Applications in Reaction Networks and Kinetic Theory

By

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A dissertation submitted in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

(Mathematics)

at the

UNIVERSITY OF WISCONSIN – MADISON

2021

Date of final oral examination: June 21, 2021

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Abstract

A chemical reaction is a process that leads to the chemical transformation of one set of chemical substances to another. Reaction networks are the mathematical models used on dictating the behaviour of the chemical systems. Reaction–diffusion systems are mathematical models which mostly correspond to the change of the concentration of chemical substances: Local Chemical Reactions and Diffusion which causes the substances to spread out over a surface in space. Kinetic theory of gases is a model of the thermodynamic behaviour of gases. The model describes a gas as a large number of identical submicroscopic particles, all of which are in constant, rapid, random motion.

In this thesis, firstly, we are interested in the properties on mass-action systems that are dynamically equivalent to complex-balanced ones and single target networks. Then, we prove the uniqueness of the weakly reversible and deficiency zero realization. Next, we show the local and global stability on the complex balanced equilibrium for some chemical reaction-diffusion systems with boundary equilibria. We also consider the instability on the corresponding boundary equilibria. Finally, we study a simple collisionless model in kinetic theory under a mixing effect of stochastic boundary damping the moments of fluctuation.

Acknowledgements

I would like to express my sincerely appreciation to many people, including my co-authors in this thesis. Chapter 2, based on [25, 47], are results of joint work with Gheorghe Craciun and Polly Yu. Sections 3.1, based on [46], is joint work with Gheorghe Craciun, Casian Pantea and Adrian Tudorascu, while Section 3.2, based on [58], is joint work with Chanwoo Kim. Finally, Chapter 4, based on [59], is joint work with Chanwoo Kim.

First, I would like to thank both my advisors, Gheorghe Craciun and Chanwoo Kim, for their support. You have been very patient with me and guide me to become a qualified math PhD. I have been touched by the passion and earnest on research from both of you. This helps me to make up my mind to choose the faculty path. Also thank you for introducing me to all interesting projects and coming up with ideas to help me to overcome difficulties. I would also like to thank David Anderson and Sigurd Angenent for their helpful discussions and encouragements when I felt confused.

I have been surrounded by many good friends. Among those from our department, Yunbai Cao and Chaojie Yuan deserve a huge thanks for helping me in both research and daily life, hanging out and enjoying delicious food together. My friends in China and Canada, thank you for sharing moments of happiness and struggles and inspiring me when I was stressed. A special thanks to my best friend, Zhongjie Zhang, for being like a brother to me. Words are powerless to express my gratitude.

I would also like to thank my parents for supporting me on this hard but worthy career path. It is my privilege to thank my fiancée, Shilu Zhang, who has been giving me constant encouragement throughout my PhD period. We first met in 2018 and she will be my wife at the end of this month.

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Notation and Symbols

$\mathbb{R}$: the real numbers

$\mathbb{R}_{>0}$ / $\mathbb{R}_{+}$: set of positive real numbers

$\mathbb{R}^n$: set of vectors indexed by n

$\mathbb{R}^n_{>0}$: set of vectors with components in $\mathbb{R}_{>0}$

$\boldsymbol{x}^{\boldsymbol{y}} := x_1^{y_1} x_2^{y_2} \cdots x_n^{y_n}$

$\log(\boldsymbol{x}) := (\log x_1, \log x_2, \ldots, \log x_n)^\top$

$\exp(\boldsymbol{x}) := (e^{x_1}, e^{x_2}, \ldots, e^{x_n})^\top$

$\boldsymbol{x} \circ \boldsymbol{y} := (x_1 y_1, x_2 y_2, \ldots, x_n y_n)^\top$

$\frac{\boldsymbol{x}}{\boldsymbol{y}} := (\frac{x_1}{y_1}, \frac{x_2}{y_2}, \ldots, \frac{x_n}{y_n})^\top$

$\langle x,\, y\rangle$: the standard scalar product of $x, y \in \mathbb{R}^n$

X^{o}: $X \subseteq \mathbb{R}^n$ is contained in some affine subspace of $\mathbb{R}^n$

∂X: boundary of the set X

Contents

Chapter 1

Introduction

Many mathematical models in biology, chemistry, physics, and engineering are obtained from nonlinear interactions between several species or populations, such as (bio)chemical reactions in a cell or a chemical reactor, population dynamics in an ecosystem, or kinetic interactions in a gas or solution [8, 22, 27, 29, 30, 37–40, 49, 56, 95, 98]. Very often, these models are generated by a graph of interactions according to specific kinetic rules; *mass-action kinetics* for reaction network models is one such example [110].

In order to describe various properties of reaction networks, it is useful to visualize them in Euclidean space as *Euclidean embedded graphs* [21]. Each vertex of the network is naturally associated to a vector in $\mathbb{R}^n$, via its stoichiometric coefficients; hence, every directed edge in the network (i.e., reaction) can be visualized as a vector between vertices of the network in $\mathbb{R}^n$. The resulting directed graph in $\mathbb{R}^n$ is called the Euclidean embedded graph of the reaction network, and its *Newton polytope* is the convex hull of its *source* vertices. A *strongly endotactic network* is essentially an "inward pointing" one: any edge originating on the boundary of the Newton polytope must point inside the polytope or along its boundary (i.e., cannot point outside the polytope), and on any face of the polytope there exists an edge that starts on that face and points away from it.

If the graph underlying the mass-action system in a given reaction network has some special properties, then the associated dynamical system is known (or conjectured) to have certain dynamical properties. There has been a great amount of work on establishing connections between the qualitative dynamics of these systems and their underlying network structures

[8, 38, 40, 43, 49, 55, 56, 110]. For example, if the underlying network is *reversible* (i.e., for every edge, there is an edge in the reverse direction), then the mass-action system admits a positive steady state for any choice of positive rate constants [17]. In addition, if the rate constants satisfy some algebraic constraints such as the Wegscheider conditions [108], the mass-action system is in a state of thermodynamic equilibrium, where the rate of any forward reaction is balanced by the rate of the reverse reaction. Such a system, said to be *detailed-balanced*, enjoys remarkable dynamical properties, like the existence of a globally defined Lyapunov function, and uniqueness of a positive steady state within every invariant polytope detemined by mass conservation laws.

Similarly, if the underlying network is *weakly reversible* (i.e., every edge is part of an oriented cycle), again the mass-action system admits a positive steady state for any choice of positive rate constants [17]. If the rate constants satisfy some algebraic constraints, the mass-action system is *complex-balanced*[38, 55, 56], a generalization of detailed-balanced. Again, the system admits a globally defined Lyapunov function, has a unique positive steady state within every invariant polytope, and is conjectured to be globally stable. This is the *Global Attractor Conjecture*, which has been proved in several cases: when the network has only one connected component [6, 18]; when the system has dimension three or less [27, 85], or when the network is *strongly endotactic* [7, 48]. In particular, some networks are always complex-balanced under mass-action kinetics, regardless of the values of rate constants: these are the weakly reversible network with deficiency zero [38, 55]. One interpretation of the deficiency zero property is that the reaction vectors span the maximal dimensional subspace possible [43].

It turns out that the same dynamical system can be generated by a multitude of reaction networks [28, 53, 61, 102, 103]. Therefore, if a system is generated by a network that does *not* enjoy a specific graphical property (e.g., not weakly reversible), we can ask whether the same system *may* be generated by a weakly reversible network. Others have asked this question before and formulated algorithms for a given number of complexes [61, 93, 102, 103] and applied the results to designing control systems [98, 104]. In order to determine whether a given system is generated by a weakly reversible or complex-balanced system, one would have to determine if it can be done using n number of complexes for all $n \geq 1$.

Compared with the ODE systems, much less is known about the corresponding reaction-diffusion models, although a number of recent papers have focused on extending the results above in the PDE setting. A promising venue for relating the PDE and ODE models is by way of space discretization (the method of lines). As proof of concept, the network $A + B \rightleftharpoons C$ was considered in [78] where it was shown that solutions of the discretized system converge to the solution of the PDE system as the space discretization grows finer. Solutions of the reaction-diffusion system $A + B \rightleftharpoons C$ have been shown to approach a positive spatially homogeneous distribution [91] via semigroup theory. Newer work uses entropy techniques to prove global asymptotic stability for other systems, including dimerization networks $2A \rightleftharpoons B$ [32] and monomolecular networks [67]. Recent results by Desvillettes, Fellner and collaborators [33,34,62] removed the requirement of equal diffusion constants, and showed that in the absence of boundary equilibria, the positive equilibrium of a general complex balanced reaction-diffusion system attracts all solutions with positive initial data. These papers also considered special cases of networks with boundary equilibria, where a detailed analysis showed that positive solutions remain globally asymptotically stable. However, the general case of systems with boundary equilibria remains open, and the analysis of such systems is on a case-by-case basis.

A recent paper by Pierre et al [87] studies the general case of a reversible reaction; the authors prove that for nonnegative initial data in $L^1 \cap L \log L$, the solution will converge to some equilibrium. If the equilibrium happens to be the unique complex-balanced equilibrium in the given stoichiometric class (as opposed to a boundary equilibrium), then it is shown that the convergence is exponential. Furthermore, if the solution is globally (in time) essentially bounded, [87] also shows that the solution converges exponentially to the complex-balanced equilibrium. In another recent paper [31], authors prove that as long as the closeness to equilibrium is measured in L^∞ norm, the convergence holds for arbitrary dimension.

Besides reaction networks and reaction-diffusion systems, kinetic theory of gases is also a widely used mathematical model. One important and active research direction in the mathematical kinetic theory is on the asymptotic behavior of its solutions as $t \to \infty$ for both the collisional models (e.g. [2, 36, 64, 69, 80, 100]) and the collisionless models (e.g. [1, 12, 73, 81]).

Due to its conceptual importance and applications, the mixing effect of the stochastic boundary has been studied in various aspects of the Boltzmann equation. In [2], Guo establishes a novel L^2-L^∞ framework to control an L^∞_x-norm of the Boltzmann equation for all basic boundary conditions (e.g. diffuse reflection, specular reflection, inflow, and bounce-back conditions). In this framework of [2], an L^∞_x-norm can be controlled directly along the generalized characteristics corresponding to the boundary condition, the bouncing billiard trajectories with stochastic boundary in the case of (1.11), without any differentiability assumption. In [3], Kim constructs initial data of the Boltzmann equation inducing the formation of singularity at the boundary and proves the propagation of such singularity along with the generalized characteristics. In [90], Esposito-Guo-Kim-Marra construct the stationary solutions of the Boltzmann equation when the boundary temperature can be non-constant. In fact, these solutions are non-equilibrium stationary states since they are not local Maxwellians. They also prove exponentially-fast asymptotical stability of such stationary states under small perturbations in L^∞_x ([90]). In [36, 88], Kim et al. construct strong solutions of Vlasov-Poisson-Boltzmann systems in convex domains with the diffuse reflection boundary and prove exponentially-fast asymptotical stability.

1.1 Overview

This introductory chapter defines all notations in reaction networks, reaction-diffusion systems and kinetic theory that are relevant to this thesis. In particular, Section 1.2 reviews what is mass-action systems and complex-balanced systems. Section 1.3 shows what is complex-balanced steady states and corresponding entropy in reaction-diffusion. Section 1.4 focuses on the diffusive boundary condition and the characteristic lines in kinetic equations.

In Chapter 2, we are interested in dynamical equivalence between reaction models and the relation between reaction rates, graph structures with complex-balanced realization. In Section 2.1, we develop a theory of dynamical equivalence between mass-action systems and weakly reversible and complex-balanced systems. In Section 2.2, we concern the class of single-target networks and prove that under mass-action kinetics, a single-target network either has a globally stable positive steady state for any choice of rate constants, or has no positive steady state for any choice of rate constants.

In Chapter 3, we work on asymptotic analysis for reaction-diffusion systems and the stability or instability on equilibria. In Section 3.1, we study the rate of convergence to the complex-balanced equilibrium for some chemical reaction-diffusion systems with boundary equilibria. In Section 3.2, I show the local instability on the boundary equilibria to a three-species system and prove the convergence to the positive equilibria as long as the initial data is closed enough to the the positive equilibrium.

Finally, in Chapter 4, we look at the convergence for the kinetic equations. In Section 4.1,we prove that exponential moments of a fluctuation of the pure transport equation decay *pointwisely* when the domain is any general strictly convex subset of $\mathbb{R}^3$ with the smooth boundary of the diffuse boundary condition.

1.2 Reaction networks

Chemical reaction networks appear at the intersection of biology, biochemistry, chemistry, engineering, and mathematics. Different notations are used in the literature; here we explain the notations used throughout this paper. Introductions to chemical reaction network theory can be found in [39, 49, 110].

Definition 1.2.1. A ***reaction network*** (or simply a ***network***) is a directed graph $G = (V_G, E_G)$ embedded in Euclidean space, with no self-loops, i.e., $V_G \subseteq \mathbb{R}^n$ and $E_G \subseteq V_G \times V_G$ and $(\boldsymbol{y}, \boldsymbol{y}) \notin E_G$ for any $\boldsymbol{y} \in V_G$. When there is no ambiguity, we simply write $G = (V, E)$.

Remark 1.2.2. Vertices are points in $\mathbb{R}^n$, so an edge $e \in E$ can be regarded as a bona fide vector in $\mathbb{R}^n$. We denote an edge $e = (\boldsymbol{y}, \boldsymbol{y}')$ as $\boldsymbol{y} \to \boldsymbol{y}'$, which is associated to a ***reaction vector*** $\boldsymbol{y}' - \boldsymbol{y} \in \mathbb{R}^n$. We also write $\boldsymbol{y} \to \boldsymbol{y}' \in G$ instead of $\boldsymbol{y} \to \boldsymbol{y}' \in E$.

The dimension n of the ambient Euclidean space is the number of chemical species involved in the reaction network G. An edge in the set E is called a ***reaction***. A vertex in V is also known as a ***reaction complex***. The ***source vertex*** of a reaction $\boldsymbol{y} \to \boldsymbol{y}'$ is the vertex $\boldsymbol{y}$, while $\boldsymbol{y}'$ is the ***product vertex***. Let $V_s \subseteq V$ denote the ***set of source vertices***, i.e., the set of vertices that is the source of some reaction.

The vector space spanned by the reaction vectors is the ***stoichiometric subspace*** $S = \text{span}_{\mathbb{R}}\{\boldsymbol{y}' - \boldsymbol{y} \colon \boldsymbol{y} \to \boldsymbol{y}' \in G\}$. For any positive vector $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$, the affine polytope $(\boldsymbol{x}_0 + S)_> = (\boldsymbol{x}_0 + S) \cap \mathbb{R}_{>0}$ is known as the ***stoichiometric compatibility class*** of $\boldsymbol{x}_0$. A reaction network G is ***reversible*** if $\boldsymbol{y}' \to \boldsymbol{y} \in G$ whenever $\boldsymbol{y} \to \boldsymbol{y}' \in G$; for simplicity, we denote such a pair of reactions by $\boldsymbol{y} \rightleftharpoons \boldsymbol{y}'$. It is ***weakly reversible*** if every connected component of G is strongly connected, i.e., every reaction $\boldsymbol{y} \to \boldsymbol{y}' \in G$ is part of an oriented cycle.

Example 1.2.3. Figure 1.1 shows a reaction network G in $\mathbb{R}^2$ with 6 vertices and 3 reactions. The reactions are

$$\boldsymbol{y}_1 \to \boldsymbol{z}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \to \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \qquad \boldsymbol{y}_2 \to \boldsymbol{z}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \to \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \qquad \boldsymbol{y}_3 \to \boldsymbol{z}_3 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \to \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The stoichiometric subspace, which is the linear span of the reaction vectors, is $\mathbb{R}^2$. In particular, any stoichiometric compatibility class is all of $\mathbb{R}^2_{>0}$. The reaction network G is neither reversible nor weakly reversible.

Example 1.2.4. Three more examples of reaction networks are presented in Figure 1.2. The

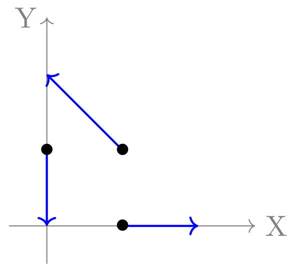


Figure 1.1: A reaction network G in $\mathbb{R}^2$ consisting of 3 reactions and 6 vertices. Under mass-action kinetics, this network gives rise to the classical Lotka–Volterra model for population dynamics.

reaction networks (a) G, (b) G', and (c) G^* share the vertices

$$\boldsymbol{y}_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \boldsymbol{y}_2 = \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \quad \boldsymbol{y}_3 = \begin{pmatrix} 3 \\ 2 \end{pmatrix}, \quad \text{and} \quad \boldsymbol{y}_4 = \begin{pmatrix} 3 \\ 0 \end{pmatrix}.$$

The reaction networks G, G^* have two additional vertices

$$\boldsymbol{y}_5 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \boldsymbol{y}_6 = \begin{pmatrix} 2 \\ 1 \end{pmatrix}.$$

The set of four reactions of G is $E_G = \{\boldsymbol{y}_1 \to \boldsymbol{y}_5, \boldsymbol{y}_2 \to \boldsymbol{y}_5, \boldsymbol{y}_3 \to \boldsymbol{y}_6, \boldsymbol{y}_4 \to \boldsymbol{y}_6\}$. The set of reactions of G' is $E_{G'} = \{\boldsymbol{y}_1 \rightleftharpoons \boldsymbol{y}_2, \boldsymbol{y}_2 \rightleftharpoons \boldsymbol{y}_3, \boldsymbol{y}_3 \rightleftharpoons \boldsymbol{y}_4, \boldsymbol{y}_4 \rightleftharpoons \boldsymbol{y}_1, \boldsymbol{y}_1 \rightleftharpoons \boldsymbol{y}_3, \boldsymbol{y}_2 \rightleftharpoons \boldsymbol{y}_4\}$. The set of reactions of G^* is $E_{G^*} = \{\boldsymbol{y}_1 \rightleftharpoons \boldsymbol{y}_5 \rightleftharpoons \boldsymbol{y}_2, \boldsymbol{y}_3 \rightleftharpoons \boldsymbol{y}_6 \rightleftharpoons \boldsymbol{y}_4, \boldsymbol{y}_5 \rightleftharpoons \boldsymbol{y}_6, \boldsymbol{y}_5 \to \boldsymbol{y}_3, \boldsymbol{y}_5 \to \boldsymbol{y}_4\}$. The networks G' and G^* are weakly reversible, and G' is also reversible. The stoichiometric subspace is $S = \mathbb{R}^2$ for all three networks.

A reaction network G is associated to a dynamical system, by assuming that each reaction $\boldsymbol{y} \to \boldsymbol{y}'$ proceeds according to a rate function $\nu_{\boldsymbol{y}\to\boldsymbol{y}'}(\boldsymbol{x})$, where $\boldsymbol{x} \in \mathbb{R}^n_{>0}$ is the vector of *concentrations* of the chemical species in the system. One of the most extensively studied kinetic systems is *mass-action kinetics*, where $\nu_{\boldsymbol{y}\to\boldsymbol{y}'}(\boldsymbol{x})$ is a monomial whose exponent vector is $\boldsymbol{y}$.

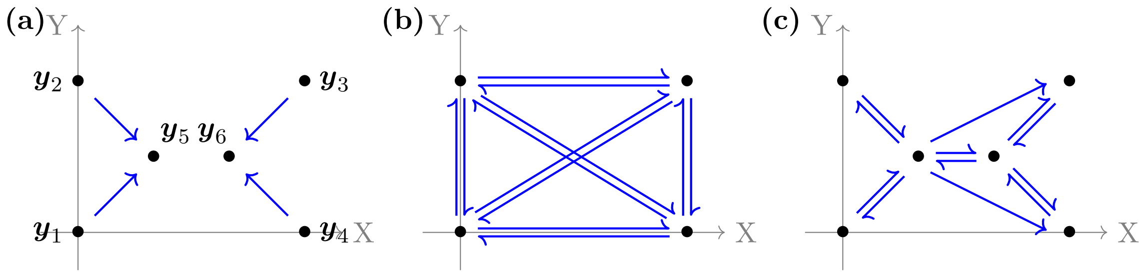


Figure 1.2: Examples of reaction networks (a) G, (b) G', and (c) G^*, with labels of vertices shown in (a). The dynamical systems generated by the network (a) can also be generated by (b) or (c) for well-chosen rate constants. Note that (b) and (c) are weakly reversible, and (b) is also reversible.

Definition 1.2.5. Let $G = (V, E)$ be a reaction network, and let $\boldsymbol{k} = (k_{\boldsymbol{y}\to\boldsymbol{y}'})_{\boldsymbol{y}\to\boldsymbol{y}'\in G} \in \mathbb{R}^E_{>0}$ be a vector of *rate constants*. We call the weighted directed graph $G_{\boldsymbol{k}}$ a ***mass-action system***, whose ***associated dynamical system*** is the system on $\mathbb{R}^n_{>0}$

$$\frac{d\boldsymbol{x}}{dt} = \sum_{\boldsymbol{y}\to\boldsymbol{y}'\in G} k_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}^{\boldsymbol{y}}(\boldsymbol{y}' - \boldsymbol{y}), \tag{1.1}$$

where $\boldsymbol{x}^{\boldsymbol{y}} = x_1^{y_1}x_2^{y_2}\cdots x_n^{y_n}$. By convention, $\boldsymbol{x}^{\boldsymbol{0}} = 1$ and it is convenient to refer to $k_{\boldsymbol{y}\to\boldsymbol{y}'}$ even when $\boldsymbol{y} \to \boldsymbol{y}' \notin G$, in which case we mean $k_{\boldsymbol{y}\to\boldsymbol{y}'} = 0$. We adopt the convention that the empty sum is $\boldsymbol{0}$, i.e., $\sum_{\boldsymbol{y}\to\boldsymbol{y}'\in\varnothing} k_{\boldsymbol{y}\to\boldsymbol{y}'}(\boldsymbol{y}' - \boldsymbol{y}) = \boldsymbol{0}$.

Example 1.2.6. We revisit Example 1.2.3 under the assumption of mass-action kinetics. The dynamical system associated to this reaction network $G = (V, E)$ for an arbitrary vector of rate constants $\boldsymbol{k} = (k_j)_{\boldsymbol{y}_j\to\boldsymbol{z}_j\in G} \in \mathbb{R}^E_{>0}$ is

$$\frac{d\boldsymbol{x}}{dt} = k_1 x \begin{pmatrix} 1 \\ 0 \end{pmatrix} + k_2 xy \begin{pmatrix} -1 \\ 1 \end{pmatrix} + k_3 y \begin{pmatrix} 0 \\ -1 \end{pmatrix} = \begin{pmatrix} k_1 x \quad - k_2 xy \\ k_2 xy - k_3 y \end{pmatrix}.$$

This is the Lotka–Volterra population dynamics model.

Given a mass-action system $G_{\boldsymbol{k}}$, (1.1) uniquely defines its associated dynamical system; however, many different reaction networks can give rise to the same dynamical system under mass-action kinetics. It has been known for a long time that if a reaction network has some special properties (e.g., reversible, weakly reversible, deficiency zero), then the mass-action system is known to have certain dynamical properties (e.g., existence of positive steady state, local and global stability). Therefore, given a mass-action system, we are interested in networks with richer structural properties that give rise to same dynamical systems. If two mass-action systems give rise to the same associated dynamical systems, we say they are *dynamically equivalent* [28, 61, 102, 103].

Definition 1.2.7. Two mass-action systems $G_{\boldsymbol{k}}$ and $G'_{\boldsymbol{k}'}$ are ***dynamically equivalent*** if

$$\sum_{\boldsymbol{y}_1 \to \boldsymbol{y}_2 \in G} k_{\boldsymbol{y}_1 \to \boldsymbol{y}_2} \boldsymbol{x}^{\boldsymbol{y}_1} (\boldsymbol{y}_2 - \boldsymbol{y}_1) \;=\; \sum_{\boldsymbol{y}'_1 \to \boldsymbol{y}'_2 \in G'} k'_{\boldsymbol{y}'_1 \to \boldsymbol{y}'_2} \boldsymbol{x}^{\boldsymbol{y}'_1} (\boldsymbol{y}'_2 - \boldsymbol{y}'_1) \tag{1.2}$$

for all $\boldsymbol{x} \in \mathbb{R}^n_{>0}$. We say that $G'_{\boldsymbol{k}'}$ is another ***realization*** of $G_{\boldsymbol{k}}$.

Remark 1.2.8. From (1.2), a necessary and sufficient condition for dynamical equivalence is

$$\sum_{\boldsymbol{y}_0 \to \boldsymbol{y} \in G} k_{\boldsymbol{y}_0 \to \boldsymbol{y}} (\boldsymbol{y} - \boldsymbol{y}_0) \;=\; \sum_{\boldsymbol{y}_0 \to \boldsymbol{y}' \in G'} k'_{\boldsymbol{y}_0 \to \boldsymbol{y}'} (\boldsymbol{y}' - \boldsymbol{y}_0) \tag{1.3}$$

for all $\boldsymbol{y}_0 \in V_G \cup V_{G'}$.

Note that in the associated dynamical system of a mass-action system, $\frac{d\boldsymbol{x}}{dt}$ belongs to the stoichiometric subspace S. Moreover, $\mathbb{R}^n_{>0}$ is forward invariant under mass-action kinetics, i.e., if $\boldsymbol{x}(0) \in \mathbb{R}^n_{>0}$, then $\boldsymbol{x}(t) \in \mathbb{R}^n_{>0}$ for all $t \geq 0$ [39]. Consequently, the trajectory $\boldsymbol{x}(t)$ is confined to the stoichiometric compatibility class $(\boldsymbol{x}(0) + S)_{>}$ for all $t \geq 0$.

Remark 1.2.9. The stoichiometric subspaces for dynamically equivalent systems can in principle be different. However, the *kinetic subspaces* for the two systems must be the same.For example, the system in Figure 1.3(a), made of the reaction $2\,\mathrm{X} \xrightarrow{k} \mathrm{X} + \mathrm{Y}$, is dynamically equivalent to the system in Figure 1.3(b), consisting of the reactions $2\,\mathrm{X} \xrightarrow{k} \mathrm{X} + \mathrm{Y}$ and $0 \xleftarrow{k'} \mathrm{Y} \xrightarrow{k'} 2\,\mathrm{Y}$. By definition, the two systems have different stoichiometric subspaces.

However, in these systems, the trajectory starting at $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$ is confined to the affine space $\boldsymbol{x}_0 + \mathbb{R}(-1,1)^T$ because their kinetic subspace is $\mathbb{R}(-1,1)^T$.

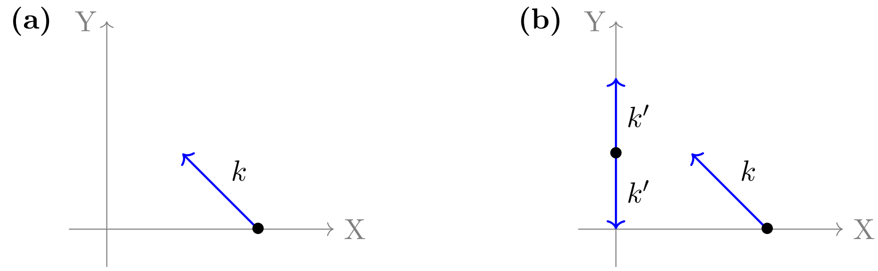


Figure 1.3: Two dynamically equivalent systems with different stoichiometric subspaces. Trajectories are confined to the same affine invariant spaces because their kinetic subspaces are the same.

Example 1.2.10. For the networks in Figure 1.2, let $k_{ij} > 0$ be the rate constant on the reaction $\boldsymbol{y}_i \to \boldsymbol{y}_j \in G$; let k'_{ij} be the rate constant on the reaction $\boldsymbol{y}_i \to \boldsymbol{y}_j \in G'$. Suppose k_{ij} and k'_{pq} satisfy the following equations:

$$
\begin{aligned}
k_{15}\begin{pmatrix}1\\1\end{pmatrix} &= k'_{12}\begin{pmatrix}0\\2\end{pmatrix} + k'_{13}\begin{pmatrix}3\\2\end{pmatrix} + k'_{14}\begin{pmatrix}3\\0\end{pmatrix},\\
k_{25}\begin{pmatrix}1\\-1\end{pmatrix} &= k'_{21}\begin{pmatrix}0\\-2\end{pmatrix} + k'_{23}\begin{pmatrix}3\\0\end{pmatrix} + k'_{24}\begin{pmatrix}3\\-2\end{pmatrix},\\
k_{36}\begin{pmatrix}-1\\-1\end{pmatrix} &= k'_{31}\begin{pmatrix}-3\\-2\end{pmatrix} + k'_{32}\begin{pmatrix}-3\\0\end{pmatrix} + k'_{34}\begin{pmatrix}0\\-2\end{pmatrix},\\
k_{46}\begin{pmatrix}-1\\1\end{pmatrix} &= k'_{41}\begin{pmatrix}-3\\0\end{pmatrix} + k'_{42}\begin{pmatrix}-3\\2\end{pmatrix} + k'_{43}\begin{pmatrix}0\\2\end{pmatrix}.
\end{aligned}
$$

Then $G_{\boldsymbol{k}}$ and $G'_{\boldsymbol{k}'}$ are dynamically equivalent. The linear constraints on the rate constants arise from vector decomposition of the reaction vectors starting at the source vertices of G and G'. In fact, if $\boldsymbol{k}$, $\boldsymbol{k}'$, and $\boldsymbol{k}^*$, where $\boldsymbol{k}^*$ is a vector of rate constants for G^*, satisfy some linear relations, the three mass-action systems $G_{\boldsymbol{k}}$, $G'_{\boldsymbol{k}'}$ and $G^*_{\boldsymbol{k}^*}$ are dynamically equivalent.

Mass-action systems give rise to very diverse dynamics. For example, weakly reversible deficiency zero mass-action systems have exactly one locally asymptotically stable steady state (within the same stoichiometric compatibility class). Yet there are other mass-action systems that have periodic orbits or limit cycles [10, 76, 89] and others that admit multiple steady states (within the same stoichiometric compatibility class) [11, 23, 24], and even chaotic dynamics [99, 110]. We refer the reader to [8, 39, 49, 110] for an introduction to mass-action systems. In this paper, we focus on several kinds of steady states of mass-action systems.

Definition 1.2.11. Let $G_{\boldsymbol{k}}$ be a mass-action system with the associated dynamical system

$$\frac{d\boldsymbol{x}}{dt} = \sum_{\boldsymbol{y}\to\boldsymbol{y}'\in G} k_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}^{\boldsymbol{y}}(\boldsymbol{y}'-\boldsymbol{y}).$$

A state $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$ is a ***positive steady state*** if

$$\frac{d\boldsymbol{x}}{dt} = \sum_{\boldsymbol{y}\to\boldsymbol{y}'\in G} k_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}_0^{\boldsymbol{y}}(\boldsymbol{y}'-\boldsymbol{y}) = \boldsymbol{0}. \tag{1.4}$$

A positive steady state $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$ is ***detailed-balanced*** if for every $\boldsymbol{y} \rightleftharpoons \boldsymbol{y}' \in G$, we have

$$k_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}_0^{\boldsymbol{y}} = k_{\boldsymbol{y}'\to\boldsymbol{y}}\boldsymbol{x}_0^{\boldsymbol{y}'}. \tag{1.5}$$

A positive steady state $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$ is ***complex-balanced*** if for every vertex $\boldsymbol{y}_0 \in V_G$, we have

$$\sum_{\boldsymbol{y}_0\to\boldsymbol{y}'\in G} k_{\boldsymbol{y}_0\to\boldsymbol{y}'}\boldsymbol{x}_0^{\boldsymbol{y}_0} = \sum_{\boldsymbol{y}\to\boldsymbol{y}_0\in G} k_{\boldsymbol{y}\to\boldsymbol{y}_0}\boldsymbol{x}_0^{\boldsymbol{y}}. \tag{1.6}$$

Intuitively, detailed balancing is when fluxes across every pair of reversible reactions are balanced; this is intimately related to the notion of microreversibility or dynamical equilibrium in physical chemistry [15, 16]. Complex balancing is when fluxes through every vertex (i.e., reaction complex) is balanced.

1.3 Reaction-diffusion system

In this section, we set up terminology and notation in reaction-diffusion systems. We also discuss some of the techniques used in this thesis and in previous work.

Now we consider $0 < T \leq \infty$ and the semilinear parabolic system

$$\mathbf{c}_t - \mathcal{D}\Delta\mathbf{c} = R(\mathbf{c}) \text{ in } \Omega \times (0,T) \tag{1.7}$$

with initial data

$$\mathbf{c}(\cdot,0) = \mathbf{c}_0 \text{ in } \Omega,$$

where $\mathbf{c} : \Omega \times [0,T) \to \mathbb{R}^n$ is the vector of concentrations at spatial position $x \in \Omega$ (an open subset of $\mathbb{R}^d$) and time $t \in [0,\infty)$, $\mathcal{D}$ is a positive definite, diagonal $n \times n$ matrix, and $R : \mathbb{R}^n \to \mathbb{R}^n$ is a vector field whose components are polynomials (determined by the chemical reactions under consideration). We exclusively consider Neumann boundary conditions throughout this work:

$$\nabla c_i \cdot \nu = 0 \text{ on } \partial\Omega \times (0,T),\ i = 1,...,n,$$

where ν is the outer normal vector to the boundary. This system can be linear and "trivial" (at least in the sense that "enough" of its equations decouple), such as

$$\begin{aligned} a_t - d_a\Delta a &= -ka, \\ b_t - d_b\Delta b &= ka \text{ in } \Omega \times (0,T), \end{aligned}$$

(which corresponds to the reaction $A \to B$ with reaction rate $k > 0$), linear and nontrivial (weakly coupled) such as

$$\begin{aligned} a_t - d_a\Delta a &= -k_1 a + k_2 b, \\ b_t - d_b\Delta b &= k_1 a - k_2 b \text{ in } \Omega \times (0,T), \end{aligned}$$

(which corresponds to $A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$), or (as soon as a reaction includes two or more reactants) nonlinear in the zero order terms (semilinear). For example, the single reaction $A + B \xrightarrow{k} C$ yields

$$\begin{aligned} a_t - d_a \Delta a &= -kab, \\ b_t - d_b \Delta b &= -kab, \\ c_t - d_c \Delta c &= kab \text{ in } \Omega \times (0, T). \end{aligned}$$

We use this last system to illustrate, rather informally, some terminology and notation. Here A, B, and C are the three *species* of the network, and $A + B$ and C are its *complexes*. The concentrations of A, B, C are non-negative functions of time and space and are collected in the *concentration vector* $\mathbf{c} = (a, b, c)$. The *reaction rate* of a reaction is given by mass-action, and is proportional to the concentration of each reactant species. The aggregate contribution of all reaction rates are collected in the vector $R(\mathbf{c}) = (-kab, -kab, kab)$. In general, this is given by

$$R(\mathbf{c}) := \sum_{y \to y'} k_{y \to y'} \mathbf{c}^y (y' - y),$$

where $k_{y \to y'}$ is the rate constant of $y \to y'$ and the summation is over all reactions $y \to y'$ in the network. Finally, $\mathcal{D} = \mathrm{diag}\{d_a, d_b, d_c\} \in M_{3\times 3}(\mathbb{R})$ denotes the diagonal matrix of diffusion constants.

In the previous example the first two equations have the benefit of being decoupled, but that feature is lost as soon as we allow for reversibility; indeed, corresponding to $A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C$ we have

$$\begin{aligned} a_t - d_a \Delta a &= -k_1 ab + k_2 c, \\ b_t - d_b \Delta b &= -k_1 ab + k_2 c, \\ c_t - d_c \Delta c &= k_1 ab - k_2 c \text{ in } \Omega \times (0, T). \end{aligned} \tag{1.8}$$

When it comes to basic questions on the existence, uniqueness, smoothness and non-negativity of solutions (if the initial data components are nonnegative), for linear systems the answers are provided in the (by now, classical) literature (see, e.g., [74]). However, complexity adds quickly as nonlinear reactions and more reactants enter the system.

In general, we say that an equilibrium point c_0 of a *reaction system* (i.e. an equilibrium of the ODE system $\mathbf{c}_t = R(\mathbf{c})$; diffusion is removed) is a *complex balanced equilibrium* if for all complexes $\bar{y}$ we have

$$\sum_{\bar{y}\to y} k_{\bar{y}\to y} c_0^{\bar{y}} = \sum_{y\to\bar{y}} k_{y\to\bar{y}} c_0^{y}.$$

In other words, the total chemical flux that exits the complex $\bar{y}$ equals the total chemical flux that enters the complex $\bar{y}$ (for any choice of $\bar{y}$). A reaction system is called *complex balanced* if it admits a positive complex balanced equilibrium. We call a reaction-diffusion system complex balanced if its corresponding reaction system is complex balanced. It was shown that all steady states of a complex balanced reaction-diffusion system are constant functions (do not depend on space), whose values equal the steady states of the corresponding complex balanced reaction system [77]. We can therefore identify the steady states (equilibria) of complex balanced reaction-diffusion systems with those of corresponding reaction systems.

Reaction systems often admit linear first integrals, called *conservation laws*; for example, the single reaction $A + B \to C$ has conservation laws $a + c = const$ and $b + c = const$. In this paper, an *accessible boundary equilibrium* of a reaction network is an equilibrium on the boundary of the positive orthant which gives the same values of the conservation laws as some phase point with strictly positive coordinates. These are the only equilibria that might be reachable from positive initial conditions, and the only ones relevant for positive solutions of the mass-action system. We note that not all equilibria on the boundary are accessible boundary equilibria. For example, $A + B \to A$ has one conservation law $a = const$. The positive a-axis $\{(a, 0)|a > 0\}$ consists of accessible boundary equilibria. On the other hand, all points $\{(0, b)|b \geq 0\}$ on the non-negative b-axis are boundary equilibria which are not accessible (the conservation law $a = 0$ is not compatible with points in the positive orthant). The distinction between accessible boundary equilibria and inaccessible ones was relevant in previous work [34], although it was not made explicit. The reaction-diffusion systems we consider in this thesis are complex-balanced with accessible boundary equilibria.

All systems arising from complex balanced reaction-diffusion systems admit a "canonical" Lyapunov functional of the relative Boltzmann entropy type. Its general form (again, see, e.g., [34]), this logarithmic free relative energy functional reads

$$E(t) := \sum_{i=1}^{n} \int_{\Omega} \left[c_i(x,t) \log \frac{c_i(x,t)}{c_{i,\infty}} - c_i(x,t) + c_{i,\infty} \right] dx,$$

where $\mathbf{c}_\infty := (c_{1,\infty}, ..., c_{n,\infty})$ is the constant vector denoting the positive complex balanced equilibrium. The entropy dissipation functional is computed by differentiating E along trajectories; that is, once all the time derivatives of concentrations are replaced by their equation specific expressions and the Neumann BC are used to integrate by parts wherever the Laplacian appears, one gets

$$D(t) := \sum_{i=1}^{n} d_i \int_{\Omega} \frac{|\nabla c_i(x,t)|^2}{c_i(x,t)} dx + \sum_{r=1}^{\rho} k_r c_\infty^{y_r} \int_{\Omega} \Phi\left(\frac{c^{y_r}}{c_\infty^{y_r}}; \frac{c^{y_r'}}{c_\infty^{y_r'}} \right) dx,$$

where ρ is the number of reactions and $\Phi(x,y) := x\log(x/y) - x + y$. Of course, one gets exponential decay to zero for E if one can prove that there exists a positive constant α such that

$$D(t) \geq \alpha E(t) \text{ for all } t \geq 0. \tag{1.9}$$

Naturally, $E(t)$ should not only be identically zero when $\mathbf{c}(t) = \mathbf{c}_\infty$, but it should also be bounded below by some increasing function of the distance (from some norm) between $\mathbf{c}(t)$ and $\mathbf{c}_\infty$.

For complex balanced systems, in the spatially isotropic case ($\mathcal{D} = 0$, so the PDE's are reduced to ODE's) recent work by Craciun [20] answers in the affirmative a long standing conjecture on the convergence to the positive equilibrium in each stoichiometric class. In the PDE case, the most general result concerns the case where there are no boundary equilibria. Very recently, Desvillettes, Fellner and Tang [34] showed that, contingent on the existence of suitable solutions (essentially, solutions that may not be classical but they are *renormalized* and do satisfy a weak entropy entropy-dissipation law), one obtains exponentially fast convergence to the equilibrium which lies in the same stoichiometric class as the initial data, which is merely assumed nonnegative and integrable over some bounded, C^2 domain in $\mathbb{R}^d$. This is also a remarkably general result in the sense that the initial concentrations are only assumed to lie in $L^1(\Omega)$. This improvement (over the previous works, where L^∞-bounds were imposed on the initial data) is achieved via the use of the Log-Sobolev inequality (see, e.g., [34]) in order to establish the *entropy-entropy dissipation inequality* (EEDI) (1.9). In all the previous works, the EEDI follows from the standard zero-average Poincaré inequality applied to the square roots of the concentration functions, combined with their uniform L^∞-bounds (in space-time). We note that (1.8) is one of the two systems studied in [32], and the authors use the uniform L^∞-bound as available in the literature (for this particular system). In [78] the authors carry out the proof in some detail (adapted from a proof in [109]), and show that the properties of the Neumann Heat Kernel involved in it hold for the discrete Neumann Heat Kernel as well.

1.4 Kinetic Theory

In this section, we are interested in a mixing effect of stochastic boundary damping the moments of fluctuation for a simple collisionless model. More precisely, we consider a *free transport* equation in a bounded domain $\Omega \subset \mathbb{R}^3$, with an initial condition $F(t,x,v)|_{t=0} = F_0(x,v)$,

$$\partial_t F + v \cdot \nabla_x F = 0, \quad \text{for } (t,x,v) \in \mathbb{R}_+ \times \Omega \times \mathbb{R}^3. \tag{1.10}$$

Throughout this thesis, we assume the domain is *smooth* and *strictly convex*: there exists a smooth function $\xi : \mathbb{R}^3 \to \mathbb{R}$ such that $\Omega = \{x \in \mathbb{R}^3 : \xi(x) < 0\}$ and $\sum_{i,j} \partial_i \partial_j \xi(x) \zeta_i \zeta_j \gtrsim |\zeta|^2$ for all $\zeta \in \mathbb{R}^3$ ([66]). The phase boundary $\gamma := \{(x,v) \in \partial\Omega \times \mathbb{R}^3\}$ is decomposed into the outgoing boundary and incoming boundary $\gamma_\pm := \{(x,v) \in \partial\Omega \times \mathbb{R}^3, n(x) \cdot v \gtrless 0\}$ with the outward normal $n(x)$ at $x \in \partial\Omega$.

We consider an *isothermal diffusive reflection* boundary condition which is the simplest model among the family of stochastic boundary conditions (see [88, 90] for the general boundary conditions)

$$F(t,x,v) = c_\mu \mu(v) \int_{n(x)\cdot v_1>0} F(t,x,v_1)\{n(x)\cdot v_1\}\mathrm{d}v_1, \quad \text{for } (t,x,v) \in \mathbb{R}_+ \times \gamma_-. \tag{1.11}$$

Here, for $c_\mu = \sqrt{2\pi}$, $c_\mu\mu(v) = c_\mu \frac{1}{(2\pi)^{3/2}} \exp\{-|v|^2/2\}$ stands for the wall Maxwellian distribution of the unit wall temperature. At the molecule level, the boundary condition (1.11) corresponds to the Markov process at the boundary ([57]). We set the total mass of the initial datum to be $\mathfrak{M} \times |\Omega|$, for some $\mathfrak{M} \geq 0$:

$$\iint_{\Omega\times\mathbb{R}^3} F_0(x,v)\mathrm{d}x\mathrm{d}v = \iint_{\Omega\times\mathbb{R}^3} \mathfrak{M}\mu(v)\mathrm{d}x\mathrm{d}v. \tag{1.12}$$

The choice of $c_\mu = \sqrt{2\pi}$ formally guarantees a null flux condition at the boundary and the conservation of mass. We are interested in a long time behavior of the fluctuation of F around the equilibrium $\mathfrak{M}\mu(v)$:

$$f(t,x,v) = F(t,x,v) - \mathfrak{M}\mu(v), \quad \text{where } \mu(v) = \frac{1}{(2\pi)^{3/2}} e^{-\frac{|v|^2}{2}}. \tag{1.13}$$

Damping induced solely by the mixing effect of the stochastic boundary is a primary subject in this thesis. It is a different mechanism of the phase mixing *without the Boltzmann collision effect*. Perhaps, the most famous result of the phase mixing is the Landau damping, which generally refers to the decay of the moments of the fluctuation or electrostatic force field for the Vlasov-Poisson system without the boundary ([1,73]). Mathematical justification of the nonlinear Landau damping has been a longstanding open question, which is recently settled in the affirmative by Mouhot-Villani in [81] for the real analytic fluctuation around spatially homogeneous equilibriums (also see [12] for the fluctuation in some Gevrey space). On the other hand, the nonlinear Landau damping around spatially inhomogeneous equilibriums is a challenging open problem. We refer to [51] for the existence of spatially inhomogeneous steady states which are linearly stable.

Perhaps, the first quantitative study on the asymptotic behavior of the fluctuation can be found in [94], in which Yu proves a decay rate of moments of the fluctuation in L^∞ when the boundary is a 1D slab using a probabilistic approach (of Markov chains of i.i.d. random variables). This approach has been successfully generalized to the multi-D cases of *symmetric* domains (a disk in 2D and a ball in 3D) in [68], in which they obtain an optimal decay rate t^{-D}. The *symmetric* assumption of the domains is essential in their proof. Under this condition, the bouncing characteristics can be formed by the independent and identically distributed (i.i.d.) random variables. Moreover, the derivatives of outgoing flux can be bounded with the symmetric condition. In general, such derivatives could blow up in general convex domains ([65, 66]) and non-convex domains ([3]). We also refer to [63, 79] for the studies on the decay of the fluctuation in $L^1_{x,v}$ when the domains have some symmetry. Recently, there is a very interesting development of the subject toward removing the symmetric assumption (we refer to [4, 13] for a more complete list of references). In [13], Bernou develops a method based on Harris' Theorem which is particularly well-suited for problems arising in L^1-type of spaces. The work of [13] inspires our work. In [4, 72], Lods and Mokhtar-Kharroubi develop a different spectral approach using the Tauberian argument. All works [4, 13, 72] address an asymptotic behavior of the fluctuation itself in some $L^1_{x,v}$-type spaces.

Chapter 2

Reaction networks

In this chapter, we first introduce the notion of flux equivalence, then we show how to determine a system can be dynamically equivalent to a complex-balanced one. In Section 2.1, we describe a computationally efficient characterization of polynomial or power-law dynamical systems that can be obtained as complex-balanced, detailed-balanced, weakly reversible, and reversible mass-action systems. In Section 2.2, we focus on single-target networks under mass-action kinetics and conclude some nice properties even these networks may have high deficiencies.

2.1 An efficient characterization of complex-balanced,detailed-balanced, and weakly reversible systems

2.1.1 Fluxes on Reaction Networks

Most dynamical systems associated to reaction networks are nonlinear [26, 56, 95]. While nonlinear dynamical systems are generally difficult to study, the analysis of reaction networks is sometimes facilitated by the linear constraints arising from the network structure and stoichiometry.

To illustrate what we mean, consider mass-action kinetics. The (generally nonlinear) dynamical system under mass-action kinetics has the form

$$\frac{d\boldsymbol{x}}{dt} = \sum_{\boldsymbol{y}\to\boldsymbol{y}'\in G} \nu_{\boldsymbol{y}\to\boldsymbol{y}'}(\boldsymbol{x})(\boldsymbol{y}' - \boldsymbol{y}),$$

where $\nu_{\boldsymbol{y}\to\boldsymbol{y}'}(\boldsymbol{x}) = k_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}^{\boldsymbol{y}}$. Once the nonlinearity is hidden inside the reaction rate function

$\nu_{\boldsymbol{y}\to\boldsymbol{y}'}(\boldsymbol{x})$, the linear structure remaining becomes apparent.

Enumerate the set of reactions, $E = \{\boldsymbol{y}_j \to \boldsymbol{y}_j'\}_{j=1}^{|E|}$, and let $\boldsymbol{\nu}(\boldsymbol{x}) = (\nu_{\boldsymbol{y}_j\to\boldsymbol{y}_j'}(\boldsymbol{x}))_{j=1}^{|E|}$ be a vector consisting of the reaction rate functions. Define the ***stoichiometric matrix*** $N \in \mathbb{R}^{n\times|E|}$ as the matrix whose jth column is the jth reaction vector $\boldsymbol{y}_j' - \boldsymbol{y}_j$. Then the dynamical system above can be written succinctly as $\frac{d\boldsymbol{x}}{dt} = N\boldsymbol{\nu}(\boldsymbol{x})$.

In order to deal with the underlying linear structure, we do not keep track of the concentrations that give rise to $\boldsymbol{\nu}(\boldsymbol{x})$ but leave it as a vector of unknowns. For this reason, we denote the value $\boldsymbol{\nu}(\boldsymbol{x})$ simply as $\boldsymbol{J}$ and call it a *flux vector*.

Definition 2.1.1. A ***flux vector*** $\boldsymbol{J} = (J_{\boldsymbol{y}\to\boldsymbol{y}'})_{\boldsymbol{y}\to\boldsymbol{y}'\in G} \in \mathbb{R}^E_{>0}$ on a reaction network $G = (V, E)$ is a vector of positive numbers. The number $J_{\boldsymbol{y}\to\boldsymbol{y}'}$ is called the ***flux*** of the reaction $\boldsymbol{y} \to \boldsymbol{y}'$, and the pair $(G, \boldsymbol{J})$ is called a ***flux system***.

As with the rate constants, it may be convenient to refer to $J_{\boldsymbol{y}\to\boldsymbol{y}'}$ even when $\boldsymbol{y} \to \boldsymbol{y}' \notin G$, in which case $J_{\boldsymbol{y}\to\boldsymbol{y}'} = 0$.

This idea of fluxes on a reaction network may be familiar to anyone who has worked with stoichiometric network analysis or flux balance analysis. One form of the analysis is to solve the linear equation $N\boldsymbol{J} = \boldsymbol{0}$, where the unknown vector $\boldsymbol{J}$ has nonnegative coordinates [83, 106]. Since we are interested in relating network structure with dynamics, if $\boldsymbol{y} \to \boldsymbol{y}' \in G$, we impose that $J_{\boldsymbol{y}\to\boldsymbol{y}'} > 0$. Also if $\boldsymbol{y} \rightleftharpoons \boldsymbol{y}'$ is a reversible reaction in G, then $J_{\boldsymbol{y}\to\boldsymbol{y}'}$ and $J_{\boldsymbol{y}'\to\boldsymbol{y}}$ are two positive components of the vector $\boldsymbol{J}$. A solution $\boldsymbol{J} > \boldsymbol{0}$ of the equation $N\boldsymbol{J} = \boldsymbol{0}$ corresponds to a positive steady state if $\boldsymbol{J} = \boldsymbol{\nu}(\boldsymbol{x}_0)$ for some $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$. We define the flux analogues of positive steady state, detailed-balanced steady state, and complex-balanced steady state.

Definition 2.1.2. A ***steady state flux*** on a network $G = (V, E)$ is a flux vector $\boldsymbol{J} \in \mathbb{R}^E_{>0}$ satisfying

$$\sum_{\boldsymbol{y}\to\boldsymbol{y}'\in G} J_{\boldsymbol{y}\to\boldsymbol{y}'}(\boldsymbol{y}' - \boldsymbol{y}) = \boldsymbol{0}. \tag{2.1}$$

A flux $\boldsymbol{J} \in \mathbb{R}^E_{>0}$ is said to be ***detailed-balanced*** if for every $\boldsymbol{y} \to \boldsymbol{y'} \in G$, we have

$$J_{\boldsymbol{y} \to \boldsymbol{y'}} = J_{\boldsymbol{y'} \to \boldsymbol{y}}. \tag{2.2}$$

A flux $\boldsymbol{J} \in \mathbb{R}^E_{>0}$ is said to be ***complex-balanced*** if for every $\boldsymbol{y}_0 \in V$, we have

$$\sum_{\boldsymbol{y}_0 \to \boldsymbol{y'} \in G} J_{\boldsymbol{y}_0 \to \boldsymbol{y'}} = \sum_{\boldsymbol{y} \to \boldsymbol{y}_0 \in G} J_{\boldsymbol{y} \to \boldsymbol{y}_0}. \tag{2.3}$$

A steady state flux is a positive vector $\boldsymbol{J}$ in $\ker N$, where the stoichiometric matrix N has the reaction vectors as its columns. As a shorthand, we refer to the flux system $(G, \boldsymbol{J})$ as detailed-balanced if $\boldsymbol{J}$ is a detailed-balanced flux on G. Similarly defined is a complex-balanced flux system on G. It will be clear from context whether a complex-balanced system refers to a mass-action system or a flux system.

Example 2.1.3. An example of a flux system $(G, \boldsymbol{J})$ is shown in Figure 2.1. The positive number labelled on each edge $\boldsymbol{y} \to \boldsymbol{y'}$ is the flux $J_{\boldsymbol{y} \to \boldsymbol{y'}}$ of that reaction.

Note that this flux system could have risen from a mass-action system. For example, suppose the numbers labelled on the edges are taken to be rate constants $\boldsymbol{k}$, and the state of the system is $\boldsymbol{x} = \mathbf{1}$. Then $(G, \boldsymbol{J})$ would be the flux system based off of the mass-action system $G_{\boldsymbol{k}}$.

There is *no unique* mass-action system that gives rise to a fixed flux system. For example, on the reaction network shown in Figure 2.1, suppose that the rate constants are taken to be

$$k'_{0 \to \text{Y}} = 3,\ k'_{\text{Y} \to \text{X}+\text{Y}} = 1,\ k'_{\text{X}+\text{Y} \to 0} = 1,$$
$$k'_{\text{Y} \to 0} = \frac{1}{2},\ k'_{\text{X}+\text{Y} \to 2\text{X}} = \frac{5}{2},\ k'_{2\text{X} \to \text{X}+\text{Y}} = 5,$$

and that the state of the system is $\boldsymbol{x}_0 = (1, 2)^T$; then it can be shown that $(G, \boldsymbol{J})$ is the flux system of the mass-action system $G_{\boldsymbol{k'}}$ at the state $\boldsymbol{x}_0$.

This flux system $(G, \boldsymbol{J})$ is complex-balanced. For example, at the vertex $(0, 1)$ corresponding to Y, there is one reaction going into it with flux value 3, and there are two reactions leaving this vertex, with sum of fluxes being $2 + 1 = 3$.

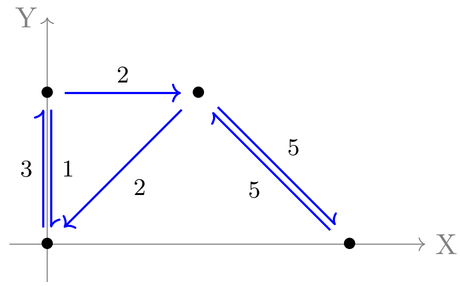


Figure 2.1: An example of a flux system. The positive numbers on any edge $\boldsymbol{y} \to \boldsymbol{y'}$ is the flux $J_{\boldsymbol{y}\to\boldsymbol{y'}}$ of that reaction. Note that this flux system is complex-balanced.

Whenever a flux vector arises from mass-action kinetics, i.e., $J_{\boldsymbol{y}\to\boldsymbol{y'}} = k_{\boldsymbol{y}\to\boldsymbol{y'}}\boldsymbol{x}^{\boldsymbol{y}}$, classical results for mass-action systems carry over to flux systems, as summarized in the following two lemmas.

Lemma 2.1.4. *Let $G_{\boldsymbol{k}}$ be a mass-action system, and fix $\boldsymbol{x} \in \mathbb{R}^n_{>0}$. For each edge $\boldsymbol{y} \to \boldsymbol{y'} \in G$, define $J_{\boldsymbol{y}\to\boldsymbol{y'}} = k_{\boldsymbol{y}\to\boldsymbol{y'}}\boldsymbol{x}^{\boldsymbol{y}}$, so that $\boldsymbol{J} = (J_{\boldsymbol{y}\to\boldsymbol{y'}})_{\boldsymbol{y}\to\boldsymbol{y'}\in G}$ is a flux vector on the network G. The following hold:*

1. *The flux vector $\boldsymbol{J}$ is a steady state flux on G if and only if $\boldsymbol{x}$ is a positive steady state of $G_{\boldsymbol{k}}$.*

2. *The flux vector $\boldsymbol{J}$ is detailed-balanced if and only if $\boldsymbol{x}$ is a detailed-balanced steady state for $G_{\boldsymbol{k}}$.*

3. *The flux vector $\boldsymbol{J}$ is complex-balanced if and only if $\boldsymbol{x}$ is a complex-balanced steady state for $G_{\boldsymbol{k}}$.*

Lemma 2.1.5. *If G admits a detailed-balanced flux, then G is reversible; if G admits a complex-balanced flux, then G is weakly reversible. If a flux is detailed-balanced on G, then it is also complex-balanced; if a flux is complex-balanced, then it is also a steady state flux.*

Proof. Let $\boldsymbol{J}$ be a flux vector on a network G — either detailed-balanced or complex-balanced or merely a steady state flux. On G, define a mass-action system $G_{\boldsymbol{k}}$ with rate constants $k_{\boldsymbol{y}\to\boldsymbol{y}'} = J_{\boldsymbol{y}\to\boldsymbol{y}'}$ for each $\boldsymbol{y} \to \boldsymbol{y}' \in G$. Then $\boldsymbol{x}_0 = (1, \cdots, 1)^T$ is a (detailed-balanced or complex-balanced or positive) steady state. Lemma 2.1.5 follows from classical results on mass-action systems [38–40, 49, 54, 55]. □

As we have seen in the previous section, some mass-action systems are dynamically equivalent; similarly there are flux equivalent systems. We define an equivalence relation for flux systems in $\mathbb{R}^n$.

Definition 2.1.6. Two flux systems $(G, \boldsymbol{J})$ and $(G', \boldsymbol{J}')$ are ***flux equivalent*** if for every vertex $\boldsymbol{y}_0 \in V_G \cup V_{G'}$, we have

$$\sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G} J_{\boldsymbol{y}_0\to\boldsymbol{y}}(\boldsymbol{y}-\boldsymbol{y}_0) = \sum_{\boldsymbol{y}_0\to\boldsymbol{y}'\in G'} J'_{\boldsymbol{y}_0\to\boldsymbol{y}'}(\boldsymbol{y}'-\boldsymbol{y}_0). \tag{2.4}$$

We denote equivalent flux systems by $(G, \boldsymbol{J}) \sim (G', \boldsymbol{J}')$ and say that $(G', \boldsymbol{J}')$ is a realization of $(G, \boldsymbol{J})$.

Lemma 2.1.7. *Flux equivalence is an equivalence relation.*

Proof. That flux equivalence is symmetric and reflexive is clear. Suppose $(G, \boldsymbol{J}) \sim (G', \boldsymbol{J}')$ and $(G', \boldsymbol{J}') \sim (G^*, \boldsymbol{J}^*)$. Transitivity follows from

$$\sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G} J_{\boldsymbol{y}_0\to\boldsymbol{y}}(\boldsymbol{y}-\boldsymbol{y}_0) = \sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G'} J'_{\boldsymbol{y}_0\to\boldsymbol{y}}(\boldsymbol{y}-\boldsymbol{y}_0) = \sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G^*} J^*_{\boldsymbol{y}_0\to\boldsymbol{y}}(\boldsymbol{y}-\boldsymbol{y}_0)$$

for any $\boldsymbol{y}_0 \in V_G \cup V_{G'} \cup V_{G^*}$. Note that if $\boldsymbol{y}_0 \notin V_{G'}$, then the sums above are all $\mathbf{0}$. □

Suppose a flux vector arises from a mass-action system; one expects the notion of dynamical equivalence to line up with that of flux equivalence.

Proposition 2.1.8. *Let $G_{\boldsymbol{k}}$, $G'_{\boldsymbol{k}'}$ be mass-action systems, and fix $\boldsymbol{x} \in \mathbb{R}^n_{>0}$. For each edge*

$\boldsymbol{y} \to \boldsymbol{y}' \in G$, let $J_{\boldsymbol{y}\to\boldsymbol{y}'} = k_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}^{\boldsymbol{y}}$, so that $\boldsymbol{J}(\boldsymbol{x}) = (J_{\boldsymbol{y}\to\boldsymbol{y}'})_{\boldsymbol{y}\to\boldsymbol{y}'\in G}$ is a flux vector on G. Similarly, define the flux vector $\boldsymbol{J}'(\boldsymbol{x}) = (J'_{\boldsymbol{y}\to\boldsymbol{y}'})_{\boldsymbol{y}\to\boldsymbol{y}'\in G'}$ on G', where $J'_{\boldsymbol{y}\to\boldsymbol{y}'} = k'_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}^{\boldsymbol{y}}$. Then the following are equivalent:

1. *The mass-action systems $G_{\boldsymbol{k}}$ and $G'_{\boldsymbol{k}'}$ are dynamically equivalent.*
2. *The flux systems $(G, \boldsymbol{J}(\boldsymbol{x}))$, $(G', \boldsymbol{J}'(\boldsymbol{x}))$ are flux equivalent for all $\boldsymbol{x} \in \mathbb{R}^n_{>0}$.*
3. *The flux systems $(G, \boldsymbol{J}(\boldsymbol{x}))$, $(G', \boldsymbol{J}'(\boldsymbol{x}))$ are flux equivalent for some $\boldsymbol{x} \in \mathbb{R}^n_{>0}$.*

Proof. It is clear that statements 1 and 2 are equivalent, and that statement 2 implies statement 3. Showing the implication of statement 1 from statement 3 will complete the proof. Let $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$ be a vector such that $(G, \boldsymbol{J}(\boldsymbol{x}_0)) \sim (G', \boldsymbol{J}'(\boldsymbol{x}_0))$. For any $\boldsymbol{y}_0 \in V_G \cup V_{G'}$ and arbitrary $\boldsymbol{x} \in \mathbb{R}^n_{>0}$, we have

$$
\begin{aligned}
&\sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G} J_{\boldsymbol{y}_0\to\boldsymbol{y}}(\boldsymbol{x})(\boldsymbol{y}-\boldsymbol{y}_0) \;-\; \sum_{\boldsymbol{y}_0\to\boldsymbol{y}'\in G'} J'_{\boldsymbol{y}_0\to\boldsymbol{y}'}(\boldsymbol{x})(\boldsymbol{y}'-\boldsymbol{y}_0)\\
&= \sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G} k_{\boldsymbol{y}_0\to\boldsymbol{y}}\boldsymbol{x}^{\boldsymbol{y}_0}(\boldsymbol{y}-\boldsymbol{y}_0) \;-\; \sum_{\boldsymbol{y}_0\to\boldsymbol{y}'\in G'} k'_{\boldsymbol{y}_0\to\boldsymbol{y}'}\boldsymbol{x}^{\boldsymbol{y}_0}(\boldsymbol{y}'-\boldsymbol{y}_0)\\
&= \frac{\boldsymbol{x}^{\boldsymbol{y}_0}}{\boldsymbol{x}_0^{\boldsymbol{y}_0}}\left(\sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G} k_{\boldsymbol{y}_0\to\boldsymbol{y}}\boldsymbol{x}_0^{\boldsymbol{y}_0}(\boldsymbol{y}-\boldsymbol{y}_0) \;-\; \sum_{\boldsymbol{y}_0\to\boldsymbol{y}'\in G'} k'_{\boldsymbol{y}_0\to\boldsymbol{y}'}\boldsymbol{x}_0^{\boldsymbol{y}_0}(\boldsymbol{y}'-\boldsymbol{y}_0)\right)\\
&= \frac{\boldsymbol{x}^{\boldsymbol{y}_0}}{\boldsymbol{x}_0^{\boldsymbol{y}_0}}\left(\sum_{\boldsymbol{y}_0\to\boldsymbol{y}\in G} J_{\boldsymbol{y}_0\to\boldsymbol{y}}(\boldsymbol{x}_0)(\boldsymbol{y}-\boldsymbol{y}_0) \;-\; \sum_{\boldsymbol{y}_0\to\boldsymbol{y}'\in G'} J'_{\boldsymbol{y}_0\to\boldsymbol{y}'}(\boldsymbol{x}_0)(\boldsymbol{y}'-\boldsymbol{y}_0)\right)\\
&= \boldsymbol{0}.
\end{aligned}
$$

□

Remark 2.1.9. The proof above holds for kinetics other than mass-action type. For each (source) vertex $\boldsymbol{y} \in V_G \cup V_{G'}$, define a rate function $\nu_{\boldsymbol{y}}\colon \mathbb{R}^n_{>0} \to \mathbb{R}_{>0}$. Then the above proposition holds when the flux vectors are defined to be $J_{\boldsymbol{y}\to\boldsymbol{y}'} = k_{\boldsymbol{y}\to\boldsymbol{y}'}\nu_{\boldsymbol{y}}(\boldsymbol{x})$ for each $\boldsymbol{y} \to \boldsymbol{y}' \in G$, and $J'_{\boldsymbol{y}\to\boldsymbol{y}'} = k'_{\boldsymbol{y}\to\boldsymbol{y}'}\nu_{\boldsymbol{y}}(\boldsymbol{x})$ for each $\boldsymbol{y} \to \boldsymbol{y}' \in G'$.

In the following proposition, we reduce a nonlinear problem about mass-action systems to a linear problem about flux systems. Instead of showing that a mass-action system is dynamically equivalent to a complex-balanced (or detailed-balanced) system, it suffices to show that an appropriately defined flux system is flux equivalent to a complex-balanced (or detailed-balanced) system.

Proposition 2.1.10. *Let $G_{\boldsymbol{k}}$ be a mass-action system, and let $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$. For each edge $\boldsymbol{y} \to \boldsymbol{y}' \in G$, define $J_{\boldsymbol{y}\to\boldsymbol{y}'} = k_{\boldsymbol{y}\to\boldsymbol{y}'}\boldsymbol{x}_0^{\boldsymbol{y}}$, so that $\boldsymbol{J} = (J_{\boldsymbol{y}\to\boldsymbol{y}'})_{\boldsymbol{y}\to\boldsymbol{y}'\in G}$ is a flux vector on the network G. Suppose $(G, \boldsymbol{J})$ is flux equivalent to $(G', \boldsymbol{J}')$, where $\boldsymbol{J}'$ is complex-balanced; then $G_{\boldsymbol{k}}$ is dynamically equivalent to a mass-action system $G'_{\boldsymbol{k}'}$, where $\boldsymbol{x}_0$ is a complex-balanced steady state for $G'_{\boldsymbol{k}'}$. Similarly, if $(G, \boldsymbol{J})$ is flux equivalent to a detailed-balanced flux system $(G', \boldsymbol{J}')$, then $G_{\boldsymbol{k}}$ is dynamically equivalent to a mass-action system $G'_{\boldsymbol{k}'}$, where $\boldsymbol{x}_0$ is a detailed-balanced steady state for $G'_{\boldsymbol{k}'}$.*

Proof. For each edge $\boldsymbol{y} \to \boldsymbol{y}' \in G'$, define its rate constant to be

$$k'_{\boldsymbol{y}\to\boldsymbol{y}'} = \frac{J'_{\boldsymbol{y}\to\boldsymbol{y}'}}{\boldsymbol{x}_0^{\boldsymbol{y}}} > 0,$$

so that $G'_{\boldsymbol{k}'}$ is a mass-action system. By Proposition 2.1.8, the mass-action systems $G_{\boldsymbol{k}}$ and $G'_{\boldsymbol{k}'}$ are dynamically equivalent, and by Lemma 2.1.4, $\boldsymbol{x}_0$ is a complex-balanced steady state if $\boldsymbol{J}'$ is a complex-balanced flux on G', and if $\boldsymbol{J}'$ is detailed-balanced on G', then $\boldsymbol{x}_0$ is a detailed-balanced steady state. □

2.1.2 Complex balancing without additional vertices

The identification of possible network structures associated to a biochemical system, say, from experimental data, is closely related to identifying key players in the system (e.g., enzymes in metabolic networks, genes in genetic networks). While the general nonuniqueness implies that network identification may often be impossible, it may still be desirable to compute equivalent systems — whether that be dynamical equivalence or flux equivalence — in order to conclude that the system has better properties than first suspected, e.g., weak reversibility or complex balance. This problem is not new [28, 102].

In recent years, the engineering community has utilized properties of mass-action systems in novel ways to designing and analyzing control systems [8, 71, 98, 104]. For example, the controllers can be added in such a way that the resulting system is a complex-balanced mass-action system; from this, one can conclude that the control system has a unique positive steady state and local stability [71, 104]. Moreover, very general results have been obtained on the stability of complex-balanced systems with delay [70].

Thus, there is strong incentive for developing effective computational methods to find structurally better dynamically equivalent systems. One approach uses linear programming, but an objective function must be chosen. To reduce the search space, one can decide to search for a realization with the maximal and minimal number of edges [61, 103]. Nonetheless, the set of vertices to be included in the reaction network must be chosen ahead of time.

In the examples of Figure 1.3, the mass-action systems systems are dynamically equivalent, but one uses an additional source vertex, whose weighted vectors sum to zero. Intuition may say that additional vertices can only improve the chance to find a network with desirable properties, as additional parameters provide extra degrees of freedom. Even if that is the case, the question of *computability* arises. Even if by adding new vertices to the network, one can produce an equivalent complex-balanced system, there is no a priori bound on the number of new vertices needed. One cannot realistically add new vertices ad infinitum.

Fortunately, we prove that *no additional vertices are needed* in order to check if a given system admits complex-balanced realizations. Thus, to check whether or not a network can admit a complex-balanced realization becomes a finite calculation, one that can be done by searching through the admissible domain as done in linear programming. Although the motivation came from mass-action systems, we prove our results in the more general setting of flux systems.

Our approach is to show that any such additional vertices in the network can be removed without changing the properties desired, namely, complex-balanced or weak reversibility. Such additional vertices will be called *virtual sources*.

Definition 2.1.11. A vertex $\boldsymbol{y}_0 \in V_s$ is a ***virtual source*** of the flux system $(G, \boldsymbol{J})$ if

$$\sum_{\boldsymbol{y}_0 \to \boldsymbol{y}' \in G} J_{\boldsymbol{y}_0 \to \boldsymbol{y}'} (\boldsymbol{y}' - \boldsymbol{y}_0) = \boldsymbol{0}, \tag{2.5}$$

where the sum is over all edges with $\boldsymbol{y}_0$ as its source.

If the flux system $(G, \boldsymbol{J})$ arises from a mass-action system, then $\boldsymbol{y}_0 \in V_s$ is a virtual source if and only if the monomial $\boldsymbol{x}^{\boldsymbol{y}_0}$ does *not* appear on the right-hand side of the associated dynamical system (1.1). For example, if we consider fluxes that arise from mass-action kinetics in the network in Figure 1.3(b), the vertex Y is a virtual source.

In this section, we prove that if a flux vector on a weakly reversible reaction network is complex-balanced and has a virtual source $\boldsymbol{y}^*$, then there is an equivalent complex-balanced flux system that does not involve $\boldsymbol{y}^*$ at all. In short, virtual sources $\boldsymbol{y}^*$ are not needed for complex balancing.

Just as an arbitrary concentration vector $\boldsymbol{x} \in \mathbb{R}^n_{>0}$ may not be a complex-balanced steady state for a weakly reversible mass-action system, so we may want to speak of fluxes that are not complex-balanced. To keep track of how far a flux vector is from being complex-balanced, we define the *potential* at a vertex to be the difference between incoming and outgoing fluxes.

Definition 2.1.12. Let $G = (V, E)$ be a reaction network, and let $\boldsymbol{J} \in \mathbb{R}^E_{>0}$ be a flux vector on G. The ***potential*** at a vertex $\boldsymbol{y}^* \in V$ is the scalar quantity

$$P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*) \ = \sum_{\boldsymbol{y} \to \boldsymbol{y}^* \in G} J_{\boldsymbol{y} \to \boldsymbol{y}^*} \ - \sum_{\boldsymbol{y}^* \to \boldsymbol{y}' \in G} J_{\boldsymbol{y}^* \to \boldsymbol{y}'}. \tag{2.6}$$

Remark 2.1.13. The flux vector $\boldsymbol{J}$ is complex-balanced on G if and only if $P_{(G,\boldsymbol{J})}(\boldsymbol{y}) = 0$ for all $\boldsymbol{y} \in V_s$. By an abuse of notation, if $\boldsymbol{y}^* \notin G$, we still refer to the potential $P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*)$ by setting it to be $P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*) = 0$.

In showing that virtual sources are not needed for complex balancing, the idea is to redirect the fluxes flowing into a virtual source $\boldsymbol{y}^*$ to other vertices while maintaining flux equivalence. If we are doing nothing more than redirecting flow of fluxes, the potential at every vertex does not change; therefore, we preserve complex balancing for the resulting flux system. This type of construction appeared first in [71] to show that new monomials were not necessary in feedback design.

We have to simultaneously keep track of the potential at each vertex and flux equivalence. We illustrate the key idea of Lemma 2.1.14 in Figure 2.2.

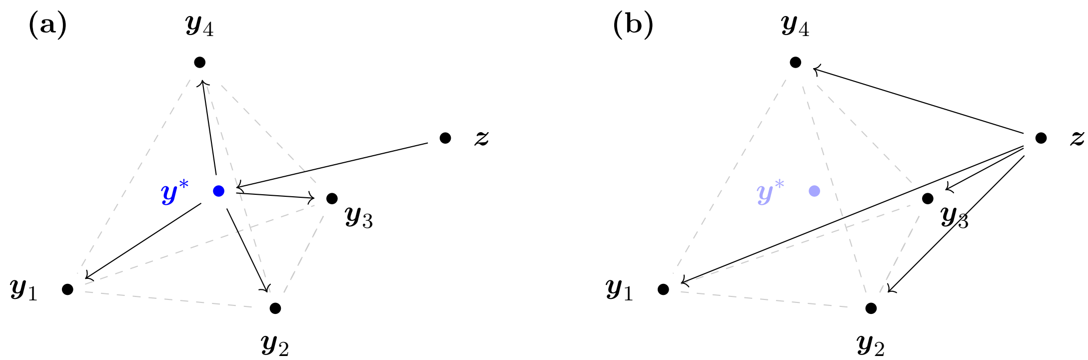


Figure 2.2: Illustrating the idea behind Lemma 2.1.14 in $\mathbb{R}^3$. (a) Assume that $\boldsymbol{y}^*$ is a virtual source in the flux system $(G, \boldsymbol{J})$. In (b) is an equivalent flux system $(G', \boldsymbol{J}')$, obtained by redirecting fluxes from $\boldsymbol{z} \to \boldsymbol{y}^* \to \boldsymbol{y}_j$ as fluxes from $\boldsymbol{z} \to \boldsymbol{y}_j$.

Lemma 2.1.14. *Consider a reaction network G consisting of the reactions $\boldsymbol{z} \to \boldsymbol{y}^*$ and $\boldsymbol{y}^* \to \boldsymbol{y}_j$ for $j = 1, 2, \ldots, M$. Suppose $\boldsymbol{y}^*$ is a virtual source for a flux system $(G, \boldsymbol{J})$ and its potential is $P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*) = 0$. Then there exists a flux equivalent system $(G', \boldsymbol{J}')$ such that $\boldsymbol{y}^* \notin V_{G'}$, and the potential at each vertex is preserved, i.e., $P_{(G,\boldsymbol{J})}(\boldsymbol{y}_j) = P_{(G',\boldsymbol{J}')}(\boldsymbol{y}_j)$ for $1 \leq j \leq M$ and $P_{(G,\boldsymbol{J})}(\boldsymbol{z}) = P_{(G',\boldsymbol{J}')}(\boldsymbol{z})$. The flux system $(G', \boldsymbol{J}')$ can be obtained constructively: remove the edges $\boldsymbol{z} \to \boldsymbol{y}^*$ and $\boldsymbol{y}^* \to \boldsymbol{y}_j$, and add the edges $\boldsymbol{z} \to \boldsymbol{y}_j$ with fluxes $J'_{\boldsymbol{z}\to\boldsymbol{y}_j} = J_{\boldsymbol{y}^*\to\boldsymbol{y}_j}$.*

Proof. For $j = 1, 2, \ldots, M$, let $\boldsymbol{w}_j = \boldsymbol{y}_j - \boldsymbol{y}^*$ and $\boldsymbol{w}_0 = \boldsymbol{z} - \boldsymbol{y}^*$ denote the reaction vectors. First, remove the edges $\boldsymbol{y}^* \to \boldsymbol{y}_j$ coming out of $\boldsymbol{y}^*$. Because $\boldsymbol{y}^*$ is a virtual source, $\sum_{j=1}^{M} J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} \boldsymbol{w}_j = \boldsymbol{0}$, so the resulting flux system is still equivalent to the original. Note that in this new flux system, only $\boldsymbol{z}$ is a source vertex.

Next, we redirect the reaction $\boldsymbol{z} \to \boldsymbol{y}^*$. Instead of the reaction $\boldsymbol{z} \to \boldsymbol{y}^*$ with flux $J_{\boldsymbol{z} \to \boldsymbol{y}^*}$, we have M reactions $\boldsymbol{z} \to \boldsymbol{y}_j$ with fluxes $J'_{\boldsymbol{z} \to \boldsymbol{y}_j} = J_{\boldsymbol{y}^* \to \boldsymbol{y}_j}$. Let $(G', \boldsymbol{J}')$ denote this newest flux system.

Recall that flux equivalence means (2.4) holds at each vertex of G and G'. Here we only need to look at the vertex $\boldsymbol{z}$ to show that $(G', \boldsymbol{J}') \sim (G, \boldsymbol{J})$. Note that $\boldsymbol{y}_j - \boldsymbol{z} = \boldsymbol{w}_j - \boldsymbol{w}_0$. From $P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*) = 0$, we also have $\sum_{j=1}^{M} J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} = J_{\boldsymbol{z} \to \boldsymbol{y}^*}$. Thus, the weighted sum of vectors coming out of $\boldsymbol{z}$ is

$$\sum_{j=1}^{M} J'_{\boldsymbol{z} \to \boldsymbol{y}_j} \left(\boldsymbol{y}_j - \boldsymbol{z}\right) = \sum_{j=1}^{M} J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} \left(\boldsymbol{w}_j - \boldsymbol{w}_0\right) = \underbrace{\sum_{j=1}^{M} J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} \boldsymbol{w}_j}_{=\,\boldsymbol{0}} - \boldsymbol{w}_0 \sum_{j=1}^{M} J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} = -J_{\boldsymbol{z} \to \boldsymbol{y}^*} \boldsymbol{w}_0,$$

and $(G', \boldsymbol{J}') \sim (G, \boldsymbol{J})$.

Finally, we prove that the potentials are unchanged. Trivially, we have

$$P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*) = P_{(G',\boldsymbol{J}')}(\boldsymbol{y}^*) = 0.$$

Also $P_{(G,\boldsymbol{J})}(\boldsymbol{y}_j) = J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} = J'_{\boldsymbol{z} \to \boldsymbol{y}_j} = P_{(G',\boldsymbol{J}')}(\boldsymbol{y}_j)$ for $j = 1, 2, \ldots, M$. Last but not least,

$$-P_{(G',\boldsymbol{J}')}(\boldsymbol{z}) = \sum_{j=1}^{M} J'_{\boldsymbol{z} \to \boldsymbol{y}_j} = \sum_{j=1}^{M} J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} = J_{\boldsymbol{z} \to \boldsymbol{y}^*} = -P_{(G,\boldsymbol{J})}(\boldsymbol{z}).$$

We have shown that the resulting flux system $(G', \boldsymbol{J}')$ is flux equivalent to the original flux system $(G, \boldsymbol{J})$, and the potential at each vertex is preserved. $\square$

Remark 2.1.15. In Lemma 2.1.14, the source vertex $\boldsymbol{z}$ may *not* be distinct from $\boldsymbol{y}_j$.

We now arrive at our main technical theorem (Theorem 2.1.16), a generalization of Lemma 2.1.14. Here, the virtual source $\boldsymbol{y}^*$ may have multiple reactions coming into it and coming out of it. The proof will be an induction on the number of edges flowing into $\boldsymbol{y}^*$. At each step, we redirect a fraction of the fluxes flowing through $\boldsymbol{y}^*$ from one incoming edge.

Theorem 2.1.16. *Let $(G, \boldsymbol{J})$ be a complex-balanced flux system on reaction network $G = (V, E)$. Suppose that $\boldsymbol{y}^* \in V$ is a virtual source. Then there exists an equivalent complex-balanced flux system $(G', \boldsymbol{J}')$ with $V_{G'} = V \setminus \{\boldsymbol{y}^*\}$. Moreover,*

$$J'_{\boldsymbol{y}_i \to \boldsymbol{y}_k} = J_{\boldsymbol{y}_i \to \boldsymbol{y}_k} + J_{\boldsymbol{y}^* \to \boldsymbol{y}_k} \frac{J_{\boldsymbol{y}_i \to \boldsymbol{y}^*}}{\sum_{\boldsymbol{y}_j \to \boldsymbol{y}^* \in G} J_{\boldsymbol{y}_j \to \boldsymbol{y}^*}} \tag{2.7}$$

for any $\boldsymbol{y}_i$ such that $\boldsymbol{y}_i \to \boldsymbol{y}^* \in G$ and any $\boldsymbol{y}_k$ such that $\boldsymbol{y}^* \to \boldsymbol{y}_k \in G$, and $J'_{\boldsymbol{y} \to \boldsymbol{y}'} = J_{\boldsymbol{y} \to \boldsymbol{y}'}$ for all other edges $\boldsymbol{y} \to \boldsymbol{y}'$.

Proof. Let N be the number of reactions with $\boldsymbol{y}^*$ as target, i.e., $N = |\{\boldsymbol{z} \to \boldsymbol{y}^* \in G\}|$. Enumerate the sources as $\boldsymbol{z}_1, \boldsymbol{z}_2, \ldots, \boldsymbol{z}_N$. Let M be the number of reactions with $\boldsymbol{y}^*$ as sources, i.e., $M = |\{\boldsymbol{y}^* \to \boldsymbol{y} \in G\}|$. Enumerate the targets as $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_M$. Since $\boldsymbol{y}^*$ is a virtual source, it is in the relative interior of the convex hull of the targets $\boldsymbol{y}_j$. From complex balancing, we have $P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*) = 0$, or

$$\sum_{j=1}^{M} J_{\boldsymbol{y}^* \to \boldsymbol{y}_j} = \sum_{i=1}^{N} J_{\boldsymbol{z}_i \to \boldsymbol{y}^*}.$$

Let $\theta = \frac{J_{\boldsymbol{z}_1 \to \boldsymbol{y}^*}}{\sum_i J_{\boldsymbol{z}_i \to \boldsymbol{y}^*}}$ be the fraction of flux to be redirected from $\boldsymbol{z}_1 \to \boldsymbol{y}^*$. We apply the construction described in Lemma 2.1.14 to the incoming edge $\boldsymbol{z}_1 \to \boldsymbol{y}^*$, and the outgoing edges $\boldsymbol{y}^* \to \boldsymbol{y}_j$ for $j = 1, 2, \ldots, M$. Let $(G', \boldsymbol{J}')$ denote the flux system after the diversion. More precisely, $J'_{\boldsymbol{z}_1\to\boldsymbol{y}^*} = 0$,

$$J'_{\boldsymbol{z}_1\to\boldsymbol{y}_j} - J_{\boldsymbol{z}_1\to\boldsymbol{y}_j} = \theta J_{\boldsymbol{y}^*\to\boldsymbol{y}_j},$$
$$J'_{\boldsymbol{y}^*\to\boldsymbol{y}_j} - J_{\boldsymbol{y}^*\to\boldsymbol{y}_j} = -\theta J_{\boldsymbol{y}^*\to\boldsymbol{y}_j},$$

and the fluxes on all other edges unchanged from $\boldsymbol{J}$.

Checking for flux equivalence at $\boldsymbol{z}_1$ before and after the diversion, we see that

$$\begin{aligned}
&(\text{Final flow from } \boldsymbol{z}_1) - (\text{Initial flow from } \boldsymbol{z}_1)\\
&= \sum_{j=1}^{M} J_{\boldsymbol{z}_1\to\boldsymbol{y}_j}(\boldsymbol{y}_j - \boldsymbol{z}_1) - J_{\boldsymbol{z}_1\to\boldsymbol{y}^*}(\boldsymbol{y}^* - \boldsymbol{z}_1)\\
&= \theta \underbrace{\sum_{j=1}^{M} J_{\boldsymbol{y}^*\to\boldsymbol{y}_j}(\boldsymbol{y}_j - \boldsymbol{y}^*)}_{=\boldsymbol{0}} + \theta \underbrace{\sum_{j=1}^{M} J_{\boldsymbol{y}^*\to\boldsymbol{y}_j}}_{=\sum_{j=1}^{N} J_{\boldsymbol{z}_i\to\boldsymbol{y}^*}} (\boldsymbol{y}^* - \boldsymbol{z}_1) - J_{\boldsymbol{z}_1\to\boldsymbol{y}^*}(\boldsymbol{y}^* - \boldsymbol{z}_1)\\
&= \boldsymbol{0}.
\end{aligned}$$

At all other vertices, the net flux is unchanged.

In terms of potentials, at $\boldsymbol{z}_1$, we have

$$P_{(G',\boldsymbol{J}')}(\boldsymbol{z}_1) - P_{(G,\boldsymbol{J})}(\boldsymbol{z}_1) = -\sum_{j=1}^{M} J'_{\boldsymbol{z}_1\to\boldsymbol{y}_j} + J_{\boldsymbol{z}_1\to\boldsymbol{y}^*} = -\theta\sum_{i=1}^{N} J_{\boldsymbol{z}_i\to\boldsymbol{y}^*} + J_{\boldsymbol{z}_1\to\boldsymbol{y}^*} = 0.$$

At each $\boldsymbol{y}_j$:

$$P_{(G',\boldsymbol{J}')}(\boldsymbol{y}_j) - P_{(G,\boldsymbol{J})}(\boldsymbol{y}_j) = \left(J'_{\boldsymbol{z}_1\to\boldsymbol{y}_j} + J'_{\boldsymbol{y}^*\to\boldsymbol{y}_j}\right) - \left(J_{\boldsymbol{z}_1\to\boldsymbol{y}_j} + J_{\boldsymbol{y}^*\to\boldsymbol{y}_j}\right) = 0.$$

At $\boldsymbol{y}^*$:

$$P_{(G',\boldsymbol{J}')}(\boldsymbol{y}^*) - P_{(G,\boldsymbol{J})}(\boldsymbol{y}^*) = -J_{\boldsymbol{z}_1\to\boldsymbol{y}^*} + \theta\sum_{j=1}^{M} J_{\boldsymbol{y}^*\to\boldsymbol{y}_j} = 0.$$

The new flux system $(G', \boldsymbol{J}')$ after diverting the flux from $\boldsymbol{z}_1 \to \boldsymbol{y}^*$ is still complex-balanced, as the potential is unchanged from those of $(G, \boldsymbol{J})$. Moreover, $(G', \boldsymbol{J}')$ and $(G, \boldsymbol{J})$ are flux equivalent. In addition, at $\boldsymbol{y}^*$, we have

$$\sum_{\boldsymbol{y}^* \to \boldsymbol{y} \in G'} J'_{\boldsymbol{y}^* \to \boldsymbol{y}}(\boldsymbol{y} - \boldsymbol{y}^*) = (1 + \theta) \sum_{\boldsymbol{y}^* \to \boldsymbol{y} \in G'} J_{\boldsymbol{y}^* \to \boldsymbol{y}}(\boldsymbol{y} - \boldsymbol{y}^*) = \boldsymbol{0},$$

i.e, $\boldsymbol{y}^*$ is a virtual source for $(G', \boldsymbol{J}')$.

Thus we have recovered all the hypotheses stated in the theorem. The only difference between $(G, \boldsymbol{J})$ and $(G', \boldsymbol{J}')$ is that G' contains $N - 1 = |\{\boldsymbol{z} \to \boldsymbol{y}^* \in G'\}|$ reactions with $\boldsymbol{y}^*$ as target vertex. By induction on the number $|\{\boldsymbol{z} \to \boldsymbol{y}^* \in G'\}|$, there exists a flux system $(G^*, \boldsymbol{J}^*)$ that is flux equivalent to $(G, \boldsymbol{J})$, and for which $\boldsymbol{J}^*$ is a complex-balanced flux on G^*. Finally, because $P_{(G^*, \boldsymbol{J}^*)}(\boldsymbol{y}^*) = 0$, but there are no incoming reactions to $\boldsymbol{y}^*$, it follows that there are no outgoing reactions from $\boldsymbol{y}^*$, i.e., $\boldsymbol{y}^* \notin V_{G^*}$. □

When does a flux system (or a reaction network) admit a complex-balanced realization? Theorