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GEOMETRIC SINGULAR PERTURBATION APPROACH TO STEADY-STATE POISSON–NERNST–PLANCK SYSTEMS*

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Abstract. Boundary value problems of a one-dimensional steady-state Poisson–Nernst–Planck (PNP) system for ion flow through a narrow membrane channel are studied. By assuming the ratio of the Debye length to a characteristic length to be small, the PNP system can be viewed as a singularly perturbed problem with multiple time scales and is analyzed using the newly developed geometric singular perturbation theory. Within the framework of dynamical systems, the global behavior is first studied in terms of limiting fast and slow systems. It is rather surprising that a *complete* set of integrals is discovered for the (nonlinear) limiting fast system. This allows a detailed description of the boundary layers for the problem. The slow system itself turns out to be a singularly perturbed one, too, which indicates that the singularly perturbed PNP system has three different time scales. A singular orbit (zeroth order approximation) of the boundary value problem is identified based on the dynamics of limiting fast and slow systems. An application of the geometric singular perturbation theory gives rise to the existence and (local) uniqueness of the boundary value problem.

Key words. singular perturbation, boundary layers, exchange lemma

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1. Introduction. Poisson–Nernst–Planck (PNP) systems serve as basic electrodiffusion equations modeling, for example, ion flow through membrane channels, and transport of holes and electrons in semiconductors (see [1, 2, 11, 14] and references therein). In the context of ion flow through a membrane channel, the flow of ions is driven by their concentration gradients and by the electric field modeled together by the Nernst–Planck equations, and the electric field is in turn governed by the ion concentrations through the Poisson equation. To motivate the one-dimensional PNP system to be studied, we give a brief account of the modeling. We will be interested in flow of two types of ions through a narrow membrane channel. For practical purposes, the narrow membrane channel through which ions flow is tubelike with a small aspect ratio and, in this regard, it is natural to approximate the channel as a one-dimensional object (see, e.g., [1, 2]). Now consider flow of two types of ions, S_1 and S_2, with valences $\alpha > 0$ and $-\beta < 0$, passing through an ion channel viewed as a line segment. Let x be the coordinate along the channel normalized from $x = 0$ to $x = 1$. Denote the concentrations of S_1 and S_2 at location x and at time t by $c_1(t, x)$ and $c_2(t, x)$. Then the electric potential $\phi(t, x)$ in the channel at time t is determined by the Poisson equation

$$\frac{\partial^2\phi}{\partial x^2} = -\frac{1}{\epsilon^2}(\alpha c_1 - \beta c_2),$$

where the parameter ϵ^2 is related to the ratio of the Debye length to a characteristic length scale. The flux densities, $\bar{J}_1$ and $\bar{J}_2$, of the two ions contributed from the concentration gradients of the two ions and the electric field satisfy the Nernst–Planck

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equations

$$D_1\left(\frac{\partial c_1}{\partial x}+\alpha c_1\frac{\partial \phi}{\partial x}\right)=-\bar{J}_1,\quad D_1\left(\frac{\partial c_2}{\partial x}-\beta c_2\frac{\partial \phi}{\partial x}\right)=-\bar{J}_2,$$

where D_1 and D_2 are the diffusion constants of ions S_1 and S_2 relative to the membrane channel, together with the conservation of mass

$$\frac{\partial c_1}{\partial t}+\frac{\partial \bar{J}_1}{\partial x}=0,\quad \frac{\partial c_2}{\partial t}+\frac{\partial \bar{J}_2}{\partial x}=0.$$

Combining the above equations, we obtain the one-dimensional PNP system as a simplified model for flow of two ions through a narrow membrane channel:

$$(1)\qquad \begin{aligned}&\epsilon^2\frac{\partial^2\phi}{\partial x^2}=-(\alpha c_1-\beta c_2),\quad \frac{\partial c_1}{\partial t}+\frac{\partial \bar{J}_1}{\partial x}=0,\quad \frac{\partial c_2}{\partial t}+\frac{\partial \bar{J}_2}{\partial x}=0,\\ &D_1\left(\frac{\partial c_1}{\partial x}+\alpha c_1\frac{\partial \phi}{\partial x}\right)=-\bar{J}_1,\quad D_1\left(\frac{\partial c_2}{\partial x}-\beta c_2\frac{\partial \phi}{\partial x}\right)=-\bar{J}_2.\end{aligned}$$

To understand the asymptotic behavior that is most relevant from a physical point of view, the first step is to study the steady-state problem. On one hand, steady-state solutions are among those that are responsible for the global structure of the full system and, on the other hand, they often represent asymptotic states of solutions of general initial conditions. In this work, we study boundary value problems of the one-dimensional steady-state PNP system. The corresponding system is

$$(2)\qquad \begin{aligned}&\epsilon^2\frac{d^2\phi}{dx^2}=-(\alpha c_1-\beta c_2),\quad \frac{dJ_1}{dx}=0,\quad \frac{dJ_2}{dx}=0,\\ &\frac{dc_1}{dx}+\alpha c_1\frac{d\phi}{dx}=-J_1,\quad \frac{dc_2}{dx}-\beta c_2\frac{d\phi}{dx}=-J_2,\end{aligned}$$

where $J_1=\bar{J}_1/D_1$ and $J_2=\bar{J}_2/D_2$, and the boundary conditions are

$$(3)\qquad \begin{aligned}&\phi(0)=v_0,\quad c_1(0)=L_1,\quad c_2(0)=L_2,\\ &\phi(1)=0,\quad c_1(1)=R_1,\quad c_2(1)=R_2.\end{aligned}$$

Many mathematical works have been done on the existence, uniqueness, and qualitative properties of boundary value problems even for high dimensional systems, and algorithms have been developed toward numerical approximations (see, e.g., [5, 6, 13, 7]). Under the assumption that $\epsilon \ll 1$, the problem can be viewed as a singularly perturbed system. Typical solutions of singularly perturbed systems exhibit different time scales; for example, boundary and internal layers (inner solutions) evolve at fast pace and regular layers (outer solutions) vary slowly. For the boundary value problems (2) and (3), there are two boundary layers, one at each end. Physically, near boundaries $x=0$ and $x=1$, the potential function $\phi(x)$ and the concentration functions $c_1(x)$ and $c_2(x)$ exhibit a large gradient or a sharp change. In [2], for $\alpha=\beta=1$, the boundary value problem was studied using the method of matched asymptotic expansions as well as numerical simulations, which provide a good quantitative and qualitative understanding of the problem.

We also treat the problem as a singularly perturbed one by assuming $\epsilon \ll 1$ but for general α and β. Our approach uses the newly developed geometric singular perturbation theory (see, e.g., [4, 8, 10, 12]). The basic ideas behind this theory for boundary value problems are

(i) to derive, based on different time scales of the system, various limiting systems for $\epsilon = 0$ and examine their dynamical structures;
(ii) to construct a singular orbit (zeroth order approximation) consisting of orbits of limiting systems, which include boundary layers, regular layers, and, sometimes, internal layers;
(iii) to show that there are true solutions near the singular orbit for $\epsilon > 0$.

Since limiting systems essentially have lower order than the full system, it is often easier to study which make (i) useful. Understanding the dynamics of limiting subsystems allows one to carry out (ii). The most difficult part is the task (iii). It requires us to investigate the interaction between the fast and slow dynamics. A successful type of results is called the exchange lemma (see, e.g., [8, 10, 15, 12]). Its objective is to track the smooth configuration of an invariant manifold as it passes regions overlapping different time scales. For boundary value problems, two invariant manifolds, say, M_L and M_R, will be tracked: M_L will be the trace of one boundary under the flow, and M_R will be the trace of the other boundary. The existence of a solution for $\epsilon > 0$ is then reduced to the nontrivial intersection of M_L and M_R. This is where the exchange lemma comes in to play the crucial role. This approach provides not only a construction of a limiting solution but also a direct verification of the validity of the limiting solution.

The rest of the paper is organized as follows. Section 2 contains three subsections. In section 2.1, the PNP system (2) is rewritten as a singularly perturbed system of first order equations, and the boundary value problem is converted to a *connecting problem*. Two systems, slow and fast systems, with different scales are first identified according to different time scales, and some general aspects of dynamical system theory are laid out for the boundary value problem. The boundary layer behavior governed by the limiting fast system is studied in section 2.2. It is rather surprising that a complete set of integrals is discovered for the nonlinear limiting fast system which allows a detailed study of the boundary layer behavior. (The physical meanings of the integrals remain unclear.) The regular layers governed by the slow flow are analyzed in section 2.3. It turns out that the slow system itself is a singularly perturbed one which is examined using again the geometric singular perturbation theory. In section 3, we construct a singular orbit of the boundary value problem and apply the exchange lemma to show the existence and uniqueness of a solution near the singular orbit. A derivation of the integrals of the fast system is given in section 4 as an appendix.

2. A dynamical system framework.

2.1. A basis of geometric singular perturbation theory. We will recast the singularly perturbed PNP system into a system of first order equations. This singularly perturbed system corresponds to the slow scale which is suitable for understanding dynamics within the membrane channel. A fast scale system can be derived through a change of scale of the independent variable x, which can be used to capture the sharp boundary behavior. Slow and fast systems of the singularly perturbed PNP system are equivalent for $\epsilon \neq 0$, but their limits are not: they provide complementary limiting information for the full system. We begin with a dynamical system formulation of the singularly perturbed PNP system (2).

Denote derivatives with respect to x by overdot symbols and introduce

$$u = \epsilon\dot{\phi}, \quad v = \beta c_2 - \alpha c_1, \quad w = \alpha^2 c_1 + \beta^2 c_2, \quad \text{and} \quad \tau = x.$$

System (2) becomes

$$\begin{aligned} &\epsilon\dot{\phi} = u, \quad \epsilon\dot{u} = v, \quad \epsilon\dot{v} = uw - \epsilon(\beta J_2 - \alpha J_1), \\ &\epsilon\dot{w} = \alpha\beta uv + (\beta-\alpha)uw - \epsilon(\alpha^2 J_1 + \beta^2 J_2), \\ &\dot{J}_1 = 0, \quad \dot{J}_2 = 0, \quad \dot{\tau} = 1. \end{aligned} \tag{4}$$

System (4) will be treated as a dynamical system with the phase space $\mathbb{R}^7$, and the independent variable x will be viewed as time. The boundary condition (3) becomes

$$\begin{aligned} \phi(0) = v_0, \quad v(0) = \beta L_2 - \alpha L_1, \quad w(0) = \alpha^2 L_1 + \beta^2 L_2, \quad \tau(0) = 0, \\ \phi(1) = 0, \quad v(1) = \beta R_2 - \alpha R_1, \quad w(1) = \alpha^2 R_1 + \beta^2 R_2, \quad \tau(1) = 1. \end{aligned} \tag{5}$$

Formulation of high order equations into dynamical systems of first order equations is not unique. For the boundary value problem considered in this paper, two issues need particular attention. One is toward the derivative of $\phi(x)$. Since $\phi(x)$ is expected to have large derivatives near the boundaries, the introduction of $u = \epsilon\dot{\phi}$ seems natural. The introduction of a new variable $\tau = x$ is a special treatment for boundary value problems. The small price paid is the addition of an extra dimension with trivial dynamics to the phase space. The apparent advantage is that, to find a solution of the boundary value problem, one needs only an orbit from one boundary to the other without worrying how much time it takes the orbit to move from one side to the other: it is automatically 1 since, as a component of the orbit, $\tau = x$ will vary from 0 to 1. The change of variables from c_1 and c_2 to v and w is motivated purely from the analysis point of view.

Observe that by setting $\epsilon = 0$ in system (4), we get $u = v = 0$. The set $\mathcal{Z}_0 = \{u = v = 0\}$ is called *the slow manifold* which supports the regular layer of the boundary value problem. The regular layer will not satisfy all conditions in (5) if $\beta L_2 - \alpha L_1 \neq 0$ or $\beta R_2 - \alpha R_1 \neq 0$, and this defect has to be remedied by boundary layers. To examine boundary layer behavior, we will now derive a system, the fast system, with a time scale different from that of (4). This will be achieved through the following rescaling of time (independent variable) for dependent variables:

$$\begin{gathered} \Phi(\xi) = \phi(\epsilon\xi),\ U(\xi) = u(\epsilon\xi),\ V(\xi) = v(\epsilon\xi),\ W(\xi) = w(\epsilon\xi), \\ I_i(\xi) = J_i(\epsilon\xi), \ \text{ and } \ T(\xi) = \tau(\epsilon\xi). \end{gathered}$$

Note that capital letters for same dependent variables are used to indicate merely different time scales. In terms of ξ, we obtain *the fast system* of (4):

$$\begin{aligned} &\Phi' = U, \quad U' = V, \quad V' = UW - \epsilon(\beta I_2 - \alpha I_1), \\ &W' = \alpha\beta UV + (\beta-\alpha)UW - \epsilon(\alpha^2 I_1 + \beta^2 I_2), \\ &I_1' = 0, \quad I_2' = 0, \quad T' = \epsilon, \end{aligned} \tag{6}$$

where the prime symbol denotes the derivative with respect to the variable ξ. The limiting fast system at $\epsilon = 0$ is

$$\begin{aligned} &\Phi' = U, \quad U' = V, \quad V' = UW, \quad W' = \alpha\beta UV + (\beta-\alpha)UW, \\ &I_1' = 0, \quad I_2' = 0, \quad T' = 0. \end{aligned} \tag{7}$$

The slow manifold $\mathcal{Z}_0$ is precisely the set of equilibria of (7).

Now let B_L and B_R be the subsets of $\mathbb{R}^7$ defined, respectively, by

$$
\begin{aligned}
B_L =& \{\phi = v_0,\ v = \beta L_2 - \alpha L_1,\ w = \alpha^2 L_1 + \beta^2 L_2,\ \tau = 0\}, \\
B_R =& \{\phi = 0,\ v = \beta R_2 - \alpha R_1,\ w = \alpha^2 R_1 + \beta^2 R_2,\ \tau = 1\}.
\end{aligned} \tag{8}
$$

The boundary value problem is then equivalent to the following *connecting problem*: finding a solution of (4) from B_L to B_R.

For $\epsilon > 0$, let M_L^ϵ be the union of all forward orbits of (4) starting from B_L and let M_R^ϵ be the union of all backward orbits starting from B_R. To obtain the existence and (local) uniqueness of a solution for the connecting problem, it thus suffices to show M_L^ϵ and M_R^ϵ intersect transversally. The intersection is exactly the orbit of a solution of the boundary value problem, and the transversality implies the local uniqueness. The strategy is to obtain a singular orbit and track the evolution of M_L^ϵ and M_R^ϵ along the singular orbit. As discussed in the introduction, a singular orbit will be a union of orbits of subsystems of (4) with different time scales.

The boundary layers will be two orbits of (7): one from B_L to $\mathcal{Z}_0$ in forward time along the stable manifold of $\mathcal{Z}_0$ and the other from B_R to $\mathcal{Z}_0$ in backward time along the unstable manifold of $\mathcal{Z}_0$. The two boundary layers will be connected by a regular layer on $\mathcal{Z}_0$, which is an orbit of a limiting system of (4). The next two subsections are devoted to the study of boundary layers and regular layers.

2.2. Fast dynamics and boundary layers. We start with the study of boundary layers governed by system (7). This system has many invariant structures that are useful for characterizing the global dynamics.

The slow manifold $\mathcal{Z}_0 = \{U = V = 0\}$ consisting entirely of equilibria of system (7) is a five-dimensional manifold of the phase space $\mathbb{R}^7$. For each equilibrium $z = (\Phi, 0, 0, W, I_1, I_2, T) \in \mathcal{Z}_0$, the linearization of system (7) has five zero eigenvalues corresponding to the dimension of $\mathcal{Z}_0$, and two eigenvalues in directions normal to $\mathcal{Z}_0$. The latter two eigenvalues and their associated eigenvectors are given by

$$
\lambda_\pm = \pm\sqrt{W} \quad \text{and} \quad n_\pm = \Big((\pm\sqrt{W})^{-1}, 1, \pm\sqrt{W}, \pm(\beta-\alpha)\sqrt{W}, 0, 0, 0\Big)^\tau. \tag{9}
$$

Thus, every equilibrium has a one-dimensional stable manifold and a one-dimensional unstable manifold. The global configurations of the stable and unstable manifolds will be needed for the boundary layer behavior. For any constants I_1^*, I_2^*, and T^*, the set $\mathcal{N} = \{I_1 = I_1^*, I_2 = I_2^*, T = T^*\}$ is a four-dimensional invariant subspace of the phase space $\mathbb{R}^7$.

Surprisingly, system (7) possesses a complete set of integrals with which the dynamics can be fully analyzed; in particular, the stable and unstable manifolds can be characterized and the behavior of boundary layers can be described in detail.

PROPOSITION 2.1. (i) *System* (7) *has a complete set of six integrals given by*

$$
\begin{aligned}
H_1 = W - (\beta-\alpha)V - \frac{\alpha\beta}{2}U^2,\ H_2 = \Phi - \frac{\ln|W+\alpha V|}{\beta}, \\
H_3 = |W+\alpha V|^\alpha |W-\beta V|^\beta,\ H_4 = I_1,\ H_5 = I_2, \quad \textit{and} \quad H_6 = T,
\end{aligned}
$$

where the argument of H_i's is $(\Phi, U, V, W, I_1, I_2, T)$.

(ii) *The stable and unstable manifolds $W^s(\mathcal{Z}_0)$ and $W^u(\mathcal{Z}_0)$ of $\mathcal{Z}_0$ are characterized as follows:*

$$
W^s(\mathcal{Z}_0) = \cup\{W^s(z^*) : z^* \in \mathcal{Z}_0\} \quad \textit{and} \quad W^u(\mathcal{Z}_0) = \cup\{W^u(z^*) : z^* \in \mathcal{Z}_0\}
$$

and, for $z^*=(\Phi^*,0,0,W^*,I_1^*,I_2^*,T^*)\in\mathcal{Z}_0$*, a point* $z=(\Phi,U,V,W,I_1,I_2,T)\in W^s(z^*)\cup W^u(z^*)$ *if and only if*

$$H_1(z)=W^*,\ H_2(z)=\Phi^*-\frac{\ln W^*}{\beta},\ H_3(z)=(W^*)^{\alpha+\beta},\ I_i=I_i^*,\ T=T^*.$$

(iii) *The stable manifold* $W^s(\mathcal{Z}_0)$ *intersects* B_L *transversally at points with*

$$U=-\mathrm{sgn}\ (\beta L_2-\alpha L_1)\sqrt{\frac{2\alpha\beta(L_1+L_2)-2(\alpha+\beta)(\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}}}{\alpha\beta}} \tag{10}$$

and arbitrary I_1 *and* I_2*, where* sgn *is the sign function. The unstable manifold* $W^u(\mathcal{Z}_0)$ *intersects* B_R *transversally at points with*

$$U=\mathrm{sgn}\ (\beta R_2-\alpha R_1)\sqrt{\frac{2\alpha\beta(R_1+R_2)-2(\alpha+\beta)(\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}}}{\alpha\beta}} \tag{11}$$

and arbitrary I_1 *and* I_2*. Let* $N_L=B_L\cap W^s(\mathcal{Z}_0)$ *and* $N_R=B_R\cap W^u(\mathcal{Z}_0)$*. Then,*

$$\omega(N_L)=\left\{\left(v_0+\frac{1}{\alpha+\beta}\ln\frac{\alpha L_1}{\beta L_2},0,0,(\alpha+\beta)(\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}},I_1,I_2,0\right)\right\},$$

$$\alpha(N_R)=\left\{\left(\frac{1}{\alpha+\beta}\ln\frac{\alpha R_1}{\beta R_2},0,0,(\alpha+\beta)(\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}},I_1,I_2,1\right)\right\}$$

for all I_1 *and* I_2*.*

Proof. The statement (i) can be verified directly (see section 4 for a derivation of H_3). The statement (ii) is a simple consequence of (i) together with the fact that $\Phi(\xi)\to\Phi^*$, $W(\xi)\to W^*$, $U(\xi)\to 0$, and $V(\xi)\to 0$ as $\xi\to\infty$ for the stable manifold and as $\xi\to-\infty$ for the unstable manifold.

For the statement (iii), we present only the proof regarding the intersection of $W^s(\mathcal{Z}_0)$ and B_L. Suppose

$$z^0=(\Phi^0,U^0,V^0,W^0,I_1^0,I_2^0,0)=(v_0,U^0,\beta L_2-\alpha L_1,\alpha^2L_1+\beta^2L_2,I_1^0,I_2^0,0)$$

is a point in $B_L\cap W^s(\mathcal{Z}_0)$. Then, using the integrals H_1, H_2, and H_3, the solution $z(\xi)=(\Phi(\xi),U(\xi),V(\xi),W(\xi),I_1^0,I_2^0,0)$ of system (7) with initial condition $z(0)=z^0$ satisfies

$$\begin{aligned}H_1(z(\xi))&=W(\xi)-(\beta-\alpha)V(\xi)-\frac{\alpha\beta}{2}U^2(\xi)=A,\\ H_2(z(\xi))&=\Phi(\xi)-\frac{\ln|W(\xi)+\alpha V(\xi)|}{\beta}=B,\\ H_3(z(\xi))&=|W(\xi)+\alpha V(\xi)|^{\alpha}|W(\xi)-\beta V(\xi)|^{\beta}=C\end{aligned}$$

for some constants A, B, and C, and for all ξ. Since $U(\xi)\to 0$ and $V(\xi)\to 0$ as $\xi\to+\infty$, $W(+\infty)=A$ from $H_1(z(\xi))=A$, and hence, $C=A^{\alpha+\beta}$ from $H_3(z(\xi))=C$. Now using the equations $H_3(z(0))=C=A^{\alpha+\beta}$ and $H_2(z(0))=B$, we have

$$A=(\alpha+\beta)(\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}},\quad B=v_0-\frac{\ln((\alpha+\beta)\beta L_2)}{\beta}.$$

Then, from $H_1(z(0)) = A$ and $H_2(z(\infty)) = B$, one has

$$U^0 = -\text{sgn }(V^0)\sqrt{\frac{2(\alpha\beta(L_1+L_2)-A)}{\alpha\beta}} \text{ and } \Phi(+\infty) = v_0 + \frac{1}{\alpha+\beta}\ln\frac{\alpha L_1}{\beta L_2}.$$

The choice of the sign for U^0 comes from the consideration that the stable eigenvector n_- in (9) has U and V components with opposite signs. Thus, B_L and $W^s(\mathcal{Z}_0)$ intersect at the points with $U = U^0$ given above, and all I_1 and I_2. If $N_L = B_L \cap W^s(\mathcal{Z}_0)$, then $\omega(N_L) = \{(\Phi(+\infty), 0, 0, W(+\infty), I_1, I_2, 0)\}$. The above formulas for $\Phi(+\infty)$ and $W(+\infty) = A$ give the desired characterization of $\omega(N_L)$. Lastly, since the stable manifold is completely characterized, one can compute its tangent space at each intersection point to verify the transversality of the intersection. It is slightly complicated but straightforward. We will omit the detail here. ∎

Part (iii) of this result implies that the boundary layer on the left end will be an orbit of (7) from $(v_0, U_L, \beta L_2 - \alpha L_1, \alpha^2 L_1 + \beta^2 L_2, I_1, I_2, 0) \in B_L$ to the point

$$z_L = \left(v_0 + \frac{1}{\alpha+\beta}\ln\frac{\alpha L_1}{\beta L_2}, 0, 0, (\alpha+\beta)(\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}}, I_1, I_2, 0\right) \in \mathcal{Z}_0,$$

where U_L is given by the display (10) and I_1 and I_2 are arbitrary at this moment, and that on the right end will be a backward orbit of (7) from the point $(0, U_R, \beta R_2 - \alpha R_1, \alpha^2 R_1 + \beta^2 R_2, I_1, I_2, 1) \in B_R$ to the point

$$z_R = \left(\frac{1}{\alpha+\beta}\ln\frac{\alpha R_1}{\beta R_2}, 0, 0, (\alpha+\beta)(\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}}, I_1, I_2, 1\right) \in \mathcal{Z}_0,$$

where U_R is given by the display (11) and I_1 and I_2 are arbitrary at this moment. It turns out that there is a unique pair of numbers I_1 and I_2 so that the corresponding points z_L and z_R can be connected by a regular layer solution on $\mathcal{Z}_0$. The regular orbit together with the two boundary layer orbits provides the singular orbit.

Remark 2.1. The integrals H_2 and H_3 imply that

$$\tilde{H}_2 = \Phi + \frac{\ln|W - \beta V|}{\alpha}$$

is also an integral which can be viewed as the symmetric part to H_2.

To find the explicit expressions of the boundary layers from B_L and B_R to $\mathcal{Z}_0$, there are certain technical difficulties. But for some special cases, for example, $\alpha = \beta$, or $\alpha = 2$ and $\beta = 1$, or $\alpha = 1$ and $\beta = 2$, the difficulty can be overcome. In particular, our results for the case $\alpha = \beta = 1$ agree with those in [2], and we provide the detail below for demonstration.

COROLLARY 2.2. *If $\alpha = \beta = 1$, then the expressions of the solutions from B_L and B_R to $\mathcal{Z}_0$ can be explicitly given.*

Proof. We will derive the solution from B_L to $\mathcal{Z}_0$ for general α and β first. Let $r = W + \alpha V$ and $s = W - \beta V$. Then, $r^\alpha s^\beta = A^{\alpha+\beta}$, where A is as in Proposition 2.1, $W = (\beta r + \alpha s)/(\alpha+\beta)$, and $V = (r - s)/(\alpha+\beta)$. Using the equations in (7), one gets

$$r' = \pm\sqrt{\frac{2\beta}{\alpha(\alpha+\beta)}}\, r\sqrt{\alpha r + \beta A^{\frac{\alpha+\beta}{\beta}} r^{-\frac{\alpha}{\beta}} - (\alpha+\beta)A}.$$

The technical difficulty mentioned above for general α and β is the integration of this equation. Once r is found, the rest can be explicitly solved. The equation can be integrated for the cases mentioned above. We now carry out the rest of the analysis for $\alpha = \beta = 1$.

Without loss of generality, we assume $L_2 > L_1$. Then, $A = 2\sqrt{L_1 L_2}$ and

$$r' = -\sqrt{r}(r - 2\sqrt{L_1 L_2}).$$

Solving the equation and using $r(0) = W(0) + V(0) = 2L_2$, one gets

$$r = \frac{A(1 + ce^{-\sqrt{A}\xi})^2}{(1 - ce^{-\sqrt{A}\xi})^2}, \quad \text{where} \;\; c = \frac{L_2^{1/4} - L_1^{1/4}}{L_2^{1/4} + L_1^{1/4}}.$$

Thus,

$$s = \frac{A^2}{r} = \frac{A(1 - ce^{-\sqrt{A}\xi})^2}{(1 + ce^{-\sqrt{A}\xi})^2}, \; W = \frac{r + s}{2} = A\left(1 + \frac{8c^2 e^{-2\sqrt{A}\xi}}{(1 - c^2 e^{-2\sqrt{A}\xi})^2}\right),$$

$$V = \frac{r - s}{2} = \frac{4Ace^{-\sqrt{A}\xi}(1 + c^2 e^{-2\sqrt{A}\xi})}{(1 - c^2 e^{-2\sqrt{A}\xi})^2}, \; U = -\sqrt{2W - 2A} = -\frac{4\sqrt{A}ce^{-\sqrt{A}\xi}}{1 - c^2 e^{-2\sqrt{A}\xi}},$$

$$\Phi = B + \ln(W + V) = v_0 + \frac{1}{2}\ln\frac{L_1}{L_2} + 2\ln\left|\frac{1 + ce^{-\sqrt{A}\xi}}{1 - ce^{-\sqrt{A}\xi}}\right|.$$

The expression for Φ is obtained by either using the integral H_2 and the solutions for V and W or by directly integrating $\Phi' = U$ from U. □

2.3. Slow dynamics and regular layers. We now examine the slow flow in the vicinity of the slow manifold $\mathcal{Z}_0 = \{u = v = 0\}$ for regular layers. If we take $\epsilon = 0$ in system (4), we get $u = v = 0$ and

$$\dot{J}_1 = 0, \; \dot{J}_2 = 0, \; \dot{\tau} = 1.$$

The information on ϕ and w is lost. This indicates that the slow flow in the vicinity of $\mathcal{Z}_0$ is itself a singular perturbation problem. To see this, we zoom into an $O(\epsilon)$-neighborhood of $\mathcal{Z}_0$ by blowing up the u and v coordinates; that is, we make a scaling $u = \epsilon p$ and $v = \epsilon q$. System (4) becomes

$$\begin{aligned} &\dot{\phi} = p, \quad \epsilon\dot{p} = q, \quad \epsilon\dot{q} = pw - (\beta J_2 - \alpha J_1), \\ &\dot{w} = \epsilon\alpha\beta pq + (\beta - \alpha)pw - (\alpha^2 J_1 + \beta^2 J_2), \\ &\dot{J}_1 = 0, \quad \dot{J}_2 = 0, \quad \dot{\tau} = 1, \end{aligned} \tag{12}$$

which is indeed a singular perturbation problem. When $\epsilon = 0$, the system reduces to

$$\begin{aligned} &\dot{\phi} = p, \quad 0 = q, \quad 0 = pw - (\beta J_2 - \alpha J_1), \\ &\dot{w} = (\beta - \alpha)pw - (\alpha^2 J_1 + \beta^2 J_2), \\ &\dot{J}_1 = 0, \quad \dot{J}_2 = 0, \quad \dot{\tau} = 1. \end{aligned} \tag{13}$$

The dynamics of ϕ and w survives in this limiting process. For this system, the slow manifold is

$$\mathcal{S}_0 = \left\{ p = \frac{\beta J_2 - \alpha J_1}{w},\ q = 0 \right\}.$$

The corresponding fast system obtained by the scaling of time

$$\Phi(\xi) = \phi(\epsilon\xi),\ P(\xi) = p(\epsilon\xi),\ Q(\xi) = q(\epsilon\xi),\ \text{ and }\ W(\xi) = w(\epsilon\xi)$$

is

$$\begin{aligned} &\Phi' = \epsilon P, \quad P' = Q, \quad Q' = PW - (\beta I_2 - \alpha I_1), \\ &W' = \epsilon^2\alpha\beta PQ + \epsilon(\beta - \alpha)PW - \epsilon(\alpha^2 I_1 + \beta^2 I_2), \\ &I_1' = 0, \quad I_2' = 0, \quad T' = 0. \end{aligned} \tag{14}$$

The limiting system of (14) when $\epsilon = 0$ is

$$\begin{aligned} &\Phi' = 0, \quad P' = Q, \quad Q' = PW - (\beta I_2 - \alpha I_1), \\ &W' = 0, \quad I_1' = 0, \quad I_2' = 0, \quad T' = 0. \end{aligned} \tag{15}$$

The slow manifold $\mathcal{S}_0$ is the set of equilibria of (15). The eigenvalues normal to $\mathcal{S}_0$ are $\lambda_\pm(p) = \pm\sqrt{W}$. In particular, the slow manifold $\mathcal{S}_0$ is normally hyperbolic, and hence, it persists for system (14) for $\epsilon > 0$ small (see [4]).

The limiting slow dynamic on $\mathcal{S}_0$ is governed by system (13), which reads

$$\dot\phi = \frac{\beta J_2 - \alpha J_1}{w}, \quad \dot w = -\alpha\beta(J_1 + J_2), \quad \dot J_i = 0, \quad \dot\tau = 1.$$

The general solution is characterized as follows: J_1 and J_2 are arbitrary constants, and

$$\begin{aligned} &\tau(x) = \tau_0 + x, \quad w(x) = \alpha_0 - \alpha\beta(J_1 + J_2)x, \\ &\phi(x) = \phi_0 - \frac{\beta J_2 - \alpha J_1}{\alpha\beta(J_1 + J_2)} \ln\left(1 - \frac{\alpha\beta(J_1 + J_2)}{\alpha_0} x\right), \end{aligned} \tag{16}$$

where $\tau_0 = \tau(0)$, $\phi(0) = \phi_0$, and $w(0) = \alpha_0$. Note that if $J_1 + J_2 = 0$, then $w(x) = \alpha_0$ and $\phi(x) = \phi_0 + (\beta J_2 - \alpha J_1)x/\alpha_0$. The latter is the limit of $\phi(x)$ in (16) as $J_1 + J_2 \to 0$. We thus use the unified formula (16) even if $J_1 + J_2 = 0$.

To identify the slow portion of the singular orbit on $\mathcal{S}_0$, we need to examine the ω-limit (resp., the α-limit) set of $M_L^\epsilon \cap W^s(\mathcal{S}_0)$ (resp., $M_R^\epsilon \cap W^u(\mathcal{S}_0)$) as $\epsilon \to 0$. To do this, we fix an $O(1)$-neighborhood of $\mathcal{S}_0$. In terms of U and V, this neighborhood is of order $O(\epsilon)$. For $\epsilon > 0$ small, the time taken in terms of ξ for M_L^ϵ and M_R^ϵ to evolve to any $O(\epsilon)$-neighborhood of $\{U = V = 0\}$ is of order $O(\epsilon|\ln\epsilon|)$. Thus, the λ-lemma (see [3]) implies that M_L^ϵ (resp., M_R^ϵ) is C^1 $O(\epsilon)$-close to M_L^0 (resp., M_R^0) in any $O(\epsilon)$-neighborhood of $\{U = V = 0\}$. Therefore, in an $O(1)$-neighborhood of $\mathcal{S}_0$ in terms of P and Q, M_L^ϵ (resp., M_R^ϵ) intersects $W^s(\mathcal{S}_0)$ (resp., $W^u(\mathcal{S}_0)$) transversally. And, by abusing the notation, if $N_L = M_L^0 \cap W^s(\mathcal{S}_0)$ and $N_R = M_R^0 \cap W^u(\mathcal{S}_0)$, then $\omega(N_L)$ and $\alpha(N_R)$ have the same descriptions as those in Proposition 2.1 with $U = V = 0$ replaced by $P = (\beta I_2 - \alpha I_1)/W$ and $Q = 0$.

The slow orbit should be one given by (16) that connects $\omega(N_L)$ and $\alpha(N_R)$. Let $\bar M_L$ (resp., $\bar M_R$) be the forward (resp., backward) image of $\omega(N_L)$ (resp., $\alpha(N_R)$) under the slow flow (13).

PROPOSITION 2.3. *$\bar{M}_L$ and $\bar{M}_R$ intersect transversally along the unique orbit given by* (16) *from $x = 0$ to $x = 1$ with*

$$\tau_0 = 0,\ \alpha_0 = (\alpha+\beta)(\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}},\ \phi_0 = v_0 + \frac{1}{\alpha+\beta}\ln\frac{\alpha L_1}{\beta L_2},$$

$$J_1 = \frac{\left(\ln\frac{R_1}{L_1} - \alpha v_0\right)\left((\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}} - (\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}}\right)}{\frac{\alpha\beta}{\alpha+\beta}\ln\frac{R_1}{L_1} + \frac{\alpha^2}{\alpha+\beta}\ln\frac{R_2}{L_2}},$$

$$J_2 = \frac{\left(\ln\frac{R_2}{L_2} + \beta v_0\right)\left((\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}} - (\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}}\right)}{\frac{\beta^2}{\alpha+\beta}\ln\frac{R_1}{L_1} + \frac{\alpha\beta}{\alpha+\beta}\ln\frac{R_2}{L_2}}.$$

Proof. We show first that $\bar{M}_L$ and $\bar{M}_R$ intersect along the orbit with the above characterization. In view of (16) and the descriptions for $\omega(N_L)$ and $\alpha(N_R)$ in Proposition 2.1, the intersection is uniquely determined by

$$\tau_0 = 0,\ \alpha_0 = w(0) = (\alpha+\beta)(\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}},$$

$$w(1) = (\alpha+\beta)(\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}},$$

$$\phi_0 = \Phi(0) = v_0 + \frac{1}{\alpha+\beta}\ln\frac{\alpha L_1}{\beta L_2},\ \Phi(1) = \frac{1}{\alpha+\beta}\ln\frac{\alpha R_1}{\beta R_2}.$$

Substituting into (16) gives

$$J_1 + J_2 = \frac{\alpha+\beta}{\alpha\beta}\left((\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}} - (\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}}\right),$$

$$\beta J_2 - \alpha J_1 = \frac{(\alpha+\beta)\left((\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}} - (\alpha R_1)^{\frac{\beta}{\alpha+\beta}}(\beta R_2)^{\frac{\alpha}{\alpha+\beta}}\right)}{\frac{\beta}{\alpha+\beta}\ln\frac{R_1}{L_1} + \frac{\alpha}{\alpha+\beta}\ln\frac{R_2}{L_2}} \times\left(v_0 + \frac{1}{\alpha+\beta}\ln\frac{L_1R_2}{L_2R_1}\right),$$

which in turn yields the expressions for J_1 and J_2. To see the transversality of the intersection, it suffices to show that $\omega(N_L)\cdot 1$ (the image of $\omega(N_L)$ under the time one map of the flow of system (13)) is transversal to $\alpha(N_R)$ on $\mathcal{S}_0 \cap \{\tau = 1\}$. If we use (ϕ, w, J_1, J_2) as a coordinate system on $\mathcal{S}_0 \cap \{\tau = 1\}$, then the set $\omega(N_L)\cdot 1$ is given by $\{(\phi(J_1, J_2), w(J_1, J_2), J_1, J_2)\}$ with

$$\phi(J_1, J_2) = v_0 + \frac{1}{\alpha+\beta}\ln\frac{\alpha L_1}{\beta L_2} - \frac{\beta J_2 - \alpha J_1}{\alpha\beta(J_1+J_2)}\ln\left(1 - \frac{\alpha\beta(J_1+J_2)}{\alpha_0}\right),$$
$$w(J_1, J_2) = (\alpha+\beta)(\alpha L_1)^{\frac{\beta}{\alpha+\beta}}(\beta L_2)^{\frac{\alpha}{\alpha+\beta}} - \alpha\beta(J_1+J_2).$$

Thus, the tangent space to $\omega(N_L)\cdot 1$ restricted on $\mathcal{S}_0 \cap \{\tau = 1\}$ is spanned by $(\phi_{J_1}, w_{J_1}, 1, 0) = (\phi_{J_1}, -\alpha\beta, 1, 0)$ and $(\phi_{J_2}, w_{J_2}, 0, 1) = (\phi_{J_2}, -\alpha\beta, 0, 1)$. In view of the display in Proposition 2.1, the tangent space to $\alpha(N_R)$ restricted on $\mathcal{S}_0 \cap \{\tau = 1\}$ is spanned by $(0,0,1,0)$ and $(0,0,0,1)$. Note that $\mathcal{S}_0 \cap \{\tau = 1\}$ is four-dimensional.

Thus, it suffices to show that the above four vectors are linearly independent or, equivalently, $\phi_{J_1} \neq \phi_{J_2}$. The latter can be verified by a direct computation. Indeed, if $J_1 + J_2 \neq 0$ at the intersection points, then

$$\phi_{J_1} - \phi_{J_2} = \frac{\alpha+\beta}{\alpha\beta(J_1+J_2)} \ln\left(1 - \frac{\alpha\beta(J_1+J_2)}{\alpha_0}\right) \neq 0;$$

if $J_1 + J_2 = 0$ at the intersection points, then $\phi(J_1, J_2) = \phi_0 + (\beta J_2 - \alpha J_1)/\alpha_0$ and hence $\phi_{J_1} - \phi_{J_2} = -(\alpha+\beta)/\alpha_0 \neq 0$. □

3. Main result. Based on the study of the limiting behavior of boundary layers and regular layers in the previous section, we can easily construct a singular orbit (zeroth order approximation) of the boundary value problem. To show that there indeed exists a true solution near the singular orbit, we apply the exchange lemma to show M_L^ϵ and M_R^ϵ intersect around the singular orbit.

We now state the existence and uniqueness result of the boundary value problem, which also provides the description of a singular orbit.

THEOREM 3.1. *Assume that $\alpha L_1 \neq \beta L_2$ and $\alpha R_1 \neq \beta R_2$. For $\epsilon > 0$ small, the connecting problem* (4), (8) *has a unique solution near a singular orbit. The singular orbit is the union of two fast orbits of system* (7) *and one slow orbit of system* (13)*; more precisely, with both $I_1 = J_1$ and $I_2 = J_2$ given in Proposition* 2.3*,*

(i) *the fast orbit representing the limiting boundary layer at $x = 0$ lies on $B_L \cap W^s(\mathcal{Z}_0)$ from B_L to $\omega(N_L) \subset \mathcal{Z}_0$, whose starting point has the U-component given by* (10) *in Proposition* 2.1*;*

(ii) *the fast orbit representing the limiting boundary layer at $x = 1$ lies on $B_R \cap W^u(\mathcal{Z}_0)$ from B_R to $\alpha(N_R) \subset \mathcal{Z}_0$, whose starting point has the U-component given by* (11) *in Proposition* 2.1*;*

(iii) *the slow orbit on $\mathcal{S}_0$ connecting the two boundary layers from $x = 0$ to $x = 1$ is displayed in* (16) *together with the quantities in Proposition* 2.3.

Proof. The singular orbit which has been studied in sections 2.2 and 2.3 is summarized in (i), (ii), and (iii) of this theorem. It remains to show the existence and uniqueness of a solution near the singular orbit for $\epsilon > 0$. Recall that M_L^ϵ (resp., M_R^ϵ) is the union of all forward (resp., backward) orbits starting from B_L (resp., B_R). It suffices to show that, for $\epsilon > 0$ small, M_L^ϵ and M_R^ϵ intersect transversally with each other around the singular orbit. We note that the assumptions $\alpha L_1 \neq \beta L_2$ and $\alpha R_1 \neq \beta R_2$ imply that the vector field of (4) is not tangent to B_L and B_R and hence, M_L^ϵ and M_R^ϵ are smooth invariant manifolds.

For $\epsilon > 0$ small, the evolutions of M_L^ϵ and M_R^ϵ from B_L and B_R, respectively, to an ϵ-neighborhood of $\mathcal{Z}_0$ along the two boundary layers are governed by system (6). Since, for system (7), M_L^0 and M_R^0 intersect $W^s(\mathcal{Z}_0)$ and $W^u(\mathcal{Z}_0)$ transversally, we have that M_L^ϵ and M_R^ϵ intersect $W^s(\mathcal{Z}_0)$ and $W^u(\mathcal{Z}_0)$ transversally. As discussed in section 2.3, in terms of the blow-up coordinates, M_L^ϵ and M_R^ϵ intersect $W^s(\mathcal{S}_0)$ and $W^u(\mathcal{S}_0)$ transversally for system (14). And, if we denote $N_L = M_L^0 \cap W^s(\mathcal{S}_0)$ and $N_R = M_R^0 \cap W^u(\mathcal{S}_0)$, then the vector field on $\mathcal{S}_0$ is not tangent to $\omega(N_L)$ and $\alpha(N_R)$. Furthermore, the traces $\bar{M}_L$ and $\bar{M}_R$ of $\omega(N_L)$ and $\alpha(N_R)$, respectively, under the slow flow on $\mathcal{S}_0$ intersect transversally. All conditions for the exchange lemma (see [15] and also [10, 8, 9]) are satisfied, and hence, M_L^ϵ and M_R^ϵ intersect transversally. The intersection has dimension

$$\dim M_L^\epsilon + \dim M_R^\epsilon - 7 = 4 + 4 - 7 = 1,$$

which is the orbit of the unique solution for the connecting problem near the singular orbit. ∎

Remark 3.1. We have considered the situation that $\alpha L_1 \neq \beta L_2$ and $\alpha R_1 \neq \beta R_2$. In the case that $\alpha L_1 = \beta L_2$ or $\alpha R_1 = \beta R_2$, then B_L or B_R is on the slow manifold $\mathcal{S}_0$ and hence there is no boundary layer at $x = 0$ or $x = 1$.

4. Appendix. A derivation of the integral H_3 in Proposition 2.1. The complete set of six integrals of system (7) in Proposition 2.1 is crucial in the quantitative investigation of the boundary layers of the boundary value problem. The integrals H_1 and H_2 are relatively easy to guess. The integral H_3, although easily verified, is discovered through several observations. It may have some general interest, and we provide a formal derivation below.

We divide the W-equation by the V-equation from system (7) to get

$$\frac{dW}{dV} = \frac{\alpha\beta V}{W} + (\beta - \alpha),$$

which is a homogeneous equation of order zero. This leads to the substitution $W = yV$. From $dW = Vdy + ydV$ and the above equation one gets

$$\left(\frac{\alpha\beta V}{yV} + (\beta - \alpha)\right) dV = Vdy + ydV \quad \text{or} \quad -\frac{dV}{V} = \frac{ydy}{y^2 - (\beta - \alpha)y - \alpha\beta}.$$

Integrating both sides, we have, for some constant C,

$$-\ln V + C = \frac{\alpha}{\alpha + \beta} \ln|y + \alpha| + \frac{\beta}{\alpha + \beta} \ln|y - \beta|,$$

or, for some constant D,

$$V = \frac{D}{|y + \alpha|^{\frac{\alpha}{\alpha+\beta}} |y - \beta|^{\frac{\beta}{\alpha+\beta}}}, \quad W = \frac{Dy}{|y + \alpha|^{\frac{\alpha}{\alpha+\beta}} |y - \beta|^{\frac{\beta}{\alpha+\beta}}}.$$

Substitute $y = W/V$ to get

$$|W + \alpha V|^{\alpha} |W - \beta V|^{\beta} = D^{\alpha+\beta}.$$

This completes the derivation of the integral H_3.

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