$, we get $u(x^*) = -\eta\frac{\partial u}{\partial \nu}(x^*) \leq 0$, and hence $u \leq u(x^*) \leq 0$ on $\overline{\Omega}$. Similarly, we obtain $u \geq 0$ in $\overline{\Omega}$, and hence $u \equiv 0$. Therefore, we conclude that $\phi_1^* \equiv \phi_2^*$ and complete the proof of Theorem 2.1. □

2.3.3 Uniform boundedness of ϕ_Λ and $c_{0,\Lambda}(\phi_\Lambda)$ under (A3)—(A4)

Lemma 2.13. *There exist positive constants $M_7 \geq 1$, M_8, and M_9 independent of Λ such that*

(a) $\max_{x\in\overline{\Omega}} c_{0,\Lambda}(\phi_\Lambda(x)) \leq M_7$ *for* $\Lambda \geq 1$.

(b) $\|\phi_\Lambda\|_{L^\infty(\Omega)} \leq M_8$ *for* $\Lambda \geq 1$.

(c) $\min_{x\in\overline{\Omega}} c_{0,\Lambda}(\phi_\Lambda(x)) \geq M_9$ *for* $\Lambda \geq 1$.

Proof. Let $M_7 = \max\left\{\frac{\tilde{\mu}_0}{\lambda_0} + \frac{\hat{\mu}_0}{\lambda_0^2}, 1\right\} \geq 1$ and $\Lambda \geq 1$. We claim that $c_{0,\Lambda}(\phi_\Lambda(x)) \leq M_7$ for $x \in \overline{\Omega}$. Suppose that $\Omega_1 = \{x \in \overline{\Omega} : c_{0,\Lambda}(\phi_\Lambda(x) > 1\}$ is nonempty. Otherwise, due to $M_7 \geq 1$, $c_{0,\Lambda}(\phi_\Lambda(x)) \leq 1 \leq M_7$ for $x \in \overline{\Omega}$, which is trivial. By (2.25) and (A4), we obtain

$$c_{0,\Lambda}(\phi_\Lambda(x)) \leq \frac{\tilde{\mu}_0}{\lambda_0} + \frac{\hat{\mu}_0}{\Lambda\lambda_0^2} \leq M_7 \quad \text{for } x \in \Omega_1.$$

Here we ahve used the fact that $\ln c_{0,\Lambda}(\phi_\Lambda(x)) > 0$ for $x \in \Omega_1$, $\Lambda \geq 1$, and $z_0 = \bar{\mu}_0 = 0$. Therefore, we complete the proof of (a).

To prove (b), let ψ be the solution to equation $-\nabla \cdot (\varepsilon\nabla\psi) = \rho_0$ with the Robin boundary condition $\psi + \eta\frac{\partial\psi}{\partial\nu} = 0$ on $\partial\Omega$, and let $\bar{\phi}_\Lambda = \phi_\Lambda - \psi$. Then function $\bar{\phi}_\Lambda$ satisfies

$$-\nabla \cdot (\varepsilon\nabla\bar{\phi}_\Lambda) = f_\Lambda(\phi_\Lambda) \quad \text{in } \Omega. \tag{2.62}$$

By (2.24), $c_{i,\Lambda}(\phi_\Lambda)$ satisfies

$$c_{i,\Lambda}(\phi_\Lambda) = (c_{0,\Lambda}(\phi_\Lambda))^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\psi - z_i\bar{\phi}_\Lambda} \quad \text{for } i = 1, \ldots, I. \tag{2.63}$$

Since ψ is independent of Λ and is continuous on $\overline{\Omega}$, then $\bar{\phi}_\Lambda$ is uniformly bounded if and only if ϕ_Λ is uniformyl bounded, and it suffices to show that $\max_{x\in\overline{\Omega}} \bar{\phi}_\Lambda(x) \leq M_8$ and $\min_{x\in\overline{\Omega}} \bar{\phi}_\Lambda \geq -M_8$ for $\Lambda \geq 1$, where M_8 is a positive constant independent of Λ.

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Now we prove that $\max_{x\in\overline{\Omega}} \bar{\phi}_\Lambda(x) \leq M_8$ for $\Lambda \geq 1$, where M_8 is a positive constant independent of Λ. Suppose by contradiction that there exists a sequence Λ_k with $\lim_{k\to\infty} \Lambda_k = \infty$ such that $\max_{\overline{\Omega}} \bar{\phi}_{\Lambda_k} \geq k$ for $k \in \mathbb{N}$. Then there exists $x_k \in \Omega$ such that $\bar{\phi}_{\Lambda_k}(x_k) = \max_{\overline{\Omega}} \bar{\phi}_{\Lambda_k}$, which implies $\nabla\bar{\phi}_{\Lambda_k}(x_k) = 0$ and $\Delta\bar{\phi}_{\Lambda_k}(x_k) \leq 0$. Note that because of the Robin boundary condition of $\bar{\phi}_{\Lambda_k}$, maximum point x_k cannot be located on the boundary $\partial\Omega$ as k sufficiently large. Hence without loss of generality, we assume each $x_k \in \Omega$ for $k \in \mathbb{N}$. For a sake of simplicity, in this proof, we set $c_{i,k} := c_{i,\Lambda_k}$, $\phi_k := \phi_{\Lambda_k}$, $f_k := f_{\Lambda_k}$, and $\bar{\phi}_k := \bar{\phi}_{\Lambda_k}$. Hence by equation (2.62) with $\nabla\bar{\phi}_k(x_k) = 0$, $\Delta\bar{\phi}_k(x_k) \leq 0$ and function ε is positive, we have

$$0 \leq -\nabla\varepsilon(x_k)\cdot\nabla\bar{\phi}_k(x_k) - \varepsilon(x_k)\Delta\bar{\phi}_k(x_k) = f_k(\phi_k(x_k)). \tag{2.64}$$

Since $f_k(\phi_k) = \sum_{i=1}^{I} z_i c_{i,k}(\phi_k)$, we can use (2.63) and (2.64) to get

$$\begin{aligned} 0 &< \sum_{z_i<0}(-z_i)[c_{0,k}(\phi_k(x_k))]^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\psi(x_k) - z_i\bar{\phi}_k(x_k)} \\ &\leq \sum_{z_i>0} z_i[c_{0,k}(\phi_k(x_k))]^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\psi(x_k) - z_i\bar{\phi}_k(x_k)}. \end{aligned} \tag{2.65}$$

Applying (a) to (2.63) for $z_i > 0$, we obtain $\lim_{k\to\infty} c_{i,k}(\phi_k(x_k)) = 0$ for all i with $z_i > 0$. Together with (2.65), it follows that

$$\lim_{k\to\infty} \sum_{z_i<0}(-z_i)[c_{0,k}(\phi_k(x_k))]^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\psi(x_k) - z_i\bar{\phi}_k(x_k)} = 0,$$

which means $\lim_{k\to\infty} c_{i,k}(\phi_k(x_k)) = 0$ for all i with $z_i < 0$. Inserting $x = x_k$ into (2.63) with $z_i < 0$, we obtain

$$c_{0,k}(\phi_k(x_k)) = [c_{i,k}(\phi_k(x_k))]^{\lambda_0/\lambda_i}[e^{\bar{\mu}_i - z_i\psi(x_k) - z_i\bar{\phi}_k(x_k)}]^{\lambda_0/\lambda_i} \to 0 \quad \text{as } k \to \infty.$$

Hence $\lim_{k\to\infty} c_{i,k}(\phi_k(x_k)) = 0$ for $i = 0, 1, \ldots, I$. By (2.24)–(2.25), we get the following contradiction:

$$0 \geq \lim_{k\to\infty} \frac{\ln(c_{0,k}(\phi_k(x_k)))}{\Lambda_k} = \lim_{k\to\infty}\left(\lambda_0\tilde{\mu}_0 + \frac{\hat{\mu}_0}{\Lambda_k} - \sum_{i=0}^{I}\lambda_0\lambda_i c_{i,k}(\phi_k(x_k))\right) = \lambda_0\tilde{\mu}_0 > 0. \tag{2.66}$$

Thus, we complete the proof and show that $\max_{x\in\overline{\Omega}} \bar{\phi}_\Lambda(x) \leq M_8$, where M_8 is a positive constant independent of Λ.

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On the other hand, we prove $\min_{\overline{\Omega}} \bar{\phi}_\Lambda \geq -M_8$ for $\Lambda \geq 1$. Suppose by contradiction that there exists a sequence Λ_k with $\lim_{k\to\infty} = \infty$ such that $\min_{\overline{\Omega}} \bar{\phi}_k \leq -k$ for $k \in \mathbb{N}$. Then there exists $x_k \in \Omega$ such that $\bar{\phi}_k(x_k) = \min_{\overline{\Omega}} \bar{\phi}_k$, which implies $\nabla\bar{\phi}_k(x_k) = 0$ and $\Delta\bar{\phi}_k(x_k) \geq 0$. Notice that because of the Robin boundary condition of $\bar{\phi}_k$, minimum point x_k cannot be located on the boundary $\partial\Omega$ as k sufficiently large. Hence without loss of generality, we assume each $x_k \in \Omega$ for $k \in \mathbb{N}$. Thus, as in (2.65), we have

$$
\begin{aligned}
0 &< \sum_{z_i>0} z_i [c_{0,k}(\phi_k(x_k))]^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\psi(x_k) - z_i\bar{\phi}_k(x_k)} \\
&\leq \sum_{z_i<0} (-z_i)[c_{0,k}(\phi_k(x_k))]^{\lambda_i/\lambda_0} e^{\bar{\mu}_i - z_i\psi(x_k) - z_i\bar{\phi}_k(x_k)}
\end{aligned}
\tag{2.67}
$$

Applying (a) to (2.63) for $z_i < 0$, we obtain $\lim_{k\to\infty} c_{i,k}(\phi_k(x_k)) = 0$ for all i with $z_i < 0$. Then (2.63) and (2.67) give $\lim_{k\to\infty} c_{i,k}(\phi_k(x_k)) = 0$ for all i with $z_i > 0$. Inserting $x = x_k$ into (2.63) with $z_i > 0$, we have $\lim_{k\to\infty} c_{0,k}(\phi_k(x_k)) = 0$, and hence $\lim_{k\to\infty} c_{i,k}(\phi_k(x_k)) = 0$ for each $i = 0, 1, \ldots, I$. As in (2.66), we also get a contradiction and complete the proof to show that $\min_{x\in\overline{\Omega}} \bar{\phi}_\Lambda(x) \geq -M_8$ for $\Lambda \geq 1$, where M_8 is a positive constant independent of Λ. Therefore, we complete the proof of (b).

Finally, we state the proof of (c). Suppose to the contrary that there exists Λ_k with $\lim_{k\to\infty} \Lambda_k = \infty$, and $x_k \in \overline{\Omega}$ is the minimum point of $c_{0,\Lambda_k}(\phi_{\Lambda_k}(x_k))$ such that $\lim_{k\to\infty} c_{0,\Lambda_k}(\phi_{\Lambda_k}(x_k)) = 0$. Notice that by (2.25), $c_{0,\Lambda}(\phi_\Lambda(x)) > 0$ for $\Lambda \geq$ and $x \in \overline{\Omega}$. Then, there exists $N_1 \in \mathbb{N}$ such that $\ln(c_{0,\Lambda_k}(\phi_{\Lambda_k}(x_k))) < 0$ for $k > N_1$. By (2.24)–(2.25) at $\phi = \phi_{\Lambda_k}(x_k)$, we get

$$
\sum_{i=0}^{I} \lambda_i c_{i,\Lambda_k}(\phi_{\Lambda_k}(x_k)) > \tilde{\mu}_0 + \frac{\hat{\mu}_0}{\Lambda_k\lambda_0} \quad \text{for } k > N_1. \tag{2.68}
$$

On the other hand, by (2.63) and (b), we obtain $\lim_{k\to\infty} c_{i,\Lambda_k}(\phi_{\Lambda_k}(x_k)) = 0$ for $i = 0, 1, \ldots, I$, which contradicits (2.68) as $k \to \infty$. Hence we complete the proof of (c) and hence complete the proof Lemma 2.13. $\square$

Remark 2.7. *By Lemma 2.13 and (2.24), we have $M_{10} \leq c_{i,\Lambda}(\phi_\Lambda(x)) \leq M_{11}$ for $x \in \overline{\Omega}$, $\Lambda \geq 1$ and $i = 0, 1, \ldots, I$, where M_{10} and M_{11} are positive constants independent of Λ. Moreover, due to $\tilde{f}_\Lambda(\phi_\Lambda) = \sum_{i=1}^{I} z_i c_{i,\Lambda}(\phi_\Lambda)$, $\|\tilde{f}_\Lambda(\phi_\Lambda)\|_{L^\infty(\overline{\Omega})} \leq M_{12}$ for $\Lambda \geq 1$, where M_{12} is a positive constant independent of Λ.*

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2.3.4 Convergence of ϕ_Λ under (A3)–(A4)

Since ϕ_Λ is the solution to equation $-\nabla\cdot(\varepsilon\nabla\phi_\Lambda)=\rho_0+f_\Lambda(\phi_\Lambda)$ in Ω with the Robin boundary condition $\phi_\Lambda+\eta\frac{\partial\phi_\Lambda}{\partial\nu}=\phi_{bd}$ on $\partial\Omega$, we use the $W^{2,p}$ estimate (cf. [2, Theorem 15.2]) to get $\|\phi_\Lambda\|_{W^{2,p}(\Omega)}\leq C(\|\rho_0+f_\Lambda(\phi_\Lambda)\|_{L^p(\Omega)}+\|\phi_{bd}\|_{W^{1,p}(\Omega)})$ for all $p>1$, where C is a positive constant independent of Λ. Hence by Remark 2.7, we have the uniform bound estimate of ϕ_Λ in $W^{2,p}$ norm. This implies that there exists a sequence of functions $\{\phi_{\Lambda_k}\}_{k=1}^{\infty}$, with $\lim\limits_{k\to\infty}\Lambda_k=\infty$, such that ϕ_{Λ_k} converges to ϕ^* weakly in $W^{2,p}(\Omega)$. By Corollary 2.9, we have the convergence of function $\tilde{f}_{\Lambda_k}$ to $\tilde{f}^*$ in $\mathcal{C}^m[-M_8,M_8]$ for $m\in\mathbb{N}$, so ϕ^* satisfies (2.20) in a weak sense, where the positive constant M_8 comes from Lemma 2.13(b). Let $w_k=\phi_{\Lambda_k}-\phi^*$, $c_{i,k}:=c_{i,\Lambda_k}$, and $f_k:=f_{\Lambda_k}$. Then by Sobolev embedding, $w_k\in\mathcal{C}^{1,\alpha}(\overline{\Omega})$ for $\alpha\in(0,1)$, and $\lim\limits_{k\to\infty}\|w_k\|_{\mathcal{C}^{1,\alpha}(\overline{\Omega})}=0$. Moreover, w_k satisfies $-\nabla\cdot(\varepsilon\nabla w_k)=f_k(w_k+\phi^*)-f^*(\phi^*)$ in Ω with the boundary condition $w_k+\eta\frac{\partial w_k}{\partial\nu}=0$ on $\partial\Omega$. Using the Schauder's estimate (cf. [38, Theorem 6.30]) with the mathematical induction, we get

$$\begin{aligned}&\|w_k\|_{\mathcal{C}^{m+2,\alpha}(\overline{\Omega})}\leq C\|f_k(w_k+\phi^*)-f^*(\phi^*)\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}\\ &\leq C'\sum_{i=1}^{I}\left(\|c_{i,k}(w_k+\phi^*)-c_i^*(w_k+\phi^*)\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}+\|c_i^*(w_k+\phi^*)-c_i^*(\phi^*)\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}\right),\end{aligned}\tag{2.69}$$

for all $m\in\mathbb{N}$ and $\alpha\in(0,1)$, where C and C' are positive constants independent of k. By Proposition 2.10(a) and induction hypothesis $\lim\limits_{k\to\infty}\|w_k\|_{\mathcal{C}^{m,\alpha}(\overline{\Omega})}=0$, we may use (2.69) to get $\lim\limits_{k\to\infty}\|w_k\|_{\mathcal{C}^{m+2,\alpha}(\overline{\Omega})}=0$, i.e. $\lim\limits_{k\to\infty}\|\phi_{\Lambda_k}-\phi^*\|_{\mathcal{C}^{m+2,\alpha}(\overline{\Omega})}=0$ for $m\in\mathbb{N}$ and $\alpha\in(0,1)$. Therefore, ϕ^* is the solution to (2.31) with the Robin boundary condition (2.15). To complete the proof of Theorem 2.2, we need to prove the following claim.

Claim 2.14. *For any $m\in\mathbb{N}$, we have $\lim\limits_{\Lambda\to\infty}\|\phi_\Lambda-\phi^*\|_{\mathcal{C}^m(\overline{\Omega})}=0$.*

Proof. Suppose that there exist the sequences $\{\Lambda_k\}$ and $\{\tilde{\Lambda}_k\}$ tending to infinity such that sequences $\{\phi_{\Lambda_k}\}$ and $\{\phi_{\tilde{\Lambda}_k}\}$ have limits ϕ_1^* and ϕ_2^*, respectively. It is clear that ϕ_1^* and ϕ_2^* satisfy (2.31) with the Robin boundary condition (2.15). Now we want to prove that $\phi_1^*\equiv\phi_2^*$. Let $u=\phi_1^*-\phi_2^*$. Subtracting (2.31) with $\phi^*=\phi_2^*$ from that with $\phi^*=\phi_1^*$, we obtain $-\nabla\cdot(\varepsilon\nabla u)=c_1(x)u$ in Ω, where

$$c_1(x)=\begin{cases}\dfrac{f^*(\phi_1^*(x))-f^*(\phi_2^*(x))}{\phi_1^*(x)-\phi_2^*(x)} & \text{if } \phi_1^*(x)\neq\phi_2^*(x);\\[2ex] \dfrac{\mathrm{d}f^*}{\mathrm{d}\phi}(\phi_1^*(x)) & \text{if } \phi_1^*(x)=\phi_2^*(x).\end{cases}$$

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By Proposition 2.10, we have $c_1 < 0$ in Ω which comes from the fact that if f is a strictly decreasing function on $\mathbb{R}$, then $\frac{f(\alpha)-f(\beta)}{\alpha-\beta} < 0$ for $\alpha \neq \beta$. Since $\nabla \cdot (\varepsilon \nabla u) + c_1(x)u = 0$ with $c_1 < 0$ in Ω, it is obvious that u cannot be a nonzero constant. Then by the strong maximum principle, we have that u attains its nonnegative maximum value and nonnpositive minimum value at the boundary point. Suppose u has nonnegative maximum value and attains its maximum value at $x^* \in \partial\Omega$. Then by the boundary condition of u which is $u + \eta\frac{\partial u}{\partial \nu} = 0$ on $\partial\Omega$, we get $u(x^*) = -\eta\frac{\partial u}{\partial \nu}(x^*) \leq 0$, and hence $u \leq u(x^*) \leq 0$ on $\overline{\Omega}$. Similarly, we obtain $u \geq 0$ in $\overline{\Omega}$, and hence $u \equiv 0$. Therefore, we conclude that $\phi_1^* \equiv \phi_2^*$ and complete the proof of Theorem 2.2. □

2.4 Numerical methods

In this section, we introduce numerical methods to solve the PB-steric equations (2.13)–(2.14) and its aossciated limiting equations (under different assumptions) with the Robin boundary condition (2.15). Throughout this section, we consider one dimensional domain $\Omega = (-1, 1)$ and assume $I = 3$, $z_0 = 0$, $z_1 = 1$, $z_2 = -1$, $z_3 = 2$, $\tilde{\mu}_0 = 1$, $\hat{\mu}_0 = 0$, $\rho_0 \equiv 0$, $\eta = \varepsilon = 0.1$, and $\phi_{bd}(\pm 1) = \pm 10$. For different assumptions, the parameters are given in Table 2.1

Assumption	Parameter
(A1) and (A2)	$\gamma = 0.1$, $\bar{\mu}_i = 0$ $(i = 0, 1, 2, 3)$
(A1)''' and (A2)	$1 - \gamma = \gamma_1 = \gamma_2 = 0.01$, $\gamma_3 = 0.97$, $\bar{\mu}_0 = \bar{\mu}_1 = 0$, $\bar{\mu}_2 = \bar{\mu}_3 = -5$
(A3) and (A4)	$\lambda_0 = \lambda_2 = \lambda_3 = 1$, $\lambda_1 = 2$, $\bar{\mu}_i = 0$ $(i = 0, 1, 2, 3)$

Table 2.1: The list of parameters under different assumptions.

To solve (2.14) and obtain the profiles of $f_\Lambda = \sum_{i=0}^{I} z_i c_{i,\Lambda}(\phi)$, we use the command `fsolve` in Matlab to perform the trust-region algorithm on the following discretized equation

$$\ln(\boldsymbol{c}_{i,\Lambda}) + z_i\boldsymbol{\phi} + \Lambda\sum_{j=0}^{I} g_{ij}\mathbf{c}_{j,\Lambda} = \Lambda\tilde{\mu}_i + \hat{\mu}_i \quad \text{for } i = 0, 1, \ldots, I, \tag{2.70}$$

where $\phi = [\phi_0, \ldots, \phi_L]^\mathsf{T}$ is the regular partition of the interval $[-10, 10]$ with $L = 1024$, and $\boldsymbol{c}_{i,\Lambda} = [c_{i,\Lambda}(\phi_0), \ldots, c_{i,\Lambda}(\phi_L)]^\mathsf{T}$. For (A1)–(A2), we use the initial data

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$c_{i,\Lambda}^{(0)} = \tilde{\mu}_0 e^{\bar{\mu}_i - z_i \phi} / H(\gamma, z_1, \ldots, z_I, \phi)$ and obtain the profiles of f_Λ, which are presented in Figure 2.1(a). Moreover, the maximum norms of $f_\Lambda - f^*$ are listed in Table 2.2, which supports Corollary 2.5.

Λ	1	10	10^2	10^3	10^4
$\|f_\Lambda - f^*\|_\infty$	5.7112E02	6.4188E01	6.7394E00	6.7950E-01	6.8010E-02

Table 2.2: The maximum norms of $f_\Lambda - f^*$ under assumptions (A1) and (A2).

For (A1)$'''$ and (A2), the initial data $c_{i,\Lambda}^{(0)}$ is given by $\dfrac{\tilde{\mu}_0 e^{\bar{\mu}_i - z_i \phi}}{1 - \gamma + \sum_{j=1}^{3} \gamma_j e^{\bar{\mu}_j - z_j \phi}}$. Then we use `fsolve` to obtain the profiles of $f_\Lambda(\phi)$ is shown in Figure 2.2(a), and the relative errors are given in Table 2.3.

nth step	2	4	8	16	32
$\Lambda = 0.5$	3.9224E-01	4.5460E-01	1.0164E00	3.5219E-01	2.6628E-01
$\Lambda = 1$	2.4876E-01	3.5486E-01	3.4606E-01	1.7767E-01	1.3938E-01
$\Lambda = 2$	2.3087E-01	1.6632E-01	4.5570E-02	1.2473E-01	6.4245E-02
$\Lambda = 4$	1.2868E-01	9.3210E-02	6.9030E-02	3.6541E-02	5.3454E-02

Table 2.3: The relative errors $\|f_\Lambda^{(n)} - f_\Lambda^{(n-1)}\|_\infty / \|f_\Lambda^{(n)}\|_\infty$ under assumptions (A1)$''$ and (A2), where $\phi_\Lambda^{(k)}$ denotes the solution after k iterations.

For (A3)–(A4), we use the initial data $c_{i,\Lambda}^{(0)} = c_i^*$, where c_i^* is the solution to limiting equation (2.28)–(2.29). Here equations (2.28)–(2.29) can be discreitzed as

$$\boldsymbol{c}_i^(\phi) = \boldsymbol{c}_0^*(\phi) \circ e^{\bar{\mu}_i - z_i \phi} \quad \text{for } i = 1, \ldots, I, \tag{2.71}$$

$$\sum_{j=0}^{I} \lambda_j (\boldsymbol{c}_0^*(\phi))^{\lambda_j / \lambda_0} \circ e^{\bar{\mu}_j - z_j \phi} = \tilde{\mu}_0. \tag{2.72}$$

Equations (2.71)–(2.72) can be solved by the command `fsolve` with the initial data $(c_i^*)^{(0)} \equiv 1$. Then we obtain the profiles of $f_\Lambda(\phi)$, which are presented in Figure 2.3(a). Moreover, we list the maximum norms of $\tilde{f}_\Lambda - \tilde{f}^*$ in Table 2.4, which supports Corollary 2.9.

Λ	1	10	10^2	10^3	10^4
$\left\|\tilde{f}_\Lambda - \tilde{f}^*\right\|_\infty$	3.4208E01	3.7875E00	3.9638E-01	3.9960E-02	3.9996E-03

Table 2.4: The maximum norms of $\tilde{f}_\Lambda - \tilde{f}^*$ under assumptions (A3)–(A4).

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To get the solution ϕ_Λ to (2.13)–(2.14), we employ the Legendre–Gauss–Lobatto (LGL) points $\{x_k\}_{k=0}^{L}$ (cf. [28]) as the partition of the interval $[-1,1]$ with $L=256$ to discrtize (2.13)–(2.14) as the following algebraic equations:

$$-\mathrm{D}_{L+1}\boldsymbol{\varepsilon}\mathrm{D}_{L+1}\boldsymbol{\phi}_\Lambda = \boldsymbol{\rho}_0 + \sum_{i=1}^{I} z_i \boldsymbol{c}_{i,\Lambda}, \tag{2.73}$$

$$\ln(\boldsymbol{c}_{i,\Lambda}) + z_i\boldsymbol{\phi}_\Lambda + \Lambda\sum_{j=0}^{I} g_{ij}\boldsymbol{c}_{j,\Lambda} = \Lambda\tilde{\mu}_i + \hat{\mu}_i \quad \text{for } i=0,1,\dots,I, \tag{2.74}$$

where $\mathrm{D}_{L+1} = [d_{ij}]_{0\le i,j\le L}$ is the matrix satisfying $\mathrm{D}_{L+1}\boldsymbol{\psi} = [\psi'(x_0),\dots,\psi'(x_L)]^\mathsf{T}$ for $\boldsymbol{\psi} = [\psi(x_0),\dots,\psi(x_L)]^\mathsf{T}$, $\boldsymbol{\varepsilon} = [\varepsilon(x_0),\dots,\varepsilon(x_L)]^\mathsf{T}$, $\boldsymbol{\rho}_0 = [\rho_0(x_0),\dots,\rho_0(x_L)]^\mathsf{T}$, $\boldsymbol{\phi}_\Lambda = [\phi_\Lambda(x_0),\dots,\phi_\Lambda(x_L)]^\mathsf{T}$, and $\boldsymbol{c}_{i,\Lambda} = [c_{i,\Lambda}(\phi_\Lambda(x_0)),\dots,c_{i,\Lambda}(\phi_\Lambda(x_L))]^\mathsf{T}$ for $i=0,1,\dots,I$. For (A1)–(A2), equations (2.73)–(2.74) can be rewritten as

$$-\mathrm{D}_{L+1}\boldsymbol{\varepsilon}\mathrm{D}_{L+1}\boldsymbol{\phi}_\Lambda = \boldsymbol{\rho}_0 + \sum_{i=1}^{I} z_i \boldsymbol{c}_{0,\Lambda} \circ e^{\bar{\mu}_i - z_i\boldsymbol{\phi}_\Lambda}, \tag{2.75}$$

$$\ln(\boldsymbol{c}_{0,\Lambda}) + \Lambda\left(1-\gamma+\frac{\gamma}{Z}\sum_{j=1}^{I} e^{\bar{\mu}_j - z_j\boldsymbol{\phi}_\Lambda}\right)\circ \boldsymbol{c}_{0,\Lambda} = \Lambda\tilde{\mu}_0 + \hat{\mu}_0. \tag{2.76}$$

On the other hand, the limiting equation of (2.19)–(2.20) (i.e., (2.23)) can be discrtized as

$$-\mathrm{D}_{L+1}\boldsymbol{\varepsilon}\mathrm{D}_{L+1}\boldsymbol{\phi}_\Lambda = \boldsymbol{\rho}_0 + \sum_{i=1}^{I} z_i \frac{\tilde{\mu}_0}{1-\gamma+\dfrac{\gamma}{Z}\displaystyle\sum_{j=1}^{I} e^{\bar{\mu}_j - z_j\boldsymbol{\phi}^*}} \circ e^{\bar{\mu}_i - z_i\boldsymbol{\phi}^*}, \tag{2.77}$$

where $\boldsymbol{\phi}^* = [\phi^*(x_0),\dots,\phi^*(x_L)]^\mathsf{T}$. In addition, we discretize the Robin boundary condition (2.15) as

$$\phi(x_0) - \eta\sum_{k=0}^{L} d_{0k}\phi(x_k) = \phi_{bd}(-1), \qquad \phi(x_L) + \eta\sum_{k=0}^{L} d_{Lk}\phi(x_k) = \phi_{bd}(1), \tag{2.78}$$

which replaces the first and last equations of (2.75) and (2.77). Then we use the command `fsolve` with the initial data $c_{0,\Lambda}\equiv 1$ and $\phi_\Lambda^{(0)} = (\phi^*)^{(0)} \equiv 0$ to obtain the profiles ϕ_Λ and $f_\Lambda(\phi_\Lambda(x))$ and their limiting functions shown in Figure 2.4. Moreover, we provide the maximum norms of $\phi_\Lambda - \phi^*$ given in Table 2.5, which supports Theorem 2.1.

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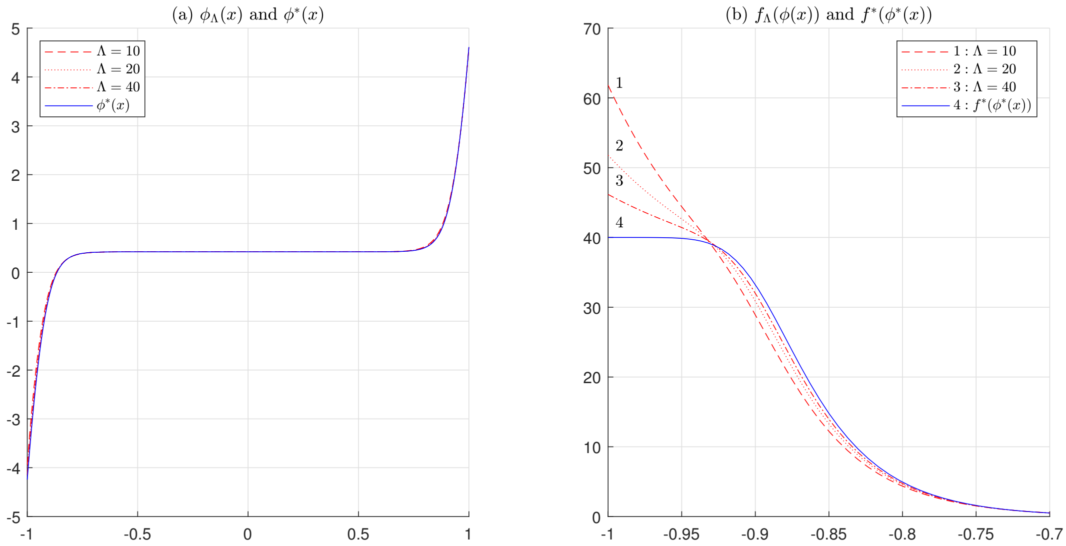

Figure 2.4: The numerical profiles of ϕ_Λ and $f_\Lambda(\phi_\Lambda(x))$ and their limiting functions under assumptions (A1)–(A2), where the red curves are the profiles of function ϕ_Λ and $f_\Lambda \circ \phi_\Lambda$ with $\Lambda = 10, 20, 40$ and the blue curve is the profiles of function ϕ^* and $f^* \circ \phi^*$.

Λ	1	10	10^2	10^3	10^4
$\|\phi_\Lambda - \phi^*\|_\infty$	1.1425E00	3.2945E-01	4.3358E-02	4.4900E-03	4.5062E-04

Table 2.5: The maximum norms of $\phi_\Lambda - \phi^*$ under assumptions (A1)–(A2).

For (A1)$'''$ and (A2), equations (2.73)–(2.74) can be denoted as

$$-\mathrm{D}_{L+1}\boldsymbol{\varepsilon}\mathrm{D}_{L+1}\boldsymbol{\phi}_\Lambda = \boldsymbol{\rho}_0 + \sum_{i=1}^{I} z_i \boldsymbol{c}_{0,\Lambda} \circ \exp(\bar{\mu}_i - z_i \boldsymbol{\phi}_\Lambda), \tag{2.79}$$

$$\ln(\boldsymbol{c}_{0,\Lambda}) + \Lambda\left(1 - \gamma + \sum_{j=1}^{I} \gamma_j \exp(\bar{\mu}_j - z_j \boldsymbol{\phi}_\Lambda)\right) \circ \boldsymbol{c}_{0,\Lambda} = \Lambda\tilde{\mu}_0 + \hat{\mu}_0. \tag{2.80}$$

For the Robin boundary condition, we replace the first and last equation of (2.79) by (2.78). Then using the command `fsolve` with the initial data $\boldsymbol{\phi}_\Lambda^{(0)} \equiv 0$ and $\boldsymbol{c}_{0,\Lambda}^{(0)} \equiv 1$, we obtain the profiles of ϕ_Λ and $f_\Lambda(\phi_\Lambda)$ in Figure 2.5. The relative erros are given in Table 2.6.

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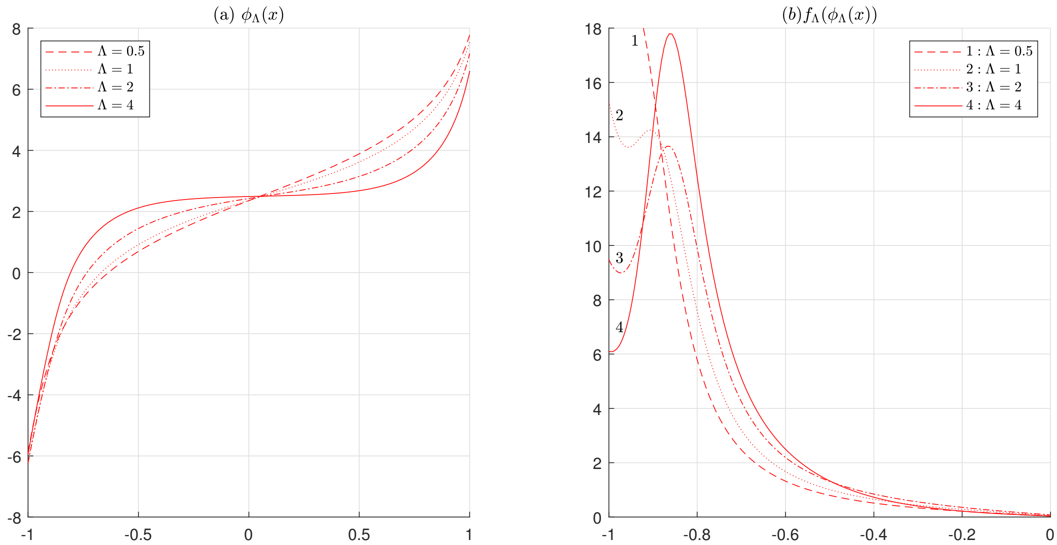

Figure 2.5: The numerical profiles of ϕ_Λ and $f_\Lambda(\phi_\Lambda(x))$ and their limiting functions under assumptions (A1)$'''$ and (A2), where the red curves are the profiles of function ϕ_Λ and $f_\Lambda \circ \phi_\Lambda$ with $\Lambda = 0.5, 1, 2, 4$.

nth step	1	2	4	8	16
$\Lambda = 0.5$	1.0929E-04	1.1032E-04	1.1049E-04	1.1081E-04	1.1148E-04
$\Lambda = 1$	1.2228E-04	1.2525E-04	1.2543E-04	1.2581E-04	1.2656E-04
$\Lambda = 2$	1.4320E-04	1.5051E-04	1.5076E-04	1.5125E-04	1.5224E-04
$\Lambda = 4$	1.7579E-04	1.8585E-04	1.8623E-04	1.8695E-04	1.8837E$-$04

Table 2.6: The relative errors $\|\phi_\Lambda^{(n)} - \phi_\Lambda^{(n-1)}\|_\infty / \|\phi_\Lambda^{(n)}\|_\infty$ under assumptions (A1)$'''$ and (A2), where $\phi_\Lambda^{(k)}$ denotes the solution after k iterations.

For (A3)–(A4), equations (2.73)–(2.74) can be denoted as

$$-\mathrm{D}_{L+1}\boldsymbol{\varepsilon}\mathrm{D}_{L+1}\boldsymbol{\phi}_\Lambda = \boldsymbol{\rho}_0 + \sum_{i=1}^{I} z_i(\boldsymbol{c}_{0,\Lambda})^{\lambda_i/\lambda_0} \circ \exp(\bar{\mu}_i - z_i\boldsymbol{\phi}_\Lambda), \tag{2.81}$$

$$\ln(\boldsymbol{c}_{0,\Lambda}) + \Lambda \sum_{j=0}^{I} \lambda_0\lambda_j(\boldsymbol{c}_{0,\Lambda})^{\lambda_j/\lambda_0} \circ \exp(\bar{\mu}_j - z_j\boldsymbol{\phi}_\Lambda) = \Lambda\lambda_0\tilde{\mu}_0 + \hat{\mu}_0. \tag{2.82}$$

On the other hand, the limiting equations of (2.26)–(2.27) (i.e., (2.31)) can be discretized as

$$-\mathrm{D}_{L+1}\boldsymbol{\varepsilon}\mathrm{D}_{L+1}\boldsymbol{\phi}^* = \boldsymbol{\rho}_0 + \sum_{i=1}^{I} z_i(\boldsymbol{c}_0^*)^{\lambda_i/\lambda_0} \circ \exp(\bar{\mu}_i - z_i\boldsymbol{\phi}^*), \tag{2.83}$$

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$$\sum_{j=0}^{I} \lambda_j (\boldsymbol{c}_0^*)^{\lambda_j/\lambda_0} \circ \exp(\bar{\mu}_j - z_j \boldsymbol{\phi}^*) = \tilde{\mu}_0, \tag{2.84}$$

For the Robin boundary condition, the first and last equations of (2.81) and (2.83) are replaced by (2.78). Using the command `fsolve` with the initial data $\boldsymbol{c}_{0,\Lambda}^{(0)} = (\boldsymbol{c}_0^*)^{(0)} \equiv 1$ and $\boldsymbol{\phi}_\Lambda^{(0)} = (\boldsymbol{\phi}^*)^{(0)} \equiv 0$, then the profiles of ϕ_Λ and $\tilde{f}_\Lambda(\phi_\Lambda)$ and their limiting functions are presented in Figure 2.6. Moreover, the maximum norms of $\phi_\Lambda - \phi^*$ are listed in Table 2.7, which supports Theorem 2.2.

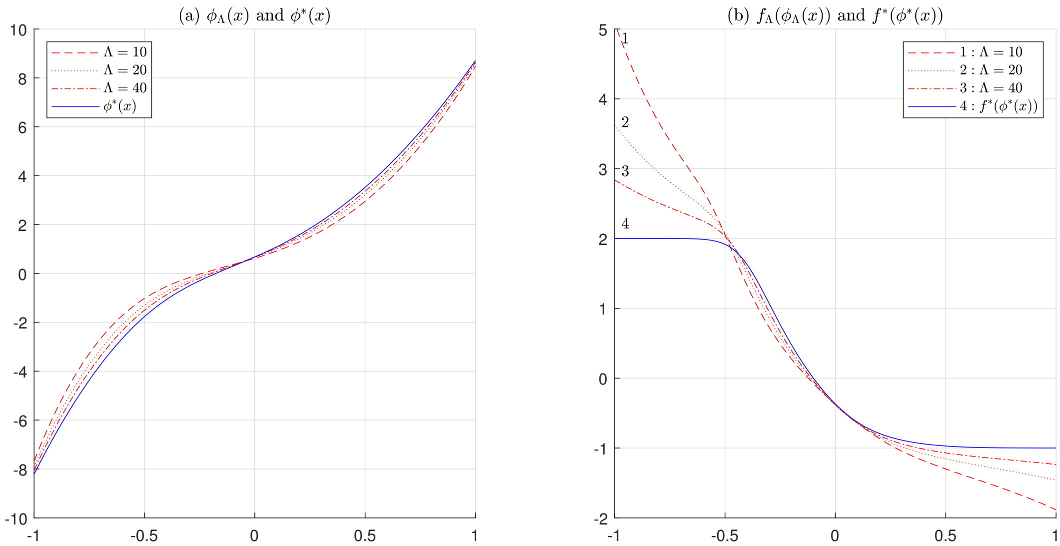

Figure 2.6: The numerical profiles of ϕ_Λ and $\tilde{f}_\Lambda(\phi_\Lambda(x))$ and their limiting functions under assumptions (A3)–(A4), where the red curves are the profiles of function ϕ_Λ and $\tilde{f}_\Lambda \circ \phi_\Lambda$ with $\Lambda = 10, 20, 40$, and the blue curves are the profiles of function ϕ^* and $\tilde{f}^* \circ \phi^*$.

Λ	1	10	10^2	10^3	10^4
$\Vert\phi_\Lambda - \phi^*\Vert_\infty$	3.4820E00	1.0872E00	1.5170E-01	1.5879E-02	1.5956E-03

Table 2.7: The maximum norms of $\phi_\Lambda - \phi^*$ under assumptions (A3)–(A4).

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Conclusions

In this chapter, we derive the PB-steric equations with a parameter Λ, and prove that as $\Lambda \to \infty$, the solution to PB-steric equations (2.13)–(2.14) converges to the solution to modified PB equations (2.3)–(2.4) and (2.5)–(2.7) under different assumptions of steric effects and chemical potentials. Equations (2.1)–(2.2), (2.3)–(2.4), and (2.5)–(2.7) were derived based on mean-field approximation (cf. [12, 80]), whereas equations (2.13)–(2.14) are derived via adding the approximate Lennard–Jones potential. We compare equations (2.1)–(2.7) and (2.13)–(2.14) in the following table to show that the PB-steric equations (2.13)–(2.14) can be regarded as a general model of PB equations.

Model	Total ionic charge density $\sum_{i=1}^{I} z_i c_i(\phi)$	$c_i(\phi)$ $(i = 0, 1, \ldots, I)$
(2.1)–(2.2)	decreasing	c_1, c_2 are monotonic, $c_0 \equiv 0$ $(I = 2)$.
(2.3)–(2.4)	decreasing	c_1, c_2 are monotonic, $c_0 \equiv 0$ $(I = 2)$.
(2.5)–(2.7)	decreasing	Some of c_i's are oscillatory; the others are monotonic. $(I \geq 2)$
(2.13)–(2.14)	oscillatory (Remark 2.4)	Some of c_i's are oscillatory; the others are monotonic. $(I = 3)$
	decreasing (Propositions 2.6 and 2.10)	Some of c_i's are oscillatory; the others are monotonic. $(I \geq 2)$

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Appendix

2A Derivation of (2.10) and (2.11)

In [84], the approximate LJ potential $\Psi_{ij,\sigma}$ between the ith ion and the jth ion can be expressed as $\Psi_{ij,\sigma}(x) = (\Psi_{ij}\chi_\sigma * \varphi_\sigma)(x)$ for $x \in \mathbb{R}^d$ and $i, j = 0, 1, \ldots, I$, where $*$ denotes the standard convolution, Ψ_{ij} is the conventional LJ potential between ith and jth ions defined by $\Psi_{ij}(x) = \dfrac{\varepsilon_{ij}(a_i + a_j)^{12}}{2|x|^{12}}$ for $x \in \mathbb{R}^d$ and $i, j = 0, 1, \ldots, I$, and $\varphi_\sigma(x)$ is the spatially band-limited function defined by $\varphi_\sigma(x) = \mathcal{F}^{-1}(1 - \chi_{\sigma^{-\gamma}}(\xi))$. Here ε_{ij} denotes energy coupling constant between the ith and the jth ions, a_0 is the radius of solvent molecules, a_i is the radius of the ith ion. In addition, χ_σ and $\chi_{\sigma^{-\gamma}}$ are the characteristic function of the exterior ball $\mathbb{R}^d - \overline{B_\sigma(0)}$ and $\mathbb{R}^d - \overline{B_{\sigma^{-\gamma}}(0)}$ for $0 < \gamma < 1$, respectively, and $\mathcal{F}^{-1}$ is the inverse Fourier transform. More precisely, the characteristic function χ_s is defined by $\chi_s(z) = 0$ if $|z| \le s; 1$ if $|z| > s$. With the approximate LJ potential, we may define the approximate energy functional $E_{LJ,\sigma}$ and show that (cf. [84])

$$E_{LJ,\sigma}[c_i, c_j] := \Lambda g_{ij} \int_{\mathbb{R}^d} c_i(x)c_j(x)\,\mathrm{d}x \sim \int_{\mathbb{R}^d} c_i(x)(\Psi_{ij} * c_j)(x)\,\mathrm{d}x = E_{LJ}[c_i, c_j], \quad (2.85)$$

where $\Lambda = a^{12}\sigma^{d-12}$ satisfies $\lim_{\sigma\to 0^+} \Lambda = \infty$, and $g_{ij} = \dfrac{\omega_d \varepsilon_{ij}}{12 - d}\dfrac{(a_i + a_j)^{12}}{a^{12}}$ denotes a dimensionless quantity. Here $a = \min\{a_i : i = 0, 1 \ldots, I\}$ and ω_d is the surface area of a d-dimensional unit ball. To derive (2.10)–(2.11), we let energy functional

$$E[c_0, c_1, \ldots, c_N, \phi] = E_{PB}[c_0, c_1, \ldots, c_I, \phi] + \frac{1}{2}\sum_{i,j=0}^{I} E_{LJ,\sigma}[c_i, c_j],$$

where $E_{LJ,\sigma}$ is defined in (2.85) and

$$E_{PB}[c_0, c_1, \cdots, c_I, \phi] = \int_{\mathbb{R}^d} \left[-\frac{1}{2}\varepsilon\, |\nabla\phi|^2 + k_B T \sum_{i=0}^{I} c_i(\ln c_i - 1) + 4\pi \left(\rho_0 + \sum_{i=1}^{I} z_i e_0 c_i \right) \phi \right] \mathrm{d}x.$$

Notice that E_{PB} is the energy functional of classical PB equation with the form $-\nabla \cdot (\varepsilon\nabla\phi) = \rho_0 + \sum_{i=1}^{I} z_i e^{\mu_i - z_i\phi}$ which can be obtained by $\delta E_{PB}/\delta\phi = 0$ and $\delta E_{PB}/\delta c_i = \mu_i$ for $i = 0, 1, \ldots, I$. Here μ_i is the chemical potential. Besides, $E_{LJ,\sigma}$ is the energy functional of the approximate LJ potentials (cf. [84]), and we may derive the equations

$$-\nabla \cdot (\varepsilon\nabla\phi) = 4\pi\rho_0 + 4\pi\sum_{i=1}^{I} z_i e_0 c_i, \quad (2.86)$$

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$$k_BT\ln(c_i) + z_ie_0\phi + \Lambda\sum_{j=0}^{I} g_{ij}c_j = \mu_i \quad \text{for } i = 0, 1, \ldots, I, \tag{2.87}$$

by $\delta E/\delta\phi = 0$ and $\delta E/\delta c_i = \mu_i$ for $i = 0, 1, \ldots, I$ when matrix (g_{ij}) is symmetric. From (2.87), constant μ_i can be expressed by

$$\mu_i = \Lambda\tilde{\mu}_i + \hat{\mu}_i \quad \text{for } i = 0, 1, \ldots, I. \tag{2.88}$$

Therefore, by (2.86)–(2.88), we have (2.10)–(2.11).

2B The existence and uniqueness of ϕ_Λ to (2.14)–(2.15)

To prove the existence of ϕ_Λ to equations (2.14)–(2.15), we study the following energy minimization problem:

$$\text{Minimize } E[\phi] := E_{\text{eq}}[\phi] + B_\eta[\phi] \quad \text{subject to } \phi \in \mathbb{H}_\eta(\Omega),$$

where the functionals

$$E_{\text{eq}}[\phi] = \frac{1}{2}\int_\Omega \varepsilon|\nabla\phi|^2\,\mathrm{d}x - \int_\Omega \rho_0\phi\,\mathrm{d}x - \int_\Omega F(\phi)\,\mathrm{d}x,$$

$$B_\eta[\phi] = \begin{cases} \dfrac{1}{2\eta}\displaystyle\int_{\partial\Omega} \varepsilon(\phi - \phi_{bd})^2\,\mathrm{d}S_x & \text{if } \eta > 0, \\ 0 & \text{if } \eta = 0, \end{cases}$$

and defined on the space

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

Here the function $F(\phi) = \int_0^\phi f(s)\,\mathrm{d}s$, and $f = f(\phi)$ is strict decreasing (cf. Propositions 2.1 and 2.7) on $\mathbb{R}$. Hence we may apply the Direct method (cf. [109]) to solve the minimization problem.

To apply the Direct method, we need the following lemma.

Lemma 2B.1. *Functional E is coercive on $H^1(\Omega)$ for $\eta > 0$.*

Proof. By Young's inequality, we have

$$B_\eta[\phi] \geq \frac{1}{4\eta}\int_{\partial\Omega} \varepsilon\phi^2\,\mathrm{d}S_x - \frac{1}{2\eta}\int_{\partial\Omega} \varepsilon\phi_{bd}^2\,\mathrm{d}S_x. \tag{2.89}$$

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By the strict decrease of f, function F is strictly concave and has an absolute maximum denoted by M_F. Hence by (2.89), we obtain

$$E[\phi] \geq C_\eta \left(\int_\Omega |\nabla\phi|^2 \, \mathrm{d}x + \int_{\partial\Omega} \phi^2 \, \mathrm{d}S_x \right) - \int_\Omega |\rho_0\phi| \, \mathrm{d}x - \frac{1}{2\eta} \int_{\partial\Omega} \varepsilon\phi_{bd}^2 \, \mathrm{d}S_x - M_F|\Omega|, \tag{2.90}$$

where $C_\eta = \frac{1}{4\eta} \min\{1, 2\eta\} \min_{\overline{\Omega}} \varepsilon > 0$ and $|\Omega|$ denotes the Lebesuge measure of Ω. Moreover, for any $\phi \in H^1(\Omega)$, Friedrichs' inequality gives

$$\int_\Omega |\nabla\phi|^2 \, \mathrm{d}x + \int_{\partial\Omega} \phi^2 \, \mathrm{d}S_x \geq C_1 \int_\Omega \phi^2 \, \mathrm{d}x, \tag{2.91}$$

where C_1 is a positive constant depending on the dimension d and the measures of Ω and $\partial\Omega$. Besides, Cauchy–Schwarz inequality gives

$$\int_\Omega |\rho_0\phi| \, \mathrm{d}x \leq \left(\int_\Omega \rho_0^2 \, \mathrm{d}x \right)^{1/2} \left(\int_\Omega \phi^2 \, \mathrm{d}x \right)^{1/2}. \tag{2.92}$$

Then by (2.90)–(2.92), Lemma 2B.1 follows. □

By Lemma 2B.1, we may prove the existence of minimizer as follows.

Proposition 2B.2. *Functional E has a minimizer $\phi \in \mathbb{H}_\eta$ for any $\eta \geq 0$.*

Proof. Suppose $\eta > 0$ and $\mathbb{H}_\eta(\Omega) = H^1(\Omega)$. By (2.90)–(2.92), $\inf_{\phi \in H^1(\Omega)} E[\phi]$ exists so there exists a minimizing sequence $\{\phi_n\}_{n=1}^\infty \subsetneq H^1(\Omega)$ such that

$$\lim_{n\to\infty} E[\phi_n] = \inf_{\phi \in H^1(\Omega)} E[\phi] := m_E.$$

Due to the coerciveness of E (see Lemma 2B.1), we have $\sup_{n\in\mathbb{N}} \|\phi_n\|_{H^1(\Omega)} < \infty$. Along with (2.90), we can get $\sup_{n\in\mathbb{N}} \|\phi_n\|_{L^2(\partial\Omega)} < \infty$. Thus, there exists a subsequence $\{\phi_{n_k}\}_{k=1}^\infty$ of $\{\phi_n\}_{n=1}^\infty$ and $\phi \in H^1(\Omega)$ such that $\phi_{n_k} \rightharpoonup \phi$ weakly in $H^1(\Omega)$ and $\phi_{n_k} \rightharpoonup \Gamma\phi$ weakly in $L^2(\partial\Omega)$ as $k \to \infty$, where $\Gamma\phi$ is the trace of ϕ on $\partial\Omega$. Since $\phi_{n_k} \rightharpoonup \phi$ weakly in $H^1(\Omega)$ implies $\nabla\phi_{n_k} \rightharpoonup \nabla\phi$ weakly in $L^2(\Omega)$, then we obtain

$$\liminf_{k\to\infty} \int_\Omega |\nabla\phi_{n_k}|^2 \, \mathrm{d}x \geq \int_\Omega |\nabla\phi|^2 \, \mathrm{d}x, \qquad \liminf_{k\to\infty} \int_{\partial\Omega} |\phi_{n_k} - \phi_{bd}|^2 \, \mathrm{d}S_x \geq \int_{\partial\Omega} |\Gamma\phi - \phi_{bd}|^2 \, \mathrm{d}S_x,$$

and

$$\lim_{k\to\infty} \phi_{n_k} = \phi \quad \text{a.e. in } \Omega.$$

Applying the Fatou's lemma, we have

$$\liminf_{k\to\infty} \int_\Omega -F(\phi_{n_k}) \, \mathrm{d}x \geq \int_\Omega -F(\phi) \, \mathrm{d}x,$$

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which gives

$$m_E = \lim_{k\to\infty} E[\phi_{n_k}] \geq E[\phi] \geq m_E,$$

and E attains its minimum m_E at $\phi \in H^1(\Omega) = \mathbb{H}_\eta(\Omega)$ for $\eta > 0$. As for $\eta = 0$ (i.e., the Dirichlet boundary condition), $B_\eta[\phi] = 0$ we may use the similar argument to prove the existence of minimizer and complete the proof. □

The minimizer of Proposition 2B.2 satisfies equation (2.14) with the Robin boundary condition (2.15) in weak sense. Now we prove the regularity of solution ϕ as follows. Because ϕ is a minimizer of the functional E on $H^1(\Omega)$, ϕ satisfies

$$\int_\Omega [\varepsilon\nabla\phi\cdot\nabla v - v\rho_0 - vf(\phi)]\,\mathrm{d}x + \frac{1}{\eta}\int_{\partial\Omega}\varepsilon(\phi-\phi_{bd})v\,\mathrm{d}S_x = 0 \tag{2.93}$$

for any $v \in H^1(\Omega)$. Let Φ be the solution to the auxiliary Poisson equation

$$-\nabla\cdot(\varepsilon\nabla\Phi) = \rho_0 + f(\phi) \quad \text{in } \Omega \tag{2.94}$$

with the Robin boundary condition $\Phi + \eta\frac{\partial\Phi}{\partial\nu} = \phi_{bd}$ on $\partial\Omega$. We multiply equation (2.94) by $(\Phi - \phi)$ and integrate it over Ω. Then applying the integration by parts, we obtain

$$\int_\Omega \varepsilon\nabla\Phi\cdot\nabla(\Phi-\phi)\,\mathrm{d}x - \int_\Omega(\Phi-\phi)[\rho_0+f(\phi)]\,\mathrm{d}x + \frac{1}{\eta}\int_{\partial\Omega}\varepsilon(\Phi-\phi_{bd})(\Phi-\phi)\,\mathrm{d}S_x = 0. \tag{2.95}$$

Here we have used the fact that $\frac{\partial\Phi}{\partial\nu} = \frac{1}{\eta}(\phi_{bd}-\Phi)$ on $\partial\Omega$. Besides, we subtract (2.93) with $v = \Phi - \phi$ from (2.95) and get

$$\int_\Omega \varepsilon|\nabla(\Phi-\phi)|^2\,\mathrm{d}x + \frac{1}{\eta}\int_{\partial\Omega}\varepsilon(\Phi-\phi)^2\,\mathrm{d}S_x = 0,$$

which implies that $\Phi \equiv \phi$ a.e. in Ω. Thus, by a standard bootstrap argument on eqation (2.94), solution ϕ becomes a classical solution. On the other hand, as for the case $\eta = 0$, we can follow a similar argument to improve the regularity of solution ϕ.

Now we prove the uniqueness of equation (2.14) with the Robin boundary condition (2.15). Suppose that $\phi_1, \phi_2 \in \mathcal{C}^\infty(\Omega)\cap\mathcal{C}^2(\overline{\Omega})$ are solutions to (2.14)–(2.15). Subtracting (2.14) with $\phi = \phi_2$ from that with $\phi = \phi_1$, we have

$$-\nabla\cdot(\varepsilon\nabla(\phi_1-\phi_2)) = f(\phi_1) - f(\phi_2) \quad \text{in } \Omega. \tag{2.96}$$

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Multiplying the equation (2.96) by $\phi_1 - \phi_2$ and integrating it over Ω, we get

$$-\int_{\partial\Omega}(\phi_1-\phi_2)\nabla\cdot(\varepsilon\nabla(\phi_1-\phi_2))\,\mathrm{d}x = \int_{\Omega}(\phi_1-\phi_2)[f(\phi_1)-f(\phi_2)]\,\mathrm{d}x.$$

Then using the integration by parts, we obtain

$$\int_{\Omega}\varepsilon|\nabla(\phi_1-\phi_2)|^2\,\mathrm{d}x + \eta\int_{\partial\Omega}\varepsilon\left|\frac{\partial(\phi_1-\phi_2)}{\partial\nu}\right|^2\mathrm{d}S_x = \int_{\Omega}(\phi_1-\phi_2)[f(\phi_1)-f(\phi_2)]\,\mathrm{d}x. \tag{2.97}$$

Here we have used the fact that $\phi_1 - \phi_2 = -\eta\frac{\partial(\phi_1-\phi_2)}{\partial\nu}$ on $\partial\Omega$, which comes from the Robin boundary condition (2.15). Due to the strict decrease of f, we note that

$$(\phi_1-\phi_2)[f(\phi_1)-f(\phi_2)] \le 0 \quad \text{in } \Omega. \tag{2.98}$$

Thus, by (2.97)–(2.98), we arrive at

$$\int_{\Omega}\varepsilon|\nabla(\phi_1-\phi_2)|^2\,\mathrm{d}x + \eta\int_{\partial\Omega}\varepsilon\left|\frac{\partial(\phi_1-\phi_2)}{\partial\nu}\right|^2\mathrm{d}S_x \le 0,$$

which implies that $\phi_1 - \phi_2$ in $\overline{\Omega}$. Therefore, we complete the proof of uniqueness of (2.14)–(2.15).

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2C An example of oscillatory f_Λ for Remark 2.4

Under the assumptions (A1)‴ and (A2), system (2.13) can be solved by

$$c_{i,\Lambda}(\phi) = \frac{W_0\left(\Lambda\left(1-\gamma+\sum_{j=1}^{3}\gamma_j e^{\bar{\mu}_j - z_j\phi}\right)e^{\Lambda\tilde{\mu}_0+\hat{\mu}_0}\right)}{\Lambda\left(1-\gamma+\sum_{j=1}^{3}\gamma_j e^{\bar{\mu}_j - z_j\phi}\right)} e^{\bar{\mu}_i - z_i\phi}$$

for $\phi \in \mathbb{R}$ and $i = 0,1,2,3$. Suppose that $\Lambda = 4$, $z_0 = 0$, $z_1 = -z_2 = 1$ $z_3 = 2$, $\bar{\mu}_0 = \bar{\mu}_1 = 0$, $\bar{\mu}_2 = \bar{\mu}_3 = -5$, $\tilde{\mu}_0 = 1$, $\hat{\mu}_0 = 0$, $\gamma = 0.99$, $\gamma_1 = \gamma_2 = 0.01$, and $\gamma_3 = 0.97$. Recall the derivative of the Lambert W function (cf. [49,93]) is $\dfrac{\mathrm{d}W_0}{\mathrm{d}x} = \dfrac{W_0(x)}{x(1+W_0(x))}$ for $x > -1/e$. Differentiating $c_{i,4}$ with respect to ϕ, we obtain

$$\begin{aligned}\frac{\mathrm{d}c_{i,4}}{\mathrm{d}\phi} &= \frac{W_0(0.04e^4(1+e^{-\phi}+e^{-5+\phi}+97e^{-5-2\phi}))}{0.04(1+e^{-\phi}+e^{-5+\phi}+97e^{-5-2\phi})}\exp(\bar{\mu}_i - z_i\phi)\\ &\times\left(\frac{(e^{-\phi}-e^{-5+\phi}+194e^{-5-2\phi})W_0(0.04e^4(1+e^{-\phi}+e^{-5+\phi}+97e^{-5-2\phi}))}{(1+e^{-\phi}+e^{-5+\phi}+97e^{-5-2\phi})(1+W_0(0.04e^4(1+e^{-\phi}+e^{-5+\phi}+97e^{-5-2\phi})))} - z_i\right)\end{aligned} \tag{2.99}$$

for $\phi \in \mathbb{R}$ and $i = 0,1,2,3$. Let $K_1 = 0.04(1+e^2+e^{-7}+97e^{-1})$ and $K_2 = e^2 - e^{-7} + 194e^{-1}$. Then we have

$$\frac{\mathrm{d}f_4}{\mathrm{d}\phi}(-2) = \frac{W_0(e^4K_1)}{K_1}\left[\frac{K_2W_0(e^4K_1)}{25K_1(1+W_0(e^4K_1))}(e^2-e^{-7}+2e^{-1}) - (e^2+e^{-7}+4e^{-1})\right]. \tag{2.100}$$

It is easy to check that $K_2/K_1 > 44$ and $3.3e^{3.3} < e^4K_1 < 3.4e^{3.4}$. Due to the monotonic increase of W_0, we have $3.3 < W_0(e^4K_1) < 3.4$. Along with (2.100), we arrive at the fact $\dfrac{\mathrm{d}f_4}{\mathrm{d}\phi}(-2) > 0$. On the other hand, from (2.99), we apply L'Hôspital's law to get $\lim_{\phi\to\infty}\dfrac{\mathrm{d}c_{1,4}}{\mathrm{d}\phi}(\phi) = 0$, $\lim_{\phi\to\infty}\dfrac{\mathrm{d}c_{2,4}}{\mathrm{d}\phi}(\phi) = 25$, $\lim_{\phi\to\infty}\dfrac{\mathrm{d}c_{3,4}}{\mathrm{d}\phi}(\phi) = 0$, which implies $\lim_{\phi\to\infty}\dfrac{\mathrm{d}f_4}{\mathrm{d}\phi}(\phi) = -25$. This shows $\dfrac{\mathrm{d}f_4}{\mathrm{d}\phi}(\phi) < 0$ when ϕ is sufficiently large. Therefore, f_4 is oscillatory and the profile of f_4 is in Figure 2.2(a).

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3 Asymptotic analysis of boundary layer solutions to Poisson–Boltzmann type equations in general bounded smooth domains

3.1 Introduction

When a charged surface (e.g., electrode, membrane, colloid) is in contact with an electrolyte, a structured layer of charge known as the electric double layer (EDL) forms. The EDL plays a crucial role in various physical, engineering, and biological systems (cf. [23, 29, 99]). It typically consists of two distinct regions:

- Stern Layer — The region closest to the surface, where ions are strongly adsorbed, governed by the surface charge density;
- Diffuse Layer — A region extending into the electrolyte, where ion distributions are influenced by electrostatic interactions and thermal fluctuations.

The behavior of the diffuse layer can be described by different types of Poisson–Boltzmann (PB) equations, including:

- The classical PB equation, which models charge screening in electrolytes (cf. [11, 33, 69]);
- The modified PB equation, which incorporates ion size effects and steric interactions (cf. [9, 12, 43, 80, 82, 88, 90]);
- The charge-conserving PB equation, which enforces global charge neutrality (cf. [34, 70, 73, 105, 112]).

To analyze the structure of the diffuse layer, we study boundary layer solutions to PB-type equations in general bounded smooth domains (including multiply connected domains). This analysis provides key insights into electrostatic interactions in complex geometries, with applications in electrochemistry, biophysics, and materials science (cf. [3, 6, 17, 22, 24, 27, 62, 114, 115]).

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The classical PB and modified PB equations can be represented by

$$-\varepsilon\Delta\phi_\varepsilon = f(\phi_\varepsilon) \quad \text{in } \Omega, \tag{3.1}$$

where $\varepsilon > 0$ is the dielectric constant and ϕ_ε is the electric potential. Here $f = f(\phi)$ is a smooth function for the total ionic charge density which satisfies the following conditions.

(F1) The function $f = f(\phi)$ is smooth, strictly decreasing in ϕ, and satisfies

$$m_f = m_f(\mathcal{K}) := \sqrt{-\max_{\phi\in\mathcal{K}} f'(\phi)} > 0 \quad \text{for any compact interval } \mathcal{K} \subseteq \mathbb{R}.$$

(F2) The function f has a unique zero point ϕ^*, i.e., $f(\phi^*) = 0$, where ϕ^* is called as reference potential (cf. [4, 41]).

For example, function $f(\phi) = \sum_{i=1}^{I} z_i c_i^{\mathrm{b}} \exp(-z_i\phi)$ describes the total ionic charge density of the classical PB equation, and satisfies conditions (F1) and (F2), where I is the number of ion species, $z_i \neq 0$ is the valence and c_i^{b} is the concentration of the ith species in the bulk (cf. [33, 69]).

The charge-conserving PB (CCPB) equation was derived from the static limit of the Poisson–Nernst–Planck equations in order to guarantee charge neutrality within electrolyte domains (cf. [112]). The CCPB equation can be denoted as

$$-\varepsilon\Delta\phi_\varepsilon = \sum_{i=1}^{I} \frac{m_i z_i \exp(-z_i\phi_\varepsilon)}{\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y} \quad \text{in } \Omega, \tag{3.2}$$

where the constant $m_i > 0$ is the total concentration of species i with valence $z_i \neq 0$ for $i = 1, \ldots, I$. For charge neutrality, we assume

$$\sum_{i=1}^{I} m_i z_i = 0. \tag{3.3}$$

Due to the integral term $\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y$, (3.2) has nonlocal nonlinearity which makes (3.2) more difficult than (3.1). Note that equation (3.2) can be denoted as $-\varepsilon\Delta\phi_\varepsilon = f_\varepsilon(\phi_\varepsilon) := \sum\limits_{i=1}^{I} z_i c_{i,\varepsilon}^{\mathrm{b}} \exp(-z_i\phi_\varepsilon)$ in Ω, which has the same form as the classical PB equation. Here $f_\varepsilon(\phi) = \sum\limits_{i=1}^{I} z_i c_{i,\varepsilon}^{\mathrm{b}} \exp(-z_i\phi)$ presents the total ionic charge density (also see (3.127)) and $c_{i,\varepsilon}^{\mathrm{b}} = m_i / \left(\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y\right)$ is the concentration of the ith ion species in the bulk.

For the general bounded smooth domain $\Omega \subseteq \mathbb{R}^d$ $(d \geq 2)$, we assume

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(D) $\Omega = \Omega_0 - \bigcup_{k=1}^{K} \Omega_k$, $K \in \mathbb{N} \cup \{0\}$ (the number of holes) and Ω_k are bounded, smooth, simply connected domains with $\Omega_k \subset\subset \Omega_0$ for $k \in \{1, \ldots, K\}$ and $\mathrm{dist}(\Omega_i, \Omega_j) > 0$ for $i, j \in \{1, \ldots, K\}$ and $i \neq j$ (see Figure 3.1). Here dist denotes the distance.

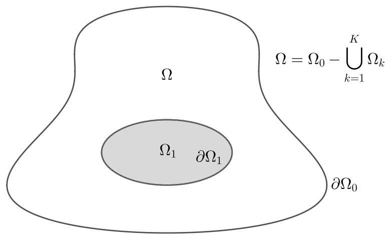

Figure 3.1: We sketch the schematic diagram of bounded smooth domain $\Omega = \Omega_0 - \bigcup_{k=1}^{K} \Omega_k$ and $K = 1$, where Ω has $(K+1)$ boundaries $\partial\Omega_k$ for $k = 0, 1, \ldots, K$.

The boundary condition of (3.1) and (3.2) is the Robin boundary condition given by

$$\phi_\varepsilon + \gamma_k \sqrt{\varepsilon} \partial_\nu \phi_\varepsilon = \phi_{bd,k} \quad \text{on } \partial\Omega_k \text{ for } k = 0, 1, \ldots, K, \tag{3.4}$$

where $\phi_{bd,k}$ is a constant for the given external electric potential, and $\gamma_k > 0$ is the ratio of Stern-layer width to the Debye screening length (cf. [8, 18, 96, 100]). As $\phi_{bd,k} = \phi^*$ for $k = 0, 1, \ldots, K$, equation (3.1) with condition (3.4) has only a trivial solution $\phi_\varepsilon \equiv \phi^*$ so we study equation (3.1) with condition (3.4) under the assumption that $\phi_{bd,k} \neq \phi^*$ for $k = 0, 1, \ldots, K$. When constants $\phi_{bd,k}$ are equal, the solution ϕ_ε to equation (3.2) with condition (3.4) is trivial. This leads us to assume that constants $\phi_{bd,k}$ are not equal. When the domain $\Omega = \Omega_0$ is simply connected (i.e., condition (D) with $K = 0$), the solution ϕ_ε to equation (3.2) with condition (3.4) is also trivial. Thus, we study equation (3.2) with condition (3.4) under the assumptions that $\phi_{bd,k}$ are not equal and the domain Ω satisfies (D) with $K \in \mathbb{N}$.

To find the boundary layer solutions to PB type equations in domain Ω, we assume $\varepsilon > 0$ (related to the Debye length) as a small parameter tending to zero (cf. [7, 31, 37, 61, 94]), and study the singular perturbation problems of (3.1) and (3.2) with the Robin boundary condition (3.4). We characterize the asymptotic expansions of solution ϕ_ε to equation (3.1) with condition (3.4) across three distinct regions based on their distance from the boundary:

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- Region I ($\Omega_{k,T,\varepsilon}$), where the distance from the boundary $\partial\Omega_k$ is at most $T\sqrt{\varepsilon}$,

- Region II ($\Omega_{k,T,\varepsilon,\beta}$), where the distance from the boundary $\partial\Omega_k$ ranges between $T\sqrt{\varepsilon}$ and ε^β,

- Region III ($\Omega_{\varepsilon,\beta}$), where the distance from the boundary $\partial\Omega$ is at least ε^β,

for given parameters $T > 0$ and $0 < \beta < 1/2$. Regions I and II are called tubular neighborhoods around $\partial\Omega_k$ (cf. [40]). A schematic illustration of these regions is shown in Figure 3.2.

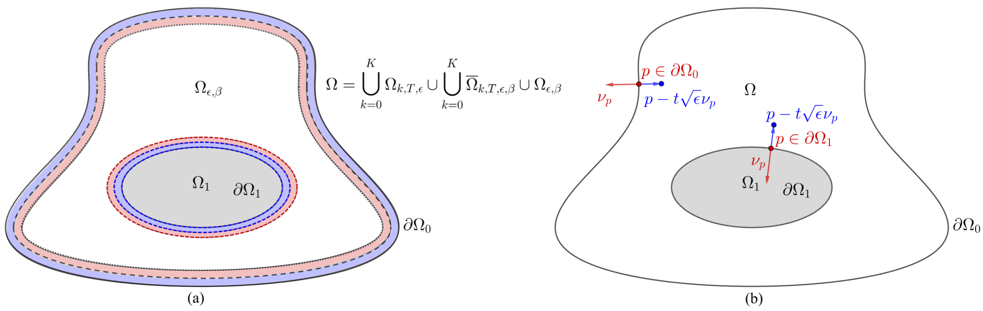

Figure 3.2: Let $0 < \beta < 1/2$, $T > 0$ and $K = 1$. In (a), we present the schematic diagram of regions $\Omega_{k,T,\varepsilon} = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega_k) < T\sqrt{\varepsilon}\}$ for $k = 0, 1$ (blue regions), $\overline{\Omega}_{k,T,\varepsilon,\beta} = \{x \in \Omega : T\sqrt{\varepsilon} \le \mathrm{dist}(x, \partial\Omega_k) \le \varepsilon^\beta\}$ for $k = 0, 1$ (red regions), and $\Omega_{\varepsilon,\beta} = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) > \varepsilon^\beta\}$ (white region) as $\varepsilon > 0$ sufficiently small. The union of these regions constitutes Ω. In (b), we sketch the point $p - t\sqrt{\varepsilon}\nu_p$ near the boundary $\partial\Omega_k$ for $k = 0, 1$, where $p \in \partial\Omega_k$ and $0 \le t \le \varepsilon^{(2\beta-1)/2}$, as $\varepsilon \to 0^+$. Here ν_p is the unit outer normal at p with respect to Ω.

The results for equation (3.1) with condition (3.4) are stated as follows.

Theorem 3.1. *Assume that (F1)–(F2) and (D) hold true, and that* $\phi_{\mathrm{bd},k} \ne \phi^*$ *for* $k = 0, 1, \ldots, K$. *Let* $\phi_\varepsilon \in \mathcal{C}^\infty(\overline{\Omega})$ *be the unique solution to equation (3.1) with condition (3.4). Let* $k \in \{0, 1, \ldots, K\}$, $p \in \partial\Omega_k$, *and* $T > 0$ *be arbitrary. Then*

(a)

$$\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_k(t) + \sqrt{\varepsilon}\Big((d-1)H(p)v_k(t) + o_\varepsilon(1)\Big), \tag{3.5}$$

$$\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\left(\frac{1}{\sqrt{\varepsilon}}u_k'(t) + (d-1)H(p)v_k'(t)\right)\nu_p + o_\varepsilon(1) \tag{3.6}$$

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for $0 \le t \le T$ *as* $\varepsilon \to 0^+$*, where* $p - t\sqrt{\varepsilon}\nu_p \in \overline{\Omega}_{k,T,\varepsilon} = \{x \in \overline{\Omega} : 0 \le \operatorname{dist}(x, \partial\Omega_k) \le T\sqrt{\varepsilon}\}$ *(see Figure 3.2). Here* $H(p)$ *and* ν_p *denote the mean curvature and unit outer normal at* p *with respect to* Ω*, respectively. The term* $o_\varepsilon(1)$*, tending to zero as* ε *goes to zero, depends on* T *but is independent of* $p \in \partial\Omega_k$*, which means*

$$\lim_{\varepsilon\to 0^+} \sup_{p\in\partial\Omega_k,\, t\in[0,T]} \left| \frac{1}{\sqrt{\varepsilon}}(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) - u_k(t)) - (d-1)H(p)v_k(t) \right| = 0,$$

$$\lim_{\varepsilon\to 0^+} \sup_{p\in\partial\Omega_k,\, t\in[0,T]} \left| \nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) + \left(\frac{1}{\sqrt{\varepsilon}} u_k'(t) + (d-1)H(p)v_k'(t) \right) \nu_p \right| = 0.$$

The functions $u_k(t)$ *and* $v_k(t)$ *are the unique solutions to*

$$u_k'' + f(u_k) = 0 \quad \text{in } (0,\infty), \tag{3.7}$$

$$u_k(0) - \gamma_k u_k'(0) = \phi_{bd,k}, \tag{3.8}$$

$$\lim_{t\to\infty} u_k(t) = \phi^*, \tag{3.9}$$

and

$$v_k'' + f'(u_k)v_k = u_k' \quad \text{in } (0,\infty), \tag{3.10}$$

$$v_k(0) - \gamma_k v_k'(0) = 0, \tag{3.11}$$

$$\lim_{t\to\infty} v_k(t) = 0. \tag{3.12}$$

(b) There exists a positive constant $\varepsilon^* > 0$ *such that*

(i)

$$|\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) - \phi^*| \le M' \exp(-Mt), \tag{3.13}$$

$$|\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p)| \le \frac{M'}{\sqrt{\varepsilon}} \exp(-Mt) \tag{3.14}$$

for $0 < \varepsilon < \varepsilon^*$*,* $0 < \beta < 1/2$ *and* $T \le t \le \varepsilon^{(2\beta-1)/2}$*, i.e.,* $p - t\sqrt{\varepsilon}\nu_p \in \overline{\Omega}_{k,T,\varepsilon,\beta} = \{x \in \Omega : T\sqrt{\varepsilon} \le \operatorname{dist}(x, \partial\Omega_k) \le \varepsilon^\beta\}$*;*

(ii)

$$|\phi_\varepsilon(x) - \phi^*| \le M' \exp\left(-M\varepsilon^{(2\beta-1)/2}\right), \tag{3.15}$$

$$|\nabla\phi_\varepsilon(x)| \le \frac{M'}{\sqrt{\varepsilon}} \exp\left(-M\varepsilon^{(2\beta-1)/2}\right) \tag{3.16}$$

for $0 < \varepsilon < \varepsilon^*$*,* $0 < \beta < 1/2$ *and* $x \in \overline{\Omega}_{\varepsilon,\beta} = \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) \ge \varepsilon^\beta\}$*.*

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Here $M > 0$ and $M' > 0$ are constants independent of ε.

Remark 3.1. *In electrostatics, the solution ϕ_ε represents the electric potential, which is of order $\mathcal{O}_\varepsilon(1)$ (cf. (3.5)), while the associated electric field $-\nabla\phi_\varepsilon$ is of order $\mathcal{O}_\varepsilon(1/\sqrt{\varepsilon})$ (cf. (3.6)) in Region I, denoted $\Omega_{k,T,\varepsilon}$. Reflecting geometric enhancement or suppression, the boundary mean curvature $H(p)$ contributes to the second-order corrections in the asymptotic expansions (3.5) and (3.6), where u_k and v_k are solutions to equations (3.7)–(3.12) and satisfy the following properties. When the external electric potential $\phi_{bd,k} > \phi^*$ and $k \in \{0, 1, \ldots, K\}$, the function $u_k(t) \in (\phi^*, \phi_{bd,k})$ is strictly decreasing for $t \in (0, \infty)$, and v_k is positive on $(0, \infty)$, strictly increasing on $(0, t_k^*)$ and strictly decreasing on (t_k^*, ∞), where $t_k^* 0$ is a constant. Conversely, when $\phi_{bd,k} < \phi^*$, $u_k(t) \in (\phi_{bd,k}, \phi^*)$ is strictly increasing for $t \in (0, \infty)$, and v_k is negative on $(0, \infty)$, strictly decreasing on $(0, t_k^*)$ and strictly increasing on (t_k^*, ∞) (cf. Propositions 3B.1 and 3C.1). The asymptotic formulas (3.5)–(3.6) thus provide approximations for the electric potential and electric field induced by an applied potential difference. In addition, the exponential decay estimates are given by (3.13)–(3.14) with respect to the variable t in Region II ($\Omega_{k,T,\varepsilon,\beta}$), and by (3.15)–(3.16) with respect to the parameter ε in Region III ($\Omega_{\varepsilon,\beta}$), highlighting the localized nature of boundary layer phenomena.*

The total ionic charge density plays crucial roles in the behavior of biological and physical systems (cf. [104]). Using formulas (3.5), (3.13)–(3.14) and (3.15)–(3.16) along with Taylor expansion of f, we derive the asymptotic expansion of the total ionic charge density $f(\phi_\varepsilon)$ as follows. Let $k \in \{0, 1, \ldots, K\}$, $p \in \partial\Omega_k$, $T > 0$, and $0 < \beta < 1/2$ be arbitrary.

- In Region I ($\Omega_{k,T,\varepsilon}$),

$$f(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p)) = f(u_k(t)) + \sqrt{\varepsilon}[(d-1)H(p)f'(u_k(t))v_k(t) + o_\varepsilon(1)] \quad (3.17)$$

  for $0 \le t \le T$;

- In Region II ($\Omega_{k,T,\varepsilon,\beta}$),

$$|f(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p))| \le M' \exp(-Mt) \quad \text{for } T \le t \le \varepsilon^{(2\beta-1)/2};$$

- In Region III ($\Omega_{\varepsilon,\beta}$),

$$|f(\phi_\varepsilon(x))| \le M' \exp(-M\varepsilon^{(2\beta-1)/2}) \quad \text{for } x \in \overline{\Omega}_{\varepsilon,\beta},$$

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as $0<\varepsilon<\varepsilon^*$, where ε^* comes from Theorem 3.1(b), M' and M are generic positive constants independent of ε. Here we have used the condition $f(\phi^*)=0$, which follows from assumption (F2).

The total ionic charge within regions $\overline{\Omega}_{k,T,\varepsilon}$, $\overline{\Omega}_{k,T,\varepsilon,\beta}$ and $\overline{\Omega}_{\varepsilon,\beta}$ can be expressed by the integral of the total ionic charge density $f(\phi_\varepsilon)$ over $\overline{\Omega}_{k,T,\varepsilon}$, $\overline{\Omega}_{k,T,\varepsilon,\beta}$ and $\overline{\Omega}_{\varepsilon,\beta}$, respectively. By Theorem 3.1, we have the following results.

Corollary 3.1. *Under the hypothesis of Theorem 3.1, if $\phi_{bd,k}>\phi^*$ (or $\phi_{bd,k}<\phi^*$), then we have*

(a) $\int_{\overline{\Omega}_{k,T,\varepsilon}} f(\phi_\varepsilon(x))\,\mathrm{d}x=\sqrt{\varepsilon}|\partial\Omega_k|(u_k'(0)-u_k'(T))$
$+\,\varepsilon(d-1)\left(\int_{\partial\Omega_k}H(p)\,\mathrm{d}S_p\right)(Tu_k'(T)+v_k'(0)-v_k'(T))+\varepsilon o_\varepsilon(1)<0$ *(or* >0*),*

(b) $\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f(\phi_\varepsilon(x))\,\mathrm{d}x=\sqrt{\varepsilon}|\partial\Omega_k|u_k'(T)$
$+\,\varepsilon(d-1)\left(\int_{\partial\Omega_k}H(p)\,\mathrm{d}S_p\right)(-Tu_k'(T)+v_k'(T))+\varepsilon o_\varepsilon(1)<0$ *(or* >0*),*

(c) $\left|\int_{\overline{\Omega}_{\varepsilon,\beta}} f(\phi_\varepsilon(x))\,\mathrm{d}x\right|\le\sqrt{\varepsilon}M'\exp\left(-M\varepsilon^{(2\beta-1)/2}\right)$

for $0<\varepsilon<\varepsilon^*$ and $0<\beta<1/2$, where $|\partial\Omega_k|$ is the surface area of $\partial\Omega_k$.

Corollary 3.1(a) and (b) imply that the total ionic charge in the near-boundary regions $\Omega_{k,T,\varepsilon}$ and $\Omega_{k,T,\varepsilon,\beta}$ is negative (or positive) when $\phi_{bd,k}>\phi^*$ (or $\phi_{bd,k}<\phi^*$), the external electric potential is greater (or less) than the reference potential. This gives a way for the redistribution of ionic species by the applied electric potential difference. Moreover,

$$0<\frac{\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f(\phi_\varepsilon(x))\,\mathrm{d}x}{\int_{\overline{\Omega}_{k,T,\varepsilon}} f(\phi_\varepsilon(x))\,\mathrm{d}x}\to\frac{u_k'(T)}{u_k'(0)-u_k'(T)}\quad\text{and}\quad\frac{|\overline{\Omega}_{k,T,\varepsilon}|}{|\overline{\Omega}_{k,T,\varepsilon,\beta}|}\to 0\quad\text{as }\varepsilon\to 0^+,\tag{3.18}$$

for $T>0$, $0<\varepsilon<1/2$ and $k=0,1,\ldots,K$. Since $u_k'(T)$ decays exponentially to zero as T goes to infinity (cf. Proposition 3B.2(a)), then (3.18) shows that for sufficiently large T, the majority of charged particles concentrate within the region $\Omega_{k,T,\varepsilon}$, whose volume satisfies $|\Omega_{k,T,\varepsilon}|\ll|\Omega_{k,T,\varepsilon,\beta}|$ as $\varepsilon\to 0^+$. In addition, Corollary 3.1(c) implies that the total ionic charge in the region $\Omega_{\varepsilon,\beta}$ decays exponentially as $\varepsilon\to 0^+$, demonstrating the emergence of electroneutrality in this bulk region. This result provides a rigorous justification for the commonly used electroneutrality assumption

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in bulk electrolyte solutions, while also quantifying the rate at which neutrality is approached in terms of the parameter β.

Analogously to Theorem 3.1, we characterize the asymptotic expansions of solution ϕ_ε to equation (3.2) with condition (3.4) across three distinct regions. The results can be stated as below.

Theorem 3.2. *Assume that the domain Ω satisfies condition (D) with $K \in \mathbb{N}$, $\phi_{bd,k}$ are not equal, and the charge neutrality condition (3.3) holds true, where $m_i > 0$ and $z_i \neq 0$ for $i = 1, \dots, I$. Let $\phi_\varepsilon \in \mathcal{C}^\infty(\overline{\Omega})$ be the unique solution to equation (3.2) with condition (3.4). Let $k \in \{0, 1, \dots, K\}$, $p \in \partial\Omega_k$, and $T > 0$ be arbitrary. Then*

(a)

$$\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_k(t) + \sqrt{\varepsilon}[(d-1)H(p)v_k(t) + w_k(t) + o_\varepsilon(1)], \tag{3.19}$$

$$\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\left(\frac{1}{\sqrt{\varepsilon}}u_k'(t) + (d-1)H(p)v_k'(t) + w_k'(t)\right)\nu_p + o_\varepsilon(1) \tag{3.20}$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$, where $p - t\sqrt{\varepsilon}\nu_p \in \overline{\Omega}_{k,T,\varepsilon}$ (see Figure 3.2). Here $H(p)$ and ν_p denote the mean curvature and the unit outer normal at p with respect to Ω, respectively. The term $o_\varepsilon(1)$, tending to zero as $\varepsilon \to 0^+$, depends on T but is independent of $p \in \partial\Omega_k$, which means

$$\lim_{\varepsilon\to 0^+} \sup_{p\in\partial\Omega_k,\, t\in[0,T]} \left|\frac{1}{\sqrt{\varepsilon}}(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) - u_k(t)) - (d-1)H(p)v_k(t) - w_k(t)\right| = 0,$$

$$\lim_{\varepsilon\to 0^+} \sup_{p\in\partial\Omega_k,\, t\in[0,T]} \left|\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) + \left(\frac{1}{\sqrt{\varepsilon}}u_k'(t) + (d-1)H(p)v_k'(t) + w_k'(t)\right)\nu_p\right| = 0.$$

The functions $u_k(t)$, $v_k(t)$, and $w_k(t)$ are the unique solutions to

$$u_k'' + f_0(u_k) = 0 \quad \text{in } (0,\infty), \tag{3.21}$$

$$u_k(0) - \gamma_k u_k'(0) = \phi_{bd,k}, \tag{3.22}$$

$$\lim_{t\to\infty} u_k(t) = \phi_0^*, \tag{3.23}$$

$$v_k'' + f_0'(u_k)v_k = u_k' \quad \text{in } (0,\infty) \tag{3.24}$$

$$v_k(0) - \gamma_k v_k'(0) = 0, \tag{3.25}$$

$$\lim_{t\to\infty} v_k(t) = 0, \tag{3.26}$$

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and

$$w_k'' + f_0'(u_k)w_k = -f_1(u_k) \quad \text{in } (0,\infty), \tag{3.27}$$

$$w_k(0) - \gamma_k w_k'(0) = 0, \tag{3.28}$$

$$\lim_{t\to\infty} w_k(t) = Q. \tag{3.29}$$

The constants ϕ_0^* and Q are determined uniquely by (3.150)–(3.151) and (3.238), respectively. The functions f_0 and f_1 are given by

$$f_0(\phi) = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi-\phi_0^*)) \quad \text{for } \phi \in \mathbb{R}, \tag{3.30}$$

$$f_1(\phi) = -Qf_0'(\phi) + \hat{f}_1(\phi) \quad \text{for } \phi \in \mathbb{R}, \tag{3.31}$$

where $|\Omega|$ is the volume of Ω, and

$$\hat{f}_1(\phi) = \frac{1}{|\Omega|}\sum_{i=1}^{I} \hat{m}_i z_i \exp(-z_i(\phi-\phi_0^*)) \quad \text{for } \phi \in \mathbb{R},$$

$$\hat{m}_i = \frac{m_i}{|\Omega|}\sum_{k=0}^{K} |\partial\Omega_k| \int_0^\infty [1-\exp(-z_i(u_k(s)-\phi_0^*))]\,\mathrm{d}s \quad \text{for } i = 1,\ldots,I.$$

Furthermore, the constant Q satisfies

$$Q = \lim_{\varepsilon\to 0^+}\frac{\phi_\varepsilon^* - \phi_0^*}{\sqrt{\varepsilon}} = \frac{\displaystyle\sum_{k=0}^{K} \frac{|\partial\Omega_k|\hat{F}_1(u_k(0)) + (d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)\left(\int_0^\infty u_k'^2(s)\,\mathrm{d}s\right)}{u_k'(0)+\gamma_k f_0(u_k(0))}}{\displaystyle\sum_{k=0}^{K}\frac{|\partial\Omega_k| f_0(u_k(0))}{u_k'(0)+\gamma_k f_0(u_k(0))}}, \tag{3.32}$$

where ϕ_ε^* is the unique zero of function f_ε for $\varepsilon > 0$ (cf. Proposition 3.14) and $\hat{F}_1(\phi) = \int_{\phi^*}^{\phi} \hat{f}_1(s)\,\mathrm{d}s = \frac{1}{|\Omega|}\sum_{i=1}^{I}\hat{m}_i[1-\exp(-z_i(\phi-\phi_0^*))]$ for $\phi\in\mathbb{R}$.

(b) *There exists a positive constant $\varepsilon^* > 0$ such that*

(i)

$$|\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) - \phi_\varepsilon^*| \le M' \exp(-Mt), \tag{3.33}$$

$$|\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p)| \le \frac{M'}{\sqrt{\varepsilon}}\exp(-Mt) \tag{3.34}$$

for $0 < \varepsilon < \varepsilon^*$, $0 < \beta < 1/2$ and $T \le t \le \varepsilon^{(2\beta-1)/2}$, i.e., $p - t\sqrt{\varepsilon}\nu_p \in \overline{\Omega}_{k,T,\varepsilon,\beta}$;

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(ii)

$$|\phi_\varepsilon(x) - \phi_\varepsilon^*| \le M' \exp\left(-M\varepsilon^{(2\beta-1)/2}\right), \tag{3.35}$$

$$|\nabla\phi_\varepsilon(x)| \le \frac{M'}{\sqrt{\varepsilon}} \exp\left(-M\varepsilon^{(2\beta-1)/2}\right) \tag{3.36}$$

for $0 < \varepsilon < \varepsilon^*$ *and* $0 < \beta < 1/2$.

Here $M > 0$ *and* $M' > 0$ *are constants independent of* ε.

The main difference of Theorems 3.1 and 3.2 comes from the integral terms in (3.2) which give the solution w_k to (3.27)–(3.29) and (3.32). This reflects the effect of nonlocal nonlinearity in (3.2).

Remark 3.2. *Recall that* $f_\varepsilon(\phi) = \sum_{i=1}^I z_i c_{i,\varepsilon}^{\mathrm{b}} \exp(-z_i\phi)$ *represents the total ionic charge density and* $c_{i,\varepsilon}^{\mathrm{b}} = m_i / \left(\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y\right)$ *is the concentration of the ith ion species in the bulk. From* (3.32), *we find*

$$c_{i,\varepsilon}^{\mathrm{b}} = c_i^{\mathrm{b}} + \sqrt{\varepsilon}\left(\frac{m_i z_i Q \exp(z_i\phi_0^*) + \hat{m}_i \exp(z_i\phi_0^*)}{|\Omega|} + o_\varepsilon(1)\right) \quad \textit{for } i = 1, \dots, I, \tag{3.37}$$

$$f_\varepsilon(\phi) = f_0(\phi) + \sqrt{\varepsilon}(f_1(\phi) + o_\varepsilon(1)) \quad \textit{for } \phi \in \mathbb{R}, \tag{3.38}$$

(cf. Remark 3.7 and (3.220) *in Section 3.3.4), where* $c_i^{\mathrm{b}} := m_i \exp(z_i\phi_0^*)/|\Omega|$ *(is the concentration of the ith ion species in the bulk) may correspond to the bulk concentration in the classical PB equation* $-\varepsilon\Delta\phi_\varepsilon = \sum_{i=1}^I z_i c_i^{\mathrm{b}} \exp(-z_i\phi_\varepsilon) = f_0(\phi_\varepsilon)$ *in* Ω. *Here* f_0 *and* f_1 *are given in* (3.30)–(3.31).

As in Remark 3.1, we have the following observation.

Remark 3.3. *In electrostatics, the solution* ϕ_ε *represents the electric potential, and its gradient* $-\nabla\phi_\varepsilon$ *represents the electric potential, with orders* $\mathcal{O}_\varepsilon(1)$ *and* $\mathcal{O}_\varepsilon(1/\sqrt{\varepsilon})$, *respectively, in the region* $\Omega_{k,T,\varepsilon}$. *Similar to Remark 3.1, the boundary curvature* $H(p)$ *contributes to the second-order corrections in the asymptotic expansions* (3.19)–(3.20), *where* u_k, v_k, *and* w_k *are the solutions to* (3.21)–(3.29) *and satisfy the following properties. When the external electric potential* $\phi_{bd,k} > \phi_0^*$ *and* $k \in \{0, 1, \dots, K\}$, *the function* $u_k(t) \in (\phi_0^*, \phi_{bd,k})$ *is strictly decreasing for* $t \in (0, \infty)$, *and* v_k *is positive on* $(0, \infty)$, *strictly increasing on* $(0, t_k^*)$ *and strictly decreasing on* (t_k^*, ∞), *where* t_k^* *is a constant. Conversely, when* $\phi_{bd,k} < \phi_0^*$, $u_k(t) \in (\phi_{bd,k}, \phi_0^*)$ *is strictly increasing*

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for $t \in (0,\infty)$, and v_k is negative on $(0,\infty)$, strictly decreasing on $(0,t_k^*)$ and strictly increasing on (t_k^*,∞) (cf. Propositions 3B.1 and 3C.1). The asymptotic formulas (3.19)–(3.20) thus provide approximations for the electric potential and electric field induced by an applied potential difference. Additionally, the exponential decay estimates are given by (3.33)–(3.34) with respect to the variable t in Region II ($\Omega_{k,T,\varepsilon,\beta}$), and by (3.35)–(3.36) with respect to the parameter ε in Region III ($\Omega_{\varepsilon,\beta}$), highlighting the localized nature of boundary layer phenomena. However, w_k, which arises from the nonlocal nonlinearity, may not behave like u_k and v_k because the constants $\hat{m}_i$ do not have the same sign.

As the previous discussion for total ionic charge density of (3.1), we use formulas (3.19), (3.33)–(3.34), (3.35)–(3.36), (3.38), and the Taylor expansions of f_0 and f_1 to derive the asymptotic expansion of the total ionic charge density $f_\varepsilon(\phi_\varepsilon)$ as follows. Let $k \in \{0,1,\dots,K\}$, $p \in \partial\Omega_k$, $T > 0$, and $0 < \beta < 1/2$ be arbitrary.

- In Region I ($\Omega_{k,T,\varepsilon}$),

$$\begin{aligned} f_\varepsilon(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p)) &= f_0(u_k(t)) \\ &\quad + \sqrt{\varepsilon}[(d-1)H(p)f_0'(u_k(t))v_k(t) + f_0'(u_k(t))w_k(t) + f_1(u_k(t)) + o_\varepsilon(1)] \end{aligned} \tag{3.39}$$

  for $0 \le t \le T$;

- In Region II ($\Omega_{k,T,\varepsilon,\beta}$),

$$|f_\varepsilon(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p))| \le M' \exp(-Mt) \quad \text{for } T \le t \le \varepsilon^{(2\beta-1)/2};$$

- In Region III ($\Omega_{\varepsilon,\beta}$),

$$|f_\varepsilon(\phi_\varepsilon(x))| \le M' \exp(-M\varepsilon^{(2\beta-1)/2}) \quad \text{for } x \in \overline{\Omega}_{\varepsilon,\beta},$$

as $0 < \varepsilon < \varepsilon^*$, where ε^* comes from Theorem 3.2(b), M' and M are generic positive constants independent of ε. Here we have used the condition $f_\varepsilon(\phi_\varepsilon^*) = 0$, which follows from Proposition 3.14, and $f_0(\phi_0^*) = 0$.

As in Corollary 3.1, we use Theorem 3.2 to derive the asymptotic expansions of total ionic charge within regions $\overline{\Omega}_{k,T,\varepsilon}$, $\overline{\Omega}_{k,T,\varepsilon,\beta}$ and $\overline{\Omega}_{\varepsilon,\beta}$ as below.

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Corollary 3.2. *Under the hypothesis of Theorem 3.2, if $\phi_{bd,k} > \phi_0^*$ (or $\phi_{bd,k} < \phi_0^*$), then we have*

(a) $\int_{\overline{\Omega}_{k,T,\varepsilon}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \sqrt{\varepsilon}|\partial\Omega_k|(u_k'(0) - u_k'(T))$
$+ \varepsilon\left[(d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)(Tu_k'(T) + v_k'(0) - v_k'(T))\right]$
$+ \varepsilon\left[|\partial\Omega_k|(w_k'(0) - w_k'(T)) + o_\varepsilon(1)\right] < 0$ *(or* > 0*),*

(b) $\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \sqrt{\varepsilon}|\partial\Omega_k|u_k'(T)$
$+ \varepsilon\left[(d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)(-Tu_k'(T) + v_k'(T))\right]$
$+ \varepsilon\left[|\partial\Omega_k|w_k'(T)\right] + \varepsilon o_\varepsilon(1)\Big] < 0$ *(or* > 0*),*

(c) $\left|\int_{\overline{\Omega}_{\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x\right| \le \sqrt{\varepsilon}M' \exp\left(-M\varepsilon^{(2\beta-1)/2}\right)$

for $0 < \varepsilon < \varepsilon^*$ *and* $0 < \beta < 1/2$*, where* $|\partial\Omega_k|$ *is the surface area of* $\partial\Omega_k$*.*

Corollary 3.2 is consistent with the charge neutrality condition (3.3), as demonstrated by equations (3.151) and (3.239) in Section 3.3. Corollary 3.2(a) and 3.2(b) also indicate that the total ionic charge in the near-boundary regions $\Omega_{k,T,\varepsilon}$ and $\Omega_{k,T,\varepsilon,\beta}$ is negative (or positive) when $\phi_{bd,k} > \phi_0^*$ (or $\phi_{bd,k} < \phi_0^*$). Such behavior is analogous to that described in Corollary 3.1, where the sign of the total ionic charge is similarly determined by the comparison between $\phi_{bd,k}$ and ϕ_0^*. This redistribution of ionic species is driven by the applied electric potential difference, consistent with the behavior in Corollary 3.1. Moreover, analogously to (3.18),

$$0 < \frac{\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x}{\int_{\overline{\Omega}_{k,T,\varepsilon}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x} \to \frac{u_k'(T)}{u_k'(0) - u_k'(T)} \quad \text{and} \quad \frac{|\overline{\Omega}_{k,T,\varepsilon}|}{|\overline{\Omega}_{k,T,\varepsilon,\beta}|} \to 0 \quad \text{as } \varepsilon \to 0^+.$$

Since $u_k'(T)$ decays exponentially to zero as $T \to \infty$ (cf. Proposition 3B.2(a)), this implies that for sufficiently large T, the majority of charged particles are concentrated within the region $\Omega_{k,T,\varepsilon}$, despite its volume being significantly smaller than that of the region $\Omega_{k,T,\varepsilon,\beta}$. Additionally, Corollary 3.2(c) implies that the total ionic charge in the region $\Omega_{\varepsilon,\beta}$ decays exponentially as $\varepsilon \to 0^+$ as in Corollary 3.1(c).

For the proof of Theorem 3.1, we first establish the uniform boundedness of the solution ϕ_ε (cf. Proposition 3.3), and then employ the principal coordinate system (cf. [38, Section 14.6]) and rescale spatial variables by $\sqrt{\varepsilon}$ to obtain the local convergence and to derive equation (3.52) in $\mathbb{R}_+^d$ with condition (3.53) (cf. Lemma 3.5). Using the exponential-type estimate of (3.52)–(3.53) (cf. Lemma 3.6) and the moving

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plane arguments (cf. Proposition 3.7), we prove the first-order asymptotic expansion of ϕ_ε (see (3.84)–(3.85)). Using the first-order asymptotic expansion, we derive the exponential-type estimate of ϕ_ε and $|\nabla\phi_\varepsilon|$ (cf. Proposition 3.9), which implies Theorem 3.1(b) holds true. For the second-order asymptotic expansion of ϕ_ε, we study $\varphi_{k,\varepsilon}(x) = \varepsilon^{-1/2}[\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})]$ for $x \in \overline{\Omega}_{k,\varepsilon,\beta} := \{x \in \overline{\Omega} : \delta_k(x) \leq \varepsilon^\beta\}$ and $k = 0, 1, \ldots, K$. We prove the uniform boundedness of $\varphi_{k,\varepsilon}$ (cf. Proposition 3.10) and the local convergence to get equation (3.112) in $\mathbb{R}^d_+$ with condition (3.113) (cf. Lemma 3.11). Using the exponential-type estimate (3.114) and the moving plane arguments (cf. Proposition 3.12), we obtain (3.5) and (3.6) in Theorem 3.1(a).

For the proof of Theorem 3.2, we rewrite equation (3.2) as $-\varepsilon\Delta\phi_\varepsilon = f_\varepsilon(\phi_\varepsilon)$ in Ω, where $f_\varepsilon(\phi) = \sum_{i=1}^I (m_i z_i / A_{i,\varepsilon}) \exp(-z_i\phi)$ for $\phi \in \mathbb{R}$, $A_{i,\varepsilon} = \int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y$ for $i = 1, \ldots, I$, and ϕ_ε is the solution to equation (3.2) with condition (3.4). In Section 3.3.1, we first prove the uniform boundedness of ϕ_ε and show that f_ε also satisfies conditions (F1)–(F2) with the unique zero ϕ^*_ε. As in the proof in Section 3.2.1, we establish the first-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$. Moreover, we also determine the unique value of ϕ^*_0 by the algebraic equations (3.150)–(3.151). However, unlike the proof of Theorem 3.1, the unique zero ϕ^*_ε of f_ε may depend on the parameter ε so it is pivotal to prove, by contradiction, the uniform boundedness of $|\phi^*_\varepsilon - \phi^*_0|/\sqrt{\varepsilon}$ (cf. Section 3.3.3). More specifically, in Section 3.3.3, under the assumption $|\phi^*_\varepsilon - \phi^*_0|/\sqrt{\varepsilon} \to \infty$ as ε goes to zero, we obtain the second-order asymptotic expansions of $A_{i,\varepsilon}$, f_ε, and ϕ_ε and the total ionic charge over three distinct regions, which contradicts the electroneutrality condition (3.3). Then in Section 3.3.4, we use the uniform boundedness of $|\phi^*_\varepsilon - \phi^*_0|/\sqrt{\varepsilon}$ to get the asymptotic expansion of $A_{i,\varepsilon}$ (see Remark 3.7). This implies that the function f_ε has the asymptotic expansion $f_\varepsilon(\phi) = f_0(\phi) + \sqrt{\varepsilon}(f_1(\phi) + o_\varepsilon(1))$ for $\phi \in \mathbb{R}$, where f_0 and f_1 are smooth functions (see (3.30)–(3.31)). Thus, equation (3.2) can be transformed into $-\varepsilon\Delta\phi_\varepsilon = f_0(\phi_\varepsilon) + \sqrt{\varepsilon}(f_1(\phi_\varepsilon) + o_\varepsilon(1))$ in Ω (cf. (3.221)), where f_0 satisfies (F1)–(F2) with a unique zero ϕ^*_0 and f_1 is bounded on any compact subsets of $\mathbb{R}$. Therefore, as in the proof of Theorem 3.1, we may apply the principal coordinate system and the moving plane arguments to prove Theorem 3.2(a).

The electric forces play a central role in the behavior of biological and physical systems (cf. [112]). In [42, 104], the Maxwell stress tensor $\mathscr{T}_\mathrm{M}$ of equation (3.1) is

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defined as

$$\mathscr{T}_{\mathrm{M}} = \varepsilon \nabla \phi_\varepsilon \otimes \nabla \phi_\varepsilon - \frac{\varepsilon}{2} |\nabla \phi_\varepsilon|^2 I_d, \tag{3.40}$$

where $\otimes$ denotes the tensor product. Then by (3.6) and (3.40), we get the Maxwell stress tensor $\mathscr{T}_{\mathrm{M}}$ at $p - t\sqrt{\varepsilon}\nu_p$:

$$\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p) = [u_k'^2(t) + 2\sqrt{\varepsilon}(d-1)H(p)u_k'(t)v_k'(t)] \left(\nu_p \otimes \nu_p - \frac{1}{2} I_d\right) + \sqrt{\varepsilon}o_\varepsilon(1)$$

for $0 \le t \le T$ and $p \in \partial\Omega_k$. By (3.265) and (3.270) with $U = u_k$, we have $u_k'^2(t) = 2(F(\phi^*) - F(u_k(t))) = -2F(u_k(t))$ for all $t \ge 0$, where $F(\phi) = \int_{\phi^*}^{\phi} f(s)\,\mathrm{d}s$ and ϕ^* is the unique zero of f. Hence

$$\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p) = [-F(u_k(t)) + \sqrt{\varepsilon}(d-1)H(p)u_k'(t)v_k'(t)](2\nu_p \otimes \nu_p - I_d) + \sqrt{\varepsilon}o_\varepsilon(1),$$

which gives

$$\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p)\nu_p = -F(u_k(t))\nu_p + \sqrt{\varepsilon}[(d-1)H(p)u_k'(t)v_k'(t)\nu_p + o_\varepsilon(1)] \tag{3.41}$$

for $0 \le t \le T$ and $p \in \partial\Omega_k$. Note that $F(u_k(t)) < 0$ for $t \ge 0$ because $F(\phi^*) = F'(\phi^*) = 0$ and $F''(\phi) = f'(\phi) < 0$ for $\phi \in \mathbb{R}$. In (3.41), $\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p)\nu_p$ is the stress tensor $\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p)$ acting on ν_p, which provides the electric force at $p - t\sqrt{\varepsilon}\nu_p$ for $0 \le t \le T$, $p \in \partial\Omega_k$, and $k \in \{0, 1, \ldots, K\}$.

For equation (3.2) with condition (3.4), we can use (3.5)–(3.12), (3.20), and (3.40) directly to derive the asymptotic formula of the Maxwell stress tensor $\mathscr{T}_{\mathrm{M}}$:

$$\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p) = \{u_k'^2(t) + 2\sqrt{\varepsilon}u_k'(t)[(d-1)H(p)v_k'(t) + w_k'(t)]\} \left(\nu_p \otimes \nu_p - \frac{1}{2} I_d\right) + \sqrt{\varepsilon}o_\varepsilon(1)$$

for $0 \le t \le T$ and $p \in \partial\Omega_k$. By (3.265) and (3.270) with $U = u_k$, we have $u_k'^2(t) = 2(F_0(\phi^*) - F_0(u_k(t))) = -2F_0(u_k(t))$ for all $t \ge 0$, where $F_0(\phi) = \int_{\phi_0^*}^{\phi} f_0(s)\,\mathrm{d}s$ and ϕ_0^* is the unique zero of f_0. Hence

$$\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p) = \{-F_0(u_k(t)) + \sqrt{\varepsilon}u_k'(t)[(d-1)H(p)v_k'(t) + w_k'(t)]\}(2\nu_p \otimes \nu_p - I_d) + \sqrt{\varepsilon}o_\varepsilon(1),$$

which implies

$$\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p)\nu_p = -F_0(u_k(t))\nu_p + \sqrt{\varepsilon}u_k'(t)\{[(d-1)H(p)v_k'(t) + w_k'(t)]\nu_p + o_\varepsilon(1)\} \tag{3.42}$$

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for $0 \le t \le T$ and $p \in \partial\Omega_k$. Note that $F_0(u_k(t)) < 0$ for $t \ge 0$ because $F_0(\phi_0^*) = F_0'(\phi_0^*) = 0$ and $F_0''(\phi) = f_0'(\phi) < 0$ for $\phi \in \mathbb{R}$. In (3.42), $\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p)\nu_p$ is the stress tensor $\mathscr{T}_{\mathrm{M}}(p - t\sqrt{\varepsilon}\nu_p)$ acting on ν_p, which provides the electric force at $p - t\sqrt{\varepsilon}\nu_p$ for $0 \le t \le T$, $p \in \partial\Omega_k$, and $k \in \{0, 1, \dots, K\}$.

Throughout the chapter we shall use the following notations.

- $\mathcal{O}_\varepsilon(1)$ is a bounded quantity independent of ε, and $o_\varepsilon(1)$ is a small quantity tending to zero as ε goes to zero.
- $\mathbb{R}^d_+ = \{(z = (z', z^d) \in \mathbb{R}^d : z^d > 0\}$, $\partial\mathbb{R}^d_+ = \{z = (z', z^d) \in \mathbb{R}^d : z^d = 0\}$, and $\overline{\mathbb{R}}^d_+ = \mathbb{R}^d_+ \cup \partial\mathbb{R}^d_+$.
- e_d stands for the unit vector in the positive direction of z^d-axis.
- $|\Omega|$ denotes the volume of Ω, and $|\partial\Omega_k|$ stands for the surface area of $\partial\Omega_k$ for $k = 0, 1, \dots, K$.
- $\Omega_{k,T,\varepsilon} = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega_k) < T\sqrt{\varepsilon}\}$, $\Omega_{k,T,\varepsilon,\beta} = \{x \in \Omega : T\sqrt{\varepsilon} < \mathrm{dist}(x, \partial\Omega_k) < \varepsilon^\beta\}$, $\Omega_{k,\varepsilon,\beta} = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega_k) < \varepsilon^\beta\}$ and $\Omega_{\varepsilon,\beta} = \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) > \varepsilon^\beta\}$, where dist denotes the distance.
- $\delta_k(x) = \mathrm{dist}(x, \partial\Omega_k)$ and $\delta(x) = \mathrm{dist}(x, \partial\Omega) = \min\{\delta_0(x), \delta_1(x), \dots, \delta_K(x)\}$.
- $\underline{\phi_{bd}} = \min\limits_{0 \le k \le K} \phi_{bd,k}$ and $\overline{\phi_{bd}} = \max\limits_{0 \le k \le K} \phi_{bd,k}$.
- $\varepsilon^* > 0$ is a sufficiently small constant, and $M > 0$ is a generic constant independent of $\varepsilon > 0$.

The rest of the chapter is organized as follows. The proofs of Theorems 3.1 and 3.2 are given in Sections 3.2 and 3.3, respectively. For the analysis of ordinary differential equations (3.7)–(3.12), (3.21)–(3.23) and (3.24)–(3.29), one may refer to Appendices 3A to 3D.

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3.2 Proof of Theorem 3.1

In this section, we derive the first- and second-order terms in the asymptotic expansion of the solution ϕ_ε to equation (3.1) with condition (3.4) near $\partial\Omega_k$ for $k = 0, 1, \ldots, K$. For the first-order term, we use the principal coordinate system (3.43) to straighten the boundary $\partial\Omega_k$ locally and rescale spatial variables by $\sqrt{\varepsilon}$ so that equations (3.1) with condition (3.4) can be transformed into (3.50)–(3.51) in the upper half-ball $B^+_{b/\sqrt{\varepsilon}}$. We then show that the solution to (3.50)–(3.51) converges (locally) to the solution to (3.52)–(3.53) in the upper half-space $\mathbb{R}^d_+$ (cf. Lemma 3.5). By the moving plane arguments on (3.52)–(3.53), we prove that the solution to (3.52)–(3.53) depends only on the single variable z^d (cf. Proposition 3.7), which is the unique solution to (3.7)–(3.9). Here we have to assume that $\phi_{bd,k}$ are constants. Hence we obtain the asymptotic expansions $\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_k(t) + o_\varepsilon(1)$ and $\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\varepsilon^{-1/2}(u_k'(t)\nu_p + o_\varepsilon(1))$ for $T > 0$, $p \in \partial\Omega_k$ and $0 \le t \le T$, where u_k is the unique solution to (3.7)–(3.9) and ν_p is the unit outer normal at p (cf. Section 3.2.1).

For the second-order term, we set $\varphi_{k,\varepsilon}(x) = \varepsilon^{-1/2}(\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon}))$ for $x \in \overline{\Omega}_{k,\varepsilon,\beta}$ and $k = 0, 1, \ldots, K$, where $\Omega_{k,\varepsilon,\beta} = \{x \in \Omega : \delta_k(x) < \varepsilon^\beta\}$ and $0 < \beta < 1/2$. Then by the exponential-type estimate of $u_{k,p}$ and ϕ_ε (cf. Lemma 3.6 and Proposition 3.9), we may prove the uniform boundedness of $\varphi_{k,\varepsilon}$ (cf. Proposition 3.10). Moreover, following similar arguments as in Section 3.2.1, we use the principal coordinate system and the moving plane arguments to prove the local convergence of $\varphi_{k,\varepsilon}$ and obtain $\varphi_{k,\varepsilon}(p - t\sqrt{\varepsilon}\nu_p) = (d-1)H(p)v_k(t) + o_\varepsilon(1)$ and $\nabla\varphi_{k,\varepsilon}(p - t\sqrt{\varepsilon}\nu_p) = -\varepsilon^{-1/2}[(d-1)H(p)v_k'(t)\nu_p + o_\varepsilon(1)]$ for $T > 0$, $p \in \partial\Omega_k$ and $0 \le t \le T$ (as $\varepsilon > 0$ sufficiently small), where v_k is the unique solution to (3.10)–(3.12) (cf. Section 3.2.2). Therefore, we obtain equations (3.5)–(3.6) and complete the proof of Theorem 3.1.

3.2.1 First-order asymptotic expansion of ϕ_ε

Equation (3.1) with the boundary condition (3.4) is the Euler–Lagrange equation of the following energy functional

$$E[\phi] = \int_\Omega \left(\frac{\varepsilon}{2}|\nabla\phi|^2 - F(\phi)\right) \mathrm{d}x + \sqrt{\varepsilon}\sum_{k=0}^{K} \frac{1}{2\gamma_k}\int_{\partial\Omega_k} (\phi - \phi_{bd,k})^2 \,\mathrm{d}S \quad \text{for } \phi \in H^1(\Omega).$$

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Since $F'' = f' < 0$ in $\mathbb{R}$, we can apply the direct method in the calculus of variations to get the unique minimizer of $E[\phi]$ over $H^1(\Omega)$ (cf. [109]). Then by the standard bootstrap argument and smoothness of f, we obtain the existence and uniqueness of the smooth solution $\phi \in \mathcal{C}^\infty(\overline{\Omega})$ to equation (3.1) with condition (3.4) (cf. [38]). Because the nonlinear term f is strictly decreasing (cf. (F1)), we can prove the uniform boundedness of the solution ϕ_ε as follows.

Proposition 3.3 (Uniform boundedness of ϕ_ε)**.** *For $\varepsilon > 0$, let $\phi_\varepsilon \in \mathcal{C}^\infty(\overline{\Omega})$ be the solution to equation* (3.1) *with condition* (3.4)*. Then $|\phi_\varepsilon(x) - \phi^*| \le C_1$ for $x \in \overline{\Omega}$ and $\varepsilon > 0$, where ϕ^* is the unique zero of f (cf. (F2)) and $C_1 > 0$ is a constant independent of ε.*

Proof. We first prove that $\phi_\varepsilon(x) \le \max\{\phi^*, \overline{\phi_{bd}}\}$ for $x \in \overline{\Omega}$ and $\varepsilon > 0$. Suppose that ϕ_ε attains its maximum value at an interior point x_0, which implies $\Delta\phi_\varepsilon(x_0) \le 0$. Then by (3.1) and (F2), we obtain $f(\phi^*) = 0 \le -\varepsilon\Delta\phi_\varepsilon(x_0) = f(\phi_\varepsilon(x_0))$. Due to the strict decrease of f (cf. (F1)), we have $\phi_\varepsilon(x_0) \le \phi^*$, which implies $\phi_\varepsilon(x) \le \phi^*$ for $x \in \overline{\Omega}$. On the other hand, we suppose that ϕ_ε attains its maximum value at a boundary point $x_0 \in \partial\Omega_{k_0}$ for some $k_0 \in \{0, 1, \dots, K\}$, which implies $\partial_\nu\phi_\varepsilon(x_0) \ge 0$. By the boundary condition (3.4) with $\gamma_{k_0} > 0$, we get

$$\phi_\varepsilon(x) \le \phi_\varepsilon(x_0) = \phi_{bd,k_0} - \gamma_{k_0}\sqrt{\varepsilon}\partial_\nu\phi_\varepsilon(x_0) \le \phi_{bd,k_0} \le \overline{\phi_{bd}} := \max_{0\le k\le K} \phi_{bd,k} \quad \text{for } x \in \overline{\Omega}.$$

Thus, $\phi_\varepsilon(x) \le \max\{\phi^*, \overline{\phi_{bd}}\}$ for $x \in \overline{\Omega}$ and $\varepsilon > 0$. Similarly, we can get $\phi_\varepsilon(x) \ge \min\{\phi^*, \underline{\phi_{bd}}\}$ for $x \in \overline{\Omega}$ and $\varepsilon > 0$, where $\underline{\phi_{bd}} := \min_{0\le k\le K} \phi_{bd,k}$. Hence $\min\{\phi^*, \underline{\phi_{bd}}\} \le \phi_\varepsilon(x) \le \max\{\phi^*, \overline{\phi_{bd}}\}$, i.e., $|\phi_\varepsilon(x) - \phi^*| \le C_1$ for $x \in \overline{\Omega}$ and $\varepsilon > 0$, where $C_1 > 0$ is a constant independent of $\varepsilon > 0$. Therefore, we complete the proof of Proposition 3.3. $\square$

Now we introduce the principal coordinate system and the associated diffeomorphism Ψ_p, which straightens the boundary portion near each point $p \in \partial\Omega_k$ for $k \in \{0, 1, \dots, K\}$. Fix $k \in \{0, 1, \dots, K\}$ arbitrarily. After a suitable rotation of the coordinate system, we may write the boundary point as $p = (p', p^d) \in \mathbb{R}^{d-1} \times \mathbb{R}$ and assume that the inner normal to $\partial\Omega_k$ at p points in the direction of the positive x^d-axis. To straighten the portion of $\partial\Omega_k$, we employ the principal coordinate system $y = (y', y^d)$ (cf. [38, Section 14.6]). Thus, there exist a neighborhood $\mathcal{N}_p$ of

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p, a constant $b'_p > 0$ (depending on p and $\partial\Omega_k$) and a smooth function $\psi_p = \psi_p(x')$ (defined for $|x' - p'| < b'_p$) satisfying

(D1) $\psi_p(p') = p^d$,

(D2) $\nabla\psi_p(p') = 0$,

(D3) $\partial\Omega_k \cap \mathcal{N}_p = \{x = (x', x^d) \in \mathbb{R}^d : x^d = \psi_p(x'),\ |x' - p'| < b'_p\}$,

(D4) $\mathcal{N}_p^+ := \Omega \cap \mathcal{N}_p = \{x = (x', x^d) \in \mathbb{R}^d : x^d > \psi_p(x'),\ |x' - p'| < b'_p\} \cap \mathcal{N}_p$ and $\overline{\mathcal{N}_p}^+ = \Psi_p(\overline{B}_b^+)$.

Here the diffeomorphism $\Psi_p : \overline{B}_b^+ \to \mathbb{R}^d$ is defined by

$$x = (x', x^d) = \Psi_p(y) = (p' + y', \psi_p(p' + y')) - y^d\nu \quad \text{for } y = (y', y^d) \in \overline{B}_b^+, \tag{3.43}$$

where $\overline{B}_b^+ = \{y = (y', y^d) \in \mathbb{R}^d : |y| \le b,\ y^d \ge 0\}$, b is a positive constant (depending on Ω) and $\nu = (\nu', \nu^d) = (\nabla\psi_p(p' + y'), -1)/\sqrt{1 + |\nabla\psi_p(p' + y')|^2}$ is the unit outer normal at $(p' + y', \psi_p(p' + y'))$ with respect to Ω (see Figure 3.3). Moreover, $y^d = \mathrm{dist}(x, \partial\Omega_k)$ and $(y', y^d) = \Psi_p^{-1}(x', x^d)$ for $x = (x', x^d) \in \overline{\mathcal{N}_p}^+$.

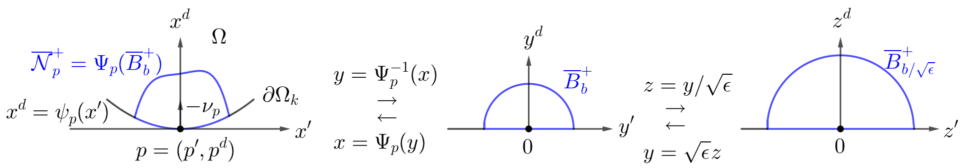

Figure 3.3: The function ψ_p describes the portion of $\partial\Omega_k$ near $p \in \partial\Omega_k$. The diffeomorphism $x = \Psi_p(y)$ maps an upper half ball $\overline{B}_b^+$ to the neighborhood $\overline{\mathcal{N}_p}^+$, and $z = y/\sqrt{\varepsilon}$ dilates $\overline{B}_b^+$ into $\overline{B}_{b/\sqrt{\varepsilon}}^+$.

By (3.43) and rescaling y by $\sqrt{\varepsilon}$, we obtain

Lemma 3.4. *For $\phi \in \mathcal{C}^\infty(\overline{\Omega})$, $p \in \partial\Omega = \bigcup_{k=0}^K \partial\Omega_k$ and $\varepsilon > 0$, let $u_{p,\varepsilon} : \overline{B}_{b/\sqrt{\varepsilon}}^+ \to \mathbb{R}$ satisfy $u_{p,\varepsilon}(z) = \phi(\Psi_p(\sqrt{\varepsilon}z))$ for $z \in \overline{B}_{b/\sqrt{\varepsilon}}^+$ (see Figure 3.3). Then $u_{p,\varepsilon} \in \mathcal{C}^\infty(\overline{B}_{b/\sqrt{\varepsilon}}^+)$, and*

$$\varepsilon\Delta_x\phi(\Psi_p(\sqrt{\varepsilon}z)) = \sum_{i,j=1}^d a_{ij}(z)\frac{\partial^2 u_{p,\varepsilon}}{\partial z^i \partial z^j}(z) + \sum_{j=1}^d b_j(z)\frac{\partial u_{p,\varepsilon}}{\partial z^j}(z) \quad \textit{for } z \in B_{b/\sqrt{\varepsilon}}^+, \tag{3.44}$$

$$\partial_{\nu_p}\phi(\Psi_p(\sqrt{\varepsilon}(z^d e_d))) = -\varepsilon^{-1/2}\partial_{z^d}u_{p,\varepsilon}(z^d e_d) \quad \textit{for } 0 \le z^d < b/\sqrt{\varepsilon}, \tag{3.45}$$

$$\phi(p - t\sqrt{\varepsilon}\nu_p) = u_{p,\varepsilon}(te_d) \quad \textit{for } 0 \le t < b/\sqrt{\varepsilon}, \tag{3.46}$$

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where e_d and ν_p are the unit vector in the positive direction of z^d-axis and the unit outer normal at p with respect to Ω, respectively. The coefficients a_{ij} and b_j satisfy

$$a_{ij}(z) = \delta_{ij} + 2\psi_{ij}\sqrt{\varepsilon}z^d + \varepsilon|z|^2\mathcal{O}(1) \quad \textit{for } 1 \le i,j \le d \textit{ and } z \in B^+_{b/\sqrt{\varepsilon}}, \tag{3.47}$$

$$b_j(z) = -\delta_{jd}\sqrt{\varepsilon}(d-1)H(p) + \varepsilon|z|\mathcal{O}(1) \quad \textit{for } 1 \le j \le d \textit{ and } z \in B^+_{b/\sqrt{\varepsilon}}. \tag{3.48}$$

Here $\delta_{ij} = \begin{cases} 1 & \textit{if } i = j \\ 0 & \textit{if } i \ne j \end{cases}$ is the Kronecker symbol, $\mathcal{O}(1)$ is a bounded quantity independent of ε and z, and

$$\psi_{ij} = \psi_{ji} := \partial_{x^i x^j}\psi_p(p') \quad \textit{for } 1 \le i,j \le d-1,$$

$$\psi_{id} = \psi_{di} := \frac{1}{2}\sum_{n=1}^{d-1}\psi_{in} \quad \textit{for } 1 \le i \le d-1,$$

$$\psi_{dd} := 0.$$

Besides, $H(p) = (d-1)^{-1}\sum_{i=1}^{d-1}\psi_{ii}$ stands for the mean curvature at the boundary point p with respect to Ω due to (D2) (see [38, (14.92)]).

Note that (3.47)–(3.48) imply that a_{ij} and b_j satisfy

$$\lim_{\varepsilon\to 0^+} a_{ij}(z) = \delta_{ij} \quad \lim_{\varepsilon\to 0^+} b_j(z) = 0 \quad \text{for } R > 0,\ 1 \le i,j \le d,\ |z| < R \text{ and } z^d > 0.$$

The proof of Lemma 3.4 follows standard calculations of the principal coordinate system (cf. [38]) so we omit it here.

To get the first-order asymptotic expansion of ϕ_ε near the boundary $\partial\Omega_k$, we define

$$u_{k,p,\varepsilon}(z) = \phi_\varepsilon(\Psi_p(\sqrt{\varepsilon}z)) \quad \text{for } z \in \overline{B}^+_{b/\sqrt{\varepsilon}},\ p \in \partial\Omega_k \text{ and } k = 0,1,\dots,K, \tag{3.49}$$

where ϕ_ε is the solution to equation (3.1) with condition (3.4). Then by (3.44), (3.45), and (3.49), $u_{k,p,\varepsilon}$ satisfies

$$\sum_{i,j=1}^{d} a_{ij}(z)\frac{\partial^2 u_{k,p,\varepsilon}}{\partial z^i \partial z^j} + \sum_{j=1}^{d} b_j(z)\frac{\partial u_{k,p,\varepsilon}}{\partial z^j} + f(u_{k,p,\varepsilon}) = 0 \qquad \text{in } B^+_{b/\sqrt{\varepsilon}}, \tag{3.50}$$

$$u_{k,p,\varepsilon} - \gamma_k\partial_{z^d}u_{k,p,\varepsilon} = \phi_{bd,k} \quad \text{on } \overline{B}^+_{b/\sqrt{\varepsilon}} \cap \partial\mathbb{R}^d_+, \tag{3.51}$$

where $\partial\mathbb{R}^d_+ = \{z = (z', z^d) \in \mathbb{R}^d : z^d = 0\}$, a_{ij} and b_j are given in (3.47)–(3.48). Based on the uniform boundedness of ϕ_ε (cf. Proposition 3.3), together with the

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standard elliptic L^q-estimate and Schauder's estimate, we obtain the $\mathcal{C}^{2,\alpha}_{\mathrm{loc}}$-estimate of $u_{k,p,\varepsilon}$. Using a diagonal process, we can prove the convergence of $u_{k,p,\varepsilon}$ in $\mathcal{C}^{2,\alpha}(\overline{B}^+_m)$ as ε tends to zero (up to a subsequence) for $m \in \mathbb{N}$. The result is stated below.

Lemma 3.5. *For any sequence $\{\varepsilon_n\}_{n=1}^\infty$ of positive numbers with $\lim_{n\to\infty} \varepsilon_n = 0$, $\alpha \in (0,1)$ and $p \in \partial\Omega_k$ ($k \in \{0,1,\ldots,K\}$), there exists a subsequence $\{\varepsilon_{nn}\}_{n=1}^\infty$ such that $\lim_{n\to\infty} \|u_{k,p,\varepsilon_{nn}} - u_{k,p}\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0$ for $m \in \mathbb{N}$, where $\overline{B}^+_m = \{z = (z', z^d) \in \mathbb{R}^d : |z| \le m,\ z^d \ge 0\}$ and $u_{k,p} \in \mathcal{C}^{2,\alpha}_{loc}(\overline{\mathbb{R}}^d_+)$ satisfies*

$$\Delta u_{k,p} + f(u_{k,p}) = 0 \qquad \text{in } \mathbb{R}^d_+, \tag{3.52}$$

$$u_{k,p} - \gamma_k \partial_{z^d} u_{k,p} = \phi_{bd,k} \quad \text{on } \partial\mathbb{R}^d_+. \tag{3.53}$$

Here $\mathbb{R}^d_+ = \{z = (z', z^d) \in \mathbb{R}^d : z^d > 0\}$.

Proof. Let $\{\varepsilon_n\}_{n=1}^\infty$ be a sequence of positive numbers with $\lim_{n\to\infty} \varepsilon_n = 0$, $\alpha \in (0,1)$, $p \in \partial\Omega_k$ and $k \in \{0,1,\ldots,K\}$. We first prove the recompactness of $\{u_{k,p,\varepsilon_n}\}_{n=1}^\infty$ in $\mathcal{C}^{2,\alpha}(\overline{B}^+_m)$ for $m \in \mathbb{N}$. Fix $m \in \mathbb{N}$ arbitrarily. Without loss of generality, we may assume that $0 < \varepsilon_n < b^2/(9m^2)$ for $n \in \mathbb{N}$. Then we have $\overline{B}^+_{3m} \subseteq \overline{B}^+_{b/\sqrt{\varepsilon_n}}$ so by (3.49), u_{k,p,ε_n} is well-defined in $\overline{B}^+_{3m}$. For the sake of simplicity, u_{k,p,ε_n} is denoted as u_{ε_n} for $n \in \mathbb{N}$. By Proposition 3.3, we have $\|u_{\varepsilon_n}\|_{L^\infty(B^+_{3m})} \le M$, which gives $\|u_{\varepsilon_n}\|_{L^q(B^+_{3m})} \le M$ and $\|f \circ u_{\varepsilon_n}\|_{L^q(B^+_{3m})} \le M$ (by the condition (F1)) for $q \ge 1$, where M is independent of n. In this proof, we use the genric constant M which is independent of n for notational convenience. Then by the standard elliptic L^q-estimates to (3.50)–(3.51) (cf. [2, 38]), we have

$$\|u_{\varepsilon_n}\|_{W^{2,q}(B^+_{2m})} \le M \left(\|u_{\varepsilon_n}\|_{L^q(B^+_{3m})} + \|f \circ u_{\varepsilon_n}\|_{L^q(B^+_{3m})} \right) \le M$$

for $q > 1$ and $n \in \mathbb{N}$. Hence by Sobolev's compact embedding theorem, we get $\|u_{\varepsilon_n}\|_{\mathcal{C}^{1,\alpha}(B^+_{2m})} \le M$ and $\{u_{\varepsilon_n}\}_{n=1}^\infty$ is precompact in $\mathcal{C}^{1,\alpha}(\overline{B}^+_{2m})$. Applying Schauder's estimate to (3.50)–(3.51) (cf. [2, 38]), we get

$$\|u_{\varepsilon_n}\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} \le M \left(\|u_{\varepsilon_n}\|_{\mathcal{C}^{0,\alpha}(\overline{B}^+_{2m})} + \|f \circ u_{\varepsilon_n}\|_{\mathcal{C}^{0,\alpha}(\overline{B}^+_{2m})} \right) \le M$$

for $n \in \mathbb{N}$, and $\{u_{\varepsilon_n}\}_{n=1}^\infty$ is precompact in $\mathcal{C}^{2,\alpha}(\overline{B}^+_m)$ for $m \in \mathbb{N}$.

Now we use the precompactness of $\{u_{\varepsilon_n}\}_{n=1}^\infty$ in $\mathcal{C}^{2,\alpha}(\overline{B}^+_m)$ for $m \in \mathbb{N}$, and the diagonal process argument to obtain the solution $u_{k,p}$ to (3.52)–(3.53). As $m = 1$, the precompactness of $\{u_{\varepsilon_n}\}_{n=1}^\infty$ in $\mathcal{C}^{2,\alpha}(\overline{B}^+_1)$ implies that there exist a subsequence

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$\{\varepsilon_{1n}\}_{n=1}^{\infty}$ of $\{\varepsilon_n\}_{n=1}^{\infty}$ and a function $u_1 \in \mathcal{C}^{2,\alpha}(\overline{B}_1^+)$ such that $\lim\limits_{n\to\infty} \|u_{\varepsilon_{1n}} - u_1\|_{\mathcal{C}^{2,\alpha}(\overline{B}_1^+)} = 0$. As $m = 2$, the precompactness of $\{u_{\varepsilon_{1n}}\}_{n=1}^{\infty}$ in $\mathcal{C}^{2,\alpha}(\overline{B}_2^+)$ implies that there exist a subsequence $\{\varepsilon_{2n}\}_{n=1}^{\infty}$ of $\{\varepsilon_{1n}\}_{n=1}^{\infty}$ and a function $u_2 \in \mathcal{C}^{2,\alpha}(\overline{B}_2^+)$ such that $\lim\limits_{n\to\infty} \|u_{\varepsilon_{2n}} - u_2\|_{\mathcal{C}^{2,\alpha}(\overline{B}_2^+)} = 0$. Note that $u_2\Big|_{\overline{B}_1^+} = u_1$ because $\{u_{\varepsilon_{2n}}\}_{n=1}^{\infty}$ is a subsequence of $\{u_{\varepsilon_{1n}}\}_{n=1}^{\infty}$. Consequently, for $m \in \mathbb{N}$, the precompactness of $\{u_{\varepsilon_{mn}}\}_{n=1}^{\infty}$ in $\mathcal{C}^{2,\alpha}(\overline{B}_m^+)$ implies that there exist a subsequence $\{\varepsilon_{(m+1)n}\}_{n=1}^{\infty}$ of $\{\varepsilon_{mn}\}_{n=1}^{\infty}$ and a function $u_{m+1} \in \mathcal{C}^{2,\alpha}(\overline{B}_{m+1}^+)$ such that $\lim\limits_{n\to\infty} \|u_{\varepsilon_{(m+1)n}} - u_{m+1}\|_{\mathcal{C}^{2,\alpha}(\overline{B}_{m+1}^+)} = 0$ and $u_{m+1}\Big|_{\overline{B}_m^+} = u_m$. Note that $\{\varepsilon_{nn}\}_{n=m}^{\infty}$ is a subsequence of $\{\varepsilon_{mn}\}_{n=1}^{\infty}$ for $m \in \mathbb{N}$. Hence $\lim\limits_{n\to\infty} \|u_{\varepsilon_{nn}} - u_m\|_{\mathcal{C}^{2,\alpha}(\overline{B}_m^+)} = 0$ for $m \in \mathbb{N}$. For $z \in \overline{\mathbb{R}}_+^d$, we define $u_{k,p}(z) = u_m(z)$, where $m \in \mathbb{N}$ is sufficiently large such that $z \in \overline{B}_m^+$. Here we have used the fact that $u_\ell\Big|_{\overline{B}_m^+} = u_m$ for $\ell \geq m$ and $\ell \in \mathbb{N}$ because of $u_{m+1}\Big|_{\overline{B}_m^+} = u_m$ for $m \in \mathbb{N}$. Clearly, $u_{k,p} \in \mathcal{C}^{2,\alpha}_{\text{loc}}(\overline{\mathbb{R}}_+^d)$ satisfies

$$u_{k,p}\Big|_{\overline{B}_m^+} = u_m \text{ and } \lim_{n\to\infty} \|u_{\varepsilon_{nn}} - u_{k,p}\|_{\mathcal{C}^{2,\alpha}(\overline{B}_m^+)} = 0 \quad \text{for } m \in \mathbb{N}. \tag{3.54}$$

Now we show that $u_{k,p}$ satisfies (3.52)–(3.53). From (3.50)–(3.51), $u_{\varepsilon_{nn}}$ satisfies

$$\sum_{i,j=1}^{d} a_{ij}(z)\frac{\partial^2 u_{\varepsilon_{nn}}}{\partial z^i \partial z^j} + \sum_{j=1}^{d} b_j(z)\frac{\partial u_{\varepsilon_{nn}}}{\partial z^j} + f(u_{\varepsilon_{nn}}) = 0 \qquad \text{in } B_m^+, \tag{3.55}$$

$$u_{\varepsilon_{nn}} - \gamma_k \frac{\partial u_{\varepsilon_{nn}}}{\partial z^d} = \phi_{bd,k} \quad \text{on } \overline{B}_m^+ \cap \partial\mathbb{R}_+^d \tag{3.56}$$

for $m, n \in \mathbb{N}$, where $B_m^+ = \{z = (z', z^d) \in \mathbb{R}^d : |z| < m,\ z^d > 0\}$. Fix $m \in \mathbb{N}$ arbitrarily and let $n \to \infty$. Then by (3.47)–(3.48) and (3.54)–(3.56), $u_{k,p}$ satisfies

$$\Delta u_{k,p} + f(u_{k,p}) = 0 \qquad \text{in } B_m^+,$$

$$u_{k,p} - \gamma_k \frac{\partial u_{k,p}}{\partial z^d} = \phi_{bd,k} \quad \text{on } \overline{B}_m^+ \cap \partial\mathbb{R}_+^d$$

for $m \in \mathbb{N}$, which implies (3.52)–(3.53). Hence we complete the proof of Lemma 3.5.

□

For the equation (3.52) together with the boundary condition (3.53), we can establish the following exponential-type estimate of $u_{k,p}$.

Lemma 3.6. *For $p \in \partial\Omega_k$ and $k \in \{0, 1, \ldots, K\}$, the solution $u_{k,p}$ to (3.52)–(3.53) satisfies*

$$|u_{k,p}(z) - \phi^*| \leq 2C_1 \exp(-C_2 z^d) \tag{3.57}$$

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for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$ *and* $z^d \geq (d-1)/(4C_2)$*, where* $C_1 > 0$ *is a constant (independent of* ε*) given in Proposition 3.3 such that* $|\phi_\varepsilon(x) - \phi^*| \leq C_1$ *for* $x \in \overline{\Omega}$*, and* $C_2 = m_f([\phi^* - C_1, \phi^* + C_1])/8 > 0$*.*

Proof. Let $\overline{z} = (\overline{z}', \overline{z}^d) \in \overline{\mathbb{R}}^d_+$ arbitrarily with $\overline{z}^d \geq (d-1)/(4C_2)$. Then let $u^\pm$ be the solution to

$$\Delta u^\pm + f(u^\pm) = 0 \qquad \text{in } B_{\overline{z}^d}(\overline{z}), \tag{3.58}$$

$$u^\pm = \phi^* \pm C_1 \quad \text{on } \partial B_{\overline{z}^d}(\overline{z}). \tag{3.59}$$

We claim that

$$u^- \leq u_{k,p} \leq u^+ \quad \text{in } \overline{B}_{\overline{z}^d}(\overline{z}). \tag{3.60}$$

We first prove $u^+ \geq u_{k,p}$ and set $\overline{u}^+_{k,p} := u^+ - u_{k,p}$ in $\overline{B}_{\overline{z}^d}(\overline{z})$. Then by (3.52) and (3.58)–(3.59), $\overline{u}^+_{k,p}$ satisfies

$$\Delta \overline{u}^+_{k,p} + c(z)\overline{u}^+_{k,p} = 0 \quad \text{in } B_{\overline{z}^d}(\overline{z}), \tag{3.61}$$

$$\overline{u}^+_{k,p} = C_1 - (u_{k,p} - \phi^*) \geq 0 \quad \text{on } \partial B_{\overline{z}^d}(\overline{z}), \tag{3.62}$$

where $c(z) = (f(u^+(z)) - f(u_{k,p}(z)))/(u^+(z) - u_{k,p}(z))$ if $u^+(z) \neq u_{k,p}(z)$; $c(z) = f'(u_{k,p}(z))$ if $u^+(z) = u_{k,p}(z)$. Here we have used (3.49), Proposition 3.3 and Lemma 3.5. Note that $c(z) < 0$ for $z \in B_{\overline{z}^d}(\overline{z})$ because f is strictly decreasing on $\mathbb{R}$ (cf. (F1)). Thus, we apply the maximum principle to (3.61)–(3.62) and obtain $\overline{u}^+_{k,p} \geq 0$ in $\overline{B}_{\overline{z}^d}(\overline{z})$, which implies $u^+ \geq u_{k,p}$ in $\overline{B}_{\overline{z}^d}(\overline{z})$. Similarly, we can prove $u^- \leq u_{k,p}$ in $B_{\overline{z}^d}(\overline{z})$, and get (3.60). Since $u^\pm$ are the radial solutions to (3.58)–(3.59), then by Proposition 3A.2 in Appendix 3A with $\varepsilon = 1$ and replacing $B_R(0)$, r, Φ_ε, Φ_{bd}, m_f by $B_{\overline{z}^d}(\overline{z})$, $|z - \overline{z}|$, $u^\pm$, $\phi^* \pm C_1$, we obtain

$$|u^\pm(z) - \phi^*| \leq 2C_1 \exp(-C_2(\overline{z}^d - |z - \overline{z}|)) \quad \text{for } z \in B_{\overline{z}^d}(\overline{z}). \tag{3.63}$$

Here we have used the fact that $\overline{z}^d \geq (d-1)/(4C_2)$. Along with (3.60) and (3.63), we obtain

$$|u_{k,p}(\overline{z}) - \phi^*| = |u_{k,p}(\overline{z}', \overline{z}^d) - \phi^*| \leq |u^\pm(\overline{z}', \overline{z}^d) - \phi^*| \leq 2C_1 \exp(-C_2\overline{z}^d)$$

for $\overline{z} \in \mathbb{R}^d_+$ and $\overline{z}^d \geq (d-1)/(4C_2)$, which gives (3.57). Therefore, we complete the proof of Lemma 3.6. □

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From Lemma 3.5, the solution $u_{k,p}$ to (3.52)–(3.53) may, a priori, depend on the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ and on the point $p \in \partial\Omega_k$. To establish the independence from the sequence and the point, we employ the moving plane arguments to prove that $u_{k,p}$ satisfies $u_{k,p}(z) = u_k(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$ (see Proposition 3.7), where u_k is the unique solution to (3.7)–(3.9), and u_k is independent of the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ and the point $p \in \partial\Omega_k$. Consequently, we improve the results of Lemma 3.5 as

$$\lim_{\varepsilon\to 0^+} \|u_{k,p,\varepsilon} - u_k\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0 \quad \text{for } m \in \mathbb{N} \text{ and } \alpha \in (0,1), \tag{3.64}$$

and

$$\lim_{\varepsilon\to 0^+} u_{k,p,\varepsilon}(z) = u_k(z^d) \quad \text{for } z = (z', z^d) \in \overline{\mathbb{R}}^d_+, \tag{3.65}$$

where $u_{k,p,\varepsilon}$ is defined in (3.49). Below are the details.

Proposition 3.7. *For $p \in \partial\Omega_k$ and $k \in \{0, 1, \ldots, K\}$, the solution $u_{k,p}$ to (3.52)–(3.53) satisfies*

(a) $u_{k,p}$ depends only on the variable z^d, i.e., $u_{k,p}(z) = u_{k,p}(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$.

(b) $u_{k,p}$ is independent of p and depends only on k, i.e., $u_{k,p}(z^d) = u_k(z^d)$ for $z^d \in [0,\infty)$, where u_k is the unique solution to (3.7)–(3.9).

Proof. To prove (a), we fix $p \in \partial\Omega_k$, $k \in \{0, 1, \ldots, K\}$ and $h \in \mathbb{R}^{d-1} - \{0\}$ arbitrarily. For notational convenience, we denote $u_{k,p}$ by u in the proof of (a). To use the moving plane arguments, we define $\tilde{u}$ by

$$\tilde{u}(z) = u(z' + h, z^d) - u(z) \quad \text{for } z = (z', z^d) \in \overline{\mathbb{R}}^d_+. \tag{3.66}$$

For the proof of (a), it suffices to show $\tilde{u} \equiv 0$, which is equivalent to showing $\sup\limits_{\overline{\mathbb{R}}^d_+} \tilde{u} = 0$ and $\inf\limits_{\overline{\mathbb{R}}^d_+} \tilde{u} = 0$. We first prove $\sup\limits_{\overline{\mathbb{R}}^d_+} \tilde{u} = 0$. Suppose by contradiction that

$$\zeta := \sup_{\overline{\mathbb{R}}^d_+} \tilde{u} > 0.$$

By (3.57) and (3.66), we have

$$|\tilde{u}(z)| \leq |u(z' + h, z^d) - \phi^*| + |u(z) - \phi^*| \leq 4C_1 \exp(-C_2 z^d)$$

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for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$ and $z^d \geq (d-1)/(4C_2)$. Clearly, there exists $L > (d-1)/(4C_2)$ such that $4C_1 \exp(-C_2 L) \leq \zeta/2$ and

$$|\tilde{u}(z)| \leq \zeta/2 \quad \text{for } z = (z', z^d) \in \mathbb{R}^d_+ \quad \text{and} \quad z^d \geq L. \tag{3.67}$$

Note that $\tilde{u}$ (defined in (3.66)) may depend on h, but L is independent of h (because C_1 and C_2 are independent of h). Thus

$$\zeta = \sup_{\mathbb{R}^d_+} \tilde{u} = \sup_{\mathbb{R}^{d-1}\times[0,L]} \tilde{u} > 0. \tag{3.68}$$

Then from (3.52)–(3.53), $\tilde{u}$ satisfies

$$\Delta \tilde{u} + c_1(z)\tilde{u} = 0 \quad \text{in } \mathbb{R}^d_+, \tag{3.69}$$

$$\tilde{u} - \gamma_k \partial_{z^d} \tilde{u} = 0 \quad \text{on } \partial\mathbb{R}^d_+, \tag{3.70}$$

where

$$c_1(z) = \begin{cases} \dfrac{f(u(z'+h, z^d)) - f(u(z))}{u(z'+h, z^d) - u(z)} & \text{if } u(z'+h, z^d) \neq u(z), \\ f'(u(z)) & \text{if } u(z'+h, z^d) = u(z). \end{cases}$$

Note that $c_1(z) < 0$ for $z \in \mathbb{R}^d_+$ because of the strict decrease of f (cf. (F1)). By the strong maximum principle applied to (3.69) in $\mathbb{R}^{d-1} \times (0, L)$ (cf. [38, Theorem 3.5]), $\tilde{u}$ has no interior maximum point in $\mathbb{R}^{d-1} \times (0, L)$. Moreover, by (3.67) and (3.68), the maximum point of $\tilde{u}$ cannot be located on $\mathbb{R}^{d-1} \times \{L\}$. On the other hand, by (3.70), the maximum point of $\tilde{u}$ cannot be located on $\partial\mathbb{R}^d_+$ because $\partial_{z^d}\tilde{u}(z', 0) = \tilde{u}(z', 0)/\gamma_k = \zeta/\gamma_k > 0$ if $(z', 0)$ is the maximum point of $\tilde{u}$, i.e., $\tilde{u}(z', 0) = \zeta$. Hence there exists a sequence $z_n = (z'_n, z^d_n) \in \mathbb{R}^{d-1} \times [0, L]$ with $\lim_{n\to\infty} |z'_n| = \infty$ and

$$\lim_{n\to\infty} z^d_n = z^d_\infty \in [0, L] \tag{3.71}$$

such that

$$\lim_{n\to\infty} \tilde{u}(z'_n, z^d_n) = \zeta. \tag{3.72}$$

Let

$$u_n(z) = u(z' + z'_n, z^d) \quad \text{for } n \in \mathbb{N} \text{ and } z = (z', z^d) \in \overline{\mathbb{R}}^d_+. \tag{3.73}$$

By the translation invariance (to z') of (3.52)–(3.53), u_n satisfies

$$\Delta u_n + f(u_n) = 0 \qquad \text{in } \mathbb{R}^d_+,$$

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$$u_n - \gamma_k \partial_{z^d} u_n = \phi_{bd,k} \quad \text{on } \partial\mathbb{R}^d_+.$$

Note that by (3.49), Proposition 3.3, and Lemma 3.5, $\|u_n\|_{L^\infty(\mathbb{R}^d_+)} \leq C_1 + |\phi^*|$ for $n \in \mathbb{N}$. Then similar to Lemma 3.5, we can apply the elliptic L^q-estimate, Sobolev's compact embedding theorem, Schauder's estimate and the diagonal process to get a subsequence $\{u_{n_{jj}}\}_{j=1}^\infty$ of $\{u_n\}_{n=1}^\infty$ such that

$$\lim_{j\to\infty} \|u_{n_{jj}} - u_\infty\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0 \quad \text{for } m \in \mathbb{N} \text{ and } \alpha \in (0,1), \tag{3.74}$$

where $u_\infty \in \mathcal{C}^{2,\alpha}_{\text{loc}}(\overline{\mathbb{R}}^d_+)$ satisfies

$$\Delta u_\infty + f(u_\infty) = 0 \qquad \text{in } \mathbb{R}^d_+, \tag{3.75}$$

$$u_\infty - \gamma_k \partial_{z^d} u_\infty = \phi_{bd,k} \quad \text{on } \partial\mathbb{R}^d_+. \tag{3.76}$$

Now we derive the contradiction and conclude that $\zeta = \sup_{\overline{\mathbb{R}}^d_+} \tilde{u} = \sup_{\mathbb{R}^{d-1}\times[0,L]} \tilde{u} = 0$ (cf. (3.68)). Let

$$\tilde{u}_\infty(z) = u_\infty(z' + h, z^d) - u_\infty(z) \quad \text{for } z = (z', z^d) \in \mathbb{R}^{d-1} \times [0, L]. \tag{3.77}$$

From (3.68), we have $\zeta \geq \tilde{u}(z)$ for $z \in \mathbb{R}^{d-1} \times [0, L]$. Then by (3.66) and (3.73) with $n = n_{jj}$, we get

$$\zeta \geq u_{n_{jj}}(z' + h, z^d) - u_{n_{jj}}(z) \quad \text{for } z \in \mathbb{R}^{d-1} \times [0, L] \text{ and } j \in \mathbb{N}. \tag{3.78}$$

We prove that ζ is the maximum value of $\tilde{u}_\infty$ as follows.

Claim 3.8. *$\tilde{u}_\infty$ attains its maximum value ζ at $(0, z^d_\infty) \in \mathbb{R}^{d-1} \times [0, L]$.*

Proof of Claim 3.8. Fix $z = (z', z^d) \in \mathbb{R}^{d-1} \times [0, L]$ arbitrarily. Then there exists $m_1 \in \mathbb{N}$ such that $z \in \overline{B}^+_{m_1}$ and $(z' + h, z^d) \in \overline{B}^+_{m_1}$. By (3.74) with $m = m_1$, we have

$$\lim_{j\to\infty} u_{n_{jj}}(z' + h, z^d) = u_\infty(z' + h, z^d) \quad \text{and} \quad \lim_{j\to\infty} u_{n_{jj}}(z) = u_\infty(z). \tag{3.79}$$

Taking $j \to \infty$ in (3.78), we use (3.77) and (3.79) to obtain

$$\zeta \geq u_\infty(z' + h, z^d) - u_\infty(z) = \tilde{u}_\infty(z). \tag{3.80}$$

By (3.71), $\lim_{j\to\infty} z^d_{n_{jj}} = z^d_\infty \in [0, L]$ and hence there exists a positive integer m_2 such that $(h, z^d_{n_{jj}}) \in \overline{B}^+_{m_2}$ and $(0, z^d_{n_{jj}}) \in \overline{B}^+_{m_2}$ for $j \in \mathbb{N}$. Then we use (3.74) with $m = m_2$ to get

$$\lim_{j\to\infty} u_{n_{jj}}(h, z^d_{n_{jj}}) = u_\infty(h, z^d_\infty) \quad \text{and} \quad \lim_{j\to\infty} u_{n_{jj}}(0, z^d_{n_{jj}}) = u_\infty(0, z^d_\infty). \tag{3.81}$$

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By (3.66), (3.72) and (3.73) with $n = n_{jj}$,

$$\zeta = \lim_{j\to\infty}[u_{n_{jj}}(h, z^d_{n_{jj}}) - u_{n_{jj}}(0, z^d_{n_{jj}})],$$

and then along with (3.77), (3.80) and (3.81), we have

$$\zeta = u_\infty(h, z^d_\infty) - u_\infty(0, z^d_\infty) = \tilde{u}_\infty(0, z^d_\infty),$$

which completes the proof of Claim 3.8. □

By (3.75)–(3.77), $\tilde{u}_\infty$ satisfies

$$\Delta\tilde{u}_\infty + c_2(z)\tilde{u}_\infty = 0 \quad \text{in } \mathbb{R}^{d-1}\times(0, L), \tag{3.82}$$

$$\tilde{u}_\infty - \gamma_k\partial_{z^d}\tilde{u}_\infty = 0 \quad \text{on } \partial\mathbb{R}^d_+, \tag{3.83}$$

where

$$c_2(z) = \begin{cases} \dfrac{f(u_\infty(z'+h, z^d)) - f(u_\infty(z))}{u_\infty(z'+h, z^d) - u_\infty(z)} & \text{if } u_\infty(z'+h, z^d) \neq u_\infty(z), \\ f'(u_\infty(z)) & \text{if } u_\infty(z'+h, z^d) = u_\infty(z). \end{cases}$$

Note that $c_2(z) < 0$ for $z \in \mathbb{R}^d_+$ because of (F1). Then by the strong maximum principle to (3.82) (cf. [38, Theorem 3.5]), the maximum point $(0, z^d_\infty)$ of $\tilde{u}_\infty$ cannot be an interior point of $\mathbb{R}^{d-1}\times(0, L)$. Hence either $z^d_\infty = 0$ or $z^d_\infty = L$. From (3.67), (3.73) with $n = n_{jj}$, (3.77) and (3.81), we have $\tilde{u}_\infty(0, L) \le \zeta/2$. Thus, by Claim 3.8, $z^d_\infty \neq L$, $z^d_\infty = 0$, $\tilde{u}_\infty(0, 0) = \zeta$ and $(0, 0)$ is the maximum point of $\tilde{u}_\infty$ in $\mathbb{R}^{d-1}\times[0, L]$. However, (3.83) gives

$$0 < \zeta = \tilde{u}_\infty(0, 0) = \gamma_k\partial_{z^d}\tilde{u}_\infty(0, 0) \le 0,$$

which leads to a contradiction. Hence we obtain $\zeta = \sup_{\mathbb{R}^d_+}\tilde{u} = 0$. Similarly, we can prove $\inf_{\mathbb{R}^d_+}\tilde{u} = 0$ by contradiction. Suppose that $\zeta' := -\inf_{\mathbb{R}^d_+}\tilde{u} > 0$. Then by (3.57) and (3.66), we have $|\tilde{u}(z)| \le \zeta'/2$ for $z = (z', z^d) \in \mathbb{R}^d_+$ and $z^d \ge L$ for some $L > 0$ independent of h, and thus $\zeta' = -\inf_{\mathbb{R}^{d-1}\times[0,L]}\tilde{u}$. Arguing as in (3.69)–(3.81), we can prove $\tilde{u}_\infty$ attains its minimum value at $(0, z^d_\infty)$, where $z^d_\infty \in [0, L]$. Then we can apply the maximum principle to (3.82)–(3.83) to get a contradiction and complete the proof of (a).

To complete the proof, it remains to prove (b). By (a), $u_{k,p} = u_{k,p}(z^d)$ solves the ordinary differential equation (3.7) with the initial condition (3.8). Moreover,

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by the exponential-type estimate (3.57), $u_{k,p}$ satisfies the asymptotic formula (3.9). Note that the equations (3.7)–(3.9) are independent of p. Hence by the uniqueness of (3.7)–(3.9) (cf. Appendix 3B), $u_{k,p}$ is independent of p; we therefore denote it by u_k for $k \in \{0, 1, \ldots, K\}$, which finalizes the proof of (b). Therefore, we complete the proof of Proposition 3.7. □

Using Proposition 3.7, we prove (3.64) and (3.65). Let $T > 0$, $k \in \{0, 1, \ldots, K\}$, and $p \in \partial\Omega_k$. Then by (3.46), (3.49), and (3.64)–(3.65), we find the first-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$:

$$\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_{k,p,\varepsilon}(te_d) = u_k(t) + o_\varepsilon(1), \tag{3.84}$$

$$\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\frac{1}{\sqrt{\varepsilon}}(u_k'(t)\nu_p + o_\varepsilon(1)) \tag{3.85}$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$.

To derive the second-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$ and capture the asymptotic behavior of the term $o_\varepsilon(1)/\sqrt{\varepsilon}$ in the next section, it is crucial to establish the following exponential-type estimates of ϕ_ε and $\nabla\phi_\varepsilon$:

Proposition 3.9 (Exponential-type estimates of ϕ_ε and $\nabla\phi_\varepsilon$). *Let Ω satisfy the uniform interior sphere condition, i.e., there exists $R > 0$ such that $B_R(p - R\nu_p) \subseteq \Omega$ and $\partial B_R(p - R\nu_p) \cap \partial\Omega = \{p\}$ for $p \in \partial\Omega$, where ν_p is the unit outer normal to $\partial\Omega$ at p. Then we have*

$$|\phi_\varepsilon(x) - \phi^*| \le 2C_1 \exp\left(-\frac{C_2\delta(x)}{\sqrt{\varepsilon}}\right), \tag{3.86}$$

$$|\nabla\phi_\varepsilon(x)| \le \frac{M}{\sqrt{\varepsilon}} \exp\left(-\frac{C_2\delta(x)}{\sqrt{2\varepsilon}}\right) \tag{3.87}$$

for $x \in \overline{\Omega}$ and $0 < \varepsilon < \varepsilon^*$, where C_1 and C_2 are positive constants given in Proposition 3.3 and Lemma 3.6, respectively. Here ε^* is a sufficiently small constant, $M > 0$ is a positive constant independent of ε, and $\delta(x) = \mathrm{dist}(x, \partial\Omega)$ for $x \in \overline{\Omega}$.

Hereafter $\varepsilon^* > 0$ is a sufficiently small constant, and $M > 0$ is a generic constant independent of $\varepsilon > 0$.

Proof of Proposition 3.9. For $x \in \Omega$, then by the uniform interior sphere condition of Ω, there exists $B_{R_0}(x_0) \subseteq \Omega$ with $R_0 \ge R$ such that $x \in B_{R_0}(x_0)$ and $\partial B_{R_0}(x_0) \cap \partial\Omega \neq \emptyset$. Note that if $\delta(x) \ge R$, then we may set $x_0 = x$ and $R_0 = \delta(x)$; if $\delta(x) < R$,

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then we take $x_0 = p_x + (x - p_x)R/|x - p_x|$ and $R_0 = R$, where $p_x \in \partial\Omega$ is the unique closest point to x. Hence we have

$$R_0 - |x - x_0| = \operatorname{dist}(x, \partial B_{R_0}(x_0)) = \delta(x) \quad \text{for } x \in \Omega. \tag{3.88}$$

To show (3.86), we let $\phi_\varepsilon^\pm$ be radial solutions to

$$-\varepsilon\Delta\phi_\varepsilon^\pm = f(\phi_\varepsilon^\pm) \qquad \text{in } B_{R_0}(x_0), \tag{3.89}$$

$$\phi_\varepsilon^\pm = \phi^* \pm C_1 \quad \text{on } \partial B_{R_0}(x_0). \tag{3.90}$$

The existence of solutions to (3.89)–(3.90) follows from the standard variational method. Now we claim

$$\phi_\varepsilon^-(x) \le \phi_\varepsilon(x) \le \phi_\varepsilon^+(x) \quad \text{for } x \in \overline{B}_{R_0}(x_0). \tag{3.91}$$

We first prove $\phi_\varepsilon^+ \ge \phi_\varepsilon$. Let $\overline{\phi}_\varepsilon^+ := \phi_\varepsilon^+ - \phi_\varepsilon$ in $\overline{B}_{R_0}(x_0)$. Then by (3.1), (3.89)–(3.90) and Proposition 3.3, $\overline{\phi}_\varepsilon^+$ satisfies

$$\varepsilon\Delta\overline{\phi}_\varepsilon^+ + c(x)\overline{\phi}_\varepsilon^+ = 0 \qquad \text{in } B_{R_0}(x_0), \tag{3.92}$$

$$\overline{\phi}_\varepsilon^+ = C_1 - (\phi_\varepsilon - \phi^*) \ge 0 \quad \text{on } \partial B_{R_0}(x_0), \tag{3.93}$$

where $c(x) = (f(\phi_\varepsilon^+(x)) - f(\phi_\varepsilon(x)))/(\phi_\varepsilon^+(x) - \phi_\varepsilon(x))$ if $\phi_\varepsilon^+(x) \ne \phi_\varepsilon(x)$; $c(x) = f'(\phi_\varepsilon(x))$ if $\phi_\varepsilon^+(x) = \phi_\varepsilon(x)$. Note that $c(x) < 0$ for $x \in B_{R_0}(x_0)$ because f is strictly decreasing on $\mathbb{R}$ (cf. (F1)). Thus, we apply the maximum principle to (3.92)–(3.93) and obtain $\overline{\phi}_\varepsilon^+ \ge 0$ in $\overline{B}_{R_0}(x_0)$, which implies $\phi_\varepsilon^+ \ge \phi_\varepsilon$ in $\overline{B}_{R_0}(x_0)$. Similarly, we prove $\phi_\varepsilon^- \le \phi_\varepsilon$ in $\overline{B}_{R_0}(x_0)$, and get (3.91). Since $\phi_\varepsilon^\pm$ are the radial solutions to (3.89)–(3.90), then by (3.88) and Proposition 3A.2 (in Appendix 3A) by replacing $B_R(0)$ with $B_{R_0}(x_0)$, we may use the fact that $R_0 \ge R$ and obtain

$$|\phi_\varepsilon^\pm(x) - \phi^*| \le 2C_1 \exp\left(-\frac{C_2 \operatorname{dist}(x, \partial B_{R_0}(x_0))}{\sqrt{\varepsilon}}\right) = 2C_1 \exp\left(-\frac{C_2\delta(x)}{\sqrt{\varepsilon}}\right) \tag{3.94}$$

for $x \in \overline{B}_{R_0}(x_0)$ and $0 < \varepsilon < 8(C_2R)^2/(d-1)^2$, which gives (3.86).

To get (3.87), we first claim

$$|\nabla\phi_\varepsilon(x)| \le M/\sqrt{\varepsilon} \quad \text{for } x \in \overline{\Omega} \quad \text{and} \quad 0 < \varepsilon < (\delta(x))^2, \tag{3.95}$$

where $M > 0$ is independent of $\varepsilon > 0$. When $x \in \partial\Omega$, we may use (3.85) to obtain (3.95). Note that $B_{\sqrt{\varepsilon}}(x_1) \subseteq \Omega$ for $x_1 \in \Omega$ and $0 < \varepsilon < (\delta(x_1))^2$. Set $y = (x - x_1)/\sqrt{\varepsilon}$

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and $\tilde{\phi}_\varepsilon(y) = \phi_\varepsilon(x_1 + \sqrt{\varepsilon}y)$. Then from (3.1), we have $-\Delta\tilde{\phi}_\varepsilon = f(\tilde{\phi}_\varepsilon)$ in $B_1(0)$. By the uniform boundedness of ϕ_ε (cf. Proposition 3.3), we can apply the elliptic L^q-estimate and obtain $\|\tilde{\phi}_\varepsilon\|_{W^{2,q}(B_{1/2}(0))} \leq M$ for $q > 1$. Using Sobolev's compact embedding theorem, we get $\|\tilde{\phi}_\varepsilon\|_{C^{1,\alpha}(B_{1/4}(0))} \leq M$ for $\alpha \in (0,1)$. In particular, we have $|\nabla\tilde{\phi}_\varepsilon(0)| \leq M$, which implies (3.95) holds true for $x \in \Omega$.

Now we prove (3.87). By (3.1), we have

$$\begin{aligned} \varepsilon\Delta|\nabla\phi_\varepsilon|^2 &= 2\varepsilon\sum_{i,j=1}^{d}\left(\frac{\partial^2\phi_\varepsilon}{\partial x^j\partial x^i}\right)^2 + 2\varepsilon\sum_{j=1}^{d}\frac{\partial\phi_\varepsilon}{\partial x^j}\frac{\partial}{\partial x^j}\Delta\phi_\varepsilon \\ &\geq -2\nabla\phi_\varepsilon\cdot\nabla(f(\phi_\varepsilon)) = -2f'(\phi_\varepsilon)|\nabla\phi_\varepsilon|^2 \quad \text{in } B_{R_0}(x_0). \end{aligned} \tag{3.96}$$

Along with Proposition 3.3 and (F1), we have $\varepsilon\Delta|\nabla\phi_\varepsilon|^2 \geq 128C_2^2|\nabla\phi_\varepsilon|^2$ in $B_{R_0}(x_0)$, where $C_2 = m_f([\phi^* - C_1, \phi^* + C_1])/8 > 0$ is given in Lemma 3.6. Let $\overline{\phi}_\varepsilon$ be the solution to $\varepsilon\Delta\overline{\phi}_\varepsilon = 128C_2^2\overline{\phi}_\varepsilon$ in $B_{R_0}(x_0)$ with the Dirichlet boundary condition $\overline{\phi}_\varepsilon = \max\limits_{\partial B_{R_0}(x_0)}|\nabla\phi_\varepsilon|^2$ on $\partial B_{R_0}(x_0)$. Then by the standard comparison principle, we obtain

$$|\nabla\phi_\varepsilon(x)|^2 \leq |\overline{\phi}_\varepsilon(x)| \leq 2\left(\max_{\partial B_{R_0}(x_0)}|\nabla\phi_\varepsilon|^2\right)\exp\left(-\frac{\sqrt{2}C_2\,\mathrm{dist}(x,\partial B_{R_0}(x_0))}{\sqrt{\varepsilon}}\right)$$

for $x \in \overline{B}_{R_0}(x_0)$ and $0 < \varepsilon < 16(C_2R)^2/(d-1)^2$. Combining (3.95), we obtain

$$|\nabla\phi_\varepsilon(x_0)| \leq \frac{M}{\sqrt{\varepsilon}}\exp\left(-\frac{C_2\delta(x_0)}{\sqrt{2\varepsilon}}\right) \quad \text{for } 0 < \varepsilon < 16(C_2R)^2/(d-1)^2,$$

which implies (3.87). Therefore, we complete the proof of Proposition 3.9. □

By Proposition 3.9, it is clear that Theorem 3.1(b) holds true.

3.2.2 Second-order asymptotic expansion of ϕ_ε in $\Omega_{k,\varepsilon}$

In this section, we prove the second-order asymptotic expansion of ϕ_ε near the boundary $\partial\Omega_k$ for $k \in \{0,1,\ldots,K\}$. Since $\mathrm{dist}(\Omega_i,\Omega_j) > 0$ for $i \neq j \in \{0,1,\ldots,K\}$ (cf. (D)), there exists $\varepsilon^* > 0$ sufficiently small such that $\mathrm{dist}(\Omega_{i,\varepsilon,\beta},\Omega_{j,\varepsilon,\beta}) \geq d_0 > 0$ for $i \neq j$ and $\Omega_{k,\varepsilon,\beta} = \{x \in \Omega : \delta_k(x) := \mathrm{dist}(x,\partial\Omega_k) < \varepsilon^\beta\}$ contains no focal points for $0 < \beta < 1/2$ and $0 < \varepsilon < \varepsilon^*$ (cf. [16]), where $d_0 > 0$ is independent of ε. Then for $x \in \overline{\Omega}_{k,\varepsilon,\beta}$, there exists a unique $p_x \in \partial\Omega_k$ (the closest point to x) and $0 \leq t_x = \delta_k(x)/\sqrt{\varepsilon} \leq \varepsilon^{(2\beta-1)/2}$ such that $x = p_x - t_x\sqrt{\varepsilon}\nu_{p_x}$, where ν_{p_x} is the unit outer normal at p_x with respect to $\Omega = \Omega_0 - \bigcup_{k=1}^K\Omega_k$. Hence (3.84)–(3.85) become

$$\phi_\varepsilon(x) = u_k(\delta_k(x)/\sqrt{\varepsilon}) + o_\varepsilon(1), \tag{3.97}$$

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$$\nabla\phi_\varepsilon(x) = -\frac{1}{\sqrt{\varepsilon}}[u_k'(\delta_k(x)/\sqrt{\varepsilon})\nu_{p_x} + o_\varepsilon(1)]. \tag{3.98}$$

For the second-order term of ϕ_ε, we use (3.97) to define the following function:

$$\varphi_{k,\varepsilon}(x) = \frac{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})}{\sqrt{\varepsilon}} \quad \text{for } x \in \overline{\Omega}_{k,\varepsilon,\beta} \text{ and } k = 0, 1, \ldots, K, \tag{3.99}$$

where u_k is the unique solution to (3.7)–(3.9), and $\delta_k(x) = \mathrm{dist}(x, \partial\Omega_k)$ for $k = 0, 1, \ldots, K$. Then by (3.1), (3.7), and (3.99), $\varphi_{k,\varepsilon}$ satisfies

$$\varepsilon\Delta\varphi_{k,\varepsilon}(x) + c_\varepsilon(x)\varphi_{k,\varepsilon}(x) = g_\varepsilon(x) \quad \text{for } x \in \Omega_{k,\varepsilon,\beta}, \tag{3.100}$$

where

$$c_\varepsilon(x) = \begin{cases} \dfrac{f(\phi_\varepsilon(x)) - f(u_k(\delta_k(x)/\sqrt{\varepsilon}))}{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})} & \text{if } \phi_\varepsilon(x) \neq u_k(\delta_k(x)/\sqrt{\varepsilon}); \\ f'(\phi_\varepsilon(x)) & \text{if } \phi_\varepsilon(x) = u_k(\delta_k(x)/\sqrt{\varepsilon}), \end{cases} \tag{3.101}$$

$$g_\varepsilon(x) = (d-1)H(p_x)u_k'(\delta_k(x)/\sqrt{\varepsilon}) + \varepsilon^\beta\mathcal{O}_\varepsilon(1). \tag{3.102}$$

Here we have used the fact that $0 \leq \delta_k(x) \leq \varepsilon^\beta$, $|\nabla\delta_k(x)| = 1$, and

$$\Delta\delta_k(x) = -\sum_{i=1}^{d-1}\frac{\kappa_i}{1-\kappa_i\delta_k(x)} = -(d-1)H(p_x) + \varepsilon^\beta\mathcal{O}_\varepsilon(1) \quad \text{for } x \in \Omega_{k,\varepsilon,\beta}, \tag{3.103}$$

where κ_i are the principal curvatures at $p_x \in \partial\Omega_k$, and $H(p_x) = (d-1)^{-1}\sum\limits_{i=1}^{d-1}\kappa_i$ is the mean curvature at $p_x \in \partial\Omega_k$ (cf. [38, Lemma 14.17]). By (F1), (3.57) and Proposition 3.3, $c_\varepsilon(x) \leq -64C_2^2 < 0$ for $x \in \overline{\Omega}_{k,\varepsilon,\beta}$, where $C_2 = m_f([\phi^* - C_1, \phi^* + C_1])/8$. Moreover, g_ε is uniformly bounded with respect to ε in $\Omega_{k,\varepsilon}$ because u_k' is bounded on $[0,\infty)$ by Proposition 3B.1 in Appendix 3B. For the boundary condition of $\varphi_{k,\varepsilon}$, we use (3.4), (3.8), (3.45) and (3.99) to get

$$\varphi_{k,\varepsilon} + \gamma_k\sqrt{\varepsilon}\partial_\nu\varphi_{k,\varepsilon} = 0 \quad \text{on } \partial\Omega_k. \tag{3.104}$$

Then we prove the uniform boundedness of $\varphi_{k,\varepsilon}$ as follows.

Proposition 3.10 (Uniform boundedness of $\varphi_{k,\varepsilon}$)**.** *There exists a constant $M > 0$ independent of ε such that $\max\limits_{\overline{\Omega}_{k,\varepsilon,\beta}}|\varphi_{k,\varepsilon}| \leq M$ for $k = 0, 1, \ldots, K$ and $0 < \varepsilon < \varepsilon^*$.*

Proof. Fix $k \in \{0, 1, \ldots, K\}$. It is equivalent to proving that $\max\limits_{\overline{\Omega}_{k,\varepsilon,\beta}}\varphi_{k,\varepsilon} \leq M$ and $\min\limits_{\overline{\Omega}_{k,\varepsilon,\beta}}\varphi_{k,\varepsilon} \geq -M$ for some constant $M > 0$ independent of ε. First, we show that

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$\max_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \le M$ for $0 < \varepsilon < \varepsilon^*$. Suppose by contradiction that there exists a sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ of positive numbers with $\lim_{n\to\infty} \varepsilon_n = 0$ and $\{x_n\}_{n=1}^{\infty} \subset \overline{\Omega}_{k,\varepsilon_n,\beta}$ such that $\varphi_{k,\varepsilon_n}(x_n) = \max_{\overline{\Omega}_{k,\varepsilon_n,\beta}} \varphi_{k,\varepsilon_n} \ge n$ for $n \in \mathbb{N}$. Since $0 < \beta < 1/2$, we may, without loss of generality, assume that $8C_1 \exp(-C_2 \varepsilon_n^{(2\beta-1)/2}) \le \sqrt{\varepsilon_n}$ for all $n \in \mathbb{N}$, where C_1 and C_2 are given in Proposition 3.3 and Lemma 3.6, respectively. Note that the maximum point x_n cannot lie on the boundary $\partial\Omega_k$ because from (3.104), $\partial_\nu \varphi_{k,\varepsilon_n}(x_n) = -\varphi_{k,\varepsilon_n}(x_n)/(\gamma_k\sqrt{\varepsilon_n}) \le -n/(\gamma_k\sqrt{\varepsilon_n}) < 0$ if the maximum point $x_n \in \partial\Omega_k$. On the other hand, by (3.57) (with Proposition 3.7) and (3.86), we have

$$|\varphi_{k,\varepsilon_n}(x)| \le \frac{|\phi_{\varepsilon_n}(x) - \phi^*| + |u_k(\delta_k(x)/\sqrt{\varepsilon_n}) - \phi^*|}{\sqrt{\varepsilon_n}} \le \frac{4C_1}{\sqrt{\varepsilon_n}} \exp\left(-C_2 \varepsilon_n^{(2\beta-1)/2}\right) \le \frac{1}{2} \tag{3.105}$$

for $\delta_k(x) = \varepsilon_n^\beta$ and $n \in \mathbb{N}$. This shows that x_n cannot lie on the boundary $\partial\Omega_{k,\varepsilon_n,\beta}$. Hence $x_n \in \Omega_{k,\varepsilon_n,\beta}$ for all $n \in \mathbb{N}$, which implies $\nabla\varphi_{k,\varepsilon_n}(x_n) = 0$ and $\Delta\varphi_{k,\varepsilon_n}(x_n) \le 0$ for $n \in \mathbb{N}$. Thus by (3.100),

$$0 \le -\varepsilon_n \Delta\varphi_{k,\varepsilon_n}(x_n) = c_{\varepsilon_n}(x_n)\varphi_{k,\varepsilon_n}(x_n) - g_{\varepsilon_n}(x_n). \tag{3.106}$$

Recall that g_ε is uniformly bounded, $\varphi_{k,\varepsilon_n}(x_n) \ge n$ for $n \in \mathbb{N}$, and $c_\varepsilon \le -64C_2^2 < 0$ in $\overline{\Omega}_{k,\varepsilon}$ for $\varepsilon > 0$. Letting $n \to \infty$, we obtain $\lim_{n\to\infty} c_{\varepsilon_n}(x_n)\varphi_{k,\varepsilon_n}(x_n) = -\infty$, which contradicts (3.106). Thus, $\max_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \le M$ for some constant $M > 0$ independent of ε. Similarly, we may use (3.57), (3.86), (3.100) and (3.104) to prove $\min_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \ge -M$ for $0 < \varepsilon < \varepsilon^*$, where $M > 0$ is independent of $\varepsilon > 0$. Therefore, we complete the proof of Proposition 3.10. □

To study the asymptotic expansion of $\varphi_{k,\varepsilon}$, we first claim that $\Psi_p(\overline{B}^+_{\varepsilon^{(2\beta+1)/2}}) \subseteq \overline{\Omega}_{k,\varepsilon,\beta}$ for $p \in \partial\Omega_k$, $k \in \{0, 1, \ldots, K\}$ and sufficiently small $\varepsilon > 0$ because

$$\delta_k(\Psi_p(y)) = |\delta_k(\Psi_p(y)) - \delta_k(p)| \le C|\Psi_p(y) - p| \le C'|y| \le \varepsilon^\beta$$

for $y \in \overline{B}^+_{\varepsilon^{(2\beta+1)/2}}$, $p \in \partial\Omega_k$, $k \in \{0, 1, \ldots, K\}$ and sufficiently small $\varepsilon > 0$, where Ψ_p is the diffeomorphism in (3.43), $C = C(\Omega)$ and $C' = C'(p, \Omega)$ are positive constants independent of y. Here we have used the facts that $\delta_k(p) = 0$, $\psi_p(p') = p^d$ (cf. (D1)) and the smoothness of ψ_p and δ_k. Hence there exists $\varepsilon^* > 0$ sufficiently small such that $\Psi_p(\overline{B}^+_{\varepsilon^{(2\beta+1)/2}}) \subset \overline{\Omega}_{k,\varepsilon,\beta} \cap \Psi_p(\overline{B}^+_b)$ for $0 < \varepsilon < \varepsilon^*$. As in Section 3.2.1, we apply

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the principal coordinate system (3.43) to the neighborhood $\Psi_p(\overline{B}^+_{\varepsilon^{(2\beta+1)/2}})$, rescale the spatial variable y by $\sqrt{\varepsilon}$ and define

$$\mathcal{W}_{k,p,\varepsilon}(z) = \varphi_{k,\varepsilon}(\Psi_p(\sqrt{\varepsilon}z)) \quad \text{for } z \in \overline{B}^+_{\varepsilon^{(2\beta-1)/2}} \text{ and } 0 < \varepsilon < \varepsilon^*. \tag{3.107}$$

Note that $\mathcal{W}_{k,p,\varepsilon}$ is well-defined due to $\Psi_p(\overline{B}^+_{\varepsilon^{(2\beta+1)/2}}) \subset \overline{\Omega}_{k,\varepsilon,\beta} \cap \Psi_p(\overline{B}^+_b)$ for $0 < \varepsilon < \varepsilon^*$.

By Lemma 3.4 and equations (3.100)–(3.104), $\mathcal{W}_{k,p,\varepsilon}$ satisfies

$$\sum_{i,j=1}^{d} a_{ij}(z)\frac{\partial^2 \mathcal{W}_{k,p,\varepsilon}}{\partial z^i \partial z^j} + \sum_{j=1}^{d} b_j(z)\frac{\partial \mathcal{W}_{k,p,\varepsilon}}{\partial z^j} + c_\varepsilon(z)\mathcal{W}_{k,p,\varepsilon} = g_\varepsilon(z) \quad \text{in } B^+_{\varepsilon^{(2\beta-1)/2}}, \tag{3.108}$$

$$\mathcal{W}_{k,p,\varepsilon} - \gamma_k \partial_{z^d}\mathcal{W}_{k,p,\varepsilon} = 0 \qquad \text{on } \overline{B}^+_{\varepsilon^{(2\beta-1)/2}} \cap \partial\mathbb{R}^d_+ \tag{3.109}$$

for $0 < \varepsilon < \varepsilon^*$, where a_{ij} and b_j are given in (3.47)–(3.48), and

$$c_\varepsilon(z) = \begin{cases} \dfrac{f(u_k(z^d) + \sqrt{\varepsilon}\mathcal{W}_{k,p,\varepsilon}(z)) - f(u_k(z^d))}{\sqrt{\varepsilon}\mathcal{W}_{k,p,\varepsilon}(z)} & \text{if } \mathcal{W}_{k,p,\varepsilon}(z) \neq 0; \\ f'(u_k(z^d)) & \text{if } \mathcal{W}_{k,p,\varepsilon}(z) = 0, \end{cases} \tag{3.110}$$

$$g_\varepsilon(z) = (d-1)H(p)u_k'(z^d) + \varepsilon^\beta \mathcal{O}_\varepsilon(1). \tag{3.111}$$

As in the proofs of Lemmas 3.5 and 3.6, we may use the uniform boundedness of $\varphi_{k,\varepsilon}$ (cf. Proposition 3.10) to prove the convergence of $\mathcal{W}_{k,p,\varepsilon}$ in $\mathcal{C}^{2,\alpha}(\overline{B}^+_m)$ as ε tends to zero (up to a subsequence) for $m \in \mathbb{N}$ and then prove the exponential-type estimate of $\mathcal{W}_{k,p}$.

Lemma 3.11. *For any sequence $\{\varepsilon_n\}_{n=1}^\infty$ of positive numbers with $\lim_{n\to\infty} \varepsilon_n = 0$, $\alpha \in (0,1)$, and $p \in \partial\Omega_k$ ($k \in \{0,1,\dots,K\}$), there exists a subsequence $\{\varepsilon_{nn}\}_{n=1}^\infty$ such that $\lim_{n\to\infty} \|\mathcal{W}_{k,p,\varepsilon_{nn}} - \mathcal{W}_{k,p}\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0$ for $m \in \mathbb{N}$, where $\mathcal{W}_{k,p} \in \mathcal{C}^{2,\alpha}_{loc}(\overline{\mathbb{R}}^d_+)$ satisfies*

$$\Delta\mathcal{W}_{k,p} + f'(u_k)\mathcal{W}_{k,p} = (d-1)H(p)u_k'(z^d) \quad \text{in } \mathbb{R}^d_+, \tag{3.112}$$

$$\mathcal{W}_{k,p} - \gamma_k\partial_{z^d}\mathcal{W}_{k,p} = 0 \quad \text{on } \partial\mathbb{R}^d_+. \tag{3.113}$$

Moreover, there exists $M > 0$ such that $\mathcal{W}_{k,p}$ satisfies

$$|\mathcal{W}_{k,p}(z) - (d-1)H(p)v_k(z^d)| \leq M\exp(-C_2 z^d) \tag{3.114}$$

for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$ and $z^d \geq (d-1)/(4C_2)$, where v_k is the solution to (3.10)–(3.12) and C_2 is given in Lemma 3.6.

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From Lemma 3.11, the solution $\mathcal{W}_{k,p}$ to (3.112)–(3.113) may, a priori depend on the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$. To establish the independence from the sequence, we apply the moving plane arguments to prove $\mathcal{W}_{k,p}(z) = \mathcal{W}_{k,p}(z^d) = (d-1)H(p)v_k(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$ (see Proposition 3.12 below), where v_k is the unique solution to (3.10)–(3.12), and v_k is independent of the choice of sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ and point $p \in \partial\Omega_k$. Therefore, the results of Lemma 3.11 can be improved as

$$\lim_{\varepsilon\to 0^+} \|\mathcal{W}_{k,p,\varepsilon} - (d-1)H(p)v_k\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0 \quad \text{for } m \in \mathbb{N} \text{ and } \alpha \in (0,1), \tag{3.115}$$

and

$$\lim_{\varepsilon\to 0^+} \mathcal{W}_{k,p,\varepsilon}(z) = (d-1)H(p)v_k(z^d) \quad \text{for } z = (z', z^d) \in \overline{\mathbb{R}}^d_+, \tag{3.116}$$

where $\mathcal{W}_{k,p,\varepsilon}$ is defined in (3.107). Below are the details.

Proposition 3.12. *For $p \in \partial\Omega_k$ and $k \in \{0,1,\dots,K\}$, the solution $\mathcal{W}_{k,p}$ to (3.112)–(3.113) satisfies*

(a) $\mathcal{W}_{k,p}$ depends only on the variable z^d, i.e., $\mathcal{W}_{k,p}(z) = \mathcal{W}_{k,p}(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$.

(b) $\mathcal{W}_{k,p}(z^d) = (d-1)H(p)v_k(z^d)$ for $z^d \in [0,\infty)$, where v_k is the unique solution to (3.10)–(3.12).

As in Proposition 3.7, we may use the moving plane arguments to prove Proposition 3.12. The proof of Proposition 3.12 is similar to that of Proposition 3.7 so we omit it here.

We may use Proposition 3.12 to prove (3.115), (3.116), and $\mathcal{W}_{k,p}(z) = (d-1)H(p)v_k(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$, where v_k is the solution to (3.10)–(3.12). Let $T > 0$, $k \in \{0,1,\dots,K\}$, and $p \in \partial\Omega_k$. Then by (3.43), (3.107), (3.115)–(3.116) and $\nabla\delta_k(p - t\sqrt{\varepsilon}\nu_p) = -\nu_p$, we have

$$\varphi_{k,\varepsilon}(p - t\sqrt{\varepsilon}\nu_p) = \mathcal{W}_{k,p,\varepsilon}(te_d) = \mathcal{W}_{k,p}(t) + o_\varepsilon(1) = (d-1)H(p)v_k(t) + o_\varepsilon(1) \tag{3.117}$$

and

$$\nabla\varphi_{k,\varepsilon}(p - t\sqrt{\varepsilon}\nu_p) = -\frac{1}{\sqrt{\varepsilon}}(\mathcal{W}'_{k,p}(t)\nu_p + o_\varepsilon(1)) = -\frac{1}{\sqrt{\varepsilon}}((d-1)H(p)v'_k(t)\nu_p + o_\varepsilon(1)) \tag{3.118}$$

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for $0 \le t \le T$ as $\varepsilon \to 0^+$. Combining (3.99), (3.107), and (3.117)–(3.118), we obtain

$$\begin{aligned}\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) &= u_k(t) + \sqrt{\varepsilon}\Big((d-1)H(p)v_k(t) + o_\varepsilon(1)\Big),\\ \nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) &= -\left(\frac{1}{\sqrt{\varepsilon}}u_k'(t) + (d-1)H(p)v_k'(t)\right)\nu_p + o_\varepsilon(1)\end{aligned}$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$, which implies (3.5)–(3.6). Therefore, we complete the proof of Theorem 3.1(a).

3.2.3 Proof of Corollary 3.1

We present the proof of Corollary 3.1. To prove (a), we integrate (3.17) over $\overline{\Omega}_{k,T,\varepsilon}$ and apply the coarea formula (see [30, 83]) to obtain

$$\int_{\overline{\Omega}_{k,T,\varepsilon}} f(\phi_\varepsilon(x))\,\mathrm{d}x = \sqrt{\varepsilon}\int_0^T\int_{\partial\Omega_k}\{f(u_k(t)) + \sqrt{\varepsilon}[(d-1)H(p)f'(u_k(t))v_k(t) + o_\varepsilon(1)]\}\mathcal{J}(t,p)\,\mathrm{d}S_p\,\mathrm{d}t, \tag{3.119}$$

where

$$\mathcal{J}(t,p) = 1 - t\sqrt{\varepsilon}(d-1)H(p) + t\sqrt{\varepsilon}o_\varepsilon(1) \quad \text{for } p \in \partial\Omega_k \text{ and } t \ge 0, \tag{3.120}$$

follows from Steiner's formula (cf. [1, 38, 40]). Combining (3.7), (3.10), and (3.119)–(3.120), we have

$$\begin{aligned}\int_{\overline{\Omega}_{k,T,\varepsilon}} f(\phi_\varepsilon(x))\,\mathrm{d}x &= \sqrt{\varepsilon}\int_0^T\int_{\partial\Omega_k} f(u_k(t))\,\mathrm{d}S_p\,\mathrm{d}t\\ &\quad + \varepsilon(d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)\left(\int_0^T [f'(u_k(t))v_k(t) - tf(u_k(t))]\,\mathrm{d}t\right) + \varepsilon o_\varepsilon(1)\\ &= -\sqrt{\varepsilon}|\partial\Omega_k|\int_0^T u_k''(t)\,\mathrm{d}t\\ &\quad + \varepsilon(d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)\left(\int_0^T [u_k'(t) - v_k''(t) + tu_k''(t)]\,\mathrm{d}t\right) + \varepsilon o_\varepsilon(1)\\ &= \sqrt{\varepsilon}|\partial\Omega_k|(u_k'(0) - u_k'(T))\\ &\quad + \varepsilon(d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)(Tu_k'(T) + v_k'(0) - v_k'(T)) + \varepsilon o_\varepsilon(1),\end{aligned}$$

which completes the proof of (a).

We now prove (b). Note that

$$\partial\Omega_{k,T,\varepsilon,\beta} = \{p - T\sqrt{\varepsilon}\nu_p \in \Omega : p \in \partial\Omega_k\} \cup \{p - \varepsilon^\beta\nu_p \in \Omega : p \in \partial\Omega_k\}$$

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is the union of two disjoint parallel surfaces to the boundary $\partial\Omega_k$. Integrating (3.1) over $\overline{\Omega}_{k,T,\varepsilon,\beta}$ and applying the divergence theorem, we obtain

$$\begin{aligned}\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f(\phi_\varepsilon(x))\,\mathrm{d}x &= -\varepsilon \int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} \Delta\phi_\varepsilon(x)\,\mathrm{d}x \\ &= -\varepsilon \int_{\partial\Omega_{k,T,\varepsilon,\beta}} \partial_{\nu_x}\phi_\varepsilon(x)\,\mathrm{d}S_x \\ &= -\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - T\sqrt{\varepsilon}\nu_p))\mathcal{J}(T,p)\,\mathrm{d}S_p \\ &\quad + \int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p-\varepsilon^\beta\nu_p))\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)\,\mathrm{d}S_p,\end{aligned} \tag{3.121}$$

where ν_x is the unit outer normal at $x \in \partial\Omega_{k,T,\varepsilon,\beta}$ with respect to $\Omega_{k,T,\varepsilon,\beta}$ and

$$\begin{aligned}&\mathcal{J}(T,p) = 1 - T\sqrt{\varepsilon}(d-1)H(p) + \sqrt{\varepsilon}o_\varepsilon(1), \\ &\mathcal{J}(\varepsilon^{(2\beta-1)/2},p) = 1 - \varepsilon^\beta(d-1)H(p) + \varepsilon^\beta o_\varepsilon(1).\end{aligned} \tag{3.122}$$

Here we have used Steiner's formula in differential geometry (cf. [1, 40]). By (3.6), we have

$$\begin{aligned}&-\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - T\sqrt{\varepsilon}\nu_p))\mathcal{J}(T,p)\,\mathrm{d}S_p \\ &= -\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - T\sqrt{\varepsilon}\nu_p))[1 - T\sqrt{\varepsilon}(d-1)H(p) + \sqrt{\varepsilon}o_\varepsilon(1)]\,\mathrm{d}S_p \\ &= \sqrt{\varepsilon}\int_{\partial\Omega_k} \{u_k'(T) + \sqrt{\varepsilon}[(d-1)H(p)v_k'(T) + o_\varepsilon(1)]\}[1 - T\sqrt{\varepsilon}(d-1)H(p) + \sqrt{\varepsilon}o_\varepsilon(1)]\,\mathrm{d}S_p \\ &= \sqrt{\varepsilon}|\partial\Omega_k|u_k'(T) + \varepsilon(d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)(-Tu_k'(T) + v_k'(T)) + \varepsilon o_\varepsilon(1).\end{aligned} \tag{3.123}$$

On the other hand, by Theorem 3.1(b,ii), we have

$$\left|\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p-\varepsilon^\beta\nu_p))\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)\,\mathrm{d}S_p\right| \leq \sqrt{\varepsilon}|\partial\Omega_k|M'\exp\left(-M\varepsilon^{(2\beta-1)/2}\right). \tag{3.124}$$

Combining (3.121)–(3.124) with $0 < \beta < 1/2$, we get (b). By an argument similar to that used in the proof of (b), one may use (3.124) to establish (c). Therefore, we complete the proof of Corollary 3.1.

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3.3 Proof of Theorem 3.2

In this section, we derive the first- and second-order asymptotic expansions of the solution ϕ_ε to equation (3.2) with condition (3.4) under the charge neutrality condition (3.3). Equation (3.2) with condition (3.4) can be denoted by

$$-\varepsilon\Delta\phi_\varepsilon = f_\varepsilon(\phi_\varepsilon) \quad \text{in } \Omega, \tag{3.125}$$

$$\phi_\varepsilon + \gamma_k\sqrt{\varepsilon}\partial_\nu\phi_\varepsilon = \phi_{bd,k} \quad \text{on } \partial\Omega_k \text{ for } k = 0, 1, \ldots, K, \tag{3.126}$$

where $f_\varepsilon = f_\varepsilon(\phi)$ is defined as

$$f_\varepsilon(\phi) = \sum_{i=1}^{I} \frac{m_i z_i}{A_{i,\varepsilon}} \exp(-z_i\phi) \quad \text{for } \phi \in \mathbb{R}, \quad \text{and} \quad A_{i,\varepsilon} = \int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y. \tag{3.127}$$

In Section 3.3.1, we prove the uniform boundedness of ϕ_ε and show that f_ε satisfies conditions (F1)–(F2) with the unique zero ϕ_ε^* for $\varepsilon > 0$. Thus, $f_\varepsilon(\phi) = f_0(\phi) + o_\varepsilon(1)$ for $\phi \in \mathbb{R}$, and (3.125) can be approximated by $-\varepsilon\Delta\phi_\varepsilon = f_0(\phi_\varepsilon) + o_\varepsilon(1)$ in Ω, where

$$f_0(\phi) = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi - \phi_0^*)) \quad \text{for } \phi \in \mathbb{R},$$

and ϕ_0^* is the pointwise limit of ϕ_ε as ε tends to zero (see Remark 3.4). Note that f_0 is strictly decreasing on $\mathbb{R}$ and has a unique zero ϕ_0^*. Hence we can use the method of Section 3.2.1 to prove the first-order asymptotic expansions $\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_k(t) + o_\varepsilon(1)$ and $\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\varepsilon^{-1/2}(u_k'(t)\nu_p + o_\varepsilon(1))$ for $T > 0$, $p \in \partial\Omega_k$, and $0 \le t \le T$, where u_k is the unique solution to (3.21)–(3.23) (cf. Section 3.3.2). To obtain the second-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$, it is essential to show the uniform boundedness of $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon}$ in Section 3.3.3. We suppose, by contradiction, that $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon} \to \infty$ as $\varepsilon \to 0^+$, and then derive the asymptotic expansions of the integral terms $A_{i,\varepsilon}$ in (3.127) and the nonlinear term f_ε. Then, as in Sections 3.2.2 and 3.2.3, we obtain the asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$, and hence the asymptotic expansions of total ionic charge over the regions $\overline{\Omega}_{k,T,\varepsilon}$, $\overline{\Omega}_{k,T,\varepsilon,\beta}$, and $\overline{\Omega}_{\varepsilon,\beta}$ (see Proposition 3.25), which contradicts the charge neutrality condition (3.3). As a result, we show $\phi_\varepsilon^* = \phi_0^* + \sqrt{\varepsilon}(Q + o_\varepsilon(1))$ (see (3.200) in Remark 3.6). In Section 3.3.4, we use $\phi_\varepsilon^* = \phi_0^* + \sqrt{\varepsilon}(Q + o_\varepsilon(1))$ and follow a similar argument of Section 3.3.3 to establish the asymptotic expansions of $A_{i,\varepsilon}$ and get the

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further asymptotic expansion of f_ε: $f_\varepsilon(\phi) = f_0(\phi) + \sqrt{\varepsilon}(f_1(\phi) + o_\varepsilon(1))$ for $\phi \in \mathbb{R}$ (cf. (3.220)), where

$$f_1(\phi) = -Q f_0'(\phi) + \hat{f}_1(\phi) \quad \text{for } \phi \in \mathbb{R}. \tag{3.128}$$

Here

$$\begin{aligned} \hat{f}_1(\phi) &= \frac{1}{|\Omega|} \sum_{i=1}^{I} \hat{m}_i z_i \exp(-z_i(\phi - \phi_0^*)) \quad \text{for } \phi \in \mathbb{R}, \\ \hat{m}_i &= \frac{m_i}{|\Omega|} \sum_{k=0}^{K} |\partial\Omega_k| \int_0^\infty [1 - \exp(-z_i(u_k(s) - \phi_0^*))] \, \mathrm{d}s \quad \text{for } i = 1, \ldots, I. \end{aligned}$$

Consequently, equation (3.125) becomes

$$-\varepsilon \Delta \phi_\varepsilon = f_0(\phi_\varepsilon) + \sqrt{\varepsilon}(f_1(\phi_\varepsilon) + o_\varepsilon(1)) \quad \text{in } \Omega,$$

and we can apply the method of Section 3.2.2 to prove the second-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$ (cf. (3.19)–(3.20)). In Section 3.3.4, using the asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$, we prove Corollary 3.2 and then apply Corollary 3.2 to determine the unique value of Q, which verifies Remark 3.6. Therefore, we complete the proof of Theorem 3.2.

3.3.1 Estimate of the solution ϕ_ε and f_ε

Equation (3.2) with the boundary condition (3.4) is the Euler–Lagrange equation of the following energy functional

$$E[\phi] = \frac{\varepsilon}{2} \int_\Omega |\nabla\phi|^2 \, \mathrm{d}x - \sum_{i=1}^{I} m_i \ln\left(\int_\Omega \exp(-z_i\phi) \, \mathrm{d}x \right) + \sqrt{\varepsilon} \sum_{k=0}^{K} \frac{1}{2\gamma_k} \int_{\partial\Omega_k} (\phi - \phi_{bd,k})^2 \, \mathrm{d}S$$

for $\phi \in H^1(\Omega)$. The existence and uniqueness of the smooth solution $\phi_\varepsilon \in \mathcal{C}^\infty(\overline{\Omega})$ was proved in [71]. Due to the charge neutrality condition (3.3), we prove the uniform boundedness of the solution ϕ_ε as follows.

Proposition 3.13 (Uniform boundedness of ϕ_ε)**.** *Assume that $\phi_{bd,k}$ are not equal and (3.3) holds true. Let $\phi_\varepsilon \in \mathcal{C}^\infty(\overline{\Omega})$ be the unique solution to equations (3.125)–(3.126). Then ϕ_ε satisfies*

$$\underline{\phi_{bd}} \le \phi_\varepsilon(x) \le \overline{\phi_{bd}} \quad \textit{for } x \in \overline{\Omega} \textit{ and } \varepsilon > 0, \tag{3.129}$$

where $\underline{\phi_{bd}} = \min_{0 \le k \le K} \phi_{bd,k}$ and $\overline{\phi_{bd}} = \max_{0 \le k \le K} \phi_{bd,k}$.

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Proof. We first prove that ϕ_ε attains its maximum value at a boundary point. Suppose by contradiction that ϕ_ε attains the maximum value at an interior point $x_0 \in \Omega$. It is clear that $\phi_\varepsilon(x_0) \geq \phi_\varepsilon(y)$ for $y \in \overline{\Omega}$ and $\Delta\phi_\varepsilon(x_0) \leq 0$. Then by (3.3) with $m_i > 0$ for $i = 1, \ldots, I$, (3.125) and (3.127),

$$0 \leq -\varepsilon\Delta\phi_\varepsilon(x_0) = \sum_{i=1}^{I} \frac{m_i z_i \exp(-z_i\phi_\varepsilon(x_0))}{\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y}$$
$$= \sum_{i=1}^{I} \frac{m_i z_i}{\int_\Omega \exp(-z_i(\phi_\varepsilon(y) - \phi_\varepsilon(x_0)))\,\mathrm{d}y} \leq \sum_{i=1}^{I} \frac{m_i z_i}{|\Omega|} = 0,$$

which implies $\phi_\varepsilon(x) = \phi_\varepsilon(x_0)$ for $x \in \overline{\Omega}$. Hence by (3.4), $\phi_{bd,k}$ are equal but this contradicts the assumption that $\phi_{bd,k}$ are not equal. Thus, ϕ_ε must attain the maximum value at a boundary point $x_{k_0} \in \partial\Omega_{k_0}$ for some $k_0 \in \{0, 1, \ldots, K\}$ and $\partial_\nu\phi_\varepsilon(x_{k_0}) \geq 0$. Moreover, from (3.4) with $\gamma_{k_0} > 0$, we obtain

$$\phi_\varepsilon(x) \leq \phi_\varepsilon(x_{k_0}) = \phi_{bd,k_0} - \gamma_{k_0}\sqrt{\varepsilon}\partial_\nu\phi_\varepsilon(x_{k_0}) \leq \phi_{bd,k_0} \leq \overline{\phi_{bd}} \quad \text{for } x \in \overline{\Omega}.$$

Similarly, we can prove that ϕ_ε attains the minimum value at a boundary point and hence $\phi_\varepsilon \geq \underline{\phi_{bd}}$ in $\overline{\Omega}$. Therefore, we complete the proof of Proposition 3.13. □

By (3.127) and Proposition 3.13, we prove f_ε satisfies conditions (F1)–(F2).

Proposition 3.14. *Assume that $\phi_{bd,k}$ are not equal and (3.3) holds true. Function $f_\varepsilon = f_\varepsilon(\phi)$ is strictly decreasing on $\mathbb{R}$ and has a unique zero denoted by $\phi_\varepsilon^* \in (\underline{\phi_{bd}}, \overline{\phi_{bd}})$ (which depends on ε). Moreover, f_ε satisfies*

$$|f_\varepsilon(\phi)| \leq M \quad \textit{for } \phi \in [\underline{\phi_{bd}}, \overline{\phi_{bd}}] \textit{ and } \varepsilon > 0, \tag{3.130}$$
$$f_\varepsilon'(\phi) \leq -C_3^2 \quad \textit{for } \phi \in \mathbb{R} \textit{ and } \varepsilon > 0, \tag{3.131}$$

where M and C_3 are positive constants independent of $\varepsilon > 0$.

Hereafter $M > 0$ denotes a generic constant independent of $\varepsilon > 0$.

Proof. By (3.129), the integral term $A_{i,\varepsilon}$ satisfies the following estimate:

$$\alpha_1 \leq A_{i,\varepsilon} = \int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y \leq \alpha_2 \quad \text{for } i = 1, \ldots, I, \tag{3.132}$$

where α_1 and α_2 are positive constants independent of ε. Note that $z_i \neq 0$ for $i = 1, \ldots, I$. Then from (3.127), we can use (3.132) to find

$$f_\varepsilon(\phi) = \sum_{i=1}^{I} \frac{m_i z_i}{A_{i,\varepsilon}} \exp(-z_i\phi) = \left(\sum_{z_i>0} + \sum_{z_i<0}\right) \frac{m_i z_i}{A_{i,\varepsilon}} \exp(-z_i\phi)$$

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$$\geq \sum_{z_i>0} \frac{m_i z_i}{\alpha_2} \exp(-z_i\phi) + \sum_{z_i<0} \frac{m_i z_i}{\alpha_1} \exp(-z_i\phi) := g_1(\phi) \quad \text{for } \phi \in \mathbb{R},$$

and

$$\begin{aligned} f_\varepsilon(\phi) &= \left(\sum_{z_i>0} + \sum_{z_i<0} \right) \frac{m_i z_i}{A_{i,\varepsilon}} \exp(-z_i\phi) \\ &\leq \sum_{z_i>0} \frac{m_i z_i}{\alpha_1} \exp(-z_i\phi) + \sum_{z_i<0} \frac{m_i z_i}{\alpha_2} \exp(-z_i\phi) := g_2(\phi) \quad \text{for } \phi \in \mathbb{R}, \end{aligned}$$

which gives

$$g_1(\phi) \leq f_\varepsilon(\phi) \leq g_2(\phi) \quad \text{for } \phi \in \mathbb{R}. \tag{3.133}$$

Clearly, g_1 and g_2 are independent of ε, strictly decreasing on $\mathbb{R}$ and

$$\lim_{\phi\to\pm\infty} g_i(\phi) = \mp\infty \quad \text{for } i = 1, 2. \tag{3.134}$$

Hence by (3.133), $g_1(\overline{\phi_{bd}}) \leq f_\varepsilon(\phi) \leq g_2(\underline{\phi_{bd}})$ for $\phi \in [\underline{\phi_{bd}}, \overline{\phi_{bd}}]$, which implies (3.130). Moreover, by (3.127) and (3.132), there exists $C_3 > 0$ independent of ε such that

$$f_\varepsilon'(\phi) = -\sum_{i=1}^{I} \frac{m_i z_i^2}{A_{i,\varepsilon}} \exp(-z_i\phi) \leq -\sum_{i=1}^{I} \frac{m_i z_i^2}{\alpha_1} \exp(-z_i\phi) \leq -C_3^2 \quad \text{for } \phi \in \mathbb{R},$$

which gives (3.131). Here $C_3^2 = \alpha_1^{-1} \min\left\{ \sum_{z_i<0} m_i z_i^2, \sum_{z_i>0} m_i z_i^2 \right\}$ comes from

$$\sum_{i=1}^{I} \frac{m_i z_i^2}{\alpha_1} \exp(-z_i\phi) \geq \sum_{z_i<0} \frac{m_i z_i^2}{\alpha_1} \quad \text{for } \phi \geq 0$$

and

$$\sum_{i=1}^{I} \frac{m_i z_i^2}{\alpha_1} \exp(-z_i\phi) \geq \sum_{z_i>0} \frac{m_i z_i^2}{\alpha_1} \quad \text{for } \phi \leq 0$$

because of $z_i z_j < 0$ for some $i, j \in \{1, \dots, I\}$. By (3.131) and (3.133)–(3.134), f_ε is strictly decreasing and has a unique zero $\phi_\varepsilon^* \in \mathbb{R}$. To complete the proof, it remains to show $\phi_\varepsilon^* \in (\underline{\phi_{bd}}, \overline{\phi_{bd}})$ for $\varepsilon > 0$. If $\phi_\varepsilon^* \geq \overline{\phi_{bd}}$ for some $\varepsilon > 0$, then by (3.129), $\phi_\varepsilon^* \geq \phi_\varepsilon(x)$ for $x \in \overline{\Omega}$. Due to the strict decrease of f_ε, we have $0 = f_\varepsilon(\phi_\varepsilon^*) \leq f_\varepsilon(\phi_\varepsilon(x))$ for $x \in \overline{\Omega}$. Then by (3.3) and (3.127), we obtain

$$0 = \int_\Omega f_\varepsilon(\phi_\varepsilon^*)\,\mathrm{d}x \leq \int_\Omega f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \int_\Omega \sum_{i=1}^{I} \frac{m_i z_i \exp(-z_i\phi_\varepsilon(x))}{\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y}\,\mathrm{d}x = \sum_{i=1}^{I} m_i z_i = 0,$$

which implies $f_\varepsilon(\phi_\varepsilon) \equiv f_\varepsilon(\phi_\varepsilon^*) = 0$ and hence $\phi_\varepsilon \equiv \phi_\varepsilon^*$ in $\overline{\Omega}$. By (3.4), $\phi_{bd,k}$ are equal but this is impossible because $\phi_{bd,k}$ are not equal. Thus $\phi_\varepsilon^* < \overline{\phi_{bd}}$ for $\varepsilon > 0$. Similarly, we can prove $\phi_\varepsilon^* > \underline{\phi_{bd}}$ for $\varepsilon > 0$. Therefore, the proof of Proposition 3.14 is complete. □

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By Propositions 3.13 and 3.14, we prove the asymptotic limit of ϕ_ε in Ω as below.

Proposition 3.15. *There exists a constant* $\phi_0^* \in [\underline{\phi_{bd}}, \overline{\phi_{bd}}]$ *such that* $\lim\limits_{\varepsilon \to 0^+} \phi_\varepsilon(x) = \phi_0^*$ *for* $x \in \Omega$ *(up to a subsequence).*

Proof. We begin by proving

$$|\nabla \phi_\varepsilon(x)| \leq M'/\sqrt{\varepsilon} \quad \text{for } x \in \Omega \text{ and } 0 < \varepsilon < (\delta(x))^2, \tag{3.135}$$

where $M' > 0$ is generic constant independent of $\varepsilon > 0$ and $\delta(x) = \mathrm{dist}(x, \partial\Omega)$ for $x \in \overline{\Omega}$. Let $x_0 \in \Omega$ be arbitrary and $B_{\sqrt{\varepsilon}}(x_0) \subseteq \Omega$ for $0 < \varepsilon < (\delta(x_0))^2$. Set $y = (x - x_0)/\sqrt{\varepsilon}$ and $\tilde{\phi}_\varepsilon(y) = \phi_\varepsilon(x_0 + \sqrt{\varepsilon} y)$. Then from (3.125), we have $-\Delta \tilde{\phi}_\varepsilon = f_\varepsilon(\tilde{\phi}_\varepsilon)$ in $B_1(0)$. By the uniform boundedness of ϕ_ε and $f_\varepsilon(\phi_\varepsilon)$ (cf. Propositions 3.13 and 3.14), we apply the elliptic L^q-estimate to obtain $\|\tilde{\phi}_\varepsilon\|_{W^{2,q}(B_{1/2}(0))} \leq M'$ for $q > 1$. Then using Sobolev's compact embedding theorem, we get $\|\tilde{\phi}_\varepsilon\|_{\mathcal{C}^{1,\alpha}(B_{1/4}(0))} \leq M'$ for $\alpha \in (0, 1)$. In particular, we have $|\nabla \tilde{\phi}_\varepsilon(0)| \leq M'$, which gives $|\nabla \phi_\varepsilon(x_0)| \leq M'/\sqrt{\varepsilon}$ and (3.135).

Suppose that Ω' is a smooth subdomain of Ω such that $\Omega' \subset\subset \Omega$. We claim that

$$|\nabla \phi_\varepsilon(x)| \leq \frac{M'}{\sqrt{\varepsilon}} \exp\left(-\frac{\sqrt{2} C_3 \,\mathrm{dist}(\Omega', \partial\Omega)}{16\sqrt{\varepsilon}}\right) \quad \text{for } x \in \Omega' \text{ and } 0 < \varepsilon < \varepsilon^*, \tag{3.136}$$

where $\varepsilon^* > 0$ is a sufficiently small constant depending on Ω' and $C_3 > 0$ is given in (3.131). Let $x_1 \in \Omega'$ be arbitrary. Clearly, $B_{R_1}(x_1) \subset\subset \Omega$ with $R_1 = \mathrm{dist}(\Omega', \partial\Omega)/2$. Then we use (3.125) to obtain

$$\begin{aligned}
\varepsilon \Delta |\nabla \phi_\varepsilon|^2 &= 2\varepsilon \sum_{i,j=1}^{d} \left(\frac{\partial^2 \phi_\varepsilon}{\partial x^j \partial x^i}\right)^2 + 2\varepsilon \sum_{j=1}^{d} \frac{\partial \phi_\varepsilon}{\partial x^j} \frac{\partial}{\partial x^j} \Delta \phi_\varepsilon \\
&\geq -2\nabla \phi_\varepsilon \cdot \nabla(f_\varepsilon(\phi_\varepsilon)) = -2 f_\varepsilon'(\phi_\varepsilon) |\nabla \phi_\varepsilon|^2 \quad \text{in } B_{R_1}(x_1).
\end{aligned}$$

Along with (3.129) and (3.131), we obtain $\varepsilon \Delta |\nabla \phi_\varepsilon|^2 \geq 2C_3^2 |\nabla \phi_\varepsilon|^2$ in $B_{R_1}(x_1)$. Let $\overline{\phi}_\varepsilon$ be the solution to $\varepsilon \Delta \overline{\phi}_\varepsilon = 2C_3^2 \overline{\phi}_\varepsilon$ in $B_{R_1}(x_1)$ with the Dirichlet boundary condition $\overline{\phi}_\varepsilon = \max\limits_{\partial B_{R_1}(x_1)} |\nabla \phi_\varepsilon|^2$. Then the standard comparison principle yields

$$|\nabla \phi_\varepsilon(x)|^2 \leq |\overline{\phi}_\varepsilon(x)| \leq 2 \left(\max_{\partial B_{R_1}(x_1)} |\nabla \phi_\varepsilon|^2\right) \exp\left(-\frac{\sqrt{2} C_3 \,\mathrm{dist}(x, \partial B_{R_1}(x_1))}{8\sqrt{\varepsilon}}\right) \tag{3.137}$$

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for $x \in \overline{B}_{R_1}(x_1)$ and $0 < \varepsilon < \varepsilon^*$. By (3.135) and (3.137), there exists $\varepsilon^* > 0$ (depending on Ω') such that

$$|\nabla\phi_\varepsilon(x_1)| \le \frac{M'}{\sqrt{\varepsilon}} \exp\left(-\frac{\sqrt{2}C_3 R_1}{8\sqrt{\varepsilon}}\right) = \frac{M'}{\sqrt{\varepsilon}} \exp\left(-\frac{\sqrt{2}C_3 \operatorname{dist}(\Omega', \partial\Omega)}{16\sqrt{\varepsilon}}\right)$$

for $0 < \varepsilon < \varepsilon^*$, which gives (3.136).

To complete the proof, let $\{\varepsilon_n\}_{n=1}^\infty$ be a sequence of positive numbers with $\lim\limits_{n\to\infty} \varepsilon_n = 0$. Since the sequence $\{\phi_{\varepsilon_n}(x_1)\}_{n=1}^\infty$ is bounded (cf. Proposition 3.13), by the Bolzano–Weierstrass theorem, there exists a subsequence $\{\varepsilon_{n_k}\}_{k=1}^\infty$ of $\{\varepsilon_n\}_{n=1}^\infty$ such that $\{\phi_{\varepsilon_{n_k}}(x_1)\}_{k=1}^\infty$ converges to a number denoted by ϕ_0^*. Let $y \in \Omega'$ arbitrarily. Then by (3.136) and Proposition 3.13, we have $|\phi_{\varepsilon_{n_k}}(y) - \phi_{\varepsilon_{n_k}}(x_1)| \to 0$ as $k \to \infty$, which implies $\lim\limits_{k\to\infty} \phi_{\varepsilon_{n_k}}(y) = \phi_0^*$. Due to the arbitrary choice of Ω', this finalizes the proof of Proposition 3.15. $\square$

Remark 3.4. *In Section 3.3.2, we will prove that $\phi_0^* \in (\underline{\phi_{bd}}, \overline{\phi_{bd}})$ is uniquely determined by the algebraic equations (3.150)–(3.151), which improves upon Proposition 3.15 to yield*

$$\lim_{\varepsilon\to 0^+} \phi_\varepsilon(x) = \phi_0^* \quad \textit{for } x \in \Omega. \tag{3.138}$$

Moreover, we will use the first-order asymptotic expansion of $\nabla\phi_\varepsilon$ near the boundary to improve the interior exponential-type estimate (3.136) (in the proof of Proposition 3.15) and obtain the global exponential-type estimate (3.161) in Proposition 3.20.

By (3.138) and the uniform boundedness of ϕ_ε (cf. Proposition 3.13), we apply Lebesgue's dominated convergence theorem to get

$$\lim_{\varepsilon\to 0^+} f_\varepsilon(\phi) = \sum_{i=1}^{I} \frac{m_i z_i \exp(-z_i\phi)}{\lim\limits_{\varepsilon\to 0^+} \displaystyle\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y} = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi - \phi_0^*)) := f_0(\phi) \tag{3.139}$$

for $\phi \in \mathbb{R}$, and

$$\lim_{\varepsilon\to 0^+} f'_\varepsilon(\phi) = -\sum_{i=1}^{I} \frac{m_i z_i^2 \exp(-z_i\phi)}{\lim\limits_{\varepsilon\to 0^+} \displaystyle\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y} = -\frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i^2 \exp(-z_i(\phi - \phi_0^*)) = f'_0(\phi) \tag{3.140}$$

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for $\phi \in \mathbb{R}$. Note that ϕ_0^* may depend on the choice of sequence $\{\varepsilon_n\}_{n=1}^{\infty}$, so may f_0. By (3.3), (3.131), and (3.139)–(3.140), it is clear that ϕ_0^* is the unique zero of f_0, and f_0 satisfies

$$f_0'(\phi) \le -C_3^2 \quad \text{for } \phi \in \mathbb{R}. \tag{3.141}$$

3.3.2 First-order asymptotic expansion of ϕ_ε

To obtain the first-order asymptotic expansion of ϕ_ε near the boundary $\partial\Omega_k$, we define

$$u_{k,p,\varepsilon}(z) = \phi_\varepsilon(\Psi_p(\sqrt{\varepsilon} z)) \quad \text{for } z \in B^+_{b/\sqrt{\varepsilon}} \text{ and } p \in \partial\Omega_k, \tag{3.142}$$

where ϕ_ε is the solution to (3.125)–(3.126) and Ψ_p is defined in (3.43). As in (3.50)–(3.51), we substitute (3.44)–(3.45) into (3.125)–(3.126) and get

$$\sum_{i,j=1}^{d} a_{ij}(z) \frac{\partial^2 u_{k,p,\varepsilon}}{\partial z^i \partial z^j} + \sum_{j=1}^{d} b_j(z) \frac{\partial u_{k,p,\varepsilon}}{\partial z^j} + f_\varepsilon(u_{k,p,\varepsilon}) = 0 \qquad \text{in } B^+_{b/\sqrt{\varepsilon}}, \tag{3.143}$$

$$u_{k,p,\varepsilon} - \gamma_k \partial_{z^d} u_{k,p,\varepsilon} = \phi_{bd,k} \quad \text{on } \overline{B}^+_{b/\sqrt{\varepsilon}} \cap \partial\mathbb{R}^d_+, \tag{3.144}$$

where a_{ij} and b_j are given in (3.47)–(3.48) and f_ε is defined in (3.127). As for Lemmas 3.5 and 3.6, we may use the uniform boundedness of ϕ_ε (cf. Proposition 3.13) and (3.139) to prove

Lemma 3.16. *For any sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ of positive numbers with $\lim_{n\to\infty} \varepsilon_n = 0$, $\alpha \in (0,1)$, and $p \in \partial\Omega_k$ ($k \in \{0,1,\dots,K\}$), there exists a subsequence $\{\varepsilon_{nn}\}_{n=1}^{\infty}$ such that $\lim_{n\to\infty} \|u_{k,p,\varepsilon_{nn}} - u_{k,p}\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0$ for $m \in \mathbb{N}$, where $u_{k,p} \in \mathcal{C}^{2,\alpha}_{loc}(\overline{\mathbb{R}}^d_+)$ satisfies*

$$\Delta u_{k,p} + f_0(u_{k,p}) = 0 \qquad \text{in } \mathbb{R}^d_+, \tag{3.145}$$

$$u_{k,p} - \gamma_k \partial_{z^d} u_{k,p} = \phi_{bd,k} \quad \text{on } \partial\mathbb{R}^d_+. \tag{3.146}$$

Moreover, $u_{k,p}$ satisfies the following exponential-type estimate

$$|u_{k,p}(z) - \phi_0^*| \le 2(\overline{\phi_{bd}} - \underline{\phi_{bd}}) \exp(-C_3 z^d/8) \tag{3.147}$$

for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$ and $z^d \ge 2(d-1)/C_3$, where ϕ_0^* is defined in Proposition 3.15 and C_3 is the positive constant given in (3.131).

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From Lemma 3.16, the solution $u_{k,p}$ to (3.145)–(3.146) may, a priori, depend on the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ and on the point $p \in \partial\Omega_k$. To establish the independence, we first use the moving plane arguments (as in Proposition 3.7) to prove that $u_{k,p}$ satisfies $u_{k,p}(z) = u_k(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$, where u_k is the unique solution to (3.21)–(3.23), and u_k is independent of the point $p \in \partial\Omega_k$. However, unlike Section 3.2, the solution u_k to (3.21)–(3.23) may still depend on the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ because ϕ_0^* (the unique zero of f_0) may depend on the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ (see Proposition 3.15). To remove the dependence on the sequence, we prove that ϕ_0^* is the unique solution to the algebraic equations (3.150)–(3.151), which are independent of the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$, in Proposition 3.18. Consequently, as in (3.64)–(3.65), we may apply Propositions 3.17 and 3.18 to prove that $u_{k,p,\varepsilon}$ (defined in (3.142)) satisfies

$$\lim_{\varepsilon\to 0^+} \|u_{k,p,\varepsilon} - u_k\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0 \quad \text{for } m \in \mathbb{N} \text{ and } \alpha \in (0,1), \tag{3.148}$$

and

$$\lim_{\varepsilon\to 0^+} u_{k,p,\varepsilon}(z) = u_k(z^d) \quad \text{for } z = (z', z^d) \in \overline{\mathbb{R}}^d_+, \tag{3.149}$$

which improve the results of Lemma 3.16. Below are the details.

Proposition 3.17. *For $p \in \partial\Omega_k$ and $k \in \{0, 1, \dots, K\}$, the solution $u_{k,p}$ to (3.145)–(3.146) satisfies*

(a) $u_{k,p}$ depends only on the variable z^d, i.e., $u_{k,p}(z) = u_{k,p}(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$.

(b) $u_{k,p}$ is independent of p and depends only on k, i.e., $u_{k,p}(z^d) = u_k(z^d)$ for $z^d \in [0, \infty)$, where u_k is the unique solution to (3.21)–(3.23).

The proof of Proposition 3.17 is similar to that of Proposition 3.7 because (3.145)–(3.146) have the same form as (3.52)–(3.53) with $f = f_0$, and f_0 satisfies (F1)–(F2) (cf. Proposition 3.15).

For the uniqueness of ϕ_0^* in Remark 3.4, we use Propositions 3.15 and 3.17 to prove

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Proposition 3.18. *The value of* $\phi_0^* \in (\underline{\phi_{bd}}, \overline{\phi_{bd}})$*, defined in Proposition 3.15, is uniquely determined by the following equations.*

$$\phi_{bd,k} - u_k(0) = \operatorname{sgn}(\phi_{bd,k} - \phi_0^*)\gamma_k \sqrt{\frac{2}{|\Omega|}\sum_{i=1}^{I} m_i[\exp(-z_i(u_k(0) - \phi_0^*)) - 1]} \quad \textit{for } k = 0, 1, \ldots, K, \tag{3.150}$$

$$\sum_{k=0}^{K} |\partial\Omega_k| u_k'(0) = \sum_{k=0}^{K} |\partial\Omega_k| \frac{\phi_{bd,k} - u_k(0)}{\gamma_k} = 0, \tag{3.151}$$

where u_k *is the unique solution to* (3.21)–(3.23)*.*

Proof. It is clear that (3.150) follows from (3.267) (in Appendix 3B) with $\Phi_{bd} = \phi_{bd,k}$, $U_0 = u_k(0)$, $\phi^* = \phi_0^*$, $\gamma = \gamma_k$ and $F(\phi) = F_0(\phi) = |\Omega|^{-1}\sum_{i=1}^{I} m_i(1 - \exp(-z_i(\phi - \phi_0^*)))$. On the other hand, we integrate (3.125) over Ω and apply the divergence theorem to get

$$\begin{aligned} \sum_{k=0}^{K} \int_{\partial\Omega_k} \frac{\phi_{bd,k} - \phi_\varepsilon}{\gamma_k}\, \mathrm{d}S &= \sqrt{\varepsilon}\int_{\partial\Omega} \partial_\nu \phi_\varepsilon \, \mathrm{d}S = \frac{1}{\sqrt{\varepsilon}}\int_\Omega \Delta\phi_\varepsilon(x)\, \mathrm{d}x \\ &= -\frac{1}{\sqrt{\varepsilon}}\int_\Omega f_\varepsilon(\phi_\varepsilon)\, \mathrm{d}x = -\frac{1}{\sqrt{\varepsilon}}\sum_{i=1}^{I} m_i z_i = 0. \end{aligned} \tag{3.152}$$

Here we have used the conditions (3.3) and (3.4). By (3.46) and (3.149), $\lim_{\varepsilon\to 0^+} \phi_\varepsilon(p) = \lim_{\varepsilon\to 0^+} u_{k,p,\varepsilon}(0) = u_k(0)$ for $p \in \partial\Omega_k$. Thus, letting $\varepsilon \to 0^+$, (3.152) implies (3.151). Hence ϕ_0^* satisfies (3.150)–(3.151).

We now prove $\phi_0^* \in (\underline{\phi_{bd}}, \overline{\phi_{bd}})$. Recall that $\phi_0^* \in [\underline{\phi_{bd}}, \overline{\phi_{bd}}]$ (cf. Proposition 3.15). If $\phi_0^* = \overline{\phi_{bd}}$, then $\phi_0^* \geq \phi_{bd,k}$ for $k = 0, 1, \ldots, K$. When $\phi_0^* = \phi_{bd,k}$, $u_k \equiv \phi_0^*$ on $[0, \infty)$; when $\phi_0^* > \phi_{bd,k}$, u_k is strictly increasing on $[0, \infty)$ and $u_k(0) > \phi_{bd,k}$ (cf. Proposition 3B.1). Thus, $u_k(0) \geq \phi_{bd,k}$ for $k = 0, 1, \ldots, K$. Along with (3.151), $u_k(0) = \phi_{bd,k}$ for $k = 0, 1, \ldots, K$, which means $\phi_0^* = \phi_{bd,k}$ for $k = 0, 1, \ldots, K$. This cannot happen because $\phi_{bd,k}$ are not equal. Hence $\phi_0^* < \overline{\phi_{bd}}$. Similarly, we can prove $\phi_0^* \neq \underline{\phi_{bd}}$. Consequently, $\phi_0^* \in (\underline{\phi_{bd}}, \overline{\phi_{bd}})$.

To complete the proof, it remains to show that algebraic equations (3.150)–(3.151) admit a unique solution ϕ_0^*. Suppose that there exist $\{\varepsilon_n\}_{n=1}^{\infty}$ and $\{\tilde{\varepsilon}_n\}_{n=1}^{\infty}$ such that $\lim_{n\to\infty} \phi_{\varepsilon_n}^* = \phi_0^*$ and $\lim_{n\to\infty} \phi_{\tilde{\varepsilon}_n}^* = \tilde{\phi}_0^*$. For $k = 0, 1, \ldots, K$, let u_k be the solutions to

$$u_k'' + f_0(u_k) = 0 \quad \text{in } (0, \infty),$$

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$$u_k(0) - \gamma_k u_k'(0) = \phi_{bd,k},$$
$$\lim_{t\to\infty} u_k(t) = \phi_0^*,$$

and let $\tilde{u}_k$ be the solutions to

$$\tilde{u}_k'' + \tilde{f}_0(\tilde{u}_k) = 0 \quad \text{in } (0,\infty),$$
$$\tilde{u}_k(0) - \gamma_k \tilde{u}_k'(0) = \phi_{bd,k},$$
$$\lim_{t\to\infty} \tilde{u}_k(t) = \tilde{\phi}_0^*.$$

where

$$f_0(\phi) = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi-\phi_0^*)) \quad \text{and} \quad \tilde{f}_0(\phi) = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi-\tilde{\phi}_0^*)) \quad \text{for } \phi \in \mathbb{R}.$$

As $\phi_0^* = \tilde{\phi}_0^*$, it is clear that $f_0 = \tilde{f}_0$ and $u_k = \tilde{u}_k$ for $k = 0,1,\dots,K$. Note that $(u_0(0), u_1(0), \dots, u_K(0), \phi_0^*)$ and $(\tilde{u}_0(0), \tilde{u}_1(0), \dots, \tilde{u}_K(0), \tilde{\phi}_0^*)$ satisfy (3.150)–(3.151). Consequently, the values of $u_k(0)$ and $\tilde{u}_k(0)$ depend on ϕ_0^* and $\tilde{\phi}_0^*$, respectively. Now we prove

Claim 3.19. *$\phi_0^* > \tilde{\phi}_0^*$ ($\phi_0^* < \tilde{\phi}_0^*$, resp.) if and only if $u_k(0) > \tilde{u}_k(0)$ ($u_k(0) < \tilde{u}_k(0)$, resp.) for all $k = 0,1,\dots,K$.*

Proof of Claim 3.19. We first suppose $\phi_0^* > \tilde{\phi}_0^*$. Let

$$g(\phi, s) = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi - s)) \quad \text{for } \phi, s \in \mathbb{R}.$$

It is obvious that $g(\phi, \phi_0^*) = f_0(\phi)$ and $g(\phi, \tilde{\phi}_0^*) = \tilde{f}_0(\phi)$ for $\phi \in \mathbb{R}$. Since

$$\partial_s g(\phi, s) = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i^2 \exp(-z_i(\phi - s)) > 0 \quad \text{for } s \in \mathbb{R},$$

the function g is increasing in s for $\phi \in \mathbb{R}$. Hence by the assumption $\phi_0^* > \tilde{\phi}_0^*$, we get

$$f_0(\phi) > \tilde{f}_0(\phi) \quad \text{for } \phi \in \mathbb{R}. \tag{3.153}$$

Suppose, to the contrary, that $u_{k_0}(0) \le \tilde{u}_{k_0}(0)$ for some $k_0 \in \{0,1,\dots,K\}$. Let $\overline{u}_{k_0} = u_{k_0} - \tilde{u}_{k_0}$ on $[0,\infty)$. Then it is easy to verify that $\overline{u}_{k_0}(0) \le 0$ and

$$\overline{u}_{k_0}'' + f_0(u_{k_0}) - \tilde{f}_0(\tilde{u}_{k_0}) = 0 \quad \text{in } (0,\infty), \tag{3.154}$$

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$$\overline{u}_{k_0}(0) - \gamma_k \overline{u}'_{k_0}(0) = 0, \tag{3.155}$$

$$\lim_{t\to\infty} \overline{u}_{k_0}(t) = \phi_0^* - \tilde{\phi}_0^* > 0. \tag{3.156}$$

Since $\overline{u}_{k_0}(0) \le 0$, we have $\overline{u}'_{k_0}(0) \le 0$ by (3.155). Moreover, since $\tilde{f}_0$ is strictly decreasing, we use (3.153)–(3.154) to obtain

$$\overline{u}''_{k_0}(0) = \tilde{f}_0(\tilde{u}_{k_0}(0)) - f_0(u_{k_0}(0)) \le \tilde{f}_0(u_{k_0}(0)) - f_0(u_{k_0}(0)) < 0.$$

Thus, by (3.156), there exists $t_1 \in (0,\infty)$ such that $\overline{u}_{k_0}(t) < 0$ on $(0,t_1)$, $\overline{u}_{k_0}(t_1) = 0$ and $\overline{u}'_{k_0}(t_1) \ge 0$. Integrating (3.154) over $[0,t_1]$, we get

$$\overline{u}'_{k_0}(t_1) - \overline{u}'_{k_0}(0) + \int_0^{t_1} [f_0(u_{k_0}(s)) - \tilde{f}_0(\tilde{u}_{k_0}(s))] \, \mathrm{d}s = 0,$$

which implies

$$\int_0^{t_1} [f_0(u_{k_0}(s)) - \tilde{f}_0(\tilde{u}_{k_0}(s))] \, \mathrm{d}s = \overline{u}'_{k_0}(0) - \overline{u}'_{k_0}(t_1) \le 0. \tag{3.157}$$

Since f_0 is strictly decreasing on $\mathbb{R}$ (cf. (3.141)) and $u_{k_0}(t) - \tilde{u}_{k_0}(t) = \overline{u}_{k_0}(t) < 0$ on $(0,t_1)$, it follows that

$$f_0(u_{k_0}(t)) - \tilde{f}_0(\tilde{u}_{k_0}(t)) > f_0(\tilde{u}_{k_0}(t)) - \tilde{f}_0(\tilde{u}_{k_0}(t)) > 0 \quad \text{for } 0 < t < t_1,$$

which contradicts (3.157). Here we have used (3.153) in the last inequality. Therefore, we arrive at $\overline{u}_k(0) > 0$, which means $u_k(0) > \tilde{u}_k(0)$ for all $k = 0,1,\ldots,K$. Similarly, we can prove $\phi_0^* < \tilde{\phi}_0^*$ implies $u_k(0) < \tilde{u}_k(0)$ and thus complete proof of Claim 3.19. □

To complete the proof of Proposition 3.18, we combine Claim 3.19 and (3.151) for u_k and $\tilde{u}_k$ to get the following contradiction:

$$0 = \sum_{k=0}^{K} |\partial\Omega_k| \frac{\phi_{bd,k} - u_k(0)}{\gamma_k} \ne \sum_{k=0}^{K} |\partial\Omega_k| \frac{\phi_{bd,k} - \tilde{u}_k(0)}{\gamma_k} = 0 \quad \text{if } \phi_0^* \ne \tilde{\phi}_0^*,$$

which implies $\phi_0^* = \tilde{\phi}_0^*$ and $u_k(0) = \tilde{u}_k(0)$. Therefore, we complete the proof of Proposition 3.18. □

Consequently, we can use (3.43), (3.46), (3.142), and (3.148)–(3.149) to obtain the first-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$:

$$\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_k(t) + o_\varepsilon(1), \tag{3.158}$$

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$$\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\frac{1}{\sqrt{\varepsilon}}(u_k'(t)\nu_p + o_\varepsilon(1)) \tag{3.159}$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$, where $T > 0$, $k \in \{0, 1, \dots, K\}$, and $p \in \partial\Omega_k$ (as in (3.84)–(3.85)).

To derive the second-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$ and capture the asymptotic behavior of the term $o_\varepsilon(1)/\sqrt{\varepsilon}$ in the subsequent analysis, it is crucial to establish the following exponential-type estimates of ϕ_ε and $\nabla\phi_\varepsilon$ analogously to Proposition 3.9:

Proposition 3.20 (Exponential-type estimates of ϕ_ε and $\nabla\phi_\varepsilon$)**.** *Under the hypothesis of Theorem 3.2, let Ω satisfy the uniform interior sphere condition, i.e., there exists $R > 0$ such that $B_R(p - R\nu_p) \subseteq \Omega$ and $\partial B_R(p - R\nu_p) \cap \partial\Omega = \{p\}$ for $p \in \partial\Omega$, where ν_p is the unit outer normal of $\partial\Omega$ at p. Then we have*

$$|\phi_\varepsilon(x) - \phi_\varepsilon^*| \le 2(\overline{\phi_{bd}} - \underline{\phi_{bd}}) \exp\left(-\frac{C_3\delta(x)}{8\sqrt{\varepsilon}}\right), \tag{3.160}$$

$$|\nabla\phi_\varepsilon| \le \frac{M'}{\sqrt{\varepsilon}} \exp\left(-\frac{M\delta(x)}{\sqrt{\varepsilon}}\right) \tag{3.161}$$

for $x \in \overline{\Omega}$ and $0 < \varepsilon < \varepsilon^*$, where C_3 (given in (3.131)) is independent of ε and ϕ_ε^* is defined in Proposition 3.14.

Proof. As in the proof of Proposition 3.9, the uniform interior sphere condition of Ω ensures that there exists $B_{R_0}(x_0) \subseteq \Omega$ with $R_0 \ge R$; hence (3.88) holds. To show (3.160), we let $\phi_\varepsilon^\pm$ be the solutions to

$$-\varepsilon\Delta\phi_\varepsilon^\pm = f_\varepsilon(\phi_\varepsilon^\pm) \qquad \text{in } B_{R_0}(x_0), \tag{3.162}$$

$$\phi_\varepsilon^\pm = \phi_\varepsilon^* \pm (\overline{\phi_{bd}} - \underline{\phi_{bd}}) \quad \text{on } \partial B_{R_0}(x_0), \tag{3.163}$$

The existence of solutions to (3.162)–(3.163) follows from the standard variational method because of the strict decrease of f_ε (cf. Proposition 3.14). Following the argument of Proposition 3.9 for (3.91), with replacing f by f_ε, we obtain $\phi_\varepsilon^- \le \phi_\varepsilon \le \phi_\varepsilon^+$ in $\overline{B}_{R_0}(x_0)$. Then by (3.88) and Proposition 3A.4 in Appendix 3A with $M = C_3$, $|\Phi_{bd} - \phi_\varepsilon^*| = \overline{\phi_{bd}} - \underline{\phi_{bd}}$ and $B_R(0) = B_{R_0}(x_0)$, we have

$$|\phi_\varepsilon^\pm(x) - \phi_\varepsilon^*| \le 2(\overline{\phi_{bd}} - \underline{\phi_{bd}}) \exp\left(-\frac{C_3\delta(x)}{8\sqrt{\varepsilon}}\right) \quad \text{for } x \in \overline{B}_{R_0}(x_0) \text{ and } 0 < \varepsilon < \varepsilon^*, \tag{3.164}$$

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which implies (3.160). As in (3.95), we can use (3.159) to improve the estimate (3.135) as $|\nabla\phi_\varepsilon(x)| \le M'/\sqrt{\varepsilon}$ for $x \in \overline{\Omega}$ and $0 < \varepsilon < (\delta(x))^2$. Then (3.161) follows from (3.131) and the standard comparison principle on (3.96) (with replacing f by f_ε). Therefore, we complete the proof of Proposition 3.20. $\square$

Recall that $\delta(x) = \operatorname{dist}(x, \partial\Omega)$. By Proposition 3.20, it is clear that Theorem 3.2(b) holds true.

3.3.3 Uniform boundedness of $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon}$

From (3.138)–(3.139) and (3.160), the first-order asymptotic expansions of ϕ_ε^*, $A_{i,\varepsilon}$, and f_ε are represented by

$$\begin{aligned}
\phi_\varepsilon^* &= \phi_0^* + o_\varepsilon(1), \\
A_{i,\varepsilon} &= |\Omega| \exp(-z_i\phi_0^*) + o_\varepsilon(1) \quad && \text{for } i = 1, \ldots, I, \\
f_\varepsilon(\phi) &= f_0(\phi) + o_\varepsilon(1) && \text{for } \phi \in \mathbb{R},
\end{aligned}$$

where $A_{i,\varepsilon} = \int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y$, $f_\varepsilon(\phi) = \sum_{i=1}^{I}(m_i z_i/A_{i,\varepsilon})\exp(-z_i\phi)$, and $f_0(\phi)$ is given in (3.30). To obtain the second-order asymptotic expansion of ϕ_ε, we require the second-order asymptotic expansions of f_ε and $A_{i,\varepsilon}$. Thus, it is necessary to show the uniform boundedness of $(\phi_\varepsilon^* - \phi_0^*)/\sqrt{\varepsilon}$.

Suppose by contradiction that there exists a sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ such that $\lim\limits_{n\to\infty} |\phi_{\varepsilon_n}^* - \phi_0^*|/\sqrt{\varepsilon_n} = \infty$ and $\lim\limits_{n\to\infty} \varepsilon_n = 0$. For notational convenience, we henceforth drop the subscript n in this section so the assumption becomes

$$\lim_{\varepsilon\to 0^+} \frac{|\phi_\varepsilon^* - \phi_0^*|}{\sqrt{\varepsilon}} = \infty. \tag{3.165}$$

A direct computation gives

$$\begin{aligned}
f_{1,\varepsilon}(\phi) &:= \frac{f_\varepsilon(\phi) - f_0(\phi)}{\phi_\varepsilon^* - \phi_0^*} \\
&= \frac{1}{\phi_\varepsilon^* - \phi_0^*} \sum_{i=1}^{I} m_i z_i \left(\frac{\exp(-z_i\phi_0^*)}{A_{i,\varepsilon}} - \frac{1}{|\Omega|} \right) \exp(-z_i(\phi - \phi_0^*)) \\
&= -\sum_{i=1}^{I} \frac{m_i z_i B_{i,\varepsilon}}{|\Omega|[|\Omega| \exp(-z_i\phi_0^*) + (\phi_\varepsilon^* - \phi_0^*)B_{i,\varepsilon}]} \exp(-z_i(\phi - \phi_0^*)) \quad \text{for } \phi \in \mathbb{R},
\end{aligned} \tag{3.166}$$

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where

$$B_{i,\varepsilon} = \frac{A_{i,\varepsilon} - |\Omega| \exp(-z_i \phi_0^*)}{\phi_\varepsilon^* - \phi_0^*} = \int_\Omega \frac{\exp(-z_i \phi_\varepsilon(y)) - \exp(-z_i \phi_0^*)}{\phi_\varepsilon^* - \phi_0^*} \, \mathrm{d}y \tag{3.167}$$

for $i = 1, \ldots, I$ and $\varepsilon > 0$. Note that $B_{i,\varepsilon}$ can be expressed by

$$B_{i,\varepsilon} = J_{i,1} + \sum_{k=0}^{K} J_{i,k,2} \quad \text{for } i = 1, \ldots, I, \tag{3.168}$$

where

$$J_{i,1} = \int_{\overline{\Omega}_{\varepsilon,\beta}} \frac{\exp(-z_i \phi_\varepsilon(y)) - \exp(-z_i \phi_0^*)}{\phi_\varepsilon^* - \phi_0^*} \, \mathrm{d}y, \tag{3.169}$$

$$J_{i,k,2} = \int_{\Omega_{k,\varepsilon,\beta}} \frac{\exp(-z_i \phi_\varepsilon(y)) - \exp(-z_i \phi_0^*)}{\phi_\varepsilon^* - \phi_0^*} \, \mathrm{d}y \quad \text{for } k = 0, 1, \ldots, K. \tag{3.170}$$

Here $\overline{\Omega}_{\varepsilon,\beta} = \{x \in \Omega : \delta(x) \geq \varepsilon^\beta\}$ and $\Omega_{k,\varepsilon,\beta} = \{x \in \Omega : \delta_k(x) < \varepsilon^\beta\}$ for $0 < \beta < 1/2$ and $k = 0, 1, \ldots, K$. Clearly, $\Omega_{k,\varepsilon,\beta}$ are disjoint for sufficiently small $\varepsilon > 0$. Then we may apply (3.160), (3.165), and (3.167) to get

Lemma 3.21. *$B_{i,\varepsilon} = -z_i \exp(-z_i \phi_0^*)|\Omega| + o_\varepsilon(1)$ for $i = 1, \ldots, I$.*

Henceforth $\varepsilon^* > 0$ is a sufficiently small constant, and M and M' are generic constants independent of ε.

Proof. Fix $i \in \{1, \ldots, I\}$. In view of (3.168), it suffices to determine the limits of $J_{i,1}$ and $J_{i,k,2}$. We begin with an analysis of $J_{i,1}$ when $z_i > 0$. By (3.160), we have

$$\exp\left[-z_i \phi_\varepsilon^* - z_i M' \exp\left(-\frac{M\delta(x)}{\sqrt{\varepsilon}}\right)\right] \leq \exp(-z_i \phi_\varepsilon(x)) \leq \exp\left[-z_i \phi_\varepsilon^* + z_i M' \exp\left(-\frac{M\delta(x)}{\sqrt{\varepsilon}}\right)\right]$$

for $x \in \overline{\Omega}$ and $0 < \varepsilon < \varepsilon^*$, which implies

$$\begin{aligned} &\exp(-z_i \phi_0^*) \left\{\exp[-z_i M' \exp(-M\delta(x)/\sqrt{\varepsilon})] \exp[-z_i(\phi_\varepsilon^* - \phi_0^*)] - 1\right\} \\ \leq& \exp(-z_i \phi_\varepsilon(x)) - \exp(-z_i \phi_0^*) \\ \leq& \exp(-z_i \phi_0^*) \left\{\exp[z_i M' \exp(-M\delta(x)/\sqrt{\varepsilon})] \exp[-z_i(\phi_\varepsilon^* - \phi_0^*)] - 1\right\} \end{aligned} \tag{3.171}$$

for $x \in \overline{\Omega}$ and $0 < \varepsilon < \varepsilon^*$. For $x \in \overline{\Omega}_{\varepsilon,\beta}$ (i.e., $\delta(x) \geq \varepsilon^\beta$) and $0 < \varepsilon < \varepsilon^*$, (3.171) becomes

$$\begin{aligned} &\exp(-z_i \phi_0^*) \left\{\exp[-z_i M' \exp(-M\varepsilon^{(2\beta-1)/2})] \exp[-z_i(\phi_\varepsilon^* - \phi_0^*)] - 1\right\} \\ \leq& \exp(-z_i \phi_\varepsilon(x)) - \exp(-z_i \phi_0^*) \\ \leq& \exp(-z_i \phi_0^*) \left\{\exp[z_i M' \exp(-M\varepsilon^{(2\beta-1)/2})] \exp[-z_i(\phi_\varepsilon^* - \phi_0^*)] - 1\right\}. \end{aligned} \tag{3.172}$$

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Now we can combine (3.169) and (3.172) to get

$$\exp(-z_i\phi_0^*)|\overline{\Omega}_{\varepsilon,\beta}|\frac{\exp[-z_iM'\exp(-M\varepsilon^{(2\beta-1)/2})]\exp[-z_i(\phi_\varepsilon^*-\phi_0^*)]-1}{\phi_\varepsilon^*-\phi_0^*}$$
$$\leq J_{i,1}\leq \exp(-z_i\phi_0^*)|\overline{\Omega}_{\varepsilon,\beta}|\frac{\exp[z_iM'\exp(-M\varepsilon^{(2\beta-1)/2})]\exp[-z_i(\phi_\varepsilon^*-\phi_0^*)]-1}{\phi_\varepsilon^*-\phi_0^*}.$$

Along with the fact that

$$\begin{aligned}&\lim_{\varepsilon\to 0^+}\frac{\exp[z_iM'\exp(-M\varepsilon^{(2\beta-1)/2})]\exp[-z_i(\phi_\varepsilon^*-\phi_0^*)]-1}{\phi_\varepsilon^*-\phi_0^*}\\ =&\lim_{\varepsilon\to 0^+}\frac{\exp[z_iM'\exp(-M\varepsilon^{(2\beta-1)/2})-z_i(\phi_\varepsilon^*-\phi_0^*)]-1}{\phi_\varepsilon^*-\phi_0^*}=-z_i,\end{aligned}$$

which follows from (3.165) and $0<\beta<1/2$, we obtain

$$J_{i,1}=-z_i\exp(-z_i\phi_0^*)|\Omega|+o_\varepsilon(1)\quad\text{for } i=1,\dots,I. \tag{3.173}$$

For the case of $z_i<0$, we can follow a similar argument to get (3.173).

Now it remains to estimate $J_{i,k,2}$. Fix $k\in\{0,1,\dots,K\}$. For $y\in\overline{\Omega}_{k,\varepsilon,\beta}$ and sufficiently small $\varepsilon>0$, there exist unique $p\in\partial\Omega_k$ and $0\leq s\leq\varepsilon^{(2\beta-1)/2}$ such that $y=p-s\sqrt{\varepsilon}\nu_p$. By the coarea formula (cf. [30, 83]), (3.170) becomes

$$\begin{aligned}J_{i,k,2}=&\int_{\Omega_{k,\varepsilon,\beta}}\frac{\exp(-z_i\phi_\varepsilon(y))-\exp(-z_i\phi_0^*)}{\phi_\varepsilon^*-\phi_0^*}\,\mathrm{d}y\\ =&\frac{\sqrt{\varepsilon}}{\phi_\varepsilon^*-\phi_0^*}\int_0^{\varepsilon^{(2\beta-1)/2}}\int_{\partial\Omega_k}[\exp(-z_i\phi_\varepsilon(p-s\sqrt{\varepsilon}\nu_p))-\exp(-z_i\phi_0^*)]\mathcal{J}(s,p)\,\mathrm{d}S_p\,\mathrm{d}s\end{aligned}$$

for $i=1,\dots,I$ and $k=0,1,\dots,K$. Along with (3.120), we have

$$|J_{i,k,2}|\leq\frac{2\sqrt{\varepsilon}}{|\phi_\varepsilon^*-\phi_0^*|}\int_0^{\varepsilon^{(2\beta-1)/2}}\int_{\partial\Omega_k}|\exp(-z_i\phi_\varepsilon(p-s\sqrt{\varepsilon}\nu_p))-\exp(-z_i\phi_0^*)|\,\mathrm{d}S_p\,\mathrm{d}s. \tag{3.174}$$

From Propositions 3.13 and 3.15, $|\phi_\varepsilon-\phi_0^*|$ is uniformly bounded in $\overline{\Omega}$ and $\varepsilon>0$, which implies that there exists $M>1$ such that $|\exp[-z_i(\phi_\varepsilon(x)-\phi_0^*)]-1|\leq M|\phi_\varepsilon(x)-\phi_0^*|$ for $x\in\overline{\Omega}$ and $0<\varepsilon<\varepsilon^*$. Then by (3.160), we get

$$\begin{aligned}|\exp(-z_i\phi_\varepsilon(x))-\exp(-z_i\phi_0^*)|&=\exp(-z_i\phi_0^*)|\exp[-z_i(\phi_\varepsilon(x)-\phi_0^*)]-1|\\ &\leq M'\exp\left(-\frac{M\delta(x)}{\sqrt{\varepsilon}}\right)+M'|\phi_\varepsilon^*-\phi_0^*|\end{aligned} \tag{3.175}$$

for $x\in\overline{\Omega}$ and $0<\varepsilon<\varepsilon^*$. Combining (3.165), (3.174) and (3.175), we arrive at

$$\begin{aligned}|J_{i,k,2}|&\leq\frac{2\sqrt{\varepsilon}}{|\phi_\varepsilon^*-\phi_0^*|}\int_0^{\varepsilon^{(2\beta-1)/2}}\int_{\partial\Omega_k}[M'\exp(-Ms)+M'|\phi_\varepsilon^*-\phi_0^*|]\,\mathrm{d}S_p\,\mathrm{d}s\\ &=\frac{M'\sqrt{\varepsilon}}{|\phi_\varepsilon^*-\phi_0^*|}(1-\exp(M\varepsilon^{(2\beta-1)/2}))+M'\varepsilon^\beta\to 0\quad\text{as }\varepsilon\to 0^+,\end{aligned} \tag{3.176}$$

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for $i = 1, \ldots, I$ and $k = 0, 1, \ldots, K$. Thus, combining (3.168), (3.173), and (3.176), we complete the proof of Lemma 3.21. $\square$

Applying Lemma 3.21 to (3.166), we obtain

$$\begin{aligned} f_{1,\varepsilon}(\phi) &= -\sum_{i=1}^{I} \frac{m_i z_i B_{i,\varepsilon}}{|\Omega|[|\Omega| \exp(-z_i \phi_0^*) + (\phi_\varepsilon^* - \phi_0^*) B_{i,\varepsilon}]} \exp(-z_i(\phi - \phi_0^*)) \\ &= \frac{1}{|\Omega|} \sum_{i=1}^{I} m_i z_i^2 \exp(-z_i(\phi - \phi_0^*)) + o_\varepsilon(1) = -f_0'(\phi) + o_\varepsilon(1), \end{aligned}$$

which implies

$$f_\varepsilon(\phi) = f_0(\phi) - (\phi_\varepsilon^* - \phi_0^*) f_0'(\phi) + (\phi_\varepsilon^* - \phi_0^*) o_\varepsilon(1) \quad \text{for } \phi \in \mathbb{R}. \tag{3.177}$$

Regarding (3.99), we now define

$$\varphi_{k,\varepsilon} = \frac{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})}{\phi_\varepsilon^* - \phi_0^*} \quad \text{for } x \in \overline{\Omega}_{k,\varepsilon,\beta} \text{ and } k = 0, 1, \ldots, K, \tag{3.178}$$

where u_k is the unique solution to (3.21)–(3.23) and $\delta_k(x) = \mathrm{dist}(x, \partial\Omega_k)$ for $k = 0, 1, \ldots, K$. Then by (3.2), (3.21), (3.103), and (3.177)–(3.178), $\varphi_{k,\varepsilon}$ satisfies

$$\varepsilon \Delta \varphi_{k,\varepsilon} + c_\varepsilon(x) \varphi_{k,\varepsilon} = f_0'(u_k(\delta_k(x)/\sqrt{\varepsilon})) + o_\varepsilon(1) \quad \text{for } x \in \overline{\Omega}_{k,\varepsilon,\beta}, \tag{3.179}$$

where

$$c_\varepsilon(x) = \begin{cases} \dfrac{f_\varepsilon(\phi_\varepsilon(x)) - f_\varepsilon(u_k(\delta_k(x)/\sqrt{\varepsilon}))}{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})} & \text{if } \phi_\varepsilon(x) \neq u_k(\delta_k(x)/\sqrt{\varepsilon}); \\ f_\varepsilon'(\phi_\varepsilon(x)) & \text{if } \phi_\varepsilon(x) = u_k(\delta_k(x)/\sqrt{\varepsilon}). \end{cases}$$

For the boundary condition of $\varphi_{k,\varepsilon}$, we use (3.4), (3.21), (3.45) and (3.178) to get

$$\varphi_{k,\varepsilon} + \gamma_k \sqrt{\varepsilon} \partial_\nu \varphi_{k,\varepsilon} = 0 \quad \text{on } \partial\Omega_k. \tag{3.180}$$

Following Proposition 3.10, we prove the uniform boundedness of $\varphi_{k,\varepsilon}$:

Proposition 3.22. *Suppose that (3.165) holds true. Then there exists a constant $M > 0$ independent of ε such that $\max_{\overline{\Omega}_{k,\varepsilon,\beta}} |\varphi_{k,\varepsilon}| \leq M$ for $k = 0, 1, \ldots, K$ and $0 < \varepsilon < \varepsilon^*$.*

Proof. Fix $k \in \{0, 1, \ldots, K\}$. It is equivalent to showing that $\max_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \leq M$ and $\min_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \geq -M$ for some constant $M > 0$ independent of ε. We first prove that

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$\max_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \leq M$ for $0 < \varepsilon < \varepsilon^*$. Suppose by contradiction that there exists a sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ of positive numbers with $\lim_{n\to\infty} \varepsilon_n = 0$ and $\{x_n\}_{n=1}^{\infty} \subset \overline{\Omega}_{k,\varepsilon_n,\beta}$ such that $\varphi_{k,\varepsilon_n}(x_n) = \max_{\overline{\Omega}_{k,\varepsilon_n,\beta}} \varphi_{k,\varepsilon_n} \geq n$ for $n \in \mathbb{N}$. Since $0 < \beta < 1/2$, we may, without loss of generality, assume that $8(\overline{\phi_{bd}} - \underline{\phi_{bd}}) \exp(-C_3 \varepsilon_n^{(2\beta-1)/2}/8) \leq |\phi^*_{\varepsilon_n} - \phi^*_0|$ for all $n \in \mathbb{N}$, , respectively. Note that the maximum point x_n cannot lie on the boundary $\partial\Omega_k$ because from (3.180), $\partial_\nu \varphi_{k,\varepsilon_n}(x_n) = -\varphi_{k,\varepsilon_n}(x_n)/(\gamma_k\sqrt{\varepsilon_n}) \leq -n/(\gamma_k\sqrt{\varepsilon_n}) < 0$ if the maximum point $x_n \in \partial\Omega_k$. On the other hand, by (3.147) (with Proposition 3.17) and (3.160), we have

$$\begin{aligned}
|\varphi_{k,\varepsilon_n}(x)| &\leq \frac{|\phi_{\varepsilon_n}(x) - \phi^*_{\varepsilon_n}| + |u_k(\delta_k(x)/\sqrt{\varepsilon_n}) - \phi^*_0| + |\phi^*_{\varepsilon_n} - \phi^*_0|}{|\phi^*_{\varepsilon_n} - \phi^*_0|} \\
&\leq 1 + \frac{4(\overline{\phi_{bd}} - \underline{\phi_{bd}})}{|\phi^*_{\varepsilon_n} - \phi^*_0|} \exp\left(-\frac{C_3}{8}\varepsilon_n^{(2\beta-1)/2}\right) \leq \frac{3}{2} \quad \text{for } \delta_k(x) = \varepsilon_n^\beta \text{ and } n \in \mathbb{N}.
\end{aligned}$$

This shows that x_n cannot lie on the boundary $\partial\Omega_{k,\varepsilon_n,\beta}$. Hence $x_n \in \Omega_{k,\varepsilon_n,\beta}$ for all $n \in \mathbb{N}$, which implies $\nabla\varphi_{k,\varepsilon_n}(x_n) = 0$ and $\Delta\varphi_{k,\varepsilon_n}(x_n) \leq 0$ for $n \in \mathbb{N}$. Thus by (3.179),

$$0 \leq -\varepsilon_n \Delta\varphi_{k,\varepsilon_n}(x_n) = c_{\varepsilon_n}(x_n)\varphi_{k,\varepsilon_n}(x_n) - f_0'(u_k(\delta_k(x)/\sqrt{\varepsilon_n})) + o_{\varepsilon_n}(1). \tag{3.181}$$

Recall that $f_0'(u_k(t))$ is uniformly bounded for $t \in [0,\infty)$, $\varphi_{k,\varepsilon_n}(x_n) \geq n$ for $n \in \mathbb{N}$, and $c_\varepsilon \leq -C_3^2 < 0$ in $\overline{\Omega}_{k,\varepsilon}$ for $\varepsilon > 0$. Letting $n \to \infty$, we obtain $\lim_{n\to\infty} c_{\varepsilon_n}(x_n)\varphi_{k,\varepsilon_n}(x_n) = -\infty$, which contradicts (3.181). Thus, $\max_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \leq M$ for some constant $M > 0$ independent of ε. Similarly, we may use (3.147), (3.160), (3.179), and (3.180) to prove $\min_{\overline{\Omega}_{k,\varepsilon,\beta}} \varphi_{k,\varepsilon} \geq -M$ for $0 < \varepsilon < \varepsilon^*$, where $M > 0$ is independent of $\varepsilon > 0$. Therefore, we complete the proof of Proposition 3.22. □

To derive a contradiction from (3.165), we study the asymptotic expansion of $\varphi_{k,\varepsilon}$ in $\Omega_{k,\varepsilon,\beta}$ and define

$$\mathcal{W}_{k,p,\varepsilon}(z) = \varphi_{k,\varepsilon}(\Psi_p(\sqrt{\varepsilon}z)) \quad \text{for } z \in \overline{B}^+_{\varepsilon^{(2\beta-1)/2}} \text{ and } 0 < \varepsilon < \varepsilon^* \tag{3.182}$$

(cf. (3.107)), where Ψ_p is given in (3.43). Similar to (3.108)–(3.111), $\mathcal{W}_{k,p,\varepsilon}$ satisfies

$$\begin{aligned}
\sum_{i,j=1}^d a_{ij}(z)\frac{\partial^2 \mathcal{W}_{k,p,\varepsilon}}{\partial z^i \partial z^j} + \sum_{j=1}^d b_j(z)\frac{\partial \mathcal{W}_{k,p,\varepsilon}}{\partial z^j} + c_\varepsilon(z)\mathcal{W}_{k,p,\varepsilon} = f_0(u_k(z^d)) + o_\varepsilon(1) \quad &\text{in } B^+_{\varepsilon^{(2\beta-1)/2}}, \\
\mathcal{W}_{k,p,\varepsilon} - \gamma_k \partial_{z^d}\mathcal{W}_{k,p,\varepsilon} = 0 \quad &\text{on } \overline{B}^+_{\varepsilon^{(2\beta-1)/2}} \cap \partial\mathbb{R}^d_+
\end{aligned}$$

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for $0 < \varepsilon < \varepsilon^*$, where a_{ij} and b_j are given in (3.47)–(3.48), and

$$c_\varepsilon(z) = \begin{cases} \dfrac{f_\varepsilon(u_k(z^d) + (\phi_\varepsilon^* - \phi_0^*)\mathcal{W}_{k,p,\varepsilon}(z)) - f_\varepsilon(u_k(z^d))}{(\phi_\varepsilon^* - \phi_0^*)\mathcal{W}_{k,p,\varepsilon}(z)} & \text{if } \mathcal{W}_{k,p,\varepsilon}(z) \neq 0; \\ f_\varepsilon'(u_k(z^d)) & \text{if } \mathcal{W}_{k,p,\varepsilon}(z) = 0. \end{cases}$$

As in Lemma 3.11 of Section 3.2.2, we use the uniform boundedness of $\varphi_{k,\varepsilon}$ (cf. Proposition 3.22) to prove

Lemma 3.23. *Suppose that (3.165) holds true. For any sequence $\{\varepsilon_n\}_{n=1}^\infty$ of positive numbers with $\lim\limits_{n\to\infty} \varepsilon_n = 0$, $\alpha \in (0,1)$, and $p \in \partial\Omega_k$ ($k \in \{0, 1, \ldots, K\}$), there exists a subsequence $\{\varepsilon_{nn}\}_{n=1}^\infty$ such that $\lim\limits_{n\to\infty} \|\mathcal{W}_{k,p,\varepsilon_{nn}} - \mathcal{W}_{k,p}\|_{\mathcal{C}^{2,\alpha}(\overline{B}_m^+)} = 0$ for $m \in \mathbb{N}$, where $\mathcal{W}_{k,p} \in \mathcal{C}^{2,\alpha}_{loc}(\overline{\mathbb{R}}^d_+)$ satisfies*

$$\Delta \mathcal{W}_{k,p} + f_0'(u_k)\mathcal{W}_{k,p} = f_0'(u_k) \quad \text{in } \mathbb{R}^d_+, \tag{3.183}$$

$$\mathcal{W}_{k,p} - \gamma_k \partial_{z^d}\mathcal{W}_{k,p} = 0 \qquad \text{on } \partial\mathbb{R}^d_+. \tag{3.184}$$

Moreover, there exists $M > 0$ such that $\mathcal{W}_{k,p}$ satisfies the following estimate

$$|\mathcal{W}_{k,p}(z) - \theta_k(z^d)| \leq M \exp(-C_3 z^d/8) \quad \text{for } z = (z', z^d) \in \overline{\mathbb{R}}^d_+ \text{ and } z^d \geq 2(d-1)/C_3, \tag{3.185}$$

where C_3 is given in (3.131) and $\theta_k = \theta_k(t)$ is the solution to ordinary differential equation

$$\theta_k'' + f_0'(u_k)\theta_k = f_0'(u_k) \quad \text{in } (0, \infty), \tag{3.186}$$

$$\theta_k(0) - \gamma_k\theta_k'(0) = 0, \tag{3.187}$$

$$\lim_{t\to\infty} \theta_k(t) = 1. \tag{3.188}$$

Remark 3.5. *By the standard linear ODE theory, the unique solution θ_k to (3.186)–(3.188) can be expressed explicitly as*

$$\theta_k(t) = 1 - \frac{u_k'(t)}{u_k'(0) + \gamma_k f_0(u_k(0))} \quad \text{for } t \geq 0. \tag{3.189}$$

By (F1)–(F2), Proposition 3B.1, together with (3.189), it follows that

$$\theta_k'(0) = \frac{f_0(u_k(0))}{u_k'(0) + \gamma_k f_0(u_k(0))} > 0. \tag{3.190}$$

From Lemma 3.23, the solution $\mathcal{W}_{k,p}$ to (3.183)–(3.184) may, a priori, depend on the sequence $\{\varepsilon_n\}_{n=1}^\infty$ and on the point. To establish the independence from the

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sequence and the point, we apply the moving plane arguments, as in Propositions 3.7 and 3.12, to prove that $\mathcal{W}_{k,p} = \mathcal{W}_{k,p}(z^d) = \theta_k(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$, where θ_k is the unique solution to (3.186)–(3.188). Here θ_k is independent of the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ and the point $p \in \partial\Omega_k$. Consequently, the results of Lemma 3.23 can be improved as

$$\lim_{\varepsilon\to 0^+} \|\mathcal{W}_{k,p} - \theta_k\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0 \quad \text{for } m \in \mathbb{N} \text{ and } \alpha \in (0,1), \tag{3.191}$$

and

$$\lim_{\varepsilon\to 0^+} \mathcal{W}_{k,p,\varepsilon}(z) = \theta_k(z^d) \quad \text{for } z = (z', z^d) \in \overline{\mathbb{R}}^d_+, \tag{3.192}$$

where $\mathcal{W}_{k,p,\varepsilon}$ is defined in (3.182). The details are provided below.

Proposition 3.24. *Suppose that (3.165) holds true. For $p \in \partial\Omega_k$ and $k \in \{0, 1, \ldots, K\}$, the solution $\mathcal{W}_{k,p}$ to (3.183)–(3.184) satisfies*

(a) $\mathcal{W}_{k,p}$ depends only on the variable z^d, i.e., $\mathcal{W}_{k,p}(z) = \mathcal{W}_{k,p}(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$.

(b) $\mathcal{W}_{k,p}$ is independent of p and depends only on k, i.e., $\mathcal{W}_{k,p}(z^d) = \theta_k(z^d)$ for $z^d \in [0,\infty)$, where θ_k is the unique solution to (3.186)–(3.188).

Proof. Following Proposition 3.12, we replace f with f_0 and apply the moving plane arguments to obtain (a). By (a), (3.185), and (3.188), $\mathcal{W}_{k,p} = \mathcal{W}_{k,p}(z^d)$ satisfies

$$\begin{aligned}
&\mathcal{W}''_{k,p} + f_0'(u_k)\mathcal{W}_{k,p} = f_0'(u_k) \quad \text{in } (0,\infty),\\
&\mathcal{W}_{k,p} - \gamma_k \mathcal{W}'_{k,p}(0) = 0,\\
&\lim_{t\to\infty} \mathcal{W}_{k,p}(t) = 1.
\end{aligned}$$

By the uniqueness of the solution to (3.186)–(3.188), it follows that $\mathcal{W}_{k,p} \equiv \theta_k$, which gives (b). This completes the proof of Proposition 3.24. □

We may use Proposition 3.24 to prove (3.191), (3.192), and $\mathcal{W}_{k,p}(z) = \theta_k(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$. Let $T > 0$, $k \in \{0, 1, \ldots, K\}$, and $p \in \partial\Omega_k$. Then, under the assumption (3.165), we can use (3.43), (3.182), (3.191)–(3.192), and $\nabla\delta_k(p - t\sqrt{\varepsilon}\nu_p) = -\nu_p$ to get

$$\varphi_{k,\varepsilon}(p - t\sqrt{\varepsilon}\nu_p) = \theta_k(t) + o_\varepsilon(1), \qquad \nabla\varphi_{k,\varepsilon}(p - t\sqrt{\varepsilon}\nu_p) = -\frac{1}{\sqrt{\varepsilon}}[\theta_k'(t)\nu_p + o_\varepsilon(1)]$$

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for $0 \le t \le T$ as $\varepsilon \to 0^+$. Together with (3.178) and (3.182), we arrive at

$$\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_k(t) + (\phi_\varepsilon^* - \phi_0^*)\theta_k(t) + (\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1), \tag{3.193}$$

$$\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\frac{1}{\sqrt{\varepsilon}}\{[u_k'(t) + (\phi_\varepsilon^* - \phi_0^*)\theta_k'(t)]\nu_p + (\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1)\} \tag{3.194}$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$.

By (3.177) and (3.193), we have

$$\begin{aligned} f_\varepsilon(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p)) &= f_0(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p)) - (\phi_\varepsilon^* - \phi_0^*)f_0'(\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p)) + (\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1) \\ &= f_0(u_k(t)) + (\phi_\varepsilon^* - \phi_0^*)f_0'(u_k(t))[\theta_k(t) - 1] + (\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1) \end{aligned} \tag{3.195}$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$. Combining (3.194)–(3.195), we then follow an argument similar to that in Section 3.2.3 to obtain

Proposition 3.25. *Suppose that* (3.165) *holds true. Then we have*

(a) $\int_{\overline{\Omega}_{k,T,\varepsilon}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \sqrt{\varepsilon}|\partial\Omega_k|(u_k'(0) - u_k'(T)) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)|\partial\Omega_k|(\theta_k'(0) - \theta_k'(T)) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1)$,

(b) $\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \sqrt{\varepsilon}|\partial\Omega_k|u_k'(T) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)|\partial\Omega_k|\theta_k'(T) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)\varepsilon o_\varepsilon(1)$,

(c) $\left|\int_{\overline{\Omega}_{\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x\right| \le \sqrt{\varepsilon}M' \exp\left(-M\varepsilon^{(2\beta-1)/2}\right)$

for $0 < \varepsilon < \varepsilon^*$ *and* $0 < \beta < 1/2$, *where* $|\partial\Omega_k|$ *is the surface area of* $\partial\Omega_k$.

Proof. Following Corollary 3.1, we begin with (a). Integrating (3.195) over $\overline{\Omega}_{k,T,\varepsilon}$ and applying the coarea formula (cf. [30, 83]) with (3.120), we get

$$\begin{aligned} \int_{\overline{\Omega}_{k,T,\varepsilon}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x &= \sqrt{\varepsilon}\int_0^T \int_{\partial\Omega_k} f_0(u_k(t))\,\mathrm{d}S_p\,\mathrm{d}t \\ &\quad + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)\int_0^T \int_{\partial\Omega_k} f_0'(u_k(t))[\theta_k(t) - 1]\,\mathrm{d}S_p\,\mathrm{d}t + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1). \end{aligned}$$

Together with (3.21) and (3.186), we obtain

$$\begin{aligned} \int_{\overline{\Omega}_{k,T,\varepsilon}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x &= \sqrt{\varepsilon}|\partial\Omega_k|\int_0^T (-u_k''(t))\,\mathrm{d}t + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)|\partial\Omega_k|\int_0^T (-\theta_k''(t))\,\mathrm{d}t + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1) \\ &= \sqrt{\varepsilon}|\partial\Omega_k|(u_k'(0) - u_k'(T)) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)|\partial\Omega_k|(\theta_k'(0) - \theta_k'(T)) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1), \end{aligned}$$

which gives (a).

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We now prove (b). As in (3.121), we integrate (3.2) over $\overline{\Omega}_{k,T,\varepsilon,\beta}$ and then apply the divergence theorem to obtain

$$
\begin{aligned}
\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x &= -\varepsilon \int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} \Delta\phi_\varepsilon(x)\,\mathrm{d}x \\
&= -\varepsilon \int_{\partial\Omega_{k,T,\varepsilon,\beta}} \partial_{\nu_x}\phi_\varepsilon(x)\,\mathrm{d}S_x \\
&= -\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - T\sqrt{\varepsilon}\nu_p))\mathcal{J}(T,p)\,\mathrm{d}S_p \\
&\quad + \int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - \varepsilon^\beta\nu_p))\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)\,\mathrm{d}S_p,
\end{aligned}
\tag{3.196}
$$

where ν_x is the unit outer normal at $x \in \partial\Omega_{k,T,\varepsilon,\beta}$ with respect to $\Omega_{k,T,\varepsilon,\beta}$, and $\mathcal{J}(T,p)$ and $\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)$ are given in (3.122). Then by (3.165) and (3.194), we have

$$
\begin{aligned}
&-\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - T\sqrt{\varepsilon}\nu_p))\mathcal{J}(T,p)\,\mathrm{d}S_p \\
&= -\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - T\sqrt{\varepsilon}\nu_p))[1 - T\sqrt{\varepsilon}(d-1)H(p) + \sqrt{\varepsilon}o_\varepsilon(1)]\,\mathrm{d}S_p \\
&= \int_{\partial\Omega_k} [\sqrt{\varepsilon}u_k'(T) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)\theta_k'(T)][1 - T\sqrt{\varepsilon}(d-1)H(p) + \sqrt{\varepsilon}o_\varepsilon(1)]\,\mathrm{d}S_p \\
&= \sqrt{\varepsilon}|\partial\Omega_k|u_k'(T) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)|\partial\Omega_k|\theta_k'(T) + \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*)o_\varepsilon(1).
\end{aligned}
\tag{3.197}
$$

On the other hand, by (3.161) in Proposition 3.20, we have

$$
\left|\int_{\partial\Omega_k} (\varepsilon\partial_{\nu_p}\phi_\varepsilon(p - \varepsilon^\beta\nu_p))\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)\,\mathrm{d}S_p\right| \leq \sqrt{\varepsilon}|\partial\Omega_k|M'\exp\left(-M\varepsilon^{(2\beta-1)/2}\right).
\tag{3.198}
$$

Combining (3.196)–(3.198) with $0 < \beta < 1/2$, we get (b). Following the argument for (b), one may use (3.198) to prove (c). Therefore, we complete the proof of Proposition 3.25. □

We are now in a position to derive a contradiction from (3.165). By (3.2)–(3.3), we observe that

$$
\int_\Omega f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \sum_{i=1}^I \frac{m_i z_i \exp(-z_i\phi_\varepsilon(x))}{\int_\Omega \exp(-z_i\phi_\varepsilon(y))\,\mathrm{d}y}\,\mathrm{d}x = \sum_{i=1}^I m_i z_i = 0,
$$

which implies

$$
\sum_{k=0}^K \int_{\overline{\Omega}_{k,T,\varepsilon}\cup\overline{\Omega}_{k,T,\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \int_{\overline{\Omega}_{\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x.
\tag{3.199}
$$

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Along with (3.151), (3.165), and Proposition 3.25, we have

$$\sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*) \sum_{k=0}^{K} |\partial\Omega_k| \theta_k'(0) = \sqrt{\varepsilon}(\phi_\varepsilon^* - \phi_0^*) o_\varepsilon(1),$$

which gives

$$\sum_{k=0}^{K} |\partial\Omega_k| \theta_k'(0) = 0.$$

However, since $\theta_k'(0) > 0$ for all $k = 0, 1, \ldots, K$ (see (3.190) in Remark 3.5), we get a contradiction, which shows (3.165) cannot hold true. Consequently, we establish the uniform boundedness of $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon}$.

Remark 3.6. *Due to the uniform boundedness of* $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon}$*, there exists a sequence* $\{\varepsilon_n\}_{n=1}^\infty$ *with* $\lim_{n\to\infty} \varepsilon_n = 0$ *and a constant* $Q \in \mathbb{R}$ *such that* $(\phi_{\varepsilon_n}^* - \phi_0^*)/\sqrt{\varepsilon_n} \to Q$ *as* $n \to \infty$*. In Section 3.3.5, we will prove that* Q *is uniquely determined by* (3.238)*, which implies*

$$\phi_\varepsilon^* = \phi_0^* + \sqrt{\varepsilon}(Q + o_\varepsilon(1)) \quad \textit{as } \varepsilon \to 0^+. \tag{3.200}$$

3.3.4 Second-order asymptotic expansion of ϕ_ε in $\Omega_{k,\varepsilon}$

In this section, we will use uniform boundedness of $|\phi_\varepsilon^* - \phi_0^*|/\sqrt{\varepsilon}$ (cf. (3.200)) to derive the second-order asymptotic expansions of ϕ_ε and $\nabla\phi_\varepsilon$. As in Section 3.3.3, we first study the second-order asymptotic expansions of f_ε and $A_{i,\varepsilon}$. A direct computation of f_ε shows

$$\begin{aligned} f_{1,\varepsilon}(\phi) &:= \frac{f_\varepsilon(\phi) - f_0(\phi)}{\sqrt{\varepsilon}} \\ &= -\sum_{i=1}^{I} \frac{m_i z_i B_{i,\varepsilon}}{|\Omega|[|\Omega| \exp(-z_i\phi_0^*) + \sqrt{\varepsilon} B_{i,\varepsilon}]} \exp(-z_i(\phi - \phi_0^*)) \quad \text{for } \phi \in \mathbb{R}, \end{aligned} \tag{3.201}$$

where

$$B_{i,\varepsilon} = \frac{A_{i,\varepsilon} - |\Omega| \exp(-z_i\phi_0^*)}{\sqrt{\varepsilon}} = \int_\Omega \frac{\exp(-z_i\phi_\varepsilon(y)) - \exp(-z_i\phi_0^*)}{\sqrt{\varepsilon}} \, dy \tag{3.202}$$

for $i = 1, \ldots, I$ and $\varepsilon > 0$. Note that $B_{i,\varepsilon}$ can be expressed by

$$B_{i,\varepsilon} = J_{i,1} + \sum_{k=0}^{K} J_{i,k,2} \quad \text{for } i = 1, \ldots, I, \tag{3.203}$$

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where

$$J_{i,1} = \int_{\overline{\Omega}_{\varepsilon,\beta}} \frac{\exp(-z_i\phi_\varepsilon(y)) - \exp(-z_i\phi_0^*)}{\sqrt{\varepsilon}}\,\mathrm{d}y, \tag{3.204}$$

$$J_{i,k,2} = \int_{\Omega_{k,\varepsilon,\beta}} \frac{\exp(-z_i\phi_\varepsilon(y)) - \exp(-z_i\phi_0^*)}{\sqrt{\varepsilon}}\,\mathrm{d}y \quad \text{for } k = 0, 1, \ldots, K. \tag{3.205}$$

Here $\overline{\Omega}_{\varepsilon,\beta} = \{x \in \Omega : \delta(x) \geq \varepsilon^\beta\}$ and $\Omega_{k,\varepsilon,\beta} = \{x \in \Omega : \delta_k(x) < \varepsilon^\beta\}$ for $0 < \beta < 1/2$ and $k = 0, 1, \ldots, K$. Clearly, $\Omega_{k,\varepsilon,\beta}$ are disjoint for sufficiently small $\varepsilon > 0$. Using (3.160), (3.202), and (3.200), we obtain the following result, similar to Lemma 3.2 in Section 3.3.3:

Lemma 3.26. *$B_{i,\varepsilon} = \exp(-z_i\phi_0^*)[-z_iQ|\Omega| - (\hat{m}_i/m_i)|\Omega|] + o_\varepsilon(1)$ for $i = 1, \ldots, I$, where u_k is the unique solution to (3.21)–(3.23), and*

$$\hat{m}_i = \frac{m_i}{|\Omega|} \sum_{k=0}^{K} |\partial\Omega_k| \int_0^\infty [\exp(-z_i(u_k(s) - \phi_0^*)) - 1]\,\mathrm{d}s \quad \textit{for } i = 1, \ldots, I.$$

Remark 3.7. *By (3.202) and Lemma 3.26, we obtain*

$$A_{i,\varepsilon} = |\Omega|\exp(-z_i\phi_0^*) + \sqrt{\varepsilon}\exp(-z_i\phi_0^*)\left(-z_iQ|\Omega| - \frac{\hat{m}_i}{m_i}|\Omega| + o_\varepsilon(1)\right) \quad \textit{for } i = 1, \ldots, I.$$

This allows us to compute the expansion of $c^{\mathrm{b}}_{i,\varepsilon} = m_i/A_{i,\varepsilon}$:

$$\begin{aligned}
c^{\mathrm{b}}_{i,\varepsilon} = \frac{m_i}{A_{i,\varepsilon}} &= \frac{m_i}{|\Omega|\exp(-z_i\phi_0^*)}\left(1 + \sqrt{\varepsilon}\left[-z_iQ - \frac{\hat{m}_i}{m_i} + o_\varepsilon(1)\right]\right)^{-1} \\
&= \frac{m_i}{|\Omega|\exp(-z_i\phi_0^*)}\left(1 + \sqrt{\varepsilon}\left[z_iQ + \frac{\hat{m}_i}{m_i} + o_\varepsilon(1)\right]\right) \\
&= c^{\mathrm{b}}_i + \sqrt{\varepsilon}\left(\frac{m_iz_iQ\exp(z_i\phi_0^*) + \hat{m}_i\exp(z_i\phi_0^*)}{|\Omega|} + o_\varepsilon(1)\right) \quad \textit{for } i = 1, \ldots, I,
\end{aligned}$$

where $c^{\mathrm{b}}_i = m_i|\Omega|^{-1}\exp(z_i\phi_0^*)$ for $i = 1, \ldots, I$.

Proof of Lemma 3.26. To prove Lemma 3.26, we analyze $J_{i,1}$ and $J_{i,k,2}$ as in Section 3.3.3. First, we compute the limit of $J_{i,1}$ using (3.160) and (3.200).

Claim 3.27. *$J_{i,1} = -z_iQ\exp(-z_i\phi_0^*)|\Omega| + o_\varepsilon(1)$ for $i = 1, \ldots, I$.*

Henceforth $\varepsilon^* > 0$ is a sufficiently small constant, and $M, M' > 0$ are generic constants independent of $\varepsilon > 0$.

Proof of Claim 3.27. Fix $i \in \{1, \ldots, I\}$. We first consider the case of $z_i > 0$. Then by (3.160), we may follow the approach of (3.171)–(3.172) in Lemma 3.21 (with $\sqrt{\varepsilon}$

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scaling instead of $\phi_\varepsilon^* - \phi_0^*$) and apply (3.200) and (3.204) to obtain

$$
\begin{aligned}
&\exp(-z_i\phi_0^*)\left|\Omega - \bigcup_{k=0}^{K}\Omega_{k,\varepsilon,\beta}\right| \frac{\exp(-z_iQ\sqrt{\varepsilon})\exp[-z_iM'\exp(-M\varepsilon^{(2\beta-1)/2}) + \sqrt{\varepsilon}o_\varepsilon(1)] - 1}{\sqrt{\varepsilon}} \\
&\leq J_{i,1} \leq \exp(-z_i\phi_0^*)\left|\Omega - \bigcup_{k=0}^{K}\Omega_{k,\varepsilon,\beta}\right| \frac{\exp(-z_iQ\sqrt{\varepsilon})\exp[z_iM'\exp(-M\varepsilon^{(2\beta-1)/2}) + \sqrt{\varepsilon}o_\varepsilon(1)] - 1}{\sqrt{\varepsilon}}.
\end{aligned}
$$

Along with the fact that

$$
\begin{aligned}
&\lim_{\varepsilon\to0^+} \frac{\exp(-z_iQ\sqrt{\varepsilon})\exp[\pm z_iM'\exp(-M\varepsilon^{(2\beta-1)/2}) + \sqrt{\varepsilon}o_\varepsilon(1)] - 1}{\sqrt{\varepsilon}} \\
&= \lim_{\varepsilon\to0^+} \frac{\exp[-z_iQ\sqrt{\varepsilon} \pm z_iM'\exp(-M\varepsilon^{(2\beta-1)/2}) + \sqrt{\varepsilon}o_\varepsilon(1)] - 1}{\sqrt{\varepsilon}} = -z_iQ,
\end{aligned}
$$

we obtain

$$
J_{i,1} = -z_iQ\exp(-z_i\phi_0^*)|\Omega| + o_\varepsilon(1) \quad \text{for } i = 1, \ldots, I.
$$

For the case of $z_i < 0$, we can follow a similar argument and complete the proof of Claim 3.27. □

To obtain the boundedness of $J_{i,k,2}$ (defined in (3.205)), we employ (3.160), (3.200), the principal coordinate system (cf. [38]), and the coarea formula (cf. [30, 83]), adapting techniques analogous to those in Section 3.3.3. Below are the details.

Claim 3.28. *There exists $M > 0$ independent of ε such that $|J_{i,k,2}| \leq M$ for $i = 1, \ldots, I$ and $k = 0, 1, \ldots, K$ and $0 < \varepsilon < \varepsilon^*$, where $\varepsilon^* > 0$ is sufficiently small.*

Proof of Claim 3.28. Similar to the analysis in Section 3.3.3, we consider $y \in \overline{\Omega}_{k,\varepsilon,\beta} = \{x \in \overline{\Omega} : \delta_k(x) \leq \varepsilon^\beta\}$. For sufficiently small $\varepsilon > 0$, the point y can be expressed as $y = p - s\sqrt{\varepsilon}\nu_p$, where $p \in \partial\Omega_k$, ν_p is the unit outer normal, and $0 \leq s \leq \varepsilon^{(2\beta-1)/2}$. Then we apply the corea formula and (3.120) to get

$$
\begin{aligned}
J_{i,k,2} &= \int_{\partial\Omega_k}\int_0^{\varepsilon^{(2\beta-1)/2}} [\exp(-z_i\phi_\varepsilon(p - s\sqrt{\varepsilon}\nu_p)) - \exp(-z_i\phi_0^*)]\{1 - s\sqrt{\varepsilon}[(d-1)H(p) + o_\varepsilon(1)]\}\,\mathrm{d}s\,\mathrm{d}S_p \\
&:= J_{i,k,3} - J_{i,k,4} \quad \text{for } i = 1, \ldots, I \text{ and } k = 0, 1, \ldots, K,
\end{aligned} \tag{3.206}
$$

where

$$
J_{i,k,3} = \int_{\partial\Omega_k}\int_0^{\varepsilon^{(2\beta-1)/2}} (\exp(-z_i\phi_\varepsilon(p - s\sqrt{\varepsilon}\nu_p)) - \exp(-z_i\phi_0^*))\,\mathrm{d}s\,\mathrm{d}S_p, \tag{3.207}
$$

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$$J_{i,k,4} = \sqrt{\varepsilon} \int_{\partial\Omega_k} \int_0^{\varepsilon^{(2\beta-1)/2}} s[\exp(-z_i\phi_\varepsilon(p - s\sqrt{\varepsilon}\nu_p)) - \exp(-z_i\phi_0^*)][(d-1)H(p) + o_\varepsilon(1)]\,\mathrm{d}s\,\mathrm{d}S_p. \tag{3.208}$$

By Propositions 3.13 and 3.15, $|\phi_\varepsilon(x) - \phi_0^*|$ is uniformly bounded for $x \in \overline{\Omega}$ and $\varepsilon > 0$, which implies that there exists $M > 1$ such that $|\exp(-z_i(\phi_\varepsilon(x) - \phi_0^*)) - 1| \leq M|\phi_\varepsilon(x) - \phi_0^*|$ for $x \in \overline{\Omega}$ and $0 < \varepsilon < \varepsilon^*$. Then by (3.160), we have

$$|\exp(-z_i\phi_\varepsilon(x)) - \exp(-z_i\phi_0^*)| \leq M' \exp\left(-M\delta(x)/\sqrt{\varepsilon}\right) + M'|\phi_\varepsilon^* - \phi_0^*| \tag{3.209}$$

for $x \in \overline{\Omega}$ and $0 < \varepsilon < \varepsilon^*$. Using (3.200) and (3.209) with $x = p - s\sqrt{\varepsilon}\nu_p$, $J_{i,k,3}$ can be estimated by

$$\begin{aligned}
|J_{i,k,3}| &= \left| \int_{\partial\Omega_k} \int_0^{\varepsilon^{(2\beta-1)/2}} \left[\exp(-z_i\phi_\varepsilon(p - s\sqrt{\varepsilon}\nu_p)) - \exp(-z_i\phi_0^*)\right]\,\mathrm{d}s\,\mathrm{d}S_p \right| \\
&\leq M' \int_0^{\varepsilon^{(2\beta-1)/2}} [\exp(-Ms) + |\phi_\varepsilon^* - \phi_0^*|]\,\mathrm{d}s \\
&= M'(1 - \exp(-M\varepsilon^{(2\beta-1)/2})) + M'\varepsilon^{(2\beta-1)/2}|\phi_\varepsilon^* - \phi_0^*| \leq M \quad \text{for } k = 0, 1, \dots, K.
\end{aligned} \tag{3.210}$$

On the other hand, due to the smoothness of $\partial\Omega_k$, there exists a positive constant M independent of ε such that $|(d-1)H(p) + o_\varepsilon(1)| \leq M$ for $0 < \varepsilon < \varepsilon^*$. Using (3.200) and (3.209) with $x = p - s\sqrt{\varepsilon}\nu_p$, $J_{i,k,4}$ can be estimated by

$$\begin{aligned}
|J_{i,k,4}| &= \sqrt{\varepsilon} \left| \int_{\partial\Omega_k} \int_0^{\varepsilon^{(2\beta-1)/2}} s[\exp(-z_i\phi_\varepsilon(p - s\sqrt{\varepsilon}\nu_p)) - \exp(-z_i\phi_0^*)][(d-1)H(p) + o_\varepsilon(1)]\,\mathrm{d}s\,\mathrm{d}S_p \right| \\
&\leq M'\sqrt{\varepsilon} \int_0^{\varepsilon^{(2\beta-1)/2}} s\,[\exp(-Ms) + |\phi_\varepsilon^* - \phi_0^*|]\,\mathrm{d}s = \sqrt{\varepsilon}\mathcal{O}_\varepsilon(1) \quad \text{for } k = 0, 1, \dots, K.
\end{aligned} \tag{3.211}$$

Combining (3.206)–(3.211), we arrive at $|J_{i,k,2}| \leq |J_{i,k,3}| + |J_{i,k,4}| \leq M$ for $0 < \varepsilon < \varepsilon^*$, which completes the proof of Claim 3.28. □

To complete the proof of Lemma 3.26, we define

$$\varphi_{k,\varepsilon}(x) = \frac{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})}{\sqrt{\varepsilon}} \quad \text{for } x \in \overline{\Omega}_{k,\varepsilon,\beta} \text{ and } k = 0, 1, \dots, K, \tag{3.212}$$

where u_k is the unique solution to (3.21)–(3.23), $\delta_k(x) = \mathrm{dist}(x, \partial\Omega_k)$ and $\overline{\Omega}_{k,\varepsilon,\beta} = \{x \in \overline{\Omega} : \delta_k(x) \leq \varepsilon^\beta\}$ for $k = 0, 1, \dots, K$. Note that (3.212) has the same form as (3.99). Following the approach of Proposition 3.10 in Section 3.3.3, we claim

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Claim 3.29. *There exists a constant $M > 0$ independent of ε such that $\max_{\overline{\Omega}_{k,\varepsilon,\beta}} |\varphi_{k,\varepsilon}| \leq M$ for $k = 0, 1, \ldots, K$ and $0 < \varepsilon < \varepsilon^*$.*

Proof of Claim 3.29. Following the method of Section 3.2.2, we derive the partial differential equation for $\varphi_{k,\varepsilon}$ in $\Omega_{k,\varepsilon,\beta}$. As in (3.100), we use (3.2), (3.21), (3.103) and (3.212) to get

$$\begin{aligned}
\varepsilon\Delta\varphi_{k,\varepsilon}(x) &= -\frac{f_\varepsilon(\phi_\varepsilon(x)) - f_0(u_k(\delta_k(x)/\sqrt{\varepsilon}))}{\sqrt{\varepsilon}} + [(d-1)H(p_x) + \varepsilon^\beta \mathcal{O}_\varepsilon(1)]u_k'(\delta_k(x)/\sqrt{\varepsilon}) \\
&= -\frac{f_\varepsilon(\phi_\varepsilon(x)) - f_\varepsilon(u_k(\delta_k(x)/\sqrt{\varepsilon}))}{\sqrt{\varepsilon}} - \frac{f_\varepsilon(u_k(\delta_k(x)/\sqrt{\varepsilon})) - f_0(u_k(\delta_k(x)/\sqrt{\varepsilon}))}{\sqrt{\varepsilon}} \\
&\quad + [(d-1)H(p_x) + \varepsilon^\beta \mathcal{O}_\varepsilon(1)]u_k'(\delta_k(x)/\sqrt{\varepsilon}) \\
&= -c_\varepsilon(x)\varphi_{k,\varepsilon} + g_\varepsilon(x) \quad \text{for } x \in \Omega_{k,\varepsilon,\beta},
\end{aligned}$$

where

$$c_\varepsilon(x) = \begin{cases} \dfrac{f_\varepsilon(\phi_\varepsilon(x)) - f_\varepsilon(u_k(\delta_k(x)/\sqrt{\varepsilon}))}{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})} & \text{if } \phi_\varepsilon(x) \neq u_k(\delta_k(x)/\sqrt{\varepsilon}); \\ f_\varepsilon'(\phi_\varepsilon(x)) & \text{if } \phi_\varepsilon(x) = u_k(\delta_k(x)/\sqrt{\varepsilon}), \end{cases} \tag{3.213}$$

$$g_\varepsilon(x) = (d-1)H(p_x)u_k'(\delta_k(x)/\sqrt{\varepsilon}) - f_{1,\varepsilon}(u_k(\delta_k(x)/\sqrt{\varepsilon})) + \varepsilon^\beta \mathcal{O}_\varepsilon(1). \tag{3.214}$$

Here we have used the definition of $f_{1,\varepsilon}$ (cf. (3.201)) and the fact that u_k' is bounded on $[0, \infty)$ (cf. Proposition 3B.1). Note that functions c_ε and g_ε are different from (3.101)–(3.102) because $f_{1,\varepsilon}$ is a nonzero function. Along with (3.4), (3.22), (3.45) and (3.144), we obtain

$$\begin{aligned}
&\varepsilon\Delta\varphi_{k,\varepsilon} + c_\varepsilon(x)\varphi_{k,\varepsilon} = g_\varepsilon(x) \quad \text{for } x \in \Omega_{k,\varepsilon}, &(3.215)\\
&\varphi_{k,\varepsilon} + \gamma_k\sqrt{\varepsilon}\partial_\nu\varphi_{k,\varepsilon} = 0 \qquad \text{on } \partial\Omega_k \quad \text{for } k = 0, 1, \ldots, K. &(3.216)
\end{aligned}$$

Note that $c_\varepsilon(x) < 0$ for $x \in \Omega_{k,\varepsilon}$ because $f_\varepsilon'(\phi) \leq -C_3^2$ for $\phi \in \mathbb{R}$ and $\varepsilon > 0$ (cf (3.131)). By (3.201), (3.203), Claims 3.27 and 3.28, $f_{1,\varepsilon}$ is uniformly bounded on the interval $[\underline{\phi_{bd}}, \overline{\phi_{bd}}]$ with respect to ε and then g_ε is uniformly bounded with respect to ε. By (3.160), (3.200) and (3.147) with Proposition 3.17, we find the following inequality:

$$\begin{aligned}
|\varphi_{k,\varepsilon}(x)| &\leq \frac{|\phi_\varepsilon(x) - \phi_0^*| + |u_k(\delta_k(x)/\sqrt{\varepsilon}) - \phi_0^*|}{\sqrt{\varepsilon}} \\
&\leq \frac{M'}{\sqrt{\varepsilon}} \exp\left(-M\varepsilon^{(2\beta-1)/2}\right) + \frac{|\phi_\varepsilon^* - \phi_0^*|}{\sqrt{\varepsilon}} \leq 2|Q| + \frac{1}{2}
\end{aligned}$$

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for $\delta_k(x) = \varepsilon^{1/8}$ as ε sufficiently small, which has the same form as (3.105) in Proposition 3.10. Hence as in Proposition 3.10, we conclude that $\varphi_{k,\varepsilon}$ is uniformly bounded in $\overline{\Omega}_{k,\varepsilon}$, i.e., there exists a positive constant M independent of ε such that $\max_{\overline{\Omega}_{k,\varepsilon}} |\varphi_{k,\varepsilon}| \le M$ for $k = 0, 1, \dots, K$ and sufficiently small $\varepsilon > 0$. Therefore, this ends the proof of Claim 3.29. □

By (3.212) and Claim 3.29, we have

$$\exp(-z_i\phi_\varepsilon(p - s\sqrt{\varepsilon}\nu_p)) = \exp(-z_i u_k(s)) + \sqrt{\varepsilon}\mathcal{O}_\varepsilon(1) \quad \text{for } 0 \le s \le \varepsilon^{(2\beta-1)/2}. \tag{3.217}$$

Thus, by (3.207) and (3.217), we get

$$\begin{aligned}
J_{i,k,3} &= \int_{\partial\Omega_k}\int_0^{\varepsilon^{(2\beta-1)/2}} [\exp(-z_i\phi_\varepsilon(p - s\sqrt{\varepsilon}\nu_p)) - \exp(-z_i\phi_0^*)]\,\mathrm{d}s\,\mathrm{d}S_p \\
&= \int_{\partial\Omega_k}\int_0^{\varepsilon^{(2\beta-1)/2}} [\exp(-z_i u_k(s)) - \exp(-z_i\phi_0^*) + \sqrt{\varepsilon}\mathcal{O}_\varepsilon(1)]\,\mathrm{d}s\,\mathrm{d}S_p \\
&= \exp(-z_i\phi_0^*)\int_{\partial\Omega_k}\int_0^{\varepsilon^{(2\beta-1)/2}} [\exp(-z_i(u_k(s) - \phi_0^*)) - 1]\,\mathrm{d}s\,\mathrm{d}S_p + \varepsilon^\beta\mathcal{O}_\varepsilon(1) \\
&= \exp(-z_i\phi_0^*)|\partial\Omega_k| \int_0^\infty [\exp(-z_i(u_k(s) - \phi_0^*)) - 1]\,\mathrm{d}s + o_\varepsilon(1) \quad \text{for } i = 1, \dots, I,
\end{aligned}$$

which implies

$$J_{i,k,3} = \exp(-z_i\phi_0^*)|\partial\Omega_k| \int_0^\infty [\exp(-z_i(u_k(s) - \phi_0^*)) - 1]\,\mathrm{d}s + o_\varepsilon(1) \quad \text{for } i = 1, \dots, I. \tag{3.218}$$

Here we have used the fact that $\int_0^\infty [\exp(-z_i(u_k(s) - \phi_0^*)) - 1]\,\mathrm{d}s$ is convergent because of (3.147) and Proposition 3.17. Therefore, we can use (3.203), (3.206)–(3.208), (3.211), (3.218) and Claim 3.27 to get

$$\begin{aligned}
B_{i,\varepsilon} &= J_{i,1} + \sum_{k=0}^K J_{i,k,2} \\
&= (-z_i Q\exp(-z_i\phi_0^*) + o_\varepsilon(1)) + \sum_{k=0}^K (J_{i,k,3} + J_{i,k,4}) \\
&= \exp(-z_i\phi_0^*)\left[-z_i Q|\Omega| + \sum_{k=0}^K |\partial\Omega_k| \int_0^\infty [\exp(-z_i(u_k(s) - \phi_0^*)) - 1]\,\mathrm{d}s\right] + o_\varepsilon(1)
\end{aligned}$$

for $i = 1, \dots, I$, and complete the proof of Lemma 3.26. □

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Applying Lemma 3.26 to (3.201), we obtain

$$\begin{aligned}
f_{1,\varepsilon}(\phi) &= -\sum_{i=1}^{I} \frac{m_i z_i B_{i,\varepsilon}}{|\Omega|[|\Omega|\exp(-z_i\phi_0^*) + \sqrt{\varepsilon}B_{i,\varepsilon}]}\exp(-z_i(\phi-\phi_0^*)) \\
&= -\sum_{i=1}^{I}\frac{m_i z_i}{|\Omega|^2}\left[-z_i Q|\Omega| + \sum_{k=0}^{K}|\partial\Omega_k|\int_0^\infty [\exp(-z_i(u_k(s)-\phi_0^*))-1]\,\mathrm{d}s\right]\exp(-z_i(\phi-\phi_0^*)) + o_\varepsilon(1) \\
&:= f_1(\phi) + o_\varepsilon(1),
\end{aligned}$$

which implies

$$f_{1,\varepsilon}(\phi) = f_1(\phi) + o_\varepsilon(1) \quad \text{for } \phi \in \mathbb{R}. \tag{3.219}$$

Note that f_1 is given in (3.128). Hence the nonlinear term f_ε of the CCPB equation (3.125) can be expressed as

$$f_\varepsilon(\phi) = f_0(\phi) + \sqrt{\varepsilon}(f_1(\phi) + o_\varepsilon(1)) \quad \text{for } \phi \in \mathbb{R}, \tag{3.220}$$

where $f_0(\phi) = |\Omega|^{-1}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi-\phi_0^*))$ (defined in (3.139)). Consequently, the CCPB equation (3.125) can be rewritten as

$$-\varepsilon\Delta\phi_\varepsilon = f_0(\phi_\varepsilon) + \sqrt{\varepsilon}(f_1(\phi_\varepsilon) + o_\varepsilon(1)) \quad \text{in } \Omega. \tag{3.221}$$

Moreover, by (3.212)–(3.216) and (3.220)–(3.221), we have

$$\varepsilon\Delta\varphi_{k,\varepsilon} + c_\varepsilon(x)\varphi_{k,\varepsilon} = g_\varepsilon(x) \quad \text{for } x \in \Omega_{k,\varepsilon,\beta}, \tag{3.222}$$

$$\varphi_{k,\varepsilon} + \gamma_k\sqrt{\varepsilon}\partial_\nu\varphi_{k,\varepsilon} = 0 \quad \text{on } \partial\Omega_k \quad \text{for } k = 0,1,\ldots,K, \tag{3.223}$$

where

$$\begin{aligned}
c_\varepsilon(x) &= \frac{f_0(\phi_\varepsilon(x)) - f_0(u_k(\delta_k(x)/\sqrt{\varepsilon}))}{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})} \\
&\quad + \sqrt{\varepsilon}\frac{f_1(\phi_\varepsilon(x)) - f_1(u_k(\delta_k(x)/\sqrt{\varepsilon})) + o_\varepsilon(1)}{\phi_\varepsilon(x) - u_k(\delta_k(x)/\sqrt{\varepsilon})} \quad \text{if } \phi_\varepsilon(x) \neq u_k(\delta_k(x)/\sqrt{\varepsilon}),
\end{aligned} \tag{3.224}$$

$$c_\varepsilon(x) = f_0'(\phi_\varepsilon(x)) + \sqrt{\varepsilon}(f_1'(\phi_\varepsilon(x)) + o_\varepsilon(1)) \quad \text{if } \phi_\varepsilon(x) = u_k(\delta_k(x)/\sqrt{\varepsilon}), \tag{3.225}$$

and

$$g_\varepsilon(x) = (d-1)H(p)u_k'(\delta_k(x)/\sqrt{\varepsilon}) - f_1(u_k(\delta_k(x)/\sqrt{\varepsilon})) + o_\varepsilon(1). \tag{3.226}$$

Here the nonzero function f_1, defined in (3.128), distinguishes (3.224)–(3.226) from (3.101)–(3.102).

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To get the asymptotic expansion of $\varphi_{k,\varepsilon}$ in $\Omega_{k,\varepsilon,\beta}$, we apply the methods of Lemma 3.11 and Proposition 3.12 (cf. Section 3.2.2) to (3.222)–(3.223) and define

$$\mathcal{W}_{k,p,\varepsilon}(z) = \varphi_{k,\varepsilon}(\Psi_p(\sqrt{\varepsilon}z)) \quad \text{for } z \in \overline{B}^+_{\varepsilon^{(2\beta-1)/2}} \text{ and } 0 < \varepsilon < \varepsilon^* \tag{3.227}$$

(cf. (3.107)) where Ψ_p is given in (3.43). Analogously to (3.108)–(3.111), $\mathcal{W}_{k,p,\varepsilon}$ satisfies

$$\sum_{i,j=1}^{d} a_{ij}(z)\frac{\partial^2 \mathcal{W}_{k,p,\varepsilon}}{\partial z^i z^j} + \sum_{j=1}^{d} b_j(z)\frac{\partial \mathcal{W}_{k,p,\varepsilon}}{\partial z^j} + c_\varepsilon(z)\mathcal{W}_{k,p,\varepsilon} = g_\varepsilon(z) \quad \text{in } B^+_{\varepsilon^{(2\beta-1)/2}},$$

$$\mathcal{W}_{k,p,\varepsilon} - \gamma_k \partial_{z^d}\mathcal{W}_{k,p,\varepsilon} = 0 \qquad \text{on } \overline{B}^+_{\varepsilon^{(2\beta-1)/2}} \cap \partial\mathbb{R}^d_+,$$

for $0 < \varepsilon < \varepsilon^*$, where a_{ij} and b_j are given in (3.47)–(3.48), and

$$\begin{aligned} c_\varepsilon(z) &= \frac{f_0(u_k(z^d) + \sqrt{\varepsilon}\mathcal{W}_{k,p,\varepsilon}(z)) - f_0(u_k(z^d))}{\sqrt{\varepsilon}\mathcal{W}_{k,p,\varepsilon}(z)} \\ &\quad + \frac{f_1(u_k(z^d) + \sqrt{\varepsilon}\mathcal{W}_{k,p,\varepsilon}(z)) - f_1(u_k(z^d)) + o_\varepsilon(1)}{\mathcal{W}_{k,p,\varepsilon}(z)} \quad \text{if } \mathcal{W}_{k,p,\varepsilon}(z) \neq 0, \\ c_\varepsilon(z) &= f_0'(u_k(z^d)) + \sqrt{\varepsilon}(f_1'(u_k(z^d)) + o_\varepsilon(1)) \quad \text{if } \mathcal{W}_{k,p,\varepsilon}(z) = 0 \end{aligned}$$

and

$$g_\varepsilon(z) = (d-1)H(p)u_k'(z^d) - f_1(u_k(z^d)) + o_\varepsilon(1).$$

As in Lemma 3.11, we use the uniform boundedness of $\varphi_{k,\varepsilon}$ (cf. Claim 3.29) to prove

Lemma 3.30. *For any sequence $\{\varepsilon_n\}_{n=1}^\infty$ of positive numbers with $\lim_{n\to\infty}\varepsilon_n = 0$, $\alpha \in (0,1)$, and $p \in \partial\Omega_k$ ($k \in \{0,1,\dots,K\}$), there exists a subsequence $\{\varepsilon_{nn}\}_{n=1}^\infty$ such that $\lim_{n\to\infty}\|\mathcal{W}_{k,p,\varepsilon_{nn}} - \mathcal{W}_{k,p}\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0$ for $m \in \mathbb{N}$, where $\mathcal{W}_{k,p} \in \mathcal{C}^{2,\alpha}_{loc}(\overline{\mathbb{R}}^d_+)$ satisfies*

$$\Delta\mathcal{W}_{k,p} + f_0'(u_k)\mathcal{W}_{k,p} = (d-1)H(p)u_k' - f_1(u_k) \quad \textit{in } \mathbb{R}^d_+, \tag{3.228}$$

$$\mathcal{W}_{k,p} - \gamma_k\partial_{z^d}\mathcal{W}_{k,p} = 0 \quad \textit{on } \partial\mathbb{R}^d_+. \tag{3.229}$$

Moreover, there exists $M > 0$ such that $\mathcal{W}_{k,p}$ satisfies the following estimate

$$|\mathcal{W}_{k,p}(z) - (d-1)H(p)v_k(z^d) - w_k(z^d)| \le M\exp(-C_3 z^d/8) \tag{3.230}$$

for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$ and $z^d \ge 2(d-1)/C_3$, where v_k and w_k are solutions to (3.24)–(3.26) and (3.27)–(3.29), respectively. In addition, the constant C_3 is given in (3.131).

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From Lemma 3.30, the solution $\mathcal{W}_{k,p}$ to (3.228)–(3.229) may, a priori, depend on the sequence $\{\varepsilon_n\}_{n=1}^{\infty}$. To establish the indepedence from the sequence, we employ the moving plane arguments, as in Proposition 3.12 to prove that $\mathcal{W}_{k,p}(z) = \mathcal{W}_{k,p}(z^d) = (d-1)H(p)v_k(z^d) + w_k(z^d)$ for $z = (z', z^d) \in \mathbb{R}^d_+$, where v_k and w_k are the unique solutions to (3.24)–(3.26) and (3.27)–(3.29). Here v_k and w_k are independent of the choice of sequence $\{\varepsilon_n\}_{n=1}^{\infty}$ and point $p \in \partial\Omega_k$. Consequently, we can improve the results of Lemma 3.30 as

$$\lim_{\varepsilon\to 0^+} \|\mathcal{W}_{k,p,\varepsilon} - (d-1)H(p)v_k - w_k\|_{\mathcal{C}^{2,\alpha}(\overline{B}^+_m)} = 0 \quad \text{for } m \in \mathbb{N} \text{ and } \alpha \in (0,1), \tag{3.231}$$

and

$$\lim_{\varepsilon\to 0^+} \mathcal{W}_{k,p,\varepsilon}(z) = (d-1)H(p)v_k(z^d) + w_k(z^d) \quad \text{for } z = (z', z^d) \in \overline{\mathbb{R}}^d_+, \tag{3.232}$$

where $\mathcal{W}_{k,p,\varepsilon}$ is defined in (3.227). The details are stated as follows.

Proposition 3.31. *For $p \in \partial\Omega_k$ and $k \in \{0, 1, \ldots, K\}$, the solution $\mathcal{W}_{k,p}$ to (3.228)–(3.229) satisfies*

(a) $\mathcal{W}_{k,p}$ depends only on the variable z^d, i.e., $\mathcal{W}_{k,p}(z) = \mathcal{W}_{k,p}(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$.

(b) $\mathcal{W}_{k,p}(z^d) = (d-1)H(p)v_k(z^d) + w_k(z^d)$ for $z^d \in [0,\infty)$, where v_k and w_k are the unique solutions to (3.24)–(3.26) and (3.27)–(3.29), respectively.

Proof. Following Proposition 3.12, we replace f with f_0 and apply the moving plane arguments to obtain (a). By (a), (3.26), (3.29), and (3.230), $\mathcal{W}_{k,p} = \mathcal{W}_{k,p}(z^d)$ satisfies

$$\begin{aligned}
&\mathcal{W}''_{k,p} + f_0'(u_k)\mathcal{W}_{k,p} = (d-1)H(p)u_k' - f_1(u_k) \quad \text{in } (0,\infty),\\
&\mathcal{W}_{k,p}(0) - \gamma_k \mathcal{W}'_{k,p}(0) = 0,\\
&\lim_{z^d\to\infty} \mathcal{W}_{k,p}(z^d) = Q.
\end{aligned}$$

By the uniqueness of solutions to (3.24)–(3.26) and (3.27)–(3.29) (cf. (3.279) and (3.293)), we can conclude that $\mathcal{W}_{k,p} \equiv (d-1)H(p)v_k + w_k$, which gives (b). This completes the proof of Proposition 3.31. ☐

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We may use Proposition 3.31 to prove (3.231), (3.232), and $\mathcal{W}_{k,p}(z) = (d-1)H(p)v_k(z^d) + w_k(z^d)$ for $z = (z', z^d) \in \overline{\mathbb{R}}^d_+$. Let $T > 0$, $k \in \{0, 1, \dots, K\}$, and $p \in \partial\Omega_k$. Analogously to (3.117)–(3.118), we use (3.43), (3.227), (3.231)–(3.232), and $\nabla\delta_k(p - t\sqrt{\varepsilon}\nu_p) = -\nu_p$ to get

$$\varphi_{k,\varepsilon}(p - t\sqrt{\varepsilon}\nu_p) = (d-1)H(p)v_k(t) + w_k(t) + o_\varepsilon(1), \tag{3.233}$$

$$\nabla\varphi_{k,p}(p - t\sqrt{\varepsilon}\nu_p) = -\frac{1}{\sqrt{\varepsilon}}\{[(d-1)H(p)v_k'(t) + w_k'(t)]\nu_p + o_\varepsilon(1)] \tag{3.234}$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$. Combining (3.212), (3.227) and (3.233)–(3.234), we arrive at

$$\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = u_k(t) + \sqrt{\varepsilon}\left((d-1)H(p)v_k(t) + w_k(t) + o_\varepsilon(1)\right),$$
$$\nabla\phi_\varepsilon(p - t\sqrt{\varepsilon}\nu_p) = -\left(\frac{1}{\sqrt{\varepsilon}}u_k'(t) + (d-1)H(p)v_k'(t) + w_k'(t)\right)\nu_p + o_\varepsilon(1)$$

for $0 \le t \le T$ as $\varepsilon \to 0^+$, which implies (3.19)–(3.20). Therefore, we complete the proof of Theorem 3.2(a).

3.3.5 Proof of Corollary 3.2

We present the proof of Corollary 3.2, following the structure of Corollary 3.1. We first prove (a). Integrating (3.39) over $\overline{\Omega}_{k,T,\varepsilon}$ and applying the coarea formula (cf. [30, 83]) with (3.120), we get

$$\begin{aligned}\int_{\overline{\Omega}_{k,T,\varepsilon}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x = \sqrt{\varepsilon}\int_{\partial\Omega_k}\int_0^T f_0(u_k(t))\,\mathrm{d}t\,\mathrm{d}S_p& \\ + (d-1)\varepsilon\int_{\partial\Omega_k}\int_0^T H(p)[f_0'(u_k(t))v_k(t) - tf_0(u_k(t))]\,\mathrm{d}t\,\mathrm{d}S_p& \\ + \varepsilon\int_{\partial\Omega_k}\int_0^T [f_0'(u_k(t))w_k(t) + f_1(u_k(t))]\,\mathrm{d}t\,\mathrm{d}S_p + \varepsilon o_\varepsilon(1).&\end{aligned}$$

Together with (3.21), (3.24), and (3.27), we obtain

$$\begin{aligned}\int_{\overline{\Omega}_{k,T,\varepsilon}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x &= \sqrt{\varepsilon}|\partial\Omega_k|\int_0^T(-u_k''(t))\,\mathrm{d}t \\ &\quad + \varepsilon\left[(d-1)\left(\int_{\partial\Omega_k}H(p)\,\mathrm{d}S_p\right)\left(\int_0^T[u_k'(t) - v_k''(t) + tu_k''(t)]\,\mathrm{d}t\right)\right. \\ &\quad \left. + |\partial\Omega_k|\int_0^T(-w_k''(t))\,\mathrm{d}t\right] + \varepsilon o_\varepsilon(1) \\ &= \sqrt{\varepsilon}|\partial\Omega_k|(u_k'(0) - u_k'(T))\end{aligned}$$

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$$+\varepsilon\left[(d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)(Tu_k'(T)+v_k'(0)-v_k'(T))\right.$$
$$\left.+|\partial\Omega_k|(w_k'(0)-w_k'(T))\right]+\varepsilon o_\varepsilon(1),$$

which gives (a).

We now prove (b) as follows. As in (3.121), we integrate (3.2) over $\overline{\Omega}_{k,T,\varepsilon,\beta}$ and apply the divergence theorem to obtain

$$\begin{aligned}\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} f_\varepsilon(\phi_\varepsilon(x))\,\mathrm{d}x &= -\varepsilon\int_{\overline{\Omega}_{k,T,\varepsilon,\beta}} \Delta\phi_\varepsilon(x)\,\mathrm{d}x \\ &= -\varepsilon\int_{\partial\Omega_{k,T,\varepsilon,\beta}} \partial_{\nu_x}\phi_\varepsilon(x)\,\mathrm{d}S_x \\ &= -\int_{\partial\Omega_k}(\varepsilon\partial_{\nu_p}\phi_\varepsilon(p-T\sqrt{\varepsilon}\nu_p))\mathcal{J}(T,p)\,\mathrm{d}S_p \\ &\quad+\int_{\partial\Omega_k}(\varepsilon\partial_{\nu_p}\phi_\varepsilon(p-\varepsilon^\beta\nu_p))\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)\,\mathrm{d}S_p,\end{aligned}\tag{3.235}$$

where ν_x is the unit outer normal at $x\in\partial\Omega_{k,T,\varepsilon,\beta}$ with respect to $\Omega_{k,T,\varepsilon,\beta}$, and $\mathcal{J}(T,p)$ and $\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)$ are given in (3.122). Then by (3.20), we have

$$\begin{aligned}&-\int_{\partial\Omega_k}(\varepsilon\partial_{\nu_p}\phi_\varepsilon(p-T\sqrt{\varepsilon}\nu_p))\mathcal{J}(T,p)\,\mathrm{d}S_p \\ &=-\int_{\partial\Omega_k}(\varepsilon\partial_{\nu_p}\phi_\varepsilon(p-T\sqrt{\varepsilon}\nu_p))[1-T\sqrt{\varepsilon}(d-1)H(p)+\sqrt{\varepsilon}o_\varepsilon(1)]\,\mathrm{d}S_p \\ &=\sqrt{\varepsilon}\int_{\partial\Omega_k}\{u_k'(T)+\sqrt{\varepsilon}(d-1)H(p)v_k'(T)+w_k'(T)+o_\varepsilon(1)]\}[1-T\sqrt{\varepsilon}(d-1)H(p)+\sqrt{\varepsilon}o_\varepsilon(1)]\,\mathrm{d}S_p \\ &=\sqrt{\varepsilon}|\partial\Omega_k|u_k'(T)+\varepsilon\left[(d-1)\left(\int_{\partial\Omega_k}H(p)\,\mathrm{d}S_p\right)(-Tu_k'(T)+v_k'(T))+|\partial\Omega_k|w_k'(T)\right]+\varepsilon o_\varepsilon(1).\end{aligned}\tag{3.236}$$

On the other hand, by Theorem 3.2(b,ii), we have

$$\left|\int_{\partial\Omega_k}(\varepsilon\partial_{\nu_p}\phi_\varepsilon(p-\varepsilon^\beta\nu_p))\mathcal{J}(\varepsilon^{(2\beta-1)/2},p)\,\mathrm{d}S_p\right|\le\sqrt{\varepsilon}|\partial\Omega_k|M'\exp\left(-M\varepsilon^{(2\beta-1)/2}\right).\tag{3.237}$$

Combining (3.235)–(3.237) with $0<\beta<1/2$, we get (b). Following the argument as in (b), one may use (3.237) to prove (c). Therefore, we complete the proof of Corollary 3.2.

As aforementioned in Remark 3.6, to complete the proof of (3.200), it is necessary

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to show that Q is uniquely determined by

$$Q = \frac{\displaystyle\sum_{k=0}^{K} \frac{|\partial\Omega_k|\hat{F}_1(u_k(0)) + (d-1)\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right)\left(\int_0^\infty u_k'^2(s)\,\mathrm{d}s\right)}{u_k'(0) + \gamma_k f_0(u_k(0))}}{\displaystyle\sum_{k=0}^{K} \frac{|\partial\Omega_k| f_0(u_k(0))}{u_k'(0) + \gamma_k f_0(u_k(0))}}. \tag{3.238}$$

Using (3.151), (3.199), and Corollary 3.2, we find

$$\varepsilon\left[(d-1)\sum_{k=0}^{K}\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right) v_k'(0) + \sum_{k=0}^{K} |\partial\Omega_k| w_k'(0)\right] = \varepsilon o_\varepsilon(1),$$

which implies

$$(d-1)\sum_{k=0}^{K}\left(\int_{\partial\Omega_k} H(p)\,\mathrm{d}S_p\right) v_k'(0) + \sum_{k=0}^{K} |\partial\Omega_k| w_k'(0) = 0. \tag{3.239}$$

By (3.25), (3.28), (3.280) (in Appendix 3C), and (3.294) (in Appendix 3D), a straightforward calculation gives (3.238). Therefore, we complete the proof of (3.200) in Remark 3.6.

Final Remark

When the Robin boundary condition (3.4) is replaced by the Dirichlet boundary condition $\phi_\varepsilon = \phi_{bd,k}$ on $\partial\Omega_k$ for $k = 0, 1, \ldots, K$ (i.e., $\gamma_k = 0$ for $k = 0, 1, \ldots, K$), the conclusions of Theorems 3.1 and 3.2 hold true, particularly the asymptotic expansions (3.5)–(3.6) and (3.19)–(3.20), remain valid. In (3.5)–(3.6) and (3.19)–(3.20), the solutions u_k, v_k and w_k to ODEs satisfy the Dirichlet boundary conditions $u_k(0) = \phi_{bd,k}$ and $v_k(0) = w_k(0) = 0$, which can be directly regarded as the Robin boundary conditions (3.8), (3.11), (3.22), (3.25) and (3.28) with $\gamma_k = 0$. By applying the maximum principle, the L^q-theory and Schauder estimate, the proofs of Theorems 3.1 and 3.2 remain valid without other modifications for the Dirichlet boundary condition except Proposition 3.18. When $\gamma_k = 0$ for all $k = 0, 1, \ldots, K$, equations (3.150)–(3.151) are replaced by

$$\sum_{k=0}^{K} |\partial\Omega_k| u_k'(0) = \sum_{k=0}^{K} |\partial\Omega_k| \operatorname{sgn}(\phi_0^* - \phi_{bd,k}) \sqrt{\frac{2}{|\Omega|}\sum_{i=1}^{I} m_i[\exp(-z_i(\phi_{bd,k} - \phi_0^*)) - 1]} = 0,$$

which determines the value of ϕ_0^* (given in (3.138)). The properties of ODEs remains true whenever $\gamma_k \geq 0$ (see Appendices 3B to 3D).

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Conclusion

In this work, we present a rigorous analysis of boundary layer solutions to Poisson–Boltzmann (PB) type equations in general smooth domains. We extend the classical boundary layer theory to multiply connected domains via the moving plane arguments, and address the challenge posed by the nonlocal nonlinearity in charge-conserving PB equations using novel integral estimates. In the near-boundary region (where the distance to the boundary is of order $\sqrt{\varepsilon}\mathcal{O}(1)$), we construct asymptotic expansions based on solutions to associated ordinary differential equations, capturing the effect of mean curvature through second-order approximations. In the far-field region, we establish exponential decay estimates, which reveal the localized nature of boundary layer phenomena. Our analysis quantifies how domain geometry, particularly mean curvature, influences electrostatic characteristics such as electric potential, electric field, total ionic charge and total ionic charge density. These results highlight the explicit dependence of electrostatic screening on geometric features and provide analytical tools for applications in electrochemistry (e.g., porous electrodes), biophysics (e.g. ion channels), and microfluidics.

Appendix

3A Exponential-type estimate of radial solution

Here we study the radial solutions $\Phi_\varepsilon = \Phi_\varepsilon(r)$ to equations (3.1) and (3.125) in the ball $B_R(0)$ with the Dirichlet boundary condition, respectively. Equation (3.1) with the Dirichlet boundary condition can be denoted as

$$-\varepsilon(r^{d-1}\Phi_\varepsilon'(r))' = r^{d-1}f(\Phi_\varepsilon(r)) \quad \text{for } r \in (0, R), \tag{3.240}$$

$$\Phi_\varepsilon'(0) = 0, \tag{3.241}$$

$$\Phi_\varepsilon(R) = \Phi_{bd}, \tag{3.242}$$

where $f \in \mathcal{C}^1(\mathbb{R})$ is a strictly decreasing function satisfying (F1)–(F2), and Φ_{bd} is a constant independent of ε. Note that if $\Phi_{bd} = \phi^*$ (ϕ^* is the unique zero of f), then by the uniqueness of (3.240)–(3.242), $\Phi_\varepsilon \equiv \phi^*$ is a trivial solution. Hence we assume $\Phi_{bd} \neq \phi^*$. By (F1)–(F2), it is easy to prove

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Proposition 3A.1. *Assume that f satisfies (F1)–(F2). Let Φ_ε be the solution to (3.240)–(3.242) for $\varepsilon > 0$.*

(a) If $\Phi_{bd} > \phi^*$, then $\Phi_\varepsilon(0) > \phi^*$ and Φ_ε is strictly increasing;

(b) if $\Phi_{bd} < \phi^*$, then $\Phi_\varepsilon(0) < \phi^*$ and Φ_ε is strictly decreasing.

Proof. To prove (a), we first assume $\Phi_{bd} > \phi^*$ and prove $\Phi_\varepsilon(0) > \phi^*$. Suppose by contradiction that $\Phi_\varepsilon(0) \le \phi^*$. If $\Phi_\varepsilon(0) = \phi^*$, then by the uniqueness of solution to (3.240)–(3.242), we have $\Phi_\varepsilon \equiv \phi^*$ on $[0, R]$, which contradicts (3.242) and $\Phi_{bd} > \phi^*$. If $\Phi_\varepsilon(0) < \phi^*$, then there exists $r_1 > 0$ such that $\Phi_\varepsilon(r) < \phi^*$ for $r \in [0, r_1)$. By (F1) and (3.240), we get $-\varepsilon(r^{d-1}\Phi_\varepsilon'(r))' > 0$ for $r \in (0, r_1)$, which implies $r^{d-1}\Phi_\varepsilon'(r)$ is decreasing on $[0, r_1)$. Thus, by (3.241), $r^{d-1}\Phi_\varepsilon'(r) \le 0$ for $r \in [0, r_1)$, which means Φ_ε is decreasing on $[0, r_1)$. Along with $\Phi_\varepsilon(0) < \phi^*$, we get $\Phi_\varepsilon(r) \le \Phi_\varepsilon(0) < \phi^*$ for $r \in [0, r_1]$. Following this process, we can extend the interval $[0, r_1]$ to $[0, R]$ so $\Phi_\varepsilon < \phi^*$ on $[0, R]$, which contradicts (3.242) and $\Phi_{bd} > \phi^*$. Hence we obtain $\Phi_\varepsilon(0) > \phi^*$.

To complete the proof of (a), it suffices to show the strict increase of Φ_ε. Since $\Phi_\varepsilon(0) > \phi^*$, there exists $r_2 > 0$ such that $\Phi_\varepsilon(r) > \phi^*$ for $r \in [0, r_2)$. Then by (F1) and (3.240), we have $-\varepsilon(r^{d-1}\Phi_\varepsilon'(r))' < 0$ for $r \in (0, r_2)$, which implies $r^{d-1}\Phi_\varepsilon'(r)$ is increasing on $[0, r_2)$. Thus, by (3.241), $r^{d-1}\Phi_\varepsilon'(r) \ge 0$ for $r \in (0, r_2)$, which means Φ_ε is increasing on $[0, r_2)$. From $\Phi_\varepsilon(0) > \phi^*$, we get $\Phi_\varepsilon(r) > \phi^*$ for $r \in [0, r_2]$. Thus, we can extend the interval $[0, r_2]$ to $[0, R]$ and Φ_ε is strictly increasing on $[0, R]$. Suppose by contradiction that there exist two distinct points $r_3 < r_4$ such that $\Phi_\varepsilon(r_3) = \Phi_\varepsilon(r_4)$. Then by mean value theorem, there exists $r_5 \in (r_3, r_4)$ such that $\Phi_\varepsilon'(r_5) = 0$. Moreover, by (3.240) and mean value theorem, there exists $r_6 \in (0, r_5)$ such that $\Phi_\varepsilon''(r_6) = 0$. Hence by (F1)–(F2) and (3.240), we get $\Phi_\varepsilon(r_6) = \phi^*$, which contradicts to the fact that $\Phi_\varepsilon(0) > \phi^*$ and Φ_ε is increasing. Thus, Φ_ε is strictly increasing, and the proof of (a) is complete.

For the proof of (b), we may follow a similar argument to (a) and complete the proof of Proposition 3A.1. □

Proposition 3A.2. *Assume that f satisfies (F1)–(F2). Let Φ_ε be the solution to (3.240)–(3.242) for $\varepsilon > 0$. Then*

$$|\Phi_\varepsilon(r) - \phi^*| \le 2|\Phi_{bd} - \phi^*| \exp\left(-\frac{m_f(R-r)}{8\sqrt{\varepsilon}}\right) \tag{3.243}$$

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for $r \in [0, R]$ *and* $0 < \varepsilon < (m_f R)^2/[8(d-1)^2]$, *where* $m_f = m_f([\min\{\phi^*, \Phi_{bd}\}, \max\{\phi^*, \Phi_{bd}\}])$ *is given in (F1).*

Proof. Let $\overline{\Phi}_\varepsilon := \Phi_\varepsilon - \phi^*$ on $[0, R]$ for $\varepsilon > 0$. Then from (3.240)–(3.242), $\overline{\Phi}_\varepsilon$ satisfies

$$\begin{aligned} &-\varepsilon(r^{d-1}\overline{\Phi}_\varepsilon'(r))' = r^{d-1} f(\phi^* + \overline{\Phi}_\varepsilon(r)) \quad \text{for } r \in (0, R), && (3.244)\\ &\overline{\Phi}_\varepsilon'(0) = 0, && (3.245)\\ &\overline{\Phi}_\varepsilon(R) = \Phi_{bd} - \phi^*. && (3.246)\end{aligned}$$

By (F1)–(F2), we have

$$\begin{aligned} f(\phi^* + \overline{\Phi}_\varepsilon(r))\overline{\Phi}_\varepsilon(r) &= \left(\int_0^1 \frac{\mathrm{d}}{\mathrm{d}s} f(\phi^* + s\overline{\Phi}_\varepsilon(r))\,\mathrm{d}s\right)\overline{\Phi}_\varepsilon(r) \\ &= \left(\int_0^1 f'(\phi^* + s\overline{\Phi}_\varepsilon(r))\,\mathrm{d}s\right)\overline{\Phi}_\varepsilon^2(r) \le -m_f^2\overline{\Phi}_\varepsilon^2(r) \end{aligned} \tag{3.247}$$

for $r \in (0, R)$. Here we have used the fact that $\overline{\Phi}_\varepsilon = \Phi_\varepsilon - \phi^*$ is uniformly bounded (cf. Proposition 3.3 also works for the Dirichlet boundary condition (3.242)). By (3.244) and (3.247), we obtain

$$\begin{aligned} \varepsilon(\overline{\Phi}_\varepsilon^2(r))'' &= 2\varepsilon\overline{\Phi}_\varepsilon'^2(r) + 2\varepsilon\overline{\Phi}_\varepsilon''(r)\overline{\Phi}_\varepsilon(r) \\ &= 2\varepsilon\overline{\Phi}_\varepsilon'^2(r) - \frac{2\varepsilon(d-1)}{r}\overline{\Phi}_\varepsilon'(r)\overline{\Phi}_\varepsilon(r) - 2f(\phi^* + \overline{\Phi}_\varepsilon(r))\overline{\Phi}_\varepsilon(r) \\ &\ge 2\varepsilon\overline{\Phi}_\varepsilon'^2(r) - \frac{2\varepsilon(d-1)}{r}\overline{\Phi}_\varepsilon'(r)\overline{\Phi}_\varepsilon(r) + 2m_f^2\overline{\Phi}_\varepsilon^2(r) \quad \text{for } r \in (0, R). \end{aligned} \tag{3.248}$$

On the other hand, by Young's inequality, we have

$$\begin{aligned} \frac{2\varepsilon(d-1)}{r}\overline{\Phi}_\varepsilon'(r)\overline{\Phi}_\varepsilon(r) &\le 2\varepsilon\overline{\Phi}_\varepsilon'^2(r) + \frac{\varepsilon(d-1)^2}{2r^2}\overline{\Phi}_\varepsilon^2(r) \\ &\le 2\varepsilon\overline{\Phi}_\varepsilon'^2(r) + \frac{8\varepsilon(d-1)^2}{R^2}\overline{\Phi}_\varepsilon^2(r) \quad \text{for } r \in [R/4, R). \end{aligned} \tag{3.249}$$

Combining (3.248) and (3.249), we get

$$\varepsilon(\overline{\Phi}_\varepsilon^2(r))'' \ge \left(2m_f^2 - \frac{8\varepsilon(d-1)^2}{R^2}\right)\overline{\Phi}_\varepsilon^2(r) \ge m_f^2\overline{\Phi}_\varepsilon^2(r) \quad \text{for } r \in [R/4, R). \tag{3.250}$$

Here we have used that $0 < \varepsilon < (m_f R)^2/[8(d-1)^2]$. Applying the comparison theorem to (3.250), it yields

$$\overline{\Phi}_\varepsilon^2(r) \le \max\{\overline{\Phi}_\varepsilon^2(R/4), \overline{\Phi}_\varepsilon^2(R)\}\left[\exp\left(-\frac{m_f(R-r)}{\sqrt{\varepsilon}}\right) + \exp\left(-\frac{m_f(r-R/4)}{\sqrt{\varepsilon}}\right)\right] \tag{3.251}$$

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for $r \in [R/4, R]$. By Proposition 3A.1, $(\overline{\Phi}_\varepsilon^2(r))' = 2\overline{\Phi}_\varepsilon'(r)\overline{\Phi}_\varepsilon(r) > 0$ on $(0, R)$, and $\overline{\Phi}^2$ is strictly increasing on $[0, R]$. Consequently, we have $\overline{\Phi}_\varepsilon^2(R/4) < \overline{\Phi}_\varepsilon^2(R) = (\Phi_{bd} - \phi^*)^2$. From (3.251), we get

$$|\overline{\Phi}_\varepsilon(r)| \leq |\Phi_{bd} - \phi^*| \left[\exp\left(-\frac{m_f(R-r)}{2\sqrt{\varepsilon}}\right) + \exp\left(-\frac{m_f R}{8\sqrt{\varepsilon}}\right)\right] \quad \text{for } r \in [3R/4, R],$$

which implies

$$|\overline{\Phi}_\varepsilon(r)| \leq 2|\Phi_{bd} - \phi^*| \exp\left(-\frac{m_f(R-r)}{2\sqrt{\varepsilon}}\right) \quad \text{for } r \in [3R/4, R]. \tag{3.252}$$

Since $\overline{\Phi}_\varepsilon^2$ is strictly increasing on $[0, R]$, $|\overline{\Phi}|$ is also strictly increasing on $[0, R]$. Then by (3.252), we have

$$|\overline{\Phi}_\varepsilon(r)| \leq |\overline{\Phi}_\varepsilon(3R/4)| \leq 2|\Phi_{bd} - \phi^*| \exp\left(-\frac{m_f R}{8\sqrt{\varepsilon}}\right) \leq 2|\Phi_{bd} - \phi^*| \exp\left(-\frac{m_f(R-r)}{8\sqrt{\varepsilon}}\right) \tag{3.253}$$

for $r \in [0, 3R/4]$. Combining (3.252) and (3.253), we arrive at (3.243) and complete the proof of Proposition 3A.2. □

Now we consider the radial solution $\Phi_\varepsilon = \Phi_\varepsilon(r)$ to equation (3.125) with the Dirichlet boundary condition, which satisfies

$$-\varepsilon(r^{d-1}\Phi_\varepsilon'(r))' = r^{d-1} f_\varepsilon(\Phi_\varepsilon(r)) \quad \text{for } r \in (0, R), \tag{3.254}$$

$$\Phi_\varepsilon'(0) = 0, \tag{3.255}$$

$$\Phi_\varepsilon(R) = \Phi_{bd}, \tag{3.256}$$

where f_ε has a unique zero $\phi_\varepsilon^* \in \mathbb{R}$ and satisfies $f_\varepsilon'(\phi) \leq -M^2 < 0$ for $\phi \in \mathbb{R}$. Note that f_ε and its zero ϕ_ε^* may depend on ε but M is independent of ε.

Analogous to Propositions 3A.1 and 3A.2 (with ϕ^* replaced by ϕ_ε^*), we can prove

Proposition 3A.3. *Assume that f_ε has a unique zero $\phi_\varepsilon^* \in \mathbb{R}$ and satisfies $f_\varepsilon'(\phi) \leq -M^2 < 0$ for $\phi \in \mathbb{R}$ and $\varepsilon > 0$, where M is independent of ε. Let Φ_ε be the solution to (3.254)–(3.256) for $\varepsilon > 0$.*

(a) If $\Phi_{bd} > \phi_\varepsilon^*$ for $\varepsilon > 0$, then $\Phi_\varepsilon(0) > \phi_\varepsilon^*$ and Φ_ε is strictly increasing for $\varepsilon > 0$;

(b) if $\Phi_{bd} < \phi_\varepsilon^*$ for $\varepsilon > 0$, then $\Phi_\varepsilon(0) < \phi_\varepsilon^*$ and Φ_ε is strictly decreasing for $\varepsilon > 0$.

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Proposition 3A.4. *Assume that f_ε has a unique zero $\phi_\varepsilon^* \in \mathbb{R}$ and satisfies $f_\varepsilon'(\phi) \le -M^2 < 0$ for $\phi \in \mathbb{R}$ and $\varepsilon > 0$, where M is independent of ε. Let Φ_ε be the solution to (3.254)–(3.256) for $\varepsilon > 0$. Then*

$$|\phi_\varepsilon(r) - \phi_\varepsilon^*| \le 2|\Phi_{bd} - \phi_\varepsilon^*| \exp\left(-\frac{M(R-r)}{8\sqrt{\varepsilon}}\right) \tag{3.257}$$

for $r \in [0, R]$ and $0 < \varepsilon < (MR)^2/[8(d-1)^2]$.

3B Properties of the solution to (3.7)–(3.9) and (3.21)–(3.23)

In this appendix, we establish the existence, uniqueness, qualitative properties, and asymptotic behaviors of solutions to (3.7)–(3.9) and (3.21)–(3.23). For the sake of simplicity, equations (3.7)–(3.9) and (3.21)–(3.23) can be represented as follows.

$$U'' + f(U) = 0 \quad \text{in } (0, \infty), \tag{3.258}$$

$$U(0) - \gamma U'(0) = \Phi_{bd}, \tag{3.259}$$

$$\lim_{t\to\infty} U(t) = \phi^*, \tag{3.260}$$

where $\gamma \ge 0$ and $\Phi_{bd} \ne \phi^*$ are fixed constants. (When $\Phi_{bd} = \phi^*$, the solution $U \equiv \phi^*$ is trivial.) Here the function $f \in \mathcal{C}^\infty(\mathbb{R})$ satisfies assumptions (F1) and (F2). It is clear that the existence and uniqueness of solution to equations (3.7)–(3.9) and (3.21)–(3.23) for $k = 0, 1, \ldots, K$ follow from that of solution to equations (3.258)–(3.260). We may approach (3.258)–(3.260) by the following initial-value problem

$$\tilde{U}'' + f(\tilde{U}) = 0 \quad \text{in } (0, \infty), \tag{3.261}$$

$$\tilde{U}(0) = U_0, \tag{3.262}$$

$$\tilde{U}'(0) = U_0', \tag{3.263}$$

where U_0 (between ϕ^* and Φ_{bd}) and U_0' are constants to be determined such that $\tilde{U} \equiv U$ on $[0, \infty)$. The existence and uniqueness of (3.261)–(3.263) follow from the standard ODE theory. From (3.259) and (3.262)–(3.263), U_0 and U_0' must satisfy

$$U_0 - \gamma U_0' = \Phi_{bd}. \tag{3.264}$$

Multiplying (3.261) by $\tilde{U}'$ and then integrating it over $[0, t]$, we can use (3.262)–(3.263) to get

$$\tilde{U}'^2(t) + 2F(\tilde{U}(t)) = U_0'^2 + 2F(U_0) \quad \text{for } t \ge 0, \tag{3.265}$$

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where $F(\phi) = \int_{\phi^*}^{\phi} f(s)\,\mathrm{d}s$ for $\phi \in \mathbb{R}$. Note that $F'(\phi^*) = f(\phi^*) = 0$ and $F''(\phi) = f'(\phi) < 0$ for $\phi \in \mathbb{R}$ (by (F1)–(F2)) so

$$0 = F(\phi^*) > F(\phi) \quad \text{for } \phi \neq \phi^*. \tag{3.266}$$

Suppose that $\lim_{t\to\infty} \tilde{U}'(t) = 0$. Then we use (3.260) and (3.264)–(3.265) to find that U_0 (between ϕ^* and Φ_{bd}) must satisfy

$$\Phi_{bd} - U_0 = \operatorname{sgn}(\Phi_{bd} - \phi^*)\gamma\sqrt{-2F(U_0)}. \tag{3.267}$$

To show that there exists a unique U_0, between ϕ^* and Φ_{bd}, satisfying (3.267), we define a function $g : \mathbb{R} \to \mathbb{R}$ by

$$g(s) = \Phi_{bd} - s - \operatorname{sgn}(\Phi_{bd} - \phi^*)\gamma\sqrt{-2F(s)} \quad \text{for } s \in \mathbb{R},$$

which is well-defined because of (3.266). Since $g(\phi^*)g(\Phi_{bd}) < 0$ and $g'(s) < 0$ for s between ϕ^* and Φ_{bd}, function g has a unique zero U_0 between ϕ^* and Φ_{bd}, which means that equation (3.267) has a unique solution. Here one may use the facts that (i) if $\Phi_{bd} > \phi^*$, then $f(s) < 0$ for $s \in (\phi^*, \Phi_{bd}]$ and (ii) if $\Phi_{bd} < \phi^*$, then $f(s) > 0$ for $s \in [\Phi_{bd}, \phi^*)$ due to (F1)–(F2). Therefore, the initial-value problem (3.261)–(3.263) can be reformulated as

$$\tilde{U}'' + f(\tilde{U}) = 0 \quad \text{in } (0, \infty), \tag{3.268}$$

$$\tilde{U}(0) = U_0, \tag{3.269}$$

$$\tilde{U}'(0) = \operatorname{sgn}(\phi^* - \Phi_{bd})\sqrt{-2F(U_0)}, \tag{3.270}$$

where U_0 (between ϕ^* and Φ_{bd}) is uniquely determined by (3.267).

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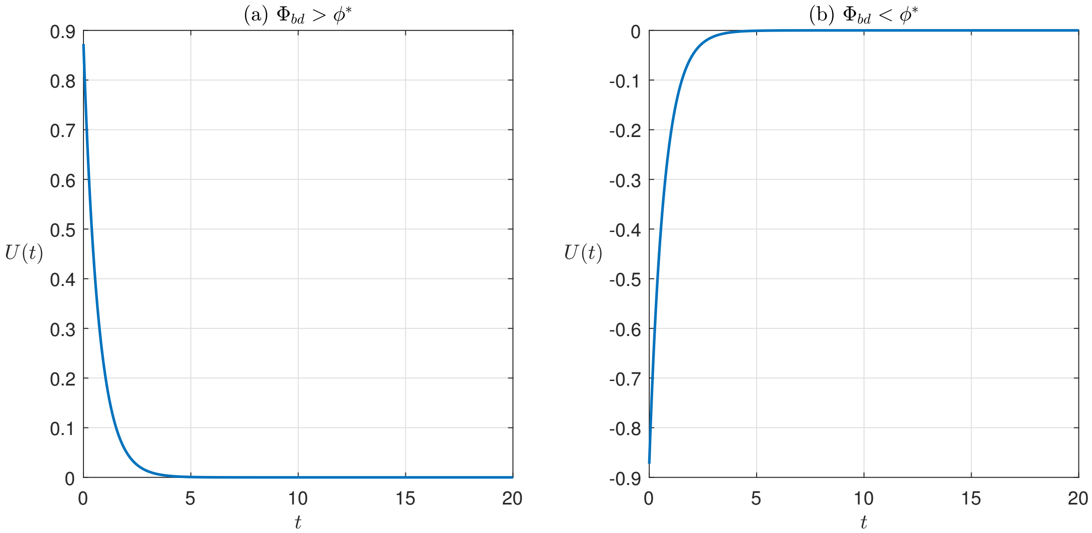

Figure 3.4: We sketch the numerical profile for the solution U to (3.258)–(3.260) for the case (a) $\Phi_{bd} = 1$ and the case (b) $\Phi_{bd} = -1$, which is consistent with Proposition 3B.1. Here $f(\phi) = \exp(\phi) - \exp(-\phi)$ and $\gamma = 0.1$.

To prove $\tilde{U} \equiv U$ on $[0, \infty)$, we need the following proposition.

Proposition 3B.1. *Let $\tilde{U}$ be the solution to* (3.268)–(3.270).

(a) If $\Phi_{bd} > \phi^*$, then $\Phi_{bd} \geq \tilde{U}(t) > \phi^*$ and $\tilde{U}'(t) < 0$ for $t \geq 0$;

(b) if $\Phi_{bd} < \phi^*$, then $\Phi_{bd} \leq \tilde{U}(t) < \phi^*$ and $\tilde{U}'(t) > 0$ for $t \geq 0$.

Proof. We first claim that $\tilde{U}'(t) \neq 0$ for $t \geq 0$. Suppose by contradiction that there exists $t_1 \in (0, \infty)$ such that $\tilde{U}'(t_1) = 0$. Multiplying (3.268) by $\tilde{U}$ and then integrating it over $[0, t]$, we obtain

$$\tilde{U}'^2(t) = \tilde{U}'^2(0) + 2(F(\tilde{U}(0)) - F(\tilde{U}(t))) = -2F(\tilde{U}(t)) \quad \text{for } t \geq 0. \tag{3.271}$$

Here we have used (3.269)–(3.270). By (3.271) and $\tilde{U}'(t_1) = 0$, we get $\tilde{U}(t_1) = \phi^*$, which implies $\tilde{U} \equiv \phi^*$ on $[t_1, \infty)$. Due to the unique continuation, $U \equiv \phi^*$ on $[0, \infty)$, which contradicts to (3.269). Hence $\tilde{U}'(t) \neq 0$ for $t \geq 0$. By (3.266) and (3.271), it is clear that $\tilde{U}(t) \neq \phi^*$ for $t \geq 0$ because $\tilde{U}'(t) \neq 0$ for $t \geq 0$.

Now we prove (a) and (b). For the case of (a), we assume that $\Phi_{bd} > \phi^*$. From (3.267) and (3.269)–(3.270), we have $\Phi_{bd} \geq \tilde{U}(0) > \phi^*$ and $\tilde{U}'(0) < 0$. Since $\tilde{U}(t) \neq \phi^*$ and $\tilde{U}'(t) \neq 0$ for $t \geq 0$, which implies $\Phi_{bd} \geq \tilde{U}(t) > \phi^*$ and $\tilde{U}'(t) < 0$ for $t \geq 0$. Thus, the proof of (a) is complete. The proof of (b) is similar to (a). Therefore, we complete the proof of Proposition 3B.1. ☐

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Now we are in the position to show that $\tilde{U}$ solves equations (3.258)–(3.260) and the uniqueness of (3.258)–(3.260), which implies $\tilde{U} \equiv U$ in $[0, \infty)$. By (3.267) and (3.269)–(3.270), we have

$$\tilde{U}(0) - \gamma \tilde{U}'(0) = U_0 \gamma \operatorname{sgn}(\phi^* - \Phi_{bd}) \sqrt{-2F(U_0)} = \Phi_{bd},$$

which means $\tilde{U}$ satisfies (3.259). By Proposition 3B.1, $\tilde{U}$ is bounded and strictly monotonic on $[0, \infty)$, which implies that there exists a constant C such that

$$\lim_{t \to \infty} \tilde{U}(t) = C.$$

Suppose by contradiction that $C \neq \phi^*$. By (3.266) and (3.269)–(3.271), we get

$$\lim_{t \to \infty} \tilde{U}'^2(t) = \tilde{U}'^2(0) + 2(F(U_0) - F(C)) = -2F(C) > 0. \tag{3.272}$$

Since $\tilde{U}'(t) \neq 0$ for $t \geq 0$, we can use (3.272) to get $\lim\limits_{t \to \infty} |\tilde{U}(t)| = \infty$, which leads to a contradiction. Thus, $\lim\limits_{t \to \infty} \tilde{U}(t) = \phi^*$, i.e., $\tilde{U}$ satisfies (3.260). Hence $\tilde{U}$ solves equations (3.258)–(3.260). To prove $\tilde{U} \equiv U$ on $[0, \infty)$, it suffices to show the uniqueness of solution to (3.258)–(3.260). Suppose that there exist two solutions U_1 and U_2 to equations (3.258)–(3.260). Let $\overline{U} = U_1 - U_2$. Then $\overline{U}$ satisfies

$$\overline{U}'' + c(t)\overline{U} = 0 \quad \text{in } (0, \infty), \tag{3.273}$$

$$\overline{U}(0) - \gamma \overline{U}'(0) = 0, \tag{3.274}$$

$$\lim_{t \to \infty} \overline{U}(t) = 0, \tag{3.275}$$

where

$$c(t) = \begin{cases} \dfrac{f(U_1(t)) - f(U_2(t))}{U_1(t) - U_2(t)} & \text{if } U_1(t) \neq U_2(t); \\ f'(U_1(t)) & \text{if } U_1(t) = U_2(t). \end{cases}$$

Note that $c(t) < 0$ for $t \geq 0$ by (F1). Thus, by the standard maximum principle, $\overline{U} \equiv 0$ on $[0, \infty)$, and we obtain the uniqueness of solution to (3.258)–(3.260). Therefore, $\tilde{U} \equiv U$ on $[0, \infty)$ and hence U satisfies Proposition 3B.1 and (3.271).

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The following result will be used in Appendix 3C to prove the existence of solution to (3.10)–(3.12) and (3.24)–(3.26).

Proposition 3B.2. *Let U be the solution to (3.258)–(3.260). Then we have*

(a) $|U'(t)| \le |U'(0)| \exp(-m_f t)$ *for* $t \ge 0$, *where* $m_f = m_f([\min\{\phi^*, \Phi_{bd}\}, \max\{\phi^*, \Phi_{bd}\}])$.

(b) $\int_0^\infty U'^2(t)\,\mathrm{d}t = \operatorname{sgn}(\phi^* - \Phi_{bd}) \int_{U_0}^{\phi^*} \sqrt{-2F(s)}\,\mathrm{d}s < \infty$.

(c) $\int_0^t (U'(s))^{-2}\,\mathrm{d}s \ge t^2 (\int_0^\infty U'^2(s)\,\mathrm{d}s)^{-1}$ *for* $t \ge 0$.

(d) $\lim_{t\to\infty} [f(U(t))/U'(t)] = -\sqrt{-f'(\phi^*)}$.

(e) $\int_0^\infty (U'(s_1))^{-2} \int_{s_1}^\infty U'^2(s_2)\,\mathrm{d}s_2\,\mathrm{d}s_1 = \infty$.

Proof. By (F1) and the standard comparison theorem, we can easily get (a). For (b), we can use the change of variable and (3.260) to obtain

$$\int_0^\infty U'^2(t)\,\mathrm{d}t = \operatorname{sgn}(\phi^* - \Phi_{bd}) \int_0^\infty \sqrt{-2F(U(t))}U'(t)\,\mathrm{d}t = \operatorname{sgn}(\phi^* - \Phi_{bd}) \int_{U_0}^{\phi^*} \sqrt{-2F(s)}\,\mathrm{d}s < \infty,$$

which gives (b). Part (c) follows directly from (b) and Cauchy–Schwarz inequality. For (d), we first note that $f(U(t))/U'(t) > 0$ for $t \ge 0$ by (F1) and Proposition 3B.1. Then applying L'Hôpital's rule, we have

$$\begin{aligned} \lim_{t\to\infty} \frac{f(U(t))}{U'(t)} &= \sqrt{\lim_{t\to\infty} \frac{[f(U(t))]^2}{U'^2(t)}} \\ &= \sqrt{\lim_{t\to\infty} \frac{2f(U(t))f'(U(t))U'(t)}{2U'(t)U''(t)}} = \sqrt{-\lim_{t\to\infty} f'(U(t))} = \sqrt{-f'(\phi^*)}, \end{aligned}$$

which implies (d). To prove (e), we combine (a), (c), (d) and (3.258) and then apply L'Hôpital's rule to get

$$\lim_{t\to\infty} U'^2(t) \int_0^t \frac{\mathrm{d}s}{U'^2(s)} = \lim_{t\to\infty} \frac{\int_0^t \frac{\mathrm{d}s}{U'^2(s)}}{\frac{1}{U'^2(t)}} = \lim_{t\to\infty} \frac{\frac{1}{U'^2(t)}}{-2\frac{U''(t)}{U'^3(t)}} = \frac{1}{2} \lim_{t\to\infty} \frac{U'(t)}{f(U(t))} = \frac{1}{2\sqrt{-f'(\phi^*)}} > 0.$$

Thus, one may apply the Fubini's theorem to get

$$\int_0^\infty \frac{1}{U'^2(s_1)} \int_{s_1}^\infty U'^2(s_2)\,\mathrm{d}s_2\,\mathrm{d}s_1 = \int_0^\infty U'^2(s_2) \int_0^{s_2} \frac{1}{U'^2(s_1)}\,\mathrm{d}s_1\,\mathrm{d}s_2 = \infty,$$

which implies (e). Therefore, the proof of Proposition 3B.2 is complete. ☐

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3C Properties of the solution to (3.10)–(3.12) and (3.24)–(3.26)

In this appendix, we establish the existence, uniqueness, and qualitative properties for solutions to (3.10)–(3.12) and (3.24)–(3.26). For the sake of simplicity, equations (3.10)–(3.12) and (3.24)–(3.26) can be represented as follows.

$$V'' + f'(U)V = U' \quad \text{in } (0,\infty), \tag{3.276}$$

$$V(0) - \gamma V'(0) = 0, \tag{3.277}$$

$$\lim_{t\to\infty} V(t) = 0, \tag{3.278}$$

where U is the solution to equations (3.258)–(3.260), $f \in \mathcal{C}^\infty(\mathbb{R})$ and $\gamma \geq 0$ are as given in (3.258)–(3.259). By standard ODE theory, the solution V to equations (3.276)–(3.278) can be represented as

$$V(t) = \frac{V_0}{U'(0)}U'(t) - U'(t)\int_0^t \frac{1}{U'^2(s_1)}\int_{s_1}^\infty U'^2(s_2)\,\mathrm{d}s_2\,\mathrm{d}s_1 \quad \text{for } t \geq 0, \tag{3.279}$$

where V_0 is given by

$$V_0 = -\frac{\gamma}{U'(0) + \gamma f(U_0)}\int_0^\infty U'^2(t)\,\mathrm{d}t. \tag{3.280}$$

Note that V_0 is well-defined due to Proposition 3B.2(b) and $U'(0) + \gamma f(U_0) \neq 0$. Clearly, (3.279) with (3.280) satisfies (3.276)–(3.277). It suffices to verify that (3.279) satisfies (3.278). By (3.258), (3.260), (F1)–(F2), Proposition 3B.2 and L'Hôpital's rule, we obtain

$$\begin{aligned}
\lim_{t\to\infty} V(t) &= \lim_{t\to\infty} \frac{\displaystyle\int_0^t \frac{1}{U'^2(s_1)}\int_{s_1}^\infty U'^2(s_2)\,\mathrm{d}s_2\,\mathrm{d}s_1}{\dfrac{1}{U'(t)}} = \lim_{t\to\infty} \frac{\dfrac{1}{U'^2(t)}\displaystyle\int_t^\infty U'^2(s_2)\,\mathrm{d}s_2}{-\dfrac{1}{U'^2(t)}U''(t)} \\
&= \lim_{t\to\infty} \frac{-\displaystyle\int_t^\infty U'^2(s)\,\mathrm{d}s}{f(U(t))} = \lim_{t\to\infty} \frac{U'^2(t)}{f'(U(t))U'(t)} = \lim_{t\to\infty} \frac{U'(t)}{f'(U(t))} = \frac{0}{f'(\phi^*)} = 0.
\end{aligned}$$

Thus, (3.279) defines a solution to (3.276)–(3.278).

Now we prove the uniqueness of the solution to (3.276)–(3.278). Suppose that there exist two solutions V and $\tilde{V}$ to (3.276)–(3.278). Let $\overline{V} = V - \tilde{V}$. Then $\overline{V}$ satisfies

$$\overline{V}'' + f'(U)\overline{V} = 0 \quad \text{in } (0,\infty), \tag{3.281}$$

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$$\overline{V}(0) - \gamma \overline{V}'(0) = 0, \tag{3.282}$$

$$\lim_{t\to\infty} \overline{V}(t) = 0. \tag{3.283}$$

Hence by (F1) and the standard maximum principle, $\overline{V} \equiv 0$ on $[0,\infty)$, and the solution to (3.276)–(3.278) must be given by (3.279).

Proposition 3C.1. *Let V be the unique solution to (3.276)–(3.278).*

(a) If $\Phi_{bd} > \phi^*$, then V is nonnegative on $[0,\infty)$, and there exists a unique $t^* \in (0,\infty)$ such that V is strictly increasing on $[0,t^*)$ and strictly decreasing on (t^*,∞). Moreover, if $\gamma > 0$, then V is positive on $[0,\infty)$.

(b) If $\Phi_{bd} < \phi^*$, then V is nonpositive on $[0,\infty)$, and there exists a unique $t^* \in (0,\infty)$ such that V is strictly decreasing on $[0,t^*)$ and strictly increasing on (t^*,∞). Moreover, if $\gamma > 0$, then V is negative on $[0,\infty)$.

Proof. We first note that

Claim 3C.2. $\lim_{t\to\infty} V'(t) = 0$.

Proof of Claim 3C.2. By (3.258) and (3.279), we have

$$V'(t) = -\frac{V_0}{U'(0)} f(U(t)) + f(U(t)) \int_0^t \frac{1}{U'^2(s_1)} \int_{s_1}^\infty U'^2(s_2)\, \mathrm{d}s_2\, \mathrm{d}s_1 - \frac{1}{U'(t)} \int_t^\infty U'^2(s)\, \mathrm{d}s.$$

By (F2), (3.258) and Proposition 3B.2(d), we apply the L'Hôpital's rule to obtain

$$\begin{aligned}
\lim_{t\to\infty} V'(t) &= \lim_{t\to\infty} \left[\frac{\displaystyle\int_0^t \frac{1}{U'^2(s_1)} \int_{s_1}^\infty U'^2(s_2)\, \mathrm{d}s_2\, \mathrm{d}s_1}{[f(U(t)]^{-1}} - \frac{\displaystyle\int_t^\infty U'^2(s)\, \mathrm{d}s}{U'(t)} \right] \\
&= \lim_{t\to\infty} \left[\frac{\displaystyle\frac{1}{U'^2(t)} \int_t^\infty U'^2(s)\, \mathrm{d}s}{[f(U(t))]^{-2} f'(U(t)) U'(t)} + \frac{U'^2(t)}{U''(t)} \right] \\
&= \frac{1}{f'(\phi^*)} \lim_{t\to\infty} \frac{\displaystyle [f(U(t))]^2 \int_t^\infty U'^2(s)\, \mathrm{d}s}{U'^3(t)} - \lim_{t\to\infty} \frac{U'^2(t)}{f(U(t))} \\
&= -\lim_{t\to\infty} \frac{\displaystyle\int_t^\infty U'^2(s)\, \mathrm{d}s}{U'(t)} = \lim_{t\to\infty} \frac{U'^2(t)}{U''(t)} = -\lim_{t\to\infty} \frac{U'^2(t)}{f(U(t))} = 0,
\end{aligned}$$

which completes the proof of Claim 3C.2. □

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We now assume $\Phi_{bd} > \phi^*$ and prove (a). By Proposition 3B.1(a), we have $U'(0) < 0$ and $f(U_0) < 0$. Along with (3.280), we get $V(0) = V_0 > 0$, and $V'(0) = -(U'(0) + \gamma f(U_0))^{-1} \int_0^\infty U'^2(t)\,\mathrm{d}t > 0$. Suppose by contradiction that there exists $t_0 \in (0, \infty)$ such that $V(t_0) \leq 0$. Since $\lim_{t\to\infty} V(t) = 0$, we may assume that V attains its minimum value at $t_0 \in (0, \infty)$, which implies $V''(t_0) \geq 0$. Then by (3.276), we have $U'(t_0) = V''(t_0) + f'(U(t_0))V(t_0) \geq 0$, which contradicts Proposition 3B.1(a). This shows that V is positive on $[0, \infty)$. Since $V'(0) > 0$ and $\lim_{t\to\infty} V(t) = 0$, there exists $t^* \in (0, \infty)$ such that V attains its maximum value at t^* and $V'(t^*) = 0$. Suppose by contradiction that there exists another maximum point t_1 such that $V'(t_1) = 0$. Without loss of generality, we may assume that $t_1 < t^*$, and there exists $t_2 \in (t_1, t^*)$ such that V attains its local minimum value at t_2 with $V'(t_2) = 0$ and $V'(t) \geq 0$ on (t_2, t^*). Integrating (3.276) over $[t, \infty)$ and using (a), we obtain

$$V'(t) = \frac{f(U(t))V(t) + \int_t^\infty U'^2(s)\,\mathrm{d}s}{-U'(t)} \quad \text{for } t \geq 0. \tag{3.284}$$

Clearly, $V'(t_2) = V'(t^*) = 0$. Let $G(t) = f(U(t))V(t) + \int_t^\infty U'^2(s)\,\mathrm{d}s$ for $t \in \mathbb{R}$. Then $G(t_2) = G(t^*) = 0$. Differentiating G gives

$$G'(t) = f'(U(t))U'(t)V(t) + f(U(t))V'(t) - U'^2(t) \quad \text{for } t \in \mathbb{R}.$$

By Proposition 3B.1(a) and (F1)–(F2), we find that $U'(t) < 0$, $f(U(t)) < 0$ and $f'(U(t)) < 0$. Since $V(t) > 0$ and $V'(t) > 0$ on (t_2, t^*), we get $G'(t) < 0$ on (t_2, t^*), which contradcits with $g(t_2) = g(t^*) = 0$. Therefore, there exists a unique $t^* \in (0, \infty)$ such that V attains its maximum value. The proof of (a) is complete.

Next we assume $\Phi_{bd} < \phi^*$ and prove (b). By Proposition 3B.1(b), we have $U'(0) > 0$ and $f(U_0) > 0$. Along with (3.280), we get $V(0) = V_0 < 0$, and $V'(0) = -(U'(0) + \gamma f(U_0))^{-1} \int_0^\infty U'^2(t)\,\mathrm{d}t < 0$. Suppose by contradiction that there exists $t_0 \in (0, \infty)$ such that $V(t_0) \geq 0$. Since $\lim_{t\to\infty} V(t) = 0$, we may assume that V attains its maximum value at $t_0 \in (0, \infty)$, which implies $V''(t_0) \leq 0$. Then by (3.276), we have $U'(t_0) = V''(t_0) + f'(U(t_0))V(t_0) \leq 0$, which contradicts to Proposition 3B.1(b). This shows that V is negative on $[0, \infty)$. Since $V'(0) < 0$ and $\lim_{t\to\infty} V(t) = 0$, there exists $t^* \in (0, \infty)$ such that V attains its minimum value at t^* and $V'(t^*) = 0$. Suppose by contradiction that there exists another minimum point t_1 such that $V'(t_1) = 0$. Then by a similar fashion of (b), we can use (3.284) to get a contradiction

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because $U'(t) > 0$, $f(U(t)) > 0$ and $f'(U(t)) < 0$ (cf. Proposition 3B.1(b) and (F1)–(F2)). Hence there exists a unique $t^* \in (0, \infty)$ such that V attains its minimum value, which implis (b). Therefore, we complete the proof of Proposition 3C.1. $\square$

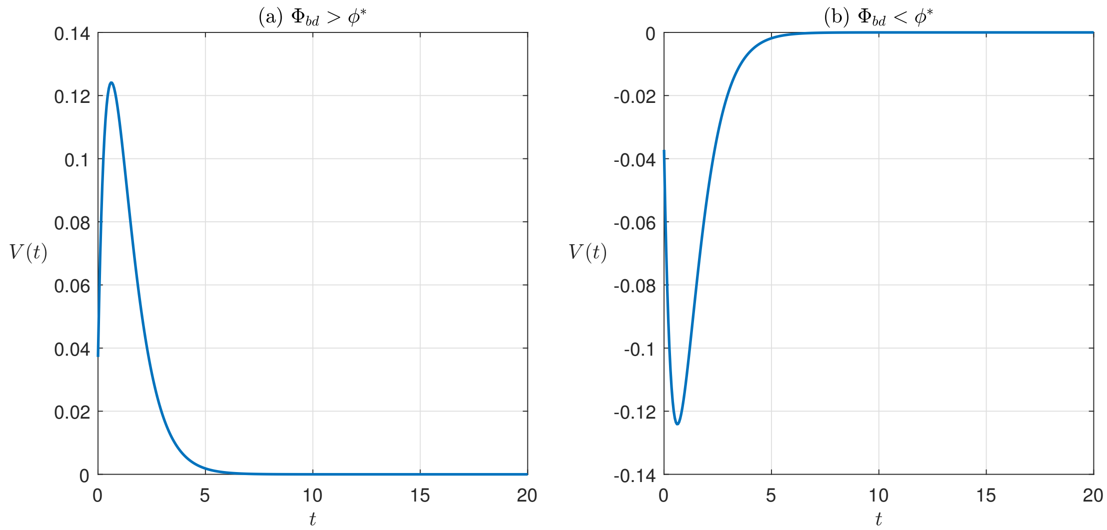

Figure 3.5: We sketch the numerical profile for the solution V to (3.276)–(3.278) for the case (a) $\Phi_{bd} = 1$ and the case (b) $\Phi_{bd} = -1$, which is consistent with Proposition 3C.1. Here $f(\phi) = \exp(\phi) - \exp(-\phi)$ and $\gamma = 0.1$.

Proposition 3C.3. *Let U and V be the unique solutions to* (3.258)–(3.260) *and* (3.276)–(3.278), *respectively. If $\Phi_{bd} \neq \phi^*$, then function $g := f(U)V + U'V'$ is negative on* $[0, \infty)$.

Proof. By (3.258), (3.276) and Proposition 3B.1, we have

$$g'(t) = f'(U(t))U'(t)V(t) + f(U(t))V'(t) + U''(t)V'(t) + U'(t)V''(t) = U'^2(t) > 0$$

for $t \geq 0$ and $\Phi_{bd} \neq \phi^*$, which implies g is strictly increasing on $[0, \infty)$. By (F2), (3.260), (3.278) and Claim 3C.2, it is clear that $\lim_{t\to\infty} g(t) = 0$. Hence $g(t) < 0$ for $t \geq 0$, and the proof of Proposition 3C.3 is complete. $\square$

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3D Properties of the solution to (3.27)–(3.29)

In this appendix, we establish the existence, uniqueness, and qualitative properties for solutions to (3.27)–(3.29).

$$w_k'' + f_0'(u_k)w_k = -f_1(u_k) \quad \text{in } (0,\infty), \tag{3.285}$$

$$w_k(0) - \gamma_k w_k'(0) = 0, \tag{3.286}$$

$$\lim_{t\to\infty} w_k(t) = Q, \tag{3.287}$$

where u_k are the solutions to equations (3.21)–(3.23), and $\gamma_k \geq 0$ are given fixed constants for $k = 0, 1, \ldots, K$. Here f_0 and f_1 are smooth functions defined by

$$f_0(\phi) = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \exp(-z_i(\phi - \phi_0^*)) \quad \text{and} \quad f_1(\phi) = -Qf_0'(\phi) + \hat{f}_1(\phi) \quad \text{for } \phi \in \mathbb{R}, \tag{3.288}$$

where $Q \in \mathbb{R}$ (defined in (3.32)), $m_i > 0$ and

$$\hat{f}_1(\phi) = \frac{1}{|\Omega|}\sum_{i=1}^{I} \hat{m}_i z_i \exp(-z_i(\phi - \phi_0^*)) \quad \text{for } \phi \in \mathbb{R}, \tag{3.289}$$

$$\hat{m}_i = \frac{m_i}{|\Omega|}\sum_{k=0}^{K} |\partial\Omega_k| \int_0^\infty [1 - \exp(-z_i(u_k(s) - \phi_0^*))]\, \mathrm{d}s \quad \text{for } i = 1, \ldots, I, \tag{3.290}$$

In addition, ϕ_0^* and $u_k(0)$ satisfy (cf. (3.150)–(3.151))

$$\phi_{bd,k} - u_k(0) = \operatorname{sgn}(\phi_{bd,k} - \phi_0^*)\gamma_k \sqrt{\frac{2}{|\Omega|}\sum_{i=1}^{I} m_i[\exp(-z_i(u_k(0) - \phi_0^*)) - 1]} \quad \text{for } k = 0, 1, \ldots, K, \tag{3.291}$$

$$\sum_{k=0}^{K} |\partial\Omega_k| u'(0) = \sum_{k=0}^{K} |\partial\Omega_k| \frac{u_k(0) - \phi_{bd,k}}{\gamma_k} = 0. \tag{3.292}$$

By standard ODE theory, the solution w_k to equations (3.285)–(3.287) can be represented as

$$w_k(t) = \frac{w_k(0)}{u_k'(0)}u_k'(t) + u_k'(t)\int_0^t \frac{Qf_0(u_k(s)) - \hat{F}_1(u_k(s))}{u_k'^2(s)}\, \mathrm{d}s \quad \text{for } t \geq 0, \tag{3.293}$$

where $w_k(0)$ and $\hat{F}_1$ are given by

$$w_k(0) = \frac{\gamma_k(Qf_0(u_k(0)) - \hat{F}_1(u_k(0)))}{u_k'(0) + \gamma_k f_0(u_k(0))}, \tag{3.294}$$

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$$\hat{F}_1(\phi) = \int_{\phi_0^*}^{\phi} \hat{f}_1(s)\,\mathrm{d}s = \frac{1}{|\Omega|}\sum_{i=1}^{I} \hat{m}_i[1-\exp(-z_i(\phi-\phi_0^*))] \quad \text{for } \phi \in \mathbb{R}. \tag{3.295}$$

Note that (3.294) is well-defined because $u_k'(0) + \gamma_k f_0(u_k(0)) \neq 0$. Clearly, (3.293) with (3.294)–(3.295) satisfies (3.285)–(3.286). To verify that (3.293) satisfies (3.287), we need the following claim.

Claim 3D.1. *Let u_k be the solution to (3.21)–(3.23), $\hat{f}_1$ and $\hat{F}_1$ defined in (3.289) and (3.295), respectively, and ϕ_0^* be the unique zero of f_0. Then we have*

(a) $\hat{f}_1(\phi_0^*) = |\Omega|^{-1}\sum_{i=1}^{I}\hat{m}_i z_i = 0$;

(b) $\left|\int_0^\infty (u_k'(s))^{-2}[Qf_0(u_k(s)) - \hat{F}_1(u_k(s))]\,\mathrm{d}s\right| = \infty$ *if* $Q \neq 0$.

Proof of Claim 3D.1. By (3.288) and $\sum_{i=1}^{I} m_i z_i = 0$ (cf. (3.3)), we have

$$\begin{aligned}
\hat{f}_1(\phi_0^*) &= \frac{1}{|\Omega|}\sum_{i=1}^{I}\hat{m}_i z_i = \frac{1}{|\Omega|}\sum_{i=1}^{I} m_i z_i \sum_{k=0}^{K}|\partial\Omega_k| \int_0^\infty [1-\exp(-z_i(u_k(s)-\phi_0^*))]\,\mathrm{d}s \\
&= \frac{1}{|\Omega|}\sum_{k=0}^{K}|\partial\Omega_k|\int_0^\infty \left(\sum_{i=1}^{I} m_i z_i - \sum_{i=1}^{I} m_i z_i \exp(-z_i(u_k(s)-\phi_0^*))\right)\mathrm{d}s \\
&= -\frac{1}{|\Omega|}\sum_{k=0}^{K}|\partial\Omega_k|\int_0^\infty f_0(u_k(s))\,\mathrm{d}s.
\end{aligned}$$

Along with (3.21)–(3.22), (3.292) and Proposition 3B.2(a), we get

$$\hat{f}_1(\phi_0^*) = \frac{1}{|\Omega|}\sum_{k=0}^{K}|\partial\Omega_k|\int_0^\infty u_k''(s)\,\mathrm{d}s = \frac{1}{|\Omega|}\sum_{k=0}^{K}|\partial\Omega_k|(-u_k'(0)) = \frac{1}{|\Omega|}\sum_{k=0}^{K}|\partial\Omega_k|\frac{\phi_{bd,k} - u_k(0)}{\gamma_k} = 0.$$

which shows (a). To prove (b), we use (3.21) and L'Hôpital's rule to get

$$\begin{aligned}
\lim_{t\to\infty}\frac{Qf_0(u_k(t)) - \hat{F}_1(u_k(t))}{u_k'^2(t)} &= \lim_{t\to\infty}\frac{Qf_0'(u_k(t))u_k'(t) - \hat{f}_1(u_k(t))u_k'(t)}{2u_k'(t)u_k''(t)} \\
&= \lim_{t\to\infty}\frac{-Qf_0'(u_k(t)) + \hat{f}_1(u_k(t))}{2f_0(u_k(t))}.
\end{aligned}$$

By (3.23)–(3.30), (3.141), Proposition 3B.1, we have $f_0(u_k(t)) \neq 0$ for $t \geq 0$ and $\lim_{t\to\infty} f_0(u_k(t)) = 0$. By (3.23), (3.141), (a) and the condition $Q \neq 0$, we get

$$\lim_{t\to\infty}(-Qf_0'(u_k(t)) + \hat{f}_1(u_k(t))) = -Qf_0'(\phi_0^*) \neq 0.$$

Hence $\left|\int_0^\infty (u_k'(s))^{-2}[Qf_0(u_k(s)) - \hat{F}_1(u_k(s))]\,\mathrm{d}s\right| = \infty$, which gives (b) and completes the proof of Claim 3D.1. □

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Now we show that (3.293) satisfies (3.287) and obtain the existence of (3.285)–(3.287). For the case that $Q \neq 0$, we can use (3.258), Claim 3D.1 and L'Hôpital's rule to get

$$
\begin{aligned}
\lim_{t\to\infty} w_k(t) &= \lim_{t\to\infty} \frac{\dfrac{w_k(0)}{u_k'(0)} + \displaystyle\int_0^t \frac{Qf_0(u_k(s)) - \hat{F}_1(u_k(s))}{u_k'^2(s)}\,\mathrm{d}s}{\dfrac{1}{u_k'(t)}} \\
&= \lim_{t\to\infty} \frac{\dfrac{Qf_0(u_k(t)) - \hat{F}_1(u_k(t))}{u_k'^2(t)}}{-\dfrac{u_k''(t)}{u_k'^2(t)}} \\
&= \lim_{t\to\infty} \frac{Qf_0(u_k(t)) - \hat{F}_1(u_k(t))}{f_0(u_k(t))} = Q + \lim_{t\to\infty} \frac{-\hat{f}_1(u_k(t))u_k'(t)}{f_0'(u_k(t))u_k'(t)} \\
&= Q - \lim_{t\to\infty} \frac{\hat{f}_1(u_k(t))}{f_0'(u_k(t))} = Q - \frac{\hat{f}_1(\phi_0^*)}{f_0'(\phi_0^*)} = Q,
\end{aligned}
\tag{3.296}
$$

which gives (3.287) for $Q \neq 0$. This shows the existence of a solution (3.285)–(3.287) for $Q \neq 0$. For the case of $Q = 0$, we define w_k^0 and $w_k^{\pm}$ by (3.293) for $Q = 0$ and $Q = \pm 1$, respectively. Then due to the linearity of (3.293) (with respect to Q), $w_k^0 = (w_k^+ + w_k^-)/2$. By (3.296) with $Q = \pm 1$, we find that $\lim_{t\to\infty} w_k^0(t) = \lim_{t\to\infty} (w_k^+(t) + w_k^-(t))/2 = (1 + (-1))/2 = 0$, which implies that w_k^0 satisfies (3.287) for $Q = 0$. Therefore, we get the existence of the solution to (3.285)–(3.287) for $Q \in \mathbb{R}$.

It remains to prove the uniqueness of the solution to (3.285)–(3.287). Suppose that there exist two solutions w_k and $\tilde{w}_k$ of (3.285)–(3.287). Let $\overline{w}_k = w_k - \tilde{w}_k$. Then $\overline{w}_k$ satisfies

$$
\begin{aligned}
&\overline{w}_k'' + f_0'(u_k)\overline{w}_k = 0 \quad \text{in } (0,\infty), \\
&\overline{w}_k(0) - \gamma_k \overline{w}_k'(0) = 0, \\
&\lim_{t\to\infty} \overline{w}_k(t) = 0.
\end{aligned}
$$

By the standard maximum principle, it is easy to obtain $\overline{w}_k \equiv 0$ on $[0,\infty)$, which gives the uniqueness of solution to (3.285)–(3.287).

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4 Near- and far-field expansions for stationary solutions to Poisson–Nernst–Planck equations[2]

4.1 Introduction

With the development of current nanotechnology in electrochemistry [46, 102], analysis of solutions to mathematical models with regulated parameters plays a more and more important role in investigating the distribution of electrostatic potential in electrolyte-like solutions (cf. [35, 48, 53, 55, 63, 91, 98, 106, 108]). In the past few decades, a key ingredient for understanding of such microscopic phenomena is the Poisson–Boltzmann equation [20, 110, 112], but which suffered from deficiencies that are well known. Different types of nonlinear electrochemistry systems (see, e.g., [19, 45, 51, 52, 54, 56, 57, 77, 84, 85, 92, 103, 105, 107]) have already been modeled and the corresponding computational confirmation is expected to reach theoretical prediction.

Among such phenomena in electrochemistry, an unstable one relates to the non-electroneutrality characterized by the localization of excess charge distributions. For instance, a faradaic current drives ions from one electrode surface to another and results in an ionic distribution which is non-uniform near the electrode surface. We refer the reader to [36, 78]. Other instabilities including the electroconvective instability in channels have been investigated; see, e.g., [86] and references therein. Despite the intensive investigation yielding detailed information and the reasonable success, little is known about the non-electroneutral phenomenon near the charged surface. In [14, 15], employing the one dimensional Poisson–Nernst–Planck (PNP) system provides an underlying framework for such phenomena, where it is reasonably assumed that all ions transport in the same direction along a tubular-like

[2]This chapter is adapted from an article co-authored with Professor Chiun-Chang Lee and my advisor, Professor Tai-Chia Lin, which has been published in [89]. I am grateful to Professor Chiun-Chang Lee for suggesting the problem and to both professors for their valuable suggestions on the manuscript. My main contributions include establishing the rigorous mathematical proofs and producing the numerical figures.

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mircodomain with finite-length so that the physical domain can be set as a one-dimensional interval $\Omega = (0,1)$. At the beginning of this work we consider the model for single-ion species which is represented as

$$\begin{cases} \dfrac{\partial p}{\partial t}(t,r) = D_p \dfrac{\partial}{\partial r}\left(\dfrac{\partial p}{\partial r}(t,r) + \dfrac{z_p \mathrm{e}_0}{k_B T} p(t,r) \dfrac{\partial u}{\partial r}(t,r)\right), \\ -\dfrac{\partial^2 u}{\partial r^2}(t,r) = \lambda(\rho_{\mathrm{f}}(r) + z_p \mathrm{e}_0 p(t,r)), \qquad (t,r) \in (0,\infty) \times (0,1), \end{cases} \tag{4.1}$$

with the no-flux boundary conditions

$$\left(\frac{\partial p}{\partial r} + \frac{z_p \mathrm{e}_0}{k_B T} p \frac{\partial u}{\partial r}\right)(t,0) = \left(\frac{\partial p}{\partial r} + \frac{z_p \mathrm{e}_0}{k_B T} p \frac{\partial u}{\partial r}\right)(t,1) = 0, \ t > 0, \tag{4.2}$$

and initial conditions $p(0,r) = p_0(r) > 0$ and $u(0,r) = u_0(r)$, for $r \in [0,1]$, which are compatible with the boundary conditions (4.2). Notice that (4.1)–(4.2) satisfies shift in variance in u and so we will set the boundary condition for u later.

Physically, u is the electrostatic potential, p is the density of cations, D_p is the diffusion coefficient, z_p is the valency of cations, e_0 is the elementary charge, k_B is the Boltzmann constant, T is the absolute temperature, and ρ_{f} is the fixed permanent charge density in the physical domain. Besides, $\lambda = d^2 \mathrm{e}_0 S/(\varepsilon_0 U_T)$ where ε_0 is the dielectric constant of the electrolyte, U_T is the thermal voltage, d is the diameter of the domain $\Omega = (0,1)$, and S is the appropriate concentration scale [97]. Note that the no-flux boundary conditions (4.2) ensure the conservation of ions, i.e.,

$$\int_0^1 p(t,r)\mathrm{d}r = \int_0^1 p_0(r)\mathrm{d}r, \ \forall\, t > 0. \tag{4.3}$$

To see the non-electroneutral phenomenon near the charged surface, λ is assumed a large positive parameter corresponding to the number of ions occupying an electrolytic region, as was studied in [14]. To basically understand the non-electroneutral phenomenon of u and p as $\lambda \gg 1$, we neglect the effect of fixed permanent charges by setting $\rho_{\mathrm{f}} = 0$ and focus mainly on their steady-state solutions. Under the standard dimensionless formulation, we may set

$$z_p = 1, \ \mathrm{e}_0/k_B T = 1, \ D_p = 1, \tag{4.4}$$

and regard λ as a positive parameter. Without loss of generality, we may assume $\int_0^1 p_0(r)\mathrm{d}r = 1$. Then by (4.3) and (4.4), the steady-states of (4.1)–(4.2) verify $u(t,r) = u_\lambda(r)$ and the nonlocal relation $p(t,r) = \frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}$ (see also, [13, equation

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(1.1) with $p = 1$], [14, Section 2.1] and [70] and references therein). As a consequence, u_λ satisfies

$$-u_\lambda''(r) = \rho_\lambda(r) := \frac{\lambda e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}, \quad r \in (0,1). \tag{4.5}$$

Physically, ρ_λ represents the net charge density of the ion species and the parameter $\int_0^1 \rho_\lambda(r)\mathrm{d}r$ denotes the total charges of ions. It should be mentioned that in [47, Chapter 10.6.1], (4.5) is named the reverse Liouville–Bratú–Gelfand (LBG) equation which can be regarded as the nonlocal LBG equation (see, e.g., [59] and references therein).

For (4.5), we consider the following condition at $r = 0$:

$$u_\lambda(0) = u_\lambda'(0) = 0, \tag{4.6}$$

as was presented in [14], where assumption $u_\lambda(0) = 0$ is actually due to a fact that equation (4.5) satisfies the shift invariance; that is, for any $c \in \mathbb{R}$, $u_\lambda + c$ also satisfies (4.5). We emphasize that such a setting immediately implies

$$u_\lambda'(1) = -\lambda. \tag{4.7}$$

This along with (4.6) asserts that there exists an interior point $r_{\mathrm{int}}^\lambda \in (0,1)$ depending on λ such that when $\lambda \to \infty$, the net charge density $\rho_\lambda(r_{\mathrm{int}}^\lambda) = -u_\lambda''(r_{\mathrm{int}}^\lambda) = u_\lambda'(0) - u_\lambda'(1) = \lambda$ asymptotically blows up. As will be clarified later, such a phenomenon occurs only when r_{int}^λ is sufficiently close to the boundary point $r = 1$ as λ tends to infinity. The boundary blow-up behavior theoretically represents the non-neutral phenomenon near the charged surface. We further refer the reader to [70, 75, 76] for the different boundary blow-up phenomena related models with multiple species under various boundary conditions.

It should be stressed that equation (4.5)–(4.6) has recently been studied by J. Cartailler et al [14], who used the phase-plane analysis to obtain the uniqueness of equation (4.5)–(4.6). A more general argument for the uniqueness can also be found in [71]. Moreover, the authors in [14] showed that as $\lambda \to \infty$, the numerical solution to (4.5)–(4.7) develops boundary layers near $r = 1$. They further studied the leading order term of the asymptotic expansions of $u_\lambda(1)$ with respect to $\lambda \gg 1$, and compared the result with their numerical simulation. *However, the more refined pointwise asymptotics for solutions, which is crucial for describing the sharp change*

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of u_λ near the boundary, remains unclear. The issue will be addressed in detail in this work.

4.1.1 Near-field and far-field expansions

The main difficulty lies in the lack of available asymptotic analysis for such singularly perturbed nonlocal models, which we shall explain as follows. Firstly, one observes from (4.5) and (4.6) that

$$u_\lambda(r),\ u_\lambda'(r),\ u_\lambda''(r) < 0 \ \text{ for } \ r \in (0,1). \tag{4.8}$$

In particular, (4.5)–(4.7) and (4.8) imply that $\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s \geq 1$ and

$$u_\lambda(1) = -\log\left(1 + \frac{\lambda}{2}\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s\right) \to -\infty \text{ as } \lambda \to \infty. \tag{4.9}$$

This illustrates the importance of the refined asymptotic expansions of $\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s$ with respect to $\lambda \gg 1$. A perspective on obtaining such asymptotics is to consider the following nonlinear eigenvalue problem with $\kappa > 0$ (see also, [14, Appendix]):

$$\begin{cases} -U_\kappa''(r) = \kappa e^{-U_\kappa(r)}, & r \in (0,1), \\ U_\kappa(0) = U_\kappa'(0) = 0. \end{cases} \tag{4.10}$$

When $\kappa \in (0, \pi^2/2)$, (4.10) has a unique solution $U_\kappa(r) = 2\log\cos(r\sqrt{\kappa/2})$ which is uniformly bounded on $[0,1]$, and $U_\kappa(1) \to -\infty$ as κ approaches $\pi^2/2$ from the left. However, when $\kappa > \pi^2/2$, (4.10) does not have solutions defined in the whole domain $(0,1)$. As a consequence, by (4.9) it is expected that a solution u_λ of (4.5)–(4.6) satisfies

$$\frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} < \frac{\pi^2}{2} \text{ for } \lambda > 0, \text{ and } \frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} \xrightarrow{\lambda\to\infty} \frac{\pi^2}{2}. \tag{4.11}$$

We will prove (4.11) rigorously and establish a more refined asymptotic expansion of $\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s$ with respect to $\lambda \gg 1$; see the detail in (4.27) and Remark 4.2. Moreover, it yields the limiting equation for (4.5)–(4.6) formally as follows:

$$\begin{cases} -U''(r) = \frac{\pi^2}{2} e^{-U(r)}, & r \in (0,1), \\ U(0) = U'(0) = 0, \end{cases} \tag{4.12}$$

and the unique solution

$$U(r) := U_{\frac{\pi^2}{2}}(r) = 2\log\cos\left(\frac{\pi}{2}r\right), \ r \in [0,1), \tag{4.13}$$

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represents the zeroth-order outer-solution to (4.5)–(4.6) with respect to $\lambda \gg 1$; see also, Remark 4.1. In passing we note that $U(r) \to -\infty$ and $U'(r) = -\pi \tan(\frac{\pi}{2}r) \to -\infty$ as $r \uparrow 1$, which formally coincide with the boundary asymptotic blow-up behavior of u_λ and u'_λ obtained respectively in (4.9) and (4.7). In summary, equation (4.5)–(4.6) is a nonlocal singularly perturbed model with small parameter $\frac{1}{\lambda}$ in front of its Laplace operator, and its limiting equation connects to a boundary blow-up problem (4.12).

What we want to point out is that the limiting model (4.12) of (4.5)–(4.6) cannot be directly obtained from applying the standard method of matched asymptotic expansions since the nonlocal coefficient $\frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}$ is involved with the parameter λ and its corresponding zeroth order outer solution $U(r)$ diverges near $r = 1$. To achieve the pointwise description of u_λ with respect to $\lambda \gg 1$, our first task is concerned with the asymptotic expansions for the solution u_λ, consisting of the near-field expansion and the far-field expansion. In order for the reader to realize the difference from the method of matched asymptotic expansions, we present the argument as follows:

- The **near-field expansion** focuses mainly on the refined asymptotics of $u_\lambda(r^\lambda_{p,\alpha})$ and $u'_\lambda(r^\lambda_{p,\alpha})$, where α and p are positive constants independent of λ, and

$$r^\lambda_{p,\alpha} = 1 - \frac{p}{\lambda^\alpha} \in (0,1), \ \ \lambda \gg 1, \tag{4.14}$$

  is sufficiently close to the boundary point $r = 1$. Let us emphasize again that as $\lambda \gg 1$, u_λ develops boundary layers and asymptotically blows up near the boundary $r = 1$ so that the asymptotic behavior of u_λ has dramatic changes in a thin neighborhood of $r = 1$. To better understand the structure of boundary layers, we are devoted to the pointwise asymptotics of $u_\lambda(r^\lambda_{p,\alpha})$ and $u'_\lambda(r^\lambda_{p,\alpha})$ with various α and p; see, for example, (4.18) and (4.19). Such a consideration essentially points out the difference between the analysis of (4.5)–(4.6) and the standard singularly perturbed equations.

- the **far-field expansion** focuses on the refined asymptotics for u_λ in $\mathcal{C}^1(K)$ as $\lambda \to \infty$, where K independent of λ is a compact subset of $[0, 1)$. We will frequently use the norm $\|\cdot\|_{\mathcal{C}^1(D)}$ defined by

$$\|f\|_{\mathcal{C}^1(D)} := \sup_D (|f| + |f'|) \tag{4.15}$$

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where D is a bounded set of $\mathbb{R}$ and $f \in \mathcal{C}^1(D)$. When $D = K$ is a compact subset of $[0,1)$, (4.15) is used for convenience to describe the asymptotic expansions of u in K.

We refer the reader to [44, 113] for the more detailed physical background of these two terminologies.

We are now in a position to draw the asymptotic behavior of u_λ. As will be presented in detail in Theorem 4.2, for any compact subset K (independent of λ) of $[0,1)$, we establish the **far-field expansion** of u_λ with the precise asymptotic expansions up to the order of $\frac{1}{\lambda^2}$:

$$u_\lambda(r) = U(r) + \pi r \left(\frac{\sin(\pi r)}{\lambda} - \frac{\pi r + 2\sin(\pi r)}{\lambda^2} \right) \sec^2\left(\frac{\pi}{2} r\right) + \frac{\widetilde{u}_\lambda(r)}{\lambda^2} \quad \text{and} \quad \sup_K |\widetilde{u}_\lambda| \xrightarrow{\lambda\to\infty} 0, \tag{4.16}$$

where U defined in (4.13) is the unique solution to (4.12). In contrast to the asymptotics of u_λ in any compact subset of $[0,1)$, our near-field analysis reveals a totally different asymptotic behaviour of u_λ near the boundary $r = 1$. In Theorem 4.3, we show that u_λ asymptotically blows up near the boundary $r = 1$ and obtain a novel asymptotics

$$u_\lambda\left(r_{p,\alpha}^\lambda\right) = \min\{2, 2\alpha\} \log \frac{1}{\lambda} + \mathcal{O}_{p,\alpha}, \tag{4.17}$$

where $\mathcal{O}_{p,\alpha}$ depends mainly on p and α and satisfies

$$\limsup_{\lambda\to\infty} |\mathcal{O}_{p,\alpha}| < \infty$$

(see Theorem 4.3 for the detailed expression of $\mathcal{O}_{p,\alpha}$). As it was mentioned previously, we shall stress that the concept of the near-field expansions focus on the pointwise asymptotic behavior of solutions sufficiently near the boundary, which is different from the standard matched inner solution. As a consequence, by (4.16) and (4.17) we know that a strong change of u_λ with $\lambda \to \infty$ merely occurs near the boundary $r = 1$, and there hold: (i) as $0 < \alpha < 1$, $\lim_{\lambda\to\infty} \frac{u_\lambda(r_{p,\alpha}^\lambda)}{\log \lambda^{-1}} = 2\alpha$ shows that the blow-up asymptotics of $u_\lambda(r_{p,\alpha}^\lambda)$ varies with α; (ii) for $0 < \alpha_1 < \alpha_2 < 1$, interior points $1 - \lambda^{-\alpha_i}$, $i = 1, 2$, are sufficiently close to the boundary, but the corresponding potential difference $|u_\lambda(1 - \lambda^{-\alpha_1}) - u_\lambda(1 - \lambda^{-\alpha_2})|$ tends to infinity as $\lambda \gg 1$. Furthermore, we show the following properties that emphasize the significant change of u_λ near the boundary $r = 1$ as $\lambda \gg 1$ (which can be obtained from (4.32), (4.34) and (4.36)):

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(A) For $r^\lambda_{p,\alpha}$ satisfying (4.14) with $0 < \alpha \le 1$, **the second order term** of $u_\lambda(r^\lambda_{p,\alpha})$ (i.e., the leading order term of $\mathcal{O}_{p,\alpha}$ as $\lambda \gg 1$) relies exactly on p; however, when $\alpha > 1$, the second order term of $u_\lambda(r^\lambda_{p,\alpha})$ is independent of p.

(B) Various potential differences $|u_\lambda(r^\lambda_{p,\alpha}) - u_\lambda(1)|$ and $|u_\lambda(r^\lambda_{p_1;\alpha}) - u_\lambda(r^\lambda_{p_2;\alpha})|$ with $p_1 \neq p_2$ can be presented as follows:

$$\lim_{\lambda\to\infty} \left|u_\lambda(r^\lambda_{p,\alpha}) - u_\lambda(1)\right| = \begin{cases} \infty, & \text{if } 0 < \alpha < 1, \\ 2\log\dfrac{p+2}{2}, & \text{if } \alpha = 1, \\ 0, & \text{if } \alpha > 1, \end{cases} \tag{4.18}$$

and

$$\lim_{\lambda\to\infty} \left|u_\lambda\left(r^\lambda_{p_1;\alpha}\right) - u_\lambda\left(r^\lambda_{p_2;\alpha}\right)\right| = \begin{cases} 2\left|\log\dfrac{p_1}{p_2}\right|, & \text{if } 0 < \alpha < 1, \\ 2\left|\log\dfrac{p_1+2}{p_2+2}\right| \in \left(0, 2\left|\log\dfrac{p_1}{p_2}\right|\right), & \text{if } \alpha = 1, \\ 0, & \text{if } \alpha > 1. \end{cases} \tag{4.19}$$

Since $\text{dist}(r^\lambda_{p,\alpha}, 1) \to 0$ and $\text{dist}(r^\lambda_{p_1;\alpha}, r^\lambda_{p_2;\alpha}) \to 0$ as $\lambda \to \infty$, (4.18) and (4.19) present that the potential u_λ has a sharp change in a quite thin region next to the boundary $r = 1$. We refer the reader to Theorem 4.3 for the asymptotic expansions (at most the exact first three order terms) of $u_\lambda(r^\lambda_{p,\alpha})$ and $u'_\lambda(r^\lambda_{p,\alpha})$ with respect to $\lambda \gg 1$.

(C) Based on (4.16) and (4.17), the far-field and near-field expansions of ρ_λ with respect to $\lambda \gg 1$ are established. Moreover, we show in Corollary 4.1 that as $\lambda \to \infty$, the net charge density $\frac{e^{-u_\lambda}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} = \frac{\rho_\lambda}{\lambda}$ behaves exactly as a Dirac measure supported at boundary point $r = 1$. This mathematically confirms that the non-neutral phenomenon occurs near the charged surface.

4.1.2 A new comparison with charge-conserving Poisson–Boltzmann equations

In this section, we pay attention to a bi-nonlocal Poisson–Boltzmann equation for monovalent binary ions (usually called the charge-conserving Poisson–Boltzmann

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equation [112])

$$v''_{\mu,\lambda}(r) = \frac{\mu e^{v_{\mu,\lambda}(r)}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{\lambda e^{-v_{\mu,\lambda}(r)}}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s}, \quad r \in (0,1), \tag{4.20}$$

with the same boundary condition of u_λ as (4.6):

$$v_{\mu,\lambda}(0) = v'_{\mu,\lambda}(0) = 0. \tag{4.21}$$

Equation (4.20) is derived from the steady-state of PNP equation for monovalent binary electrolytes (cf. [70,73,74,76]), where μ and λ are positive parameters related to the total number of anions and cations, respectively. When we take a formal look at the case $0 < \mu \ll \lambda$, i.e., the total number of cations is great larger than that of anions, it seems that equation (4.20)–(4.21) approaches equation (4.5)–(4.6). However, since the rigorous asymptotic behavior of those nonlocal terms are unknown, it is not obvious that $0 < \mu \ll \lambda$ implies $\frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \ll \frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s}$. Hence, a question is naturally raised:

(Q) *Assume that μ depends on λ. What does the relation between μ and λ make*

$$\lim_{\lambda\to\infty} \|v_{\mu,\lambda} - u_\lambda\|_{\mathcal{C}^1([0,1])} = 0 \tag{4.22}$$

hold? Here $\|\cdot\|_{\mathcal{C}([0,1])}$ is defined in (4.15) with $K = [0,1]$.

Let us first make a brief review on (4.20)–(4.21) and point out the difficulty in studying the question (Q). It is known (cf. [70,76]) that for the case

$$\mu = \gamma\lambda \xrightarrow{\lambda\to\infty} \infty \quad (\gamma > 0 \text{ independent of } \lambda), \tag{4.23}$$

there holds $\lim_{\lambda\to\infty} |v_{\mu,\lambda}| = 0$ exponentially in any compact subset K of $[0,1)$. Moreover, under (4.23), by following the similar arguments as in [76, (2.23)], we have that $\frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s}$ and $\frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s}$ are divergent as $\lambda \to \infty$ since

$$\frac{\mu}{\lambda\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \to \gamma \quad \text{and} \quad \frac{1}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} \to \gamma \quad \text{as } \lambda \to \infty.$$

In this case, the asymptotic behavior of $v_{\mu,\lambda}$ is totally different from that of u_λ since $\lim_{\lambda\to\infty}\sup_K |u_\lambda - U| = 0$ (see (4.16)) and $\lim_{\lambda\to\infty} \frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} = 0$ (see (4.27)). As a consequence, (4.22) never holds under the condition (4.23). We shall stress that the study of (Q) is different from the case in most recent work [76] since the main

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analysis technique in [76] needs the constraint (4.23). Because of the limitation of analysis technique in these literatures, as $\lambda \to \infty$, the asymptotic behavior of the nonlocal coefficient $\frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s}$ and $v_{\mu,\lambda}$ without assumption (4.23) remains unknown.

We take an essential viewpoint to answer question (Q). Thanks to the inverse Hölder type estimate established in [75, (3.8)], we have, for $\mu > 0$ and $\lambda > 0$, the estimate $1 \leq \int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s \int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s \leq \max\{\frac{\lambda}{\mu}, \frac{\mu}{\lambda}\}$. This implies, for $\lambda > \mu > 0$,

$$\mu^2 \leq \frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \cdot \frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} \leq \mu\lambda. \tag{4.24}$$

When $\lambda > 0$ is fixed and $\mu \to 0^+$, equation (4.20)–(4.21) of $v_{\mu,\lambda}$ formally approaches equation (4.5)–(4.6) of u_λ since (4.24) implies $\lim_{\mu\to 0^+} \frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} = 0$. However, when $\lambda \to \infty$ and $\mu \to 0^+$ independently, it is not intuitive to claim $\frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \to 0$ because we do not have the further information about $\mu\lambda$. From another viewpoint, if we first assume that μ depends on λ and (4.22) holds, then we have $\frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} \sim \frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} \to \frac{\pi^2}{2}$ as $\lambda \to \infty$ (cf. (4.27)). Along with (4.24), we find that the condition

$$\lim_{\lambda\to\infty} \mu\lambda = 0 \tag{4.25}$$

verifies $\lim_{\lambda\to\infty} \frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} = 0$, together with $v_{\mu,\lambda}(r) \leq v_{\mu,\lambda}(0) = 0$ (cf. Lemma 4.3), we obtain

$$\max_{[0,1]} \frac{\mu e^{v_{\mu,\lambda}}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} = \frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \to 0 \text{ as } \lambda \to \infty,$$

and equation (4.20) formally approaches equation (4.5). The following theorem confirms such an observation and establishes convergence of $v_{\mu,\lambda}$ with $\mu \to 0$. In particular, (4.25) is a sufficient condition for (4.22).

Theorem 4.1. *For $\lambda > \mu > 0$, let $v_{\mu,\lambda} \in \mathcal{C}^2([0,1])$ be the unique solution to (4.20)–(4.21) (cf. [71, 76]), and let $u_\lambda \in \mathcal{C}^2([0,1])$ be the unique solution to (4.5)–(4.6). Then both $v_{\mu,\lambda}$ and u_λ are monotonically decreasing, but $v_{\mu,\lambda} - u_\lambda$ is monotonically increasing. Moreover, we have:*

(a) Assume (4.25). Then (4.22) is achieved.

(b) For $\lambda > 0$ fixed, there holds

$$\lim_{\mu\to 0^+} \|v_{\mu,\lambda} - u_\lambda\|_{\mathcal{C}^1([0,1])} = 0.$$

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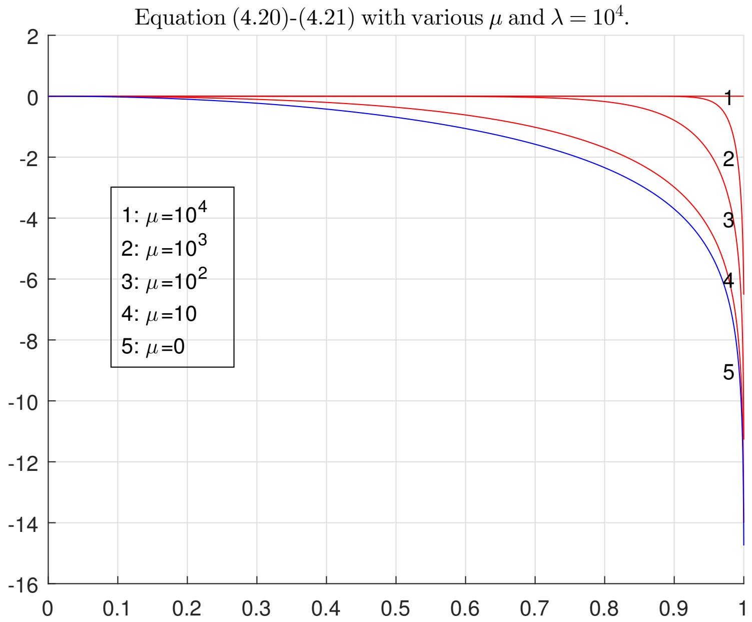

Figure 4.1: For $\lambda > 0$ fixed, equation (4.20)–(4.21) of $v_{\mu,\lambda}$ approximates equation (4.5)–(4.6) of u_λ as μ tends to zero. Given $\lambda = 10^4$, the curve 1–5 are associated with $\mu = 10^4, 10^3, 10^2, 10, 0$, respectively. Note that the curve 1 presents the neutrality ($\mu = \lambda = 10^4$), which implies $v_{\mu,\lambda} \equiv 0$.

Here we provide a numerical result to support Theorem 4.1(b) in Figure 4.1. Setting $w_{\mu,\lambda} := v_{\mu,\lambda} - u_\lambda$, we obtain

$$w''_{\mu,\lambda}(r) = e^{-v_{\mu,\lambda}(r)} W_{\mu,\lambda}(r) \text{ with } W_{\mu,\lambda}(r) = \frac{\mu e^{2v_{\mu,\lambda}(r)}}{\int_0^1 e^{v_{\mu,\lambda}(s)} \mathrm{d}s} - \frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)} \mathrm{d}s} + \frac{\lambda e^{w_{\mu,\lambda}(r)}}{\int_0^1 e^{-u_\lambda(s)} \mathrm{d}s}.$$

We shall briefly sketch the proof of Theorem 4.1 as follows.

- The basic properties of $v_{\mu,\lambda}$ and w_λ will be stated in Section 4.4.1. Furthermore, in Lemma 4.4 we carefully deal with $W_{\mu,\lambda}$ for the case $\lambda > \mu > 0$, and show that $w_{\mu,\lambda}$ has neither local maximum nor local minimum in $(0, 1)$. Along with $w'_{\mu,\lambda}(1) = v'_{\mu,\lambda}(1) - u'_\lambda(1) = \mu > 0$, this particularly shows the monotonic increase of $w_{\mu,\lambda}$ with r.

- A significant idea for proving Theorem 4.1(a) and (b) is to establish the following estimates:

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(1) For $w_{\mu,\lambda}$, we obtain

$$0 \leq \max_{[0,1]} w_{\mu,\lambda} = w_{\mu,\lambda}(1) < \log\left(\left(1-\frac{\mu}{\lambda}\right)^2 + \mu\lambda \underbrace{\left(2-\frac{\mu}{\lambda}\right)\frac{e^{-u_\lambda(1)}}{\lambda^2}}_{\substack{\text{uniformly bounded} \\ \text{as } \lambda\to\infty}}\right) \xrightarrow[\mu\lambda\to 0]{\lambda \text{ fixed or } \lambda\to\infty} 0 \tag{4.26}$$

(cf. (4.78)–(4.79) for $\lambda \to \infty$; (4.85) for $\lambda > 0$ fixed). Here we shall stress that in (4.26), the condition (4.25) seems optimal since $\lim\limits_{\lambda\to\infty} \frac{e^{-u_\lambda(1)}}{\lambda^2} = \pi^{-2}$ (see (4.31)).

(2) For $w'_{\mu,\lambda}$, we obtain

$$\max_{[0,1]} w'^2_{\mu,\lambda} := w'^2_{\mu,\lambda}(r^*_{\mu,\lambda}) \leq -\frac{\mu(2e^{v_{\mu,\lambda}(r^*_{\mu,\lambda})}-1)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \lambda\left(\frac{1}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\right) \xrightarrow[\mu\lambda\to 0]{\lambda \text{ fixed or } \lambda\to\infty} 0$$

(cf. (4.83) and Lemma 4.6 for $\lambda\to\infty$; (4.88)–(4.89) for $\lambda > 0$ fixed).

Consequently, we obtain $\lim\limits_{\substack{\lambda \text{ fixed or } \lambda\to\infty \\ \mu\lambda\to 0}} \|w_{\mu,\lambda}\|_{C^1([0,1])} = 0$. The detailed proof of Theorem 4.1 will be stated in Sections 4.4.2–4.4.4.

In Theorems 4.2–4.3 below, we will establish the refined far-field and near-field expansions for u_λ with respect to $\lambda \gg 1$. Combining Theorem 4.1(a) with Theorems 4.2–4.3, we can obtain refined asymptotic expansions of $v_{\mu,\lambda}$ as $\lambda \gg 1$ and $0 < \mu\lambda \ll 1$. Various asymptotics of $v_{\mu,\lambda}$ and u_λ can be presented as follows.

$$v_{\mu,\lambda} \xrightarrow[\lambda \text{ fixed and } \mu\to 0]{\text{(uniformly)}} u_\lambda \xrightarrow[\lambda\to\infty]{\text{(pointwise)}} U := \lim_{\lambda\to\infty} u_\lambda$$

$$v_{\mu,\lambda} - u_\lambda \xrightarrow[\lambda\to\infty \text{ and } \mu\lambda\to 0]{\text{(uniformly)}} 0$$

Organization of the chapter. The rest of the chapter is organized as follows. In Section 4.2 we will state the main results about the far-field expansions and the near-field expansions of u_λ in Theorems 4.2 and 4.3, respectively. Based on such asymptotic expansions, we establish in Corollary 4.1 for the refined asymptotic expansions of ρ_λ and the related concentration phenomenon of $\frac{\rho_\lambda}{\lambda}$ as $\lambda\to\infty$. Afterwards, we prove Theorems 4.2–4.3 and Corollary 4.1 in Section 4.3. We shall stress that Theorem 4.3 plays a crucial role in the proof of Theorem 4.1. In Section 4.4.1 we introduce some basic properties of $v_{\mu,\lambda}$. For Theorem 4.1, we will state

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the proof of (a) in Sections 4.4.2–4.4.3 and the proof of (b) in Section 4.4.4. Finally, we provide an application to calculating the capacitances and discuss such result in Section 4.5.

4.2 The main results of (4.5)–(4.6)

Throughout the whole chapter, we denote o_λ as the quantity tending to zero as λ goes to infinity. We are now in a position to state the main results about the far-field and near-field expansions of the solution to (4.5)–(4.6) as follows.

Theorem 4.2 (Far-field expansions of u_λ). *For $\lambda > 0$, let $u_\lambda \in \mathcal{C}^2([0,1])$ be the unique solution to (4.5)–(4.6). Then as $\lambda \gg 1$,*

$$\int_0^1 e^{-u_\lambda(s)} \mathrm{d}s = \frac{2}{\pi^2}\left(\lambda + 4 + \frac{4}{\lambda}(1+o_\lambda)\right) \to \infty. \tag{4.27}$$

Moreover, for any compact subset K of $[0,1)$, there holds

$$\lambda^2 \left\| u_\lambda(r) - U(r) - \pi r \left(\frac{\sin(\pi r)}{\lambda} - \frac{\pi r + 2\sin(\pi r)}{\lambda^2}\right) \sec^2\left(\frac{\pi}{2} r\right) \right\|_{\mathcal{C}^1(K)} \xrightarrow{\lambda\to\infty} 0, \tag{4.28}$$

where $U(r) = 2\log\cos\left(\frac{\pi}{2}r\right)$ is the unique solution to (4.12) and $\|\cdot\|_{\mathcal{C}^1(K)}$ is defined in (4.15).

Remark 4.1. (4.28) *gives the precise first three terms of $u_\lambda(r)$ and $u'_\lambda(r)$ with respect to $\lambda \gg 1$, for $r \in [0,1)$:*

$$\begin{aligned} u_\lambda(r) &= U(r) + \pi r \left(\frac{\sin(\pi r)}{\lambda} - \frac{\pi r + 2\sin(\pi r)}{\lambda^2}\right)\sec^2\left(\frac{\pi}{2}r\right) + O\left(\frac{1}{\lambda^3}\right), \\ u'_\lambda &= U'(r) + \frac{2\pi\tan(\pi r/2) + \pi^2 r\sec^2(\pi r/2)}{\lambda} \\ &\quad - \frac{4\pi\tan(\pi r/2) + 4\pi^2 r\sec^2(\pi r/2) + \pi^3 r^2 \sec^2(\pi r/2)\tan(\pi r/2)}{\lambda^2} + O\left(\frac{1}{\lambda^3}\right) \end{aligned} \tag{4.29}$$

In particular, one obtains

$$\lim_{\lambda\to\infty} u_\lambda(r) = U(r) \ \text{ and } \ \lim_{\lambda\to\infty} u'_\lambda(r) = U'(r) = -\pi\tan\left(\frac{\pi}{2}r\right). \tag{4.30}$$

We stress that (4.30) can be derived directly from [14]. However, the argument in [14] seems difficult to establish (4.29) due to the lack of (4.44).

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Theorem 4.3 (Near-field expansions of u_λ). *Under the same hypotheses as in Theorem 4.2, as $\lambda \gg 1$, we have*

$$u_\lambda(1) = 2\log\frac{1}{\lambda} + 2\log\pi - \frac{4}{\lambda}(1 + o_\lambda). \tag{4.31}$$

Moreover, for α, $p > 0$ independent of λ, $u_\lambda(r^\lambda_{p,\alpha})$ asymptotically blows up, which is depicted as follows:

(a) If $\alpha > 2$, i.e., $\lambda^2 \mathrm{dist}(r^\lambda_{p,\alpha}, 1) \to 0$, then $u_\lambda\left(r^\lambda_{p,\alpha}\right) = -2\log\lambda + 2\log\pi - \frac{4}{\lambda}(1+o_\lambda)$, which shares the same first three terms with $u_\lambda(1)$, and $u'_\lambda(r^\lambda_{p,\alpha})$ and $u'_\lambda(1)$ shares the same leading order term, which asymptotically blows up. In particular, $\left|u'_\lambda(r^\lambda_{p,\alpha}) - u'_\lambda(1)\right| \to 0$ as $\lambda \to \infty$.

(b) If $1 < \alpha \leq 2$, then

(b1) $u_\lambda(r^\lambda_{p,\alpha})$ and $u_\lambda(1)$ share the same first two terms:

$$u_\lambda(r^\lambda_{p,\alpha}) = 2\log\frac{1}{\lambda} + 2\log\pi + \begin{cases} \dfrac{p-4}{\lambda}(1+o_\lambda) & \text{if } \alpha = 2, \\ \dfrac{p}{\lambda^{\alpha-1}}(1+o_\lambda) & \text{if } \alpha \in (1,2). \end{cases} \tag{4.32}$$

(b2) $u'_\lambda(r^\lambda_{p,\alpha})$ and $u'_\lambda(1)$ share the same leading order term:

$$u'_\lambda(r^\lambda_{p,\alpha}) = -\lambda + \frac{p}{2}\lambda^{2-\alpha}(1+o_\lambda), \quad \alpha \in (1,2]. \tag{4.33}$$

Hence, the effect of p and α occurs at the third order term of $u_\lambda(r^\lambda_{p,\alpha})$ and the second order term $u'_\lambda(r^\lambda_{p,\alpha})$.

(c) If $\alpha = 1$, then

(c1) $u_\lambda(r^\lambda_{p,\alpha})$ and $u_\lambda(1)$ share the same leading order terms:

$$u_\lambda(r^\lambda_{p,\alpha}) = 2\log\frac{1}{\lambda} + 2\log\frac{(p+2)\pi}{2} - \frac{4}{\lambda}(1+o_\lambda). \tag{4.34}$$

(c2) The leading order term of $u'_\lambda(r^\lambda_{p,\alpha})$ depends on p:

$$u'_\lambda(r^\lambda_{p,\alpha}) = -\frac{2}{p+2}\lambda + o_\lambda. \tag{4.35}$$

Hence, the effect of p occurs at the second order term of $u_\lambda(r^\lambda_{p,\alpha})$ and the leading order term of $u'_\lambda(r^\lambda_{p,\alpha})$.

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(d) *If* $0 < \alpha < 1$, *then*

(d1) *The leading order term of* $u_\lambda(r^\lambda_{p,\alpha})$ *depends on* α *and second order term depends on* p:

$$u_\lambda(r^\lambda_{p,\alpha}) = 2\alpha \log \frac{1}{\lambda} + 2 \log \frac{p\pi}{2} + o_\lambda. \tag{4.36}$$

(d2) *The leading order term of* $u'_\lambda(r^\lambda_{p,\alpha})$ *depends on* p *and* α:

$$u'_\lambda(r^\lambda_{p,\alpha}) = -\frac{2}{p}\lambda^\alpha + o_\lambda. \tag{4.37}$$

Thanks to Theorems 4.2 and 4.3, we are able to obtain the pointwise asymptotics of $\lambda^{-1}\rho_\lambda$. Moreover, we have (cf. (4.38) and (4.39)) that as $\lambda \gg 1$:

- For $0 < \alpha < 1/2$, $\sup\limits_{[0,r^\lambda_{p,\alpha}]} \lambda^{-1}\rho_\lambda$ and $\sup\limits_{[0,r^\lambda_{p,\alpha}]} \lambda^{-1}u'^2_\lambda$ tend to zero.
- For $\alpha = 1/2$, $\lambda^{-1}\rho_\lambda(r^\lambda_{p,\alpha})$ and $\lambda^{-1}u'^2_\lambda(r^\lambda_{p,\alpha})$ are bounded and have positive lower bound.
- For $\alpha > 1/2$, $\lambda^{-1}\rho_\lambda(r^\lambda_{p,\alpha})$ and $\lambda^{-1}u'^2_\lambda(r^\lambda_{p,\alpha})$ asymptotically blow up.

More precisely, we obtain the refined far-field and near-field expansions of the net charge density ρ_λ and the boundary concentration phenomena of $\lambda^{-1}\rho_\lambda$ and $\lambda^{-1}u'^2_\lambda$, which are stated as follows.

Corollary 4.1. *Under the same hypotheses as in Theorem 4.2, as* λ *approaches infinity, we have*

(a) *(Far-field expansions of* ρ_λ*) For any compact subset* K *(independent of* λ*) of* $[0, 1)$,

$$\rho_\lambda(r) = \frac{\pi^2}{2}\sec^2\left(\frac{\pi}{2}r\right) - \frac{1}{\lambda}\left[2\pi^2\sec^2\left(\frac{\pi}{2}r\right) + \pi^3\sec^2\left(\frac{\pi}{2}r\right)\tan\left(\frac{\pi}{2}r\right)\right](1 + o_\lambda) \tag{4.38}$$

uniformly in K.

(b) *(Near-field expansions of* ρ_λ*) The asymptotics of* ρ_λ *near the boundary is depicted as follows:*

$$\rho_\lambda(r^\lambda_{p,\alpha}) = \begin{cases} \dfrac{\lambda^2}{2}(1 + o_\lambda) & \text{if } \alpha \in (1, \infty), \\ \dfrac{2\lambda^2}{(p+2)^2}(1 + o_\lambda) & \text{if } \alpha = 1, \\ \dfrac{2\lambda^{2\alpha}}{p^2}(1 + o_\lambda) & \text{if } \alpha \in (0, 1). \end{cases} \tag{4.39}$$

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(c) *(Concentration phenomenon) Both $\lambda^{-1}\rho_\lambda$ and $(2\lambda)^{-1}u_\lambda'^2$ behave exactly as Dirac measures supported at boundary point $r=1$, i.e.,*

$$\lim_{\lambda\to\infty}\int_0^1 \frac{\rho_\lambda(r)}{\lambda}h(r)\mathrm{d}r = h(1), \tag{4.40}$$

$$\lim_{\lambda\to\infty}\int_0^1 \frac{u_\lambda'^2(r)}{2\lambda}h(r)\mathrm{d}r = h(1), \tag{4.41}$$

for any continuous function $h:[0,1]\to\mathbb{R}$ independent of λ.

4.3 Proof of Theorems 4.2 and 4.3 and Corollary 4.1

It is well-known (cf. [14, Appendix]) that u_λ and ρ_λ can be expressed as

$$u_\lambda(r) = 2\log\cos\left(\sqrt{\frac{J_\lambda}{2}}r\right) \quad \text{and} \quad \rho_\lambda(r) = J_\lambda \sec^2\left(\sqrt{\frac{J_\lambda}{2}}r\right) \quad \text{for } r\in[0,1], \tag{4.42}$$

where

$$J_\lambda = \frac{\lambda}{I_\lambda} < \frac{\pi^2}{2}, \quad \text{and} \quad I_\lambda = \int_0^1 e^{-u_\lambda(s)}\mathrm{d}s. \tag{4.43}$$

To study the asymptotic behaviour of u_λ, it suffices to establish the refined asymptotic expansions of I_λ and J_λ which are stated as follows.

Lemma 4.2. *Under the same hypothesis in Theorem 4.2, we have*

$$J_\lambda = \pi^2\left(\frac{1}{2} - \frac{2}{\lambda} + \frac{6}{\lambda^2} - \frac{48-2\pi^2}{3\lambda^3}(1+o_\lambda)\right) \quad \text{as } \lambda \gg 1. \tag{4.44}$$

The proof of Lemma 4.2 is elementary so we state it in Appendix.

Remark 4.2. *Since (4.5) has a unique solution u_λ and corresponds to the nonlinear eigenvalue problem (4.10) with $(U_\kappa,\kappa)=(u_\lambda,J_\lambda)$, this results in $\frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} < \frac{\pi^2}{2}$ for any positive λ. We want to point out that (4.44) implies a squeezed estimate*

$$\pi^2\left(\frac{1}{2} - \frac{2}{\lambda} + \frac{6-\varepsilon}{\lambda^2}\right) < \frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} < \pi^2\left(\frac{1}{2} - \frac{2}{\lambda} + \frac{6}{\lambda^2}\right) \quad \text{as } \lambda > \lambda(\varepsilon),$$

for any sufficiently small $\varepsilon>0$, where $\lambda(\varepsilon)$ is a positive constant depending on ε.

Now, we are in a position to state the proof of Theorem 4.2.

Proof of Theorem 4.2. (4.27) follows from (4.44) since we have

$$I_\lambda = \frac{\lambda}{J_\lambda} = \frac{2\lambda}{\pi^2}\left(1 - \frac{4}{\lambda} + \frac{12}{\lambda^2}(1+o_{\boldsymbol{\lambda}})\right)^{-1} = \frac{2}{\pi^2}\left(\lambda + 4 + \frac{4}{\lambda}(1+o_\lambda)\right).$$

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To prove (4.28), we need to establish the precise first third order terms of $u_\lambda(r)$ and $u'_\lambda(r)$ in K. Firstly, by (4.42) and (4.44), there holds that

$$u_\lambda(r) = 2\log\cos\left(\frac{\pi}{2}r - \frac{\pi}{\lambda}r + \frac{2\pi}{\lambda^2}r(1+o_\lambda)\right) \text{ uniformly in } K, \text{ as } \lambda \to \infty. \tag{4.45}$$

Note that $r \in K$ is independent of λ. For a sake of convenience, let us set

$$\xi(r) = -\frac{\pi}{\lambda}r + \frac{2\pi}{\lambda^2}r(1+o_\lambda). \tag{4.46}$$

Then, as $\lambda \to \infty$, we have $\xi(r) \to 0$ and

$$2\log\cos\left(\frac{\pi}{2}r + \xi(r)\right) = 2\log\cos\left(\frac{\pi}{2}r\right) - 2\xi(r)\tan\left(\frac{\pi}{2}r\right) - \xi^2(r)\sec^2\left(\frac{\pi}{2}r\right) + o(\xi^3(r)), \tag{4.47}$$

uniformly in K. (4.47) can be obtained directly from the Taylor expansions so we omit the detailed derivation. As a consequence, by (4.45)–(4.47),

$$\begin{aligned} u_\lambda(r) =& 2\log\cos\left(\frac{\pi}{2}r\right) + \frac{2\pi r}{\lambda}\tan\left(\frac{\pi}{2}r\right) - \frac{\pi r}{\lambda^2}\left(4\tan\left(\frac{\pi}{2}r\right) + \pi r\sec^2\left(\frac{\pi}{2}r\right)\right)(1+o_\lambda) \\ =& 2\log\cos\left(\frac{\pi}{2}r\right) + \pi r\sec^2\left(\frac{\pi}{2}r\right)\left(\frac{\sin(\pi r)}{\lambda} - \frac{\pi r + 2\sin(\pi r)}{\lambda^2}\right)(1+o_\lambda), \end{aligned} \tag{4.48}$$

which gives the precise first third order terms of $u_\lambda(r)$.

On the other hand, differentiating (4.42) to r gives

$$u'_\lambda(r) = -2\sqrt{\frac{J_\lambda}{2}}\tan\left(\sqrt{\frac{J_\lambda}{2}}r\right). \tag{4.49}$$

Hence, by virtue of (4.44), (4.46) and (4.49), an expansion of $u'_\lambda(r)$ with respect to $\lambda \gg 1$ can be expressed as

$$\begin{aligned} u'_\lambda(r) =& \left(-\pi + \frac{2\pi}{\lambda} - \frac{4\pi}{\lambda^2}(1+o_\lambda)\right)\tan\left(\frac{\pi}{2}r - \frac{\pi}{\lambda}r + \frac{2\pi}{\lambda^2}r(1+o_\lambda)\right) \\ =& -\pi\tan\left(\frac{\pi}{2}r\right) + \frac{\pi^2 r + \pi\sin(\pi r)}{\lambda}\sec^2\left(\frac{\pi}{2}r\right) \\ & - \frac{\pi}{\lambda^2}\left[4\tan\left(\frac{\pi}{2}r\right) + 4\pi r\sec^2\left(\frac{\pi}{2}r\right) + \pi^2 r^2\sec^2\left(\frac{\pi}{2}r\right)\tan\left(\frac{\pi}{2}r\right)\right](1+o_\lambda), \end{aligned} \tag{4.50}$$

uniformly in K. Here we have used the approximation

$$\tan\left(\frac{\pi}{2}r + \xi(r)\right) = \tan\left(\frac{\pi}{2}r\right) + \xi(r)\sec^2\left(\frac{\pi}{2}r\right) + \xi^2(r)\sec^2\left(\frac{\pi}{2}r\right)\tan\left(\frac{\pi}{2}r\right) + o(\xi^3(r)).$$

Therefore, (4.28) follows immediately from (4.48) and (4.50), and we complete the proof of Theorem 4.2. $\square$

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4.3.1 Proof of Theorem 4.3

(4.31) follows from (4.9) and (4.43)–(4.44). By (4.42) and (4.49), we have

$$u_\lambda(r_{p,\alpha}^\lambda) = 2\log\cos\left(r_{p,\alpha}^\lambda\sqrt{\frac{J_\lambda}{2}}\right) = 2\log\sin\left(\frac{\pi}{2} - r_{p,\alpha}^\lambda\sqrt{\frac{J_\lambda}{2}}\right), \tag{4.51}$$

and

$$u_\lambda'(r_{p,\alpha}^\lambda) = -\sqrt{2J_\lambda}\tan\left(r_{p,\alpha}^\lambda\sqrt{\frac{J_\lambda}{2}}\right), \tag{4.52}$$

where $r_{p,\alpha}^\lambda$ is defined in (4.14). On the other hand, by (4.14) and (4.44), we have

$$r_{p,\alpha}^\lambda\sqrt{\frac{J_\lambda}{2}} = \left(1-\frac{p}{\lambda^\alpha}\right)\left(\frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda)\right). \tag{4.53}$$

Note that the asymptotic expansion of $r_{p,\alpha}^\lambda\sqrt{J_\lambda/2}$ varies with α. To obtain the refined asymptotic expansions of (4.51) and (4.52), we shall deal with the asymptotics of $r_{p,\alpha}^\lambda\sqrt{J_\lambda/2}$ under situations $\alpha>2$, $1<\alpha\le 2$, $\alpha=1$ and $0<\alpha<1$ individually.

Case 1. $\alpha > 2$**:**

In this case, we have $0<\frac{1}{\lambda^\alpha}\ll\frac{1}{\lambda^2}$ as $\lambda\gg 1$. Hence,

$$r_{p,\alpha}^\lambda\sqrt{\frac{J_\lambda}{2}} = \left(1-\frac{p}{\lambda^\alpha}\right)\left(\frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda)\right) = \frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda). \tag{4.54}$$

Along with (4.51), one may make appropriate manipulations to obtain

$$u_\lambda\left(r_{p,\alpha}^\lambda\right) = 2\log\sin\left(\frac{\pi}{\lambda}-\frac{2\pi}{\lambda^2}(1+o_\lambda)\right) = \log\frac{1}{\lambda^2}+\log\pi^2-\frac{4}{\lambda}(1+o_\lambda). \tag{4.55}$$

On the other hand, by (4.52), (4.54) and Taylor expansions of the cotangent function, one may check that

$$\begin{aligned} u_\lambda'(r_{p,\alpha}^\lambda) &= \left(-\pi+\frac{2\pi}{\lambda}-\frac{4\pi}{\lambda^2}(1+o_\lambda)\right)\tan\left[\left(1-\frac{p}{\lambda^\alpha}\right)\left(\frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda)\right)\right] \\ &= \left(-\pi+\frac{2\pi}{\lambda}-\frac{4\pi}{\lambda^2}(1+o_\lambda)\right)\cot\left(\frac{\pi}{\lambda}-\frac{2\pi}{\lambda^2}(1+o_\lambda)\right) = -\lambda+o_\lambda. \end{aligned} \tag{4.56}$$

Therefore, Theorem 4.3(a) follows from (4.55) and (4.56).

Case 2. $1<\alpha\le 2$**:**

In this case, (4.53) gives

$$r_{p,\alpha}^\lambda\sqrt{\frac{J_\lambda}{2}} = \left(1-\frac{p}{\lambda^\alpha}\right)\left(\frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda)\right) = \frac{\pi}{2}-\frac{\pi}{\lambda}-\frac{p\pi}{2\lambda^\alpha}+\frac{2\pi}{\lambda^2}(1+o_\lambda). \tag{4.57}$$

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Along with (4.51) one obtains

$$\begin{aligned} u_\lambda(r_{p,\alpha}^\lambda) =& 2\log\left(\frac{\pi}{\lambda}+\frac{p\pi}{2\lambda^\alpha}-\frac{2\pi}{\lambda^2}(1+o_\lambda)\right) = 2\log\frac{\pi}{\lambda}+2\log\left(1+\frac{p}{2\lambda^{\alpha-1}}-\frac{2}{\lambda}(1+o_\lambda)\right) \\ =& \log\frac{1}{\lambda^2}+\log\pi^2+\begin{cases}\dfrac{p-4}{\lambda}(1+o_\lambda) & \text{if } \alpha=2, \\ \dfrac{p}{\lambda^{\alpha-1}}(1+o_\lambda) & \text{if } \alpha\in(1,2)\,, \end{cases}\end{aligned}$$

and (4.32) immediately follows from this result. Combining (4.52) with (4.57) and following similar argument, we get (4.33) and complete the proof of Theorem 4.3(b).

Case 3. $\alpha = 1$:

In this case, (4.53) becomes

$$r_{p,\alpha}^\lambda\sqrt{\frac{J_\lambda}{2}} = \left(1-\frac{p}{\lambda}\right)\left(\frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda)\right) = \frac{\pi}{2}-\frac{(p+2)\pi}{2\lambda}+\frac{(p+2)\pi}{\lambda^2}(1+o_\lambda). \tag{4.58}$$

Hence, by inserting (4.58) into (4.51) and following the similar argument as in (4.55), we obtain

$$u_\lambda(r_{p,\alpha}^\lambda) = 2\log\sin\left(\frac{(p+2)\pi}{2\lambda}-\frac{(p+2)\pi}{\lambda^2}(1+o_\lambda)\right) = \log\frac{1}{\lambda^2}+\log\frac{(p+2)^2\pi^2}{4}-\frac{4}{\lambda}(1+o_\lambda).$$

This implies (4.34). Finally, (4.35) can be obtained from (4.52) and (4.58). The proof of Theorem 4.3(c) is complete.

Case 4. $0 < \alpha < 1$:

We want to emphasize that due to $0 < \frac{1}{\lambda} \ll \frac{1}{\lambda^\alpha}$ as $\lambda \gg 1$, the asymptotics of $u_\lambda(r_{p,\alpha}^\lambda)$ is more complicated than previous three cases.

Firstly, by plugging (4.53) into (4.51), one may obtain

$$\begin{aligned} u_\lambda(r_{p,\alpha}^\lambda) =& 2\log\sin\left(\frac{p\pi}{2\lambda^\alpha}+\frac{\pi}{\lambda}(1+o_\lambda)\right) \\ =& 2\log\left[\left(\frac{p\pi}{2\lambda^\alpha}+\frac{\pi}{\lambda}(1+o_\lambda)\right)-\frac{1}{6}\left(\frac{p\pi}{2\lambda^\alpha}+\frac{\pi}{\lambda}(1+o_\lambda)\right)^3(1+o_\lambda)\right]. \end{aligned} \tag{4.59}$$

Note also that $\frac{1}{\lambda^{3\alpha}} \ll \frac{1}{\lambda}$ as $3\alpha > 1$, and $\frac{1}{\lambda^{3\alpha}} \gg \frac{1}{\lambda}$ as $0 < 3\alpha < 1$. We shall deal with (4.59) under three situations $0 < \alpha < 1/3$, $\alpha = 1/3$ and $\alpha > 1/3$. After simple

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calculations, we can establish the precise first three terms of $u_\lambda(r^\lambda_{p,\alpha})$ as follows:

$$
\begin{aligned}
u_\lambda(r^\lambda_{p,\alpha}) &= \begin{cases} 2\log\left(\dfrac{p\pi}{2\lambda^\alpha}+\dfrac{\pi}{\lambda}(1+o_\lambda)\right) & \text{if } \alpha\in(1/3,1),\\ 2\log\left(\dfrac{p\pi}{2\lambda^\alpha}+\dfrac{48\pi-p^3\pi^3}{48\lambda}(1+o_\lambda)\right) & \text{if } \alpha=1/3,\\ 2\log\left(\dfrac{p\pi}{2\lambda^\alpha}-\dfrac{p^3\pi^3}{48\lambda^{3\alpha}}(1+o_\lambda)\right) & \text{if } \alpha\in(0,1/3), \end{cases}\\
&= \log\frac{1}{\lambda^{2\alpha}}+\log\frac{p^2\pi^2}{4}(1+o_\lambda).
\end{aligned}
$$

Thus, we obtain (4.36).

To prove (4.37), we shall deal with the asymptotics of (4.52) with $0<\alpha<1$. The argument is similar as the previous cases. Indeed, by (4.53) one may check that

$$
\begin{aligned}
\tan\left(r^\lambda_{p,\alpha}\sqrt{\frac{J_\lambda}{2}}\right) &= \tan\left[\left(1-\frac{p}{\lambda^\alpha}\right)\left(\frac{\pi}{2}-\frac{\pi}{\lambda}(1+o_\lambda)\right)\right] = \cot\left(\frac{p\pi}{2\lambda^\alpha}+\frac{\pi}{\lambda}(1+o_\lambda)\right)\\
&= \frac{1}{\frac{p\pi}{2\lambda^\alpha}+\frac{\pi}{\lambda}(1+o_\lambda)} = \frac{2\lambda^\alpha}{p\pi}+o_\lambda.
\end{aligned}
\tag{4.60}
$$

Combining (4.44), (4.52) and (4.60), we obtain

$$
u'_\lambda(r^\lambda_{p,\alpha}) = \left(-\pi+\frac{2\pi}{\lambda}(1+o_\lambda)\right)\left(\frac{2\lambda^\alpha}{p\pi}+o_\lambda\right) = -\frac{2}{p}\lambda^\alpha+o_\lambda.
$$

Therefore, we get (4.37) and complete the proof of Theorem 4.3.

4.3.2 Proof of Corollary 4.1

(4.38) follows from the combination of (4.42) and (4.44) as follows:

$$
\begin{aligned}
\rho_\lambda(r) &= \left(\frac{\pi^2}{2}-\frac{2\pi^2}{\lambda}+\frac{6\pi^2}{\lambda^2}(1+o_\lambda)\right)\sec^2\left(\frac{\pi r}{2}-\frac{\pi r}{\lambda}+\frac{2\pi r}{\lambda^2}(1+o_\lambda)\right)\\
&= \frac{\pi^2}{2}\sec^2\left(\frac{\pi}{2}r\right)-\frac{1}{\lambda}\left[2\pi^2\sec^2\left(\frac{\pi}{2}r\right)+\pi^3\sec^2\left(\frac{\pi}{2}r\right)\tan\left(\frac{\pi}{2}r\right)\right](1+o_\lambda),
\end{aligned}
$$

This completes the proof of Corollary 4.1(a).

Now, we shall prove (4.39). Putting $r=r^\lambda_{p,\alpha}$ into the expression of ρ_λ in (4.42) and using (4.44), we can obtain

$$
\begin{aligned}
\rho_\lambda(r^\lambda_{p,\alpha}) &= J_\lambda\sec^2\left(r^\lambda_{p,\alpha}\sqrt{\frac{J_\lambda}{2}}\right)\\
&= \left(\frac{\pi^2}{2}-\frac{2\pi^2}{\lambda}+\frac{6\pi^2}{\lambda^2}(1+o_\lambda)\right)\sec^2\left[\left(\frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda)\right)\left(1-\frac{p}{\lambda^\alpha}\right)\right].
\end{aligned}
\tag{4.61}
$$

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Note that the expansion of $\left(\frac{\pi}{2}-\frac{\pi}{\lambda}+\frac{2\pi}{\lambda^2}(1+o_\lambda)\right)\left(1-\frac{p}{\lambda^\alpha}\right)$ depends variously on $\alpha\in(0,1)$, $\alpha=1$ and $\alpha\in(1,\infty)$. Firstly, we deal with (4.61) for the case of $0<\alpha<1$ and obtain

$$\begin{aligned}\rho_\lambda(r^\lambda_{p,\alpha}) &= \left(\frac{\pi^2}{2}-\frac{2\pi^2}{\lambda}+\frac{6\pi^2}{\lambda^2}(1+o_\lambda)\right)\sec^2\left(\frac{\pi}{2}-\frac{p\pi}{2\lambda^\alpha}+\frac{\pi}{\lambda}(1+o_\lambda)\right)\\ &= \frac{2\lambda^{2\alpha}}{p^2}(1+o_\lambda),\end{aligned}$$

Here we have used the standard expansion of the cosecant function to obtain the last identity. Hence, we obtain (4.39) for the case of $0<\alpha<1$. By a similar argument, we can also prove (4.39) for the two cases $\alpha=1$ and $\alpha>1$, and the proof of Corollary 4.1(b) is complete.

It remains to prove Corollary 4.1(c). Note that $\lim_{\lambda\to\infty}\frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}=0$ (by (4.27)). Along with (4.5), we arrive at

$$\limsup_{\lambda\to\infty}\left(\frac{\rho_\lambda(r)h(r)}{\lambda}-\frac{u_\lambda'^2(r)h(r)}{2\lambda}\right)=\lim_{\lambda\to\infty}\frac{h(r)}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}=0 \text{ uniformly on } [0,1] \text{ as } \lambda\to\infty,$$

where h is a continuous function on $[0,1]$. This indicates that (4.40) and (4.41) are equivalent. Hence, it suffices to claim (4.40), i.e.,

$$\lim_{\lambda\to\infty}\int_0^1\frac{e^{-u_\lambda(r)}h(r)}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\mathrm{d}r=h(1). \tag{4.62}$$

Let $\kappa\in(0,1)$ be fixed. Then we observe that

$$\begin{aligned}\left|\int_0^1\frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}h(r)\mathrm{d}r-h(1)\right| &= \left|\left(\int_0^{1-\lambda^{-\kappa}}+\int_{1-\lambda^{-\kappa}}^1\right)\frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}(h(r)-h(1))\mathrm{d}r\right|\\ &\le 2\max_{r\in[0,1]}|h(r)|\left(\int_0^{1-\lambda^{-\kappa}}\frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\mathrm{d}r\right)\\ &\quad+\max_{r\in[1-\lambda^{-\kappa},1]}|h(r)-h(1)|\left(\int_{1-\lambda^{-\kappa}}^1\frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\mathrm{d}r\right).\end{aligned} \tag{4.63}$$

Moreover, from (4.5) and Theorem 4.2(d), a direct computation gives

$$\lim_{\lambda\to\infty}\int_{1-\lambda^{-\kappa}}^1\frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\mathrm{d}r=-\lim_{\lambda\to\infty}\int_{1-\lambda^{-\kappa}}^1\frac{u_\lambda''(r)}{\lambda}\mathrm{d}r=\lim_{\lambda\to\infty}\frac{u_\lambda'(1-\lambda^{-\kappa})-u_\lambda'(1)}{\lambda}=1,$$

which also implies

$$\lim_{\lambda\to\infty}\int_0^{1-\lambda^{-\kappa}}\frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\mathrm{d}r=0. \tag{4.64}$$

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Finally, we notice that the continuity of h implies $\lim_{\lambda\to\infty} \max_{r\in[1-\lambda^{-\kappa},1]} |h(r)-h(1)| = 0$. As a consequence, (4.62) immediately follows (4.63)–(4.64) and we prove Corollary 4.1(c).

Therefore, the proof of Corollary 4.1 is completed.

4.4 Proof of Theorem 4.1

In order to deal with the convergence of the $v_{\mu,\lambda} - u_\lambda$ with respect to $\mu\lambda \to 0^+$, throughout the whole section we shall set

$$w_{\mu,\lambda} := v_{\mu,\lambda} - u_\lambda. \tag{4.65}$$

Subtracting (4.5) from (4.20) and using (4.65) gives

$$w''_{\mu,\lambda}(r) = \frac{\mu e^{v_{\mu,\lambda}(r)}}{\int_0^1 e^{v_{\mu,\lambda}(s)} \mathrm{d}s} + \lambda \left(\frac{e^{-u_\lambda(r)}}{\int_0^1 e^{-u_\lambda(s)} \mathrm{d}s} - \frac{e^{-v_{\mu,\lambda}(r)}}{\int_0^1 e^{-v_{\mu,\lambda}(s)} \mathrm{d}s} \right) \tag{4.66}$$

and

$$w''_{\mu,\lambda}(r) = e^{-v_{\mu,\lambda}(r)} \left(\frac{\mu e^{2v_{\mu,\lambda}(r)}}{\int_0^1 e^{v_{\mu,\lambda}(s)} \mathrm{d}s} - \frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)} \mathrm{d}s} + \frac{\lambda e^{w_{\mu,\lambda}(r)}}{\int_0^1 e^{-u_\lambda(s)} \mathrm{d}s} \right). \tag{4.67}$$

We will sometimes use identity (4.66) or identity (4.67) to estimate $w_{\mu,\lambda}$ and $w'_{\mu,\lambda}$ for a sake of convenience.

Since we know that both u_λ and $v_{\mu,\lambda}$ are strictly decreasing on $[0,1]$ (by Lemma 4.3), the main difficulty of Theorem 4.1 is to obtain the monotonicity of $w_{\mu,\lambda}$, which will be presented in Lemma 4.4. To complete the proof of Theorem 4.1(a), in Sections 4.4.2 and 4.4.3, we will prove

$$\lim_{\substack{\lambda\to\infty \\ \mu\lambda\to 0}} \max_{[0,1]} |w_{\mu,\lambda}| = 0 \tag{4.68}$$

and

$$\lim_{\substack{\lambda\to\infty \\ \mu\lambda\to 0}} \max_{[0,1]} \left|w'_{\mu,\lambda}\right| = 0, \tag{4.69}$$

respectively. When $\lambda > 0$ is fixed and $\mu \to 0^+$, the proof of Theorem 4.1(b) is based on preliminary estimates in Sections 4.4.1 to 4.4.3. We will briefly state the proof in Section 4.4.4.

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4.4.1 Some basic properties

Since $\lambda > \mu > 0$, one can follow the same argument as in [70, Proposition 2.1] and [76, Lemma 2.1] to obtain $v''_{\mu,\lambda}(r) = \frac{\mu e^{v_{\mu,\lambda}(r)}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{\lambda e^{-v_{\mu,\lambda}(r)}}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} < 0$ for all $r \in (0,1]$. Along with (4.21), it yields

$$v'_{\mu,\lambda}(r) < v'_{\mu,\lambda}(0) = 0 \text{ and } v_{\mu,\lambda}(r) < v_{\mu,\lambda}(0) = 0 \text{ for all } r \in (0,1].$$

As a consequence, we obtain the following property.

Lemma 4.3. *For $\lambda > \mu > 0$, let $v_{\mu,\lambda} \in \mathcal{C}^2([0,1])$ be the unique solution to (4.20)–(4.21). Then $v_{\mu,\lambda}$ is strictly decreasing and strictly concave downward on $[0,1]$.*

Lemma 4.3 and (4.8) present that $v_{\mu,\lambda}$ and u_λ are strictly decreasing on $[0,1]$, but do not provide further information for $w_{\mu,\lambda} := v_{\mu,\lambda} - u_\lambda$. To prove (4.68), we need two crucial lemmas. Firstly, we obtain that $v_{\mu,\lambda} > u_\lambda$ on $(0,1]$ and $w_{\mu,\lambda}$ is **monotonically increasing** as $\lambda > \mu > 0$, which is stated as follows.

Lemma 4.4. *For $0 < \mu < \lambda$, $w_{\mu,\lambda}$ defined in (4.65) is positive and monotonically increasing on $(0,1]$. In particular, $w_{\mu,\lambda}$ attains its maximum value at the boundary point $r = 1$.*

Proof. Due to the continuity of $w_{\mu,\lambda}$, there exists $r_1 \in [0,1]$ such that $w_{\mu,\lambda}$ attains its minimum value at $r = r_1$. Since $w'_{\mu,\lambda}(1) = \mu > 0$, we have $r_1 \in [0,1)$.

We first show $r_1 = 0$. Suppose by contradiction that $r_1 \in (0,1)$, which implies that $w_{\mu,\lambda}(r_1) \le 0$, $w'_{\mu,\lambda}(r_1) = 0$ and $w''_{\mu,\lambda}(r_1) \ge 0$. Since $v_{\mu,\lambda}(r_1) < v_{\mu,\lambda}(0) = 0$ (by Lemma 4.3) and $w_{\mu,\lambda}(r_1) \le 0$, it is easy to obtain

$$\frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} > \frac{\mu e^{2v_{\mu,\lambda}(r_1)}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \frac{\lambda e^{w_{\mu,\lambda}(r_1)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}. \tag{4.70}$$

Along with (4.67), we find

$$\begin{aligned} w''_{\mu,\lambda}(0) &= \frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{\lambda}{\int_0^1 e^{u_\lambda(s)}\mathrm{d}s} + \frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} \\ &> \frac{\mu e^{2v_{\mu,\lambda}(r_1)}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{\lambda}{\int_0^1 e^{u_\lambda(s)}\mathrm{d}s} + \frac{\lambda e^{w_{\mu,\lambda}(r_1)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} = e^{v_{\mu,\lambda}(r_1)} w''_{\mu,\lambda}(r_1) > 0. \end{aligned} \tag{4.71}$$

Recall that $w'_{\mu,\lambda}(0) = 0$. Hence, by (4.71), there exists $r_2 \in (0, r_1)$ such that $w_{\mu,\lambda}(r_2) = \max_{[0,r_1]} w_{\mu,\lambda} > 0$. In particular,

$$w''_{\mu,\lambda}(r_2) \le 0. \tag{4.72}$$

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Since $v_{\mu,\lambda}(r_2) > v_{\mu,\lambda}(r_1)$ and $w_{\mu,\lambda}(r_2) > 0 \geq w_{\mu,\lambda}(r_1)$, we can repeat the same argument as in (4.70) to obtain

$$\frac{\mu e^{2v_{\mu,\lambda}(r_2)}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \frac{\lambda e^{w_{\mu,\lambda}(r_2)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} > \frac{\mu e^{2v_{\mu,\lambda}(r_1)}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \frac{\lambda e^{w_{\mu,\lambda}(r_1)}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}.$$

Along with (4.67), we can follow the similar argument as in (4.71) to get $w''_{\mu,\lambda}(r_2) > 0$, which contradicts (4.72). Thus, $r_1 = 0$ and $w_{\mu,\lambda} \geq 0$ on $[0, 1]$.

Next, we want to show that $w_{\mu,\lambda}$ attains its absolute maximum value at $r = 1$. Suppose by contradiction that there exists $r_3 \in (0, 1)$ such that $w_{\mu,\lambda}$ attains its local maximum at $r = r_3$. In particular, $w_{\mu,\lambda}(r_3) > 0$ and $w''_{\mu,\lambda}(r_3) \leq 0$, and there exists $\delta^* > 0$ such that $w_{\mu,\lambda}(r) \leq w_{\mu,\lambda}(r_3)$ and $w'_{\mu,\lambda}(r) \leq 0$ for $r \in (r_3, r_3 + \delta^*)$. On the other hand, since $w'_{\mu,\lambda}(1) = \mu > 0$, there exists $r_4 \in (r_3, 1)$ such that $w_{\mu,\lambda}$ attains its local minimum at $r = r_4$ with $w''_{\mu,\lambda}(r_4) \geq 0$. Note that $w_{\mu,\lambda}(r_4) \leq w_{\mu,\lambda}(r_3)$ and $v_{\mu,\lambda}(r_4) < v_{\mu,\lambda}(r_3)$. Thus, we can apply the similar argument as in (4.70) and (4.71) to get $w''_{\mu,\lambda}(r_3) > 0$, which contradicts the fact $w''_{\mu,\lambda}(r_3) \leq 0$. As a consequence, $w_{\mu,\lambda}$ attains its maximum value at $r = 1$. Furthermore, throughout the above argument, we also prove that $w_{\mu,\lambda}$ has neither local maximum nor local minimum, and $w'_{\mu,\lambda}$ preserves the same sign. Consequently, $w_{\mu,\lambda}$ is monotonically increasing since $w_{\mu,\lambda}(0) < w_{\mu,\lambda}(1)$. Therefore, we complete the proof of Lemma 4.4. □

4.4.2 Proof of (4.68)

Thanks to Lemma 4.4, it suffices to show that $w_{\mu,\lambda}(1)$ tends to zero as $\lambda \to \infty$ and $\mu\lambda \to 0$.

Lemma 4.5. *If* $\lim\limits_{\lambda\to\infty} \mu\lambda = 0$, *then*

$$\lim_{\lambda\to\infty} w_{\mu,\lambda}(1) = 0. \tag{4.73}$$

Proof. Multiplying (4.5) by u'_λ and integrating the expression over $[0, r]$ gives

$$\frac{1}{2}u'^2_\lambda(r) = \frac{\lambda(e^{-u_\lambda(r)} - 1)}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} \quad \text{for } r \in [0, 1]\,. \tag{4.74}$$

Applying the same argument to (4.20), we have

$$\frac{1}{2}v'^2_{\mu,\lambda}(r) = \frac{\mu(e^{v_{\mu,\lambda}(r)} - 1)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \frac{\lambda(e^{-v_{\mu,\lambda}(r)} - 1)}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} \quad \text{for } r \in [0, 1]\,. \tag{4.75}$$

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Putting $r=1$ into (4.74) and (4.75), one arrives at

$$\begin{aligned}\left(1-\frac{\mu}{\lambda}\right)^2 &= \frac{v'^2_{\mu,\lambda}(1)}{u'^2_\lambda(1)} \\ &= \frac{\mu}{\lambda}\frac{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s}\frac{e^{v_{\mu,\lambda}(1)}-1}{e^{-u_\lambda(1)}-1}+\frac{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s}\frac{e^{-v_{\mu,\lambda}(1)}-1}{e^{-u_\lambda(1)}-1} \\ &< \frac{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s}\frac{e^{-w_{\mu,\lambda}(1)}-e^{u_\lambda(1)}}{1-e^{u_\lambda(1)}}.\end{aligned} \tag{4.76}$$

Here we have used (4.65) and the fact $v_{\mu,\lambda}(1)<0$. Since $-v_{\mu,\lambda}\geq -w_{\mu,\lambda}(1)-u_\lambda$ on $[0,1]$ (cf. Lemma 4.4), we have

$$e^{-w_{\mu,\lambda}(1)} \leq \frac{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}. \tag{4.77}$$

Along with (4.76), we can obtain

$$\left(1-\frac{\mu}{\lambda}\right)^2 < \frac{1-e^{w_{\mu,\lambda}(1)+u_\lambda(1)}}{1-e^{u_\lambda(1)}},$$

which implies

$$1\leq e^{w_{\mu,\lambda}(1)} < \left(1-\frac{\mu}{\lambda}\right)^2+\left(2-\frac{\mu}{\lambda}\right)\frac{\mu}{\lambda}e^{-u_\lambda(1)}. \tag{4.78}$$

Note finally that (4.31) implies the uniform boundness of $\frac{e^{-u_\lambda(1)}}{\lambda^2}$ with respect to $\lambda\gg 1$. Along with $\lim\limits_{\lambda\to\infty}\mu\lambda=0$, we get

$$\lim_{\lambda\to\infty}\frac{\mu}{\lambda}e^{-u_\lambda(1)}=0. \tag{4.79}$$

Combining (4.78) with (4.79), we deduce (4.73) and complete the proof of Lemma 4.5.

□

Applying Finally, by Lemmas 4.4 and 4.5, it is easy to see $\lim\limits_{\substack{\lambda\to\infty \\ \mu\lambda\to 0}}\max\limits_{r\in[0,1]}|w_{\mu,\lambda}(r)| = \lim\limits_{\substack{\lambda\to\infty \\ \mu\lambda\to 0}} w_{\mu,\lambda}(1)=0$, which gives (4.68).

4.4.3 Proof of (4.69)

Note that $w'_{\mu,\lambda}\geq 0$, $w'_{\mu,\lambda}(0)=0$ and $\lim\limits_{\lambda\to\infty}w'_{\mu,\lambda}(1)=\lim\limits_{\lambda\to\infty}\mu=0$. For $\lambda\gg 1\gg\mu>0$, we may assume that $w'_{\mu,\lambda}$ attains its maximum value at interior point $r^*_{\mu,\lambda}$. It suffices to claim

$$\lim_{\substack{\lambda\to\infty \\ \mu\lambda\to 0}} w'_{\mu,\lambda}(r^*_{\mu,\lambda})=0. \tag{4.80}$$

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Claim of (4.80). Firstly, by $w''_{\mu,\lambda}(r^*_{\mu,\lambda}) = 0$ and (4.66), we have

$$0 = w''_{\mu,\lambda}(r^*_{\mu,\lambda}) = \frac{\mu e^{v_{\mu,\lambda}(r^*_{\mu,\lambda})}}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{\lambda e^{-v_{\mu,\lambda}(r^*_{\mu,\lambda})}}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} + \frac{\lambda e^{-u_\lambda(r^*_{\mu,\lambda})}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}. \tag{4.81}$$

On the other hand, subtracting (4.74) from (4.75) gives

$$\frac{1}{2}\left(v'^2_{\mu,\lambda}(r) - u'^2_\lambda(r)\right) = \frac{\mu(e^{v_{\mu,\lambda}(r)} - 1)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \frac{\lambda(e^{-v_{\mu,\lambda}(r)} - 1)}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{\lambda(e^{-u_\lambda(r)} - 1)}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}. \tag{4.82}$$

Putting $r = r^*_{\mu,\lambda}$ into (4.82) and using (4.81), we observe that

$$\begin{aligned}
\frac{1}{2}w'_{\mu,\lambda}(r^*_{\mu,\lambda})(v'_{\mu,\lambda}(r^*_{\mu,\lambda}) + u'_\lambda(r^*_{\mu,\lambda})) &= \frac{1}{2}\left(v'^2_{\mu,\lambda}(r^*_{\mu,\lambda}) - u'^2_\lambda(r^*_{\mu,\lambda})\right) \\
&= \frac{\mu\left(e^{v_{\mu,\lambda}(r^*_{\mu,\lambda})} - 1\right)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \lambda\left(\frac{e^{-v_{\mu,\lambda}(r^*_{\mu,\lambda})}}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{e^{-u_\lambda(r^*_{\mu,\lambda})}}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\right) \\
&\quad - \lambda\left(\frac{1}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\right) \\
&= \frac{\mu(2e^{v_{\mu,\lambda}(r^*_{\mu,\lambda})} - 1)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} - \lambda\left(\frac{1}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\right).
\end{aligned}$$

Since $0 \le w'_{\mu,\lambda} = v'_{\mu,\lambda} - u'_\lambda \le -\left(v'_{\mu,\lambda} + u'_\lambda\right)$, we have

$$\begin{aligned}
w'^2_{\mu,\lambda}(r^*_{\mu,\lambda}) &\le -w'_{\mu,\lambda}(r^*_{\mu,\lambda})(v'_{\mu,\lambda}(r^*_{\mu,\lambda}) + u'_\lambda(r^*_{\mu,\lambda})) \\
&= -\frac{2\mu(2e^{v_{\mu,\lambda}(r^*_{\mu,\lambda})} - 1)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + 2\lambda\left(\frac{1}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\right).
\end{aligned} \tag{4.83}$$

To deal with (4.83), we need the following lemma.

Lemma 4.6. *There hold*

(i) $$\lim_{\substack{\lambda\to\infty \\ \mu\lambda\to 0}} \lambda\left(\frac{1}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\right) = 0.$$

(ii) $$\lim_{\substack{\lambda\to\infty \\ \mu\lambda\to 0}} \frac{\mu\left(2e^{v_{\mu,\lambda}(r^*_{\mu,\lambda})} - 1\right)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} = 0.$$

Proof. From Lemma 4.4 and (4.77), we have

$$\frac{\lambda}{\int_0^1 e^{-u_\mu(s)}\mathrm{d}s} < \frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} < \frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s} e^{w_{\mu,\lambda}(1)}. \tag{4.84}$$

By (4.27), (4.84) and Lemma 4.5, we get Lemma 4.6(i).

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On the other hand, note that $\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s \int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s \geq 1$ (by Hölder's inequality). This along with (4.27) and Lemma 4.4 immediately implies

$$0 < \frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \leq \mu \int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s \leq \mu \int_0^1 e^{-u_\lambda(s)}\mathrm{d}s = \frac{2\mu\lambda}{\pi^2}(1+o_\lambda) \xrightarrow{\mu\lambda\to 0} 0.$$

Since $v_{\mu,\lambda} \leq 0$ (by Lemma 4.3), we obtain

$$\left| \frac{\mu\left(2e^{v_{\mu,\lambda}(r^*_{\mu,\lambda})} - 1\right)}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \right| \leq \frac{3\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} \to 0 \quad \text{as } \lambda \to \infty.$$

This proves Lemma 4.6(ii). Therefore, the proof of Lemma 4.6 is completed. □

Finally, by (4.83) and Lemma 4.6, we arrive at (4.80) and complete the proof of (4.69).

4.4.4 Proof of Theorem 4.1(b)

In this section, we fix $\lambda > 0$. Note that Lemmas 4.3–4.4 and the estimates (4.74)–(4.78) still hold for $\lambda > \mu > 0$. Hence, as $\mu \to 0^+$, we have

$$1 \leq e^{w_{\mu,\lambda}(1)} < \left(1 - \frac{\mu}{\lambda}\right)^2 + \left(2 - \frac{\mu}{\lambda}\right)\frac{\mu}{\lambda}e^{-u_\lambda(1)} \xrightarrow[\mu\to 0^+]{\lambda>0 \text{ fixed}} 1. \tag{4.85}$$

Here we have used the fact that $u_\lambda(1)$ is independent of μ. As a consequence, by (4.85) and the monotonicity of $w_{\mu,\lambda}$ (cf. Lemma 4.4), we arrive at

$$\lim_{\mu\to 0^+} \max_{[0,1]} |w_{\mu,\lambda}| = 0. \tag{4.86}$$

It remains to claim

$$\lim_{\mu\to 0^+} \max_{[0,1]} |w'_{\mu,\lambda}| = 0. \tag{4.87}$$

We assume that $w'_{\mu,\lambda}$ attains its maximum value at $r = r^*_\mu$. If $r_\mu \in (0,1)$, then one may check that (4.81)–(4.83) with $r^*_{\mu,\lambda} = r^*_\mu$ still hold for $\lambda > \mu > 0$. Moreover, by (4.84) and (4.86), we obtain

$$\lim_{\mu\to 0^+} \frac{\lambda}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} = \frac{\lambda}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}. \tag{4.88}$$

This along with (4.83) yields

$$w'^2_{\mu,\lambda}(r^*_\mu) \leq \frac{\mu}{\int_0^1 e^{v_{\mu,\lambda}(s)}\mathrm{d}s} + \lambda\left(\frac{1}{\int_0^1 e^{-v_{\mu,\lambda}(s)}\mathrm{d}s} - \frac{1}{\int_0^1 e^{-u_\lambda(s)}\mathrm{d}s}\right) \xrightarrow[\mu\to 0^+]{\lambda>0 \text{ fixed}} 0. \tag{4.89}$$

Therefore, we obtain (4.87) and complete the proof of Theorem 4.1(b).

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4.5 Applications and discussion

In this section we provide an application to calculating capacitances for the doubler-layer capacitantors in single-ion electrolyte solutions. As was studied in [76, Section 6], we define a quantity $\mathscr{C}^+(u_\lambda; K)$ related to the capacitance in a physical region $K_{\lambda;\alpha} \subset [0,1]$ as

$$\mathscr{C}^+(u_\lambda; K_{\lambda;\alpha}) := \frac{\left|\int_{K_{\lambda;\alpha}} \lambda^{-1}\rho_\lambda(r)\mathrm{d}r\right|}{\max\limits_{x,y\in \overline{K_{\lambda;\alpha}}} |u_\lambda(x) - u_\lambda(y)|}. \tag{4.90}$$

For a sake of simplicity, we shall set $K_{\lambda;\alpha} = [r^\lambda_{p,\alpha}, 1]$. We show that when $K_{\lambda;\alpha}$ attached to the boundary (the charge surface) has the thickness of the order $\lambda^{-\alpha}$ and $\alpha \geq 1$, $\mathscr{C}^+(u_\lambda; K_{\lambda;\alpha})$ has a positive infimum as λ tends to infinity. However, if the thickness of $K_{\lambda;\alpha}$ is far larger compared to the order λ^{-1} as $\lambda \gg 1$, then $\mathscr{C}^+(u_\lambda; K_{\lambda;\alpha})$ tends to zero. Such results are based on the following refined asymptotics of $\mathscr{C}^+(u_\lambda; [r^\lambda_{p,\alpha}, 1])$.

Theorem 4.4. *Under the same hypothese as in Theorem 4.2, as $\lambda \gg 1$ and $p > 0$, the asymptotic expansions of $\mathscr{C}^+(u_\lambda; [r^\lambda_{p,\alpha}, 1])$ are precisely depicted as follows:*

(a) If $\alpha > 1$, then

$$\mathscr{C}^+\left(u_\lambda; [r^\lambda_{p,\alpha}, 1]\right) = \frac{1}{2} + \left(-\frac{p}{8\lambda^{\alpha-1}}\chi_1(\alpha) + \frac{\pi^2}{2\lambda^2}\chi_2(\alpha)\right)(1 + o_\lambda),$$

where

$$\chi_1(\alpha) = \begin{cases} 0, & \text{if } \alpha > 3, \\ 1, & \text{if } 1 < \alpha \leq 3, \end{cases} \quad \text{and} \quad \chi_2(\alpha) = \begin{cases} 1, & \text{if } \alpha \geq 3, \\ 0, & \text{if } 1 < \alpha < 3. \end{cases}$$

Note that $\chi_1(\alpha) = \chi_2(\alpha) = 1$ as $\alpha = 3$.

(b) If $\alpha = 1$, then

$$\mathscr{C}^+\left(u_\lambda; [r^\lambda_{p,\alpha}, 1]\right) = \frac{p}{2(p+2)\log\left(1 + \frac{p}{2}\right)}\left(1 + \frac{H}{\lambda^2}(1 + o_\lambda)\right),$$

where H is defined by

$$H = \frac{\pi^2(p^2 + 6p + 12)}{6(p+2)} + \frac{p^2\pi^2(p+6)}{24(p+2)\log\left(1 + \frac{p}{2}\right)}.$$

(c) If $0 < \alpha < 1$, then

$$\mathscr{C}^+\left(u_\lambda; [r^\lambda_{p,\alpha}, 1]\right) = \frac{1}{\log \lambda^{2-2\alpha}}(1 + o_\lambda).$$

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Since the proof of Theorem 4.4 requires a huge amount of elementary computations based on refined asymptotics of u_λ and u'_λ in Theorem 4.3, we omit the details.

Finally, we make brief summaries for Theorem 4.4 as follows.

- For $r^\lambda_{p,\alpha}$ defined in (4.14), we have

$$\mathscr{C}^+(u_\lambda;[r^\lambda_{p,\alpha},1]) = \begin{cases} \dfrac{1}{2}(1+o_\lambda) & \text{for } \alpha > 1, \\ \dfrac{p}{2(p+2)\log\left(1+\dfrac{p}{2}\right)}(1+o_\lambda) & \text{for } \alpha = 1, \\ \dfrac{1}{\log \lambda^{2-2\alpha}}(1+o_\lambda) & \text{for } 0 < \alpha < 1. \end{cases} \tag{4.91}$$

- For $r \in [0,1)$ independent of λ, $\mathscr{C}^+(u_\lambda;[r,1]) \sim \dfrac{1}{\log \lambda^2}$ tending to zero.

Note that in (4.91), $g\,(p) := \frac{p}{2(p+2)\log\left(1+\frac{p}{2}\right)}$ is strictly increasing to the variable $p > 0$ and $\lim\limits_{p\to\infty} g\,(p) = \frac{1}{2}$. Since the amount of electrical energy which the capacitor can store depends on its capacitance, (4.91) confirms an important property of the "double-layer capacitance" that the corresponding capacitance (4.90) of the electrostatic model (4.5)–(4.6) stores much more energy in thinner region attached to the charged surface.

Before closing this section, we want to stress that the double-layer capacitance in binary electrolytes has been introduced in [76, Theorem 6.1]. Let us consider the same region $[r^\lambda_{p,\alpha},1]$ having the thickness $O(\lambda^{-\alpha})$ with $\alpha \geq 1$ attached to the charged surface and explain why we are interested in calculating the corresponding capacitance in single-ion electrolytes. A reason is that for binary electrolytes, the maximum potential difference in $[r^\lambda_{p,\alpha},1]$ is too small to get the precise value of $\lim\limits_{\lambda\to\infty} \mathscr{C}^+(u_\lambda;[r^\lambda_{p,\alpha},1])$. However, for the case of single-ion electrolytes, we exactly obtain the precise value of $\lim\limits_{\lambda\to\infty} \mathscr{C}^+(u_\lambda;[r^\lambda_{p,\alpha},1])$ shown in (4.91). Such a result provides a practical application for calculating the double-layer capacitance in electrolytes [32].

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Appendix

4A Proof of Lemma 4.2

In this appendix, we state the proof of Lemma 4.2.

By (4.42) and (4.43), one may check that

$$I_\lambda = \int_0^1 e^{-u_\lambda(s)} ds = \int_0^1 \sec^2\left(\sqrt{\frac{J_\lambda}{2}} r\right) dr = \sqrt{\frac{2}{J_\lambda}} \tan\sqrt{\frac{J_\lambda}{2}},$$

which implies

$$\frac{\sqrt{2J_\lambda}}{\lambda} = \cot\sqrt{\frac{J_\lambda}{2}} = \tan\left(\frac{\pi}{2} - \sqrt{\frac{J_\lambda}{2}}\right). \tag{4.92}$$

We shall now establish the precise first third order terms of the asymptotic expansion of J_λ with respect to $\lambda \gg 1$. Firstly, by (4.43) we have $0 < J_\lambda < \pi^2/2$ for all $\lambda > 0$. Along with (4.92), it immediately yields

$$\lim_{\lambda\to\infty} J_\lambda = \frac{\pi^2}{2}.$$

This gives the precise leading order term of J_λ with respect to $\lambda \gg 1$. Moreover, applying the approximation $\tan s = s + o(s)$ for $s = \frac{\pi}{2} - \sqrt{\frac{J_\lambda}{2}} \to 0$ to the right-hand side of (4.92), one obtains

$$\frac{\sqrt{2J_\lambda}}{\lambda} = \left(\frac{\pi}{2} - \sqrt{\frac{J_\lambda}{2}}\right)(1 + o_\lambda). \tag{4.93}$$

To deal with the second order term of J_λ with respect to $\lambda \gg 1$, let us set

$$a_\lambda = \left(J_\lambda - \frac{\pi^2}{2}\right)\lambda.$$

Then we can express the asymptotic expansion of $\sqrt{\frac{J_\lambda}{2}}$ as

$$\sqrt{\frac{J_\lambda}{2}} = \sqrt{\frac{\pi^2}{4} + \frac{a_\lambda}{2\lambda}} = \frac{\pi}{2} + \frac{a_\lambda}{2\pi\lambda}(1 + o_\lambda).$$

Along with (4.93) arrives at $\frac{\pi}{2} + \frac{a_\lambda}{2\pi\lambda}(1+o_\lambda) = \frac{\lambda}{2}\left(\frac{\pi}{2} - \sqrt{\frac{J_\lambda}{2}}\right)(1+o_\lambda) = -\frac{a_\lambda}{4\pi}(1+o_\lambda)$, and consequently $a_\lambda = -2\pi^2 + o_\lambda$, as $\lambda \gg 1$, which stands the second order term of expansion of J_λ. As a conclusion,

$$J_\lambda = \frac{\pi^2}{2} - \frac{2\pi^2}{\lambda}(1 + o_\lambda). \tag{4.94}$$

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To further get the precise third order term of J_λ with respect to λ, we consider the difference between J_λ and its first two order terms shown in the right-hand side of (4.94) and set

$$b_\lambda = \left(J_\lambda - \frac{\pi^2}{2} + \frac{2\pi^2}{\lambda} \right) \lambda^2.$$

Then we have

$$\sqrt{\frac{J_\lambda}{2}} = \sqrt{\frac{\pi^2}{4} - \frac{\pi^2}{\lambda} + \frac{b_\lambda}{2\lambda^2}} = \frac{\pi}{2} - \frac{\pi}{\lambda} + \frac{1}{\lambda^2} \left(\frac{b_\lambda}{2\pi} - \pi \right) (1 + o_\lambda) \,. \tag{4.95}$$

Rewriting (4.93) as $\sqrt{\frac{J_\lambda}{2}} = \frac{\lambda}{2} \left(\frac{\pi}{2} - \sqrt{\frac{J_\lambda}{2}} \right) (1 + o_\lambda)$ and putting (4.95) into this expression, after a simple calculation we can get

$$b_\lambda = 6\pi^2 + o_\lambda, \text{ as } \lambda \gg 1.$$

Similarly, to obtain the precise the fourth order term of J_λ with respect to λ, we set

$$c_\lambda = \lambda^3 \left(J_\lambda - \frac{\pi^2}{2} + \frac{2\pi^2}{\lambda} - \frac{6\pi^2}{\lambda^2} \right) . \tag{4.96}$$

One may follow same argument to get

$$c_\lambda = -16\pi^2 + \frac{2\pi^4}{3} + o_\lambda, \text{ as } \lambda \gg 1 \tag{4.97}$$

Therefore, (4.44) directly follows from (4.96) and (4.97), and the proof of Lemma 4.2 is complete.

doi:10.6342/NTU202501331

參考文獻

[1] E. Abbena, A. Gray, and L. Vanhecke, *Steiner's formula for the volume of a parallel hypersurface in a riemannian manifold*, Annali Sc. Norm. Sup. Pisa, 8 (1981), pp. 473–493, https://www.numdam.org/item/ASNSP_1981_4_8_3_473_0

[2] S. Agmon, A. Douglis, and L. Nirenberg, *Estimates near the boundary for solutions of elliptic partial differential equations satisfying general boundary conditions. I*, Commun. Pure Appl., 12 (1959), pp. 623–727, https://doi.org/10.1002/cpa.3160120405

[3] M. D. Altman, J. P. Bardhan, J. K. White, and B. Tidor, *Accurate solution of multi-region continuum biomolecule electrostatic problems using the linearized Poisson–Boltzmann equation with curved boundary elements*, J. Comput. Chem., 30 (2009), pp. 132–153, https://doi.org/10.1002/jcc.21027

[4] D. Andelman, *Electrostatic Properties of Membrances: The Poisson–Boltzmann Theory.* in Structure and Dynamics of Membrances, R. Lipowsku and E. Sackmann, eds., vol. 1, North-Holland, 1995, pp. 603–642, https://doi.org/10.1016/S1383-8121(06)80005-9

[5] P. B. Balbuena and K. E. Gubbins, *Theoretical interpretation of adsorption behavior of simple fluids in slit pores*, Langmuir, 9 (1993), pp. 1801–1814, https://doi.org/10.1021/la00031a031

[6] N. A. Baker, *Poisson–Boltzmann Methods for Biomolecular Electrostatics.* in Numerical Computer Methods, Part D, L. Brand and M. L. Johnson, eds., vol. 383, Academic Press, 2004, pp. 94–118, https://doi.org/10.1016/S0076-6879(04)83005-2

doi:10.6342/NTU202501331

[7] V. Barcilon, D.-P. Chen, R. S. Eisenberg, and J. W. Jerome, *Qualitative properties of steady-state Poisson–Nernst–Planck systems: perturbation and simulation study*, SIAM J. Appl. Math., 57 (1997) pp. 631–648, https://doi.org/10.1137/S0036139995312149

[8] M. Z. Bazant, K. T. Chu, and B. J. Bayly, *Current-voltage relations for electrochemical thin films*, SIAM J. Appl. Math., 65 (2005) pp. 1463–1484, https://doi.org/10.1137/040609938

[9] M. Z. Bazant, B. D. Storey, and A. A. Kornshev, *Double Layer in Ionic Liquids: Overscreening versus Crowding*, Phys. Rev. Lett., 106 (2011), 046102, https://doi.org/10.1103/PhysRevLett.106.046102

[10] J. J. Bikerman, *Structure and capacity of electrical double layer*, Philos. Mag., 7 (1942), pp. 384–397, https://doi.org/10.1080/14786444208520813

[11] R. Blossey, *The Poisson–Boltzmann Equation: An Introduction*, Springer–Verlag, 2023, https://doi.org/10.1007/978-3-031-24782-8

[12] I. Borukhov and D. Andelman, *Steric Effects in Electrolytes: A Modified Poisson–Boltzmann Equation*, Phys. Rev. Lett., 79 (1997), pp. 435–438, https://doi.org/10.1103/PhysRevLett.79.435

[13] J. A. Carrillo, *On a nonlocal elliptic equation with decreasing nonlinearity arising in plasma physics and heat conduction*, Nonlinear Anal. TMA., 32 (1998), pp. 97–115, https://doi.org/10.1016/S0362-546X(97)00455-0

[14] J. Cartailler, Z. Schuss, and D. Holcman, *Analysis of the Poisson–Nernst–Planck equation in a ball for modeling the Voltage–Current relation in neurobiological microdomains*, Physica D, 339 (2017), pp. 39–48, https://doi.org/10.1016/j.physd.2016.09.001

[15] J. Cartailler, Z. Schuss, and D. Holcman, *Electrostatics of non-neutral biological microdomains*, Scientific Reports, 7 (2017), 11269, https://doi.org/10.1038/s41598-017-11590-6

doi:10.6342/NTU202501331

[16] T. E. Cecil, *Focal Points and Support Functions in Affine Differential Geometry*, Geometriae Dedicata, 50 (1994), pp. 291–300, https://doi.org/10.1007/BF01267871

[17] B. M. N. Clarke and P. J. Stiles, *Finite electric boundary-layer solutions of a generalized Poisson–Boltzmann equation*, Proc. R. Soc. A, 471 (2015), 24, https://doi.org/10.1098/rspa.2015.0024

[18] S. Das and S. Chakraborty, *Effect of Conductivity Variations within the Electric Double Layer on the Streaming Potential Estimation in Narrow Fluidic Confinements*, Langmuir, 26 (2010), pp. 11589–11596, https://doi.org/10.1021/la1009237

[19] H. David and S. Zeev, *The Poisson–Nernst–Planck Equations in a Ball*, Asymptotics of Elliptic and Parabolic PDEs, and their Applications in Statistical Physics, Computational Neuroscience, and Biophysics (2018), pp. 341–383, https://doi.org/10.1007/978-3-319-76895-3_10

[20] P. Debye and E. Hückel, *Zur Theorie der Elektrolyte. I. Gefrierpunktserniedrigung und verwandte Erscheinungen*, Physikalische Zeitschrift, 24 (1923), pp. 185–206, https://doi.org/10.1007/978-3-642-94260-0_9

[21] K. Deimling, *Nonlinear Functional Analysis*, Springer-Verlag, Berlin, 1973, https://doi.org/10.1007/978-3-662-00547-7

[22] F. Dong, B. Olsen, and N. A. Baker, *Computational Methods for Biomolecular Electrostatics.* in Biophysical Tools for Biologists, Volume One: In Vitro Techniques, J. J. Correia, and H. W. Detrich, III, eds., vol. 84, Academic Press, 2008, ch. 26, pp. 843–870, https://doi.org/10.1016/S0091-679X(07)84026-X

[23] A. H. B. Dourado, *Electric Double Layer: The Good, the Bad, and the Beauty*, Electrochem, 3 (2022), pp. 789–808, https://doi.org/10.3390/electrochem3040052

[24] B. B. Eakins, S. D. Patel, A. P. Kalra, V. Rezania, K. Shankar, and J. A. Tuszynski, *Modeling Microtubule Counterion Distributions and*

doi:10.6342/NTU202501331

Conductivity Using the Poisson-Boltzmann Equation, Front. Mol. Biosci., 8 (2021), 650757, https://doi.org/10.3389/fmolb.2021.650757

[25] B. Eisenberg, *Proteins, channels and crowded ions*, Biophys. Chem., 100 (2003), pp. 507–517, https://doi.org/10.1016/S0301-4622(02)00302-2

[26] B. Eisenberg, *Interacting ions in biophysics: Real is not ideal*, Biophys. J., 104 (2013), pp. 1849–1866, https://doi.org/10.1016/j.bpj.2013.03.049

[27] J. J. Elisea-Espinoza, E. Gonzaález-Tovar, and G. I. Guerrero-García, *Theoretical description of the electrical double layer for a mixture of n ionic species with arbitrary size and charge asymmetries. I. Spherical geometry*, J. Chem. Phys., 158 (2023), 224111, https://doi.org/10.1063/5.0151140

[28] G. I. El-Baghdady, M. S. El-Azab, and W. S. El-Beshbeshy, *Legendre-Gauss-Lobatto pseudo-spectral method for one-dimensional advection-diffusion equation*, Sohag J. Math., 2 (2015), pp. 29–35, http://dx.doi.org/10.12785/sjm/020105

[29] D. F. Evans and H. Wennerström, *The Colloidal Domain: Where Physics, Chemistry, Biology, and Technology Meet* (2nd ed.), VCH Publishers, 1999.

[30] L. C. Evans and R. F. Gariepy, *Measure Theory and Fine Properties of Functions: Revised Edition*, CRC Press, 2015, https://doi.org/10.1201/b18333

[31] K. Fellner and V. A. Kovtunenko, *A singularly perturbed nonlinear Poisson–Boltzmann equation: uniform and super-asymptotic expansions*, Math. Methods Appl. Sci., 38 (2015), pp. 3575–3586, https://doi.org/10.1002/mma.3593

[32] G. Feng, D. Jiang, and P. T. Cummings, *Curvature effect on the capacitance of electric double layers at ionic liquid/onion-like carbon interfaces*, J. Chem. Theory Comput., 8 (2012), pp. 1058–1063, https://doi.org/10.1021/ct200914j

doi:10.6342/NTU202501331

[33] F. Fogolari, A. Brigo, and H. Molinari, *The Poisson–Boltzmann equation for biomolecular electrostatics: a tool for structural biology*, J. Mol. Recognit., 15 (2002), pp. 377–392, https://doi.org/10.1002/jmr.577

[34] M. A. Fontelos and K. B. Gamboa, *On the structure of double layers in Poisson–Boltzmann equation*, Discrete Cont. Dyn. Syst. - B, 17 (2012), pp. 1939–1967, https://doi.org/10.3934/dcdsb.2012.17.1939

[35] A. Flavell, J. Kabre, and X. Li, *An energy-preserving discretization for the Poisson–Nernst–Planck equations*, J. Comput. Electron., 16 (2017), pp. 431–441, https://doi.org/10.1007/s10825-017-0969-8

[36] A. Friedman and K. Tintarev, *Boundary asymptotics for solutions of the Poisson–Boltzmann equation*, J. Differ. Equ., 69 (1987), pp. 15–38, https://doi.org/10.1016/0022-0396(87)90100-8

[37] M. A. Gebbie, H. A. Dobbs, M. Valtiner, and J. N. Israelachvili, *Long-range electrostatic screening in ionic liquids*, PNSA, 112 (2015), pp. 7432–7437, https://doi.org/10.1073/pnas.1508366112

[38] D. Gilbarg and N. Trudinger, *Elliptic Partial Differential Equations of Second Order*, Springer–Verlag, 1977, https://doi.org/10.1007/978-3-642-61798-0

[39] D. Gillespie, *A review of steric interactions of ions: Why some theories succeed and others fail to account for ion size*, Microfluid Nanofluid, 18 (2015), pp. 717–738, https://doi.org/10.1007/s10404-014-1489-5

[40] A. Gray, *Tubes* (2nd ed.), Springer Basel AG, 2004, https://doi.org/10.1007/978-3-0348-7966-8

[41] C. G. Gray and P. J. Stiles, *Nonlinear electrostatics: the Poisson–Boltzmann equation*, Eur. J. Phys., 39 (2018), 053002, https://doi.org/10.1088/1361-6404/aaca5a

[42] D. J. Griffiths, *Introduction to Electrodynamics* (4th ed.), Cambridge University Press, 2017, https://doi.org/10.1017/9781108333511

doi:10.6342/NTU202501331

[43] P. Grochowski and J. Trylska, *Continuum molecular electrostatics, salt effects, and counterion binding—A review of the Poisson–Boltzmann theory and its modifications*, Biopolymers, 89 (2007), pp. 93–113, https://doi.org/10.1002/bip.20877

[44] M. Han and X. Xing, *Renormalized Surface Charge Density for a Strongly Charged Plate in Asymmetric Electrolytes: Exact Asymptotic Expansion in Poisson Boltzmann Theory*, J. Stat. Phys., 151 (2013), pp. 1121–1139, https://doi.org/10.1007/s10955-013-0751-7

[45] J. Hineman and R. Ryham, *Very weak solutions for Poisson–Nernst–Planck system*, Nonlinear Anal., 115 (2015), pp. 12–24, https://doi.org/10.1016/j.na.2014.11.018

[46] D. Holcman and R. Yuste, *The new nanophysiology: regulation of ionic flow in neuronal subcompartments*, Nat. Rev. Neurosci., 16 (2015), pp. 685–692, https://doi.org/10.1038/nrn4022

[47] D. Holcman and Z. Schuss, *Asymptotics of Elliptic and Parabolic PDEs*, Springer, 2018, https://doi.org/10.1007/978-3-319-76895-3

[48] B. Honig and A. Nichols, *Classical electrostatics in biology and chemistry*, Science, 268 (1995), pp. 1144–1149, https://doi.org/10.1126/science.7761829

[49] A. Hoorfar and M. Hassani, *Inequalities on the Lambert W function and hyperpower function*, JIPAM, 9 (2008), pp. 93–113, http://eudml.org/doc/130024

[50] T.-L. Horng, T.-C. Lin, C. Liu, and B. Eisenberg, *PNP equations with steric effects: A model of ion flow through channels*, J. Phys. Chem. B, 116 (2012), pp. 11422–11441, https://doi.org/10.1021/jp305273n

[51] C.-Y. Hsieh, Y. Hyon, H. Lee, T.-C. Lin, and C. Liu, *Transport of charged particles: entropy production and maximum dissipation principle*, J. Math. Anal. Appl., 422 (2015), pp. 309–336, https://doi.org/10.1016/j.jmaa.2014.07.078

doi:10.6342/NTU202501331

[52] C.-Y. Hsieh and T.-C. Lin, *Exponential decay estimates for the stability of boundary layer solutions to Poisson-Nernst-Planck systems: one spatial dimension case*, SIAM J. Math. Anal., 47 (2015), pp. 3442–3465, https://doi.org/10.1137/140994095

[53] C.-Y. Hsieh, *Stability of radial solutions of the Poisson–Nernst–Planck system in annular domains*, Discrete Contin. Dyn. Syst. Ser. B, 24 (2019), pp. 2657–2681, https://doi.org/10.3934/dcdsb.2018269

[54] C.-Y. Hsieh, *Global existence of solutions for the Poisson–Nernst–Planck system with steric effects*, Nonlinear Anal. Real World Appl., 50 (2019), pp. 34–54, https://doi.org/10.1016/j.nonrwa.2019.04.001

[55] Y. Hyon, B. Eisenberg, and C. Liu, *A mathematical model for the hard sphere repulsion in ionic solutions*, Commun. Math. Sci., 9 (2011), pp. 459–475, https://doi.org/10.4310/CMS.2011.v9.n2.a5

[56] Y. Hyon, B. Eisenber, and C. Liu, *An energetic variational approach to ion channel dynamics*, Math. Meth. Appl. Sci., 37 (2014), pp. 952–961, https://doi.org/10.1002/mma.2852

[57] Y. Hyon, D.Y. Kwak, and C. Liu, *Energetic variational approach in complex fluids: maximum dissipation principle*, Discrete Contin. Dyn. Syst., 26 (2010), pp. 1291–1304, https://doi.org/10.3934/dcds.2010.26.1291

[58] B. Huang, S. Maset, and K. Bohinc, *Interaction between charged cylinders in electrolyte solution; Excluded volume effect*, J. Phys. Chem. B, 121 (2017), pp. 9013–9023, https://doi.org/10.1021/acs.jpcb.7b05444

[59] J. Jacobsen and K. Schmitt, *The Liouville–Bratu–Gelfand Problem for Radial Operators*, J. Differ. Equ., 184 (2002), pp. 283–298, https://doi.org/10.1006/jdeq.2001.4151

[60] I. Kalcher, J. C. F. Schulz, and J. Dzubiella, *Ion-specific excluded-volume correlations and solvation forces*, Phys. Rev. Lett., 104 (2010), 097802, https://doi.org/10.1103/PhysRevLett.104.097802

doi:10.6342/NTU202501331

[61] V. Kamysbayev, V. Srivastava, N. B. Ludwig, O. J. Borkiewicz, H. Zhang, J. Ilavsky, B. Lee, K. W. Chapman, S. Vaikuntanathan, and D. V. Talapin, *Nanocrystals in Molten Salts and Ionic Liquids: Experimental Observation of Ionic Correlations Extending beyond the Debye Length*, ACS Nano, 13 (2019), pp. 5760–5770, https://doi.org/10.1021/acsnano.9b01292

[62] A. Khlyupin, I. Nesterova, and K. Gerke, *Molecular scale roughness effects on electric double layer structure in asymmetric ionic liquids*, Electrochimica Acta, 450 (2023), 142261, https://doi.org/10.1016/j.electacta.2023.142261

[63] C. Khripin, A. Jagota, and C.-Y. Hui, *Electric fields in an electrolyte solution near a strip of fixed potential*, J. Chem. Phys., 123 (2005), 134705, https://doi.org/10.1063/1.2043067

[64] E. Kierlik and M. L. Rosinberg. *Density-functional theory for inhomogeneous fluids: Adsorption of binary mixtures*, Phys. Rev. A, 44 (1991), pp. 5025–5037, https://doi.org/10.1103/PhysRevA.44.5025

[65] B. K. Klein, C. F. Anderson, and M. T. Record, *Comparison of Poisson-Boltzmann and condensation model expressions for the colligative properties of cylindrical polyions*, Biopolymers, 20 (1981), pp. 2263–2280, https://doi.org/10.1002/bip.1981.360201018

[66] C. Köhn, D. van Laethem, J. Deconinck, and A. Hubin, *A simulation study of steric effects on the anodic dissolution at high current densities*, Mater. Corros., 72 (2020), pp. 610–619, https://doi.org/10.1002/maco.202012051

[67] A. A. Kornyshev, *Double-layer in ioninc liquids: Paradigm change*, J. Phys. Chem. B, 111 (2007), pp. 5545–5557, https://doi.org/10.1021/jp067857o

[68] S. G. Krantz and H. R. Parks, *The Implicit Function Theorem: History, Theory, and Applications*, Birkhäuser, Basel, 2002, https://doi.org/10.1007/978-1-4614-5981-1

doi:10.6342/NTU202501331

[69] G. Lamm, *The Poisson–Boltzmann equation*, In *Reviews in Computational Chemistry*, K. B. Lipkowitz, R. Larter, and T. R. Cundari, eds., vol. 19, John Wiley & Sons, Ltd., 2003, ch. 4, pp. 147–365, https://doi.org/10.1002/0471466638.ch4

[70] C.-C. Lee, H. Lee, Y. Hyon, T.-C. Lin, and C. Liu, *New Poisson–Boltzmann type equations: one-dimensional solutions*, Nonlinearity, 24 (2011), pp. 431–458, https://doi.org/10.1088/0951-7715/24/2/004

[71] C.-C. Lee, *The charge conserving Poisson–Boltzmann equations: Existence, uniqueness, and maximum principle*, J. Math. Phys., 55 (2014), 051503, https://doi.org/10.1063/1.4878492

[72] J. W. Lee, R. H. Nilson, J. A. Templeton, S. K. Griffiths, A. Kung, and B. M. Wong, *Comparison of molecular dynamics with classical density functional and Poisson-Boltzmann theories of the electric double layer in nanochannels*, J. Chem. Theory Comput., 8 (2012), pp. 2012–2022, https://doi.org/10.1021/ct3001156

[73] C.-C. Lee, H. Lee, Y. Hyon, T.-C. Lin, and C. Liu, *Boundary Layer Solution of Charge Conserving Poisson–Boltzmann Equations: One-Dimensional Case*, Comm. Math. Sci., 14 (2016), pp. 911–940, https://doi.org/10.4310/CMS.2016.v14.n4.a2

[74] C.-C. Lee, *Asymptotic analysis of charge conserving Poisson–Boltzmann equations with variable dielectric coefficients*, Discrete Contin. Dyn. Syst. Ser. A, 36 (2016), pp. 3251–3276, https://doi.org/10.3934/dcds.2016.36.3251

[75] C.-C. Lee and R. J. Ryham, *Boundary asymptotics for a non-neutral electrochemistry model with small Debye length*, Z. Angew. Math. Phys., 69 (2018), pp. 41–53, https://doi.org/10.1007/s00033-018-0931-z

[76] C.-C. Lee, *Thin layer analysis of a non-local model for the double layer structure*, J. Differ. Equ., 266 (2019), pp. 742–802, https://doi.org/10.1016/j.jde.2018.07.055

doi:10.6342/NTU202501331

[77] C.-C. Lee, *Domain-size effects on boundary layers of a nonlocal sinh–Gordon equation*, Nonlinear. Anal., 202 (2021), 112141, https://doi.org/10.1016/j.na.2020.112141

[78] M. Lee and K.-Y. Chan, *Non-neutrality in a charged slit pore*, Chem. Phys. Lett., 275 (1997), pp. 56–62, https://doi.org/10.1016/S0009-2614(97)00737-9

[79] B. Leimkuhler and C. Matthews, *Molecular Dynamics with Deterministic and Stochastic Numerical Methods*, Springer, New York, 2015, https://doi.org/10.1007/978-3-319-16375-8

[80] Bo Li, *Continuum electrostatics for ionic solutions with non-uniform ionic sizes*, Nonlinearity, 22 (2009), pp. 811–833, https://doi.org/10.1088/0951-7715/22/4/007

[81] Bo Li, *Minimization of electrostatic free energy and the Poisson-Boltzmann equation for molecular solvation with implicit solvent*, SIAM J. Math. Anal., 40 (2009), pp. 2536–2566, https://doi.org/10.1137/080712350

[82] Bo Li, P. Liu, Z. Xu, and S. Zhou, *Ionic size effects: generalized Boltzmann distributions, counterion stratification and modified Debye length*, Nonlinearity, 26 (2013), pp. 2899–2922, https://doi.org/10.1088/0951-7715/26/10/2899

[83] F.-H. Lin and X. P. Yang, *Geometric Measure Theory: An Introduction*, International Press of Boston, Inc, 2002.

[84] T.-C. Lin and B. Eisenberg, *A new approach to the Lennard-Jones potential and a new model: PNP-steric equations*, Commun. Math., 12 (2014), pp. 149–173, https://dx.doi.org/10.4310/CMS.2014.v12.n1.a7

[85] T.-C. Lin and B. Eisenberg, *Multiple solutions of steady-state Poisson–Nernst–Planck equations with steric effects*, Nonlinearity, 28 (2015), pp. 2053–2080, https://doi.org/10.1088/0951-7715/28/7/2053

doi:10.6342/NTU202501331

[86] W. Liu, Y. Zhou, and P. Shi, *Shear electroconvective instability in electrodialysis channel under extreme depletion and its scaling laws*, Phys. Rev. E, 101 (2020), 043105, https://doi.org/10.1103/PhysRevE.101.043105

[87] B. Z. Lu, Y. C. Zhou, M. J. Holst, and J. A. McCammon, *Recent progress in numerical methods for the Poisson-Boltzmann equation in biophysical applications*, Commun. Comput. Phys., 3 (2008), pp. 973–1009, https://doi.org/2008-CiCP-7885

[88] B. Lu and Y. C. Zhou, *Poisson–Nernst–Planck Equations for Simulating Biomolecular Diffusion-Reaction Processes II: Size Effects on Ionic Distributions and Diffusion-Reaction Rates*, Biophys. J., 100 (2011), pp. 2475–2485, https://doi.org/10.1016/j.bpj.2011.03.059

[89] J.-H. Lyu, C.-C. Lee and T.-C. Lin, *Near- and far-field expansions for stationary solutions of Poisson-Nernst-Planck equations*, Math. Methods Appl. Sci., 44 (2021), pp. 10837–10860, https://doi.org/10.1002/mma.7453

[90] J.-H. Lyu and T.-C. Lin, *PB-steric equations: A general model of PB equations*, SIAM J. Applied Math., 83 (2023), pp. 1603–1622, https://doi.org/10.1137/22M1516270

[91] A. Mamonov, R. Coalson, A. Nitzan, and M. Kurnikova, *The role of the dielectric barrier in narrow biological channels: a novel composite approach to modeling single channel currents*, Biophys. J., 84 (2003), pp. 3646–3661, https://doi.org/10.1016/S0006-3495(03)75095-4

[92] N. Martinov, D. Ouroushev, and E. Chelevie, *New types of polarisation following from the nonlinear spherical radial Poisson-Boltzmann equation*, J. Phys. A: Math. Gen., 19 (1986), pp. 1327–1332, https://doi.org/10.1088/0305-4470/19/8/014

[93] I. Mező, *The Lambert W Function: Its Generalizations and Applications*, Chapman and Hall, London, 2022, https://doi.org/10.1201/9781003168102

doi:10.6342/NTU202501331

[94] Y. Mori, J. W. Jerome, and C. S. Peskin, *A three-dimensional model of cellular electrical activity*, Bull. Inst. Math. Acad. Sin., 2 (2007), pp. 367–390, https://www.math.sinica.edu.tw/bulletins/20072/2007212.pdf

[95] R. H. Nilson and S.K. Griffiths, *Influence of atomistic physics on electro-osmotic flow: An analysis based on density functional theory*, J. Chem. Phys., 125 (2006), 164510, https://doi.org/10.1063/1.2358684

[96] L. H. Olesen, H. Bruus, and A. Ajdari, *ac electrokinetic micropumps: The effect of geometrical confinement, Faradaic current injection, and nonlinear surface capacitance*, Phys. Rev. E, 73 (2006), 056313, https://doi.org/10.1103/PhysRevE.73.056313

[97] J. H. Park and J. W. Jerome, *Qualitative properties of steady-state Poisson–Nernst–Planck systems: mathematical study*, SIAM J. Appl. Math., 57 (2017), pp. 609–630, https://www.jstor.org/stable/2951898

[98] J. L. G. Pestana and D. H. Eckhardt, *An approximate analytic solution to the three-dimensional Poisson–Boltzmann equation*, J. Phys. A: Math. Theor., 40 (2007), pp. 12001–12006, https://doi.org/10.1088/1751-8113/40/39/019

[99] D. N. Petsev, F. van Swol, and L. J. D. Frink, *Molecular Theory of Electric Double Layers*, IOP Publishing, 2021, https://doi.org/10.1088/978-0-7503-2276-8

[100] F. Plouraboué and H.-C. Chang, *Attraction between two similar particles in an electrolyte: effects of Stern layer absorption*, An Acad Bras Cienc, 82 (2010), pp. 95–108, https://doi.org/10.1590/S0001-37652010000100009

[101] D. C. Rapaport, *The Art of Molecular Dynamics Simulation*, Cambridge University Press, Cambridge, 1995, https://doi.org/10.1017/CBO9780511816581

[102] R. A. Rica, R. Ziano, D. Salerno, F. Mantegazza, and D. Brogioli, *Thermodynamic relation between voltage concentration dependence and*

doi:10.6342/NTU202501331

salt adsorption in electrochemical cells, Phys. Rev. Lett., 109 (2012), 156103, https://doi.org/10.1103/PhysRevLett.109.156103

[103] S. M. Rubinstein, G. Manukyan, A. Staicu, I. Rubinstein, B. Zaltzman, R. G. H. Lammertink, F. Mugele, and M. Wessling, *Direct observation of a nonequilibrium electro-osmotic instability*, Phys. Rev. Lett., 101 (2008), 236101, https://doi.org/10.1103/PhysRevLett.101.236101

[104] W. B. Russel, D. A. Saville, and W. R. Schowalter, *Colloidal Dispersions*, Cambridge Univ. Press, 1989, https://doi.org/10.1017/CBO9780511608810

[105] R. Ryham, C. Liu, and Z.-Q. Wang, *On electro-kinetic fluids: One dimensional configurations*, Discrete Cont. Dyn. Syst. - B, 6 (2006), pp. 357–371, https://doi.org/10.3934/dcdsb.2006.6.357

[106] L. Samaj and E. Trizac, *Effective charge of cylindrical and spherical colloids immersed in an electrolyte: the quasi-planar limit*, J. Phys. A: Math. Theor., 48 (2015), 265003, https://doi.org/10.1088/1751-8113/48/26/265003

[107] A. Singer, D. Gillespie, J. Norbury, and R. S. Eisenberg, *Singular perturbation analysis of the steady–state Poisson–Nernst–Planck system: applications to ion channels*, European J. Appl. Math., 19 (2008), pp. 541–560, https://doi.org/10.1017/S0956792508007596

[108] A. R. Stinchcombe, Y. Mori, and C. S. Peskin, *Well-Posed Treatment of Space-Charge Layers in the Electroneutral Limit of Electrodiffusion*, Commun. Pure Appl. Math., 69 (2016), pp. 2221–2249, https://doi.org/10.1002/cpa.21611

[109] M. Struwe, *Variational Methods: Applications to Nonlinear Partial Differential Equations and Hamiltonian Systems*, Springer, 2008, https://doi.org/10.1007/978-3-540-74013-1

[110] H. Sugioka, *Ion-conserving Poisson–Boltzmann theory*, Phys. Rev. E, 86 (2012), 016318, https://doi.org/10.1103/PhysRevE.86.016318

doi:10.6342/NTU202501331

[111] Z. Tang, L. E. Scriven, and H. T. Davis, *A three-component model of the electrical double layer*, J. Chem. Phys., 97 (1992), pp. 494–503, https://doi.org/10.1063/1.463595

[112] L. Wan, S. Xu, M. Liao, C. Liu, and P. Sheng, *Self-Consistent Approach to Global Charge Neutrality in Electrokinetics: A Surface Potential Trap Model*, Phys. Rev. X, 4 (2014), 011042, https://doi.org/10.1103/PhysRevX.4.011042

[113] X. Xing, *Poisson–Boltzmann theory for two parallel uniformly charged plates*, Phys. Rev. E, 83 (2011), 041410, https://doi.org/10.1103/PhysRevE.83.041410

[114] Y. Yang, J. Walz, and P. Pintauro, *Curvature effects on electric double-layer forces, Part 1. — Comparisons with parallel plate geometry*, J. Chem. Soc. Farady trans., 91 (1995), pp. 2827–2836, https://doi.org/10.1039/FT9959102827

[115] Y. Yang, J. Walz, and P. Pintauro, *Curvature effects on electric double-layer forces, Part 2. — Dependence of forces on cavity radius and relative permittivity*, J. Chem. Soc. Farady trans., 93 (1997), pp. 603–611, https://doi.org/10.1039/A607031K

[116] F. Ziebert, M. Z. Bazant, and D. Lacoste, *Effective zero-thickness model for a conductive membrane driven by an electric field*, Phys. Rev. E, 81 (2010), 031912, https://doi.org/10.1103/PhysRevE.81.031912

[117] S. Zhou, Z. Wang, and B. Li, *Mean-field description of ionic size effects with nonuniform ionic sizes: A numerical approach*, Phys. Rev. E, 84 (2011), 021901, https://doi.org/10.1103/PhysRevE.84.021901

doi:10.6342/NTU202501331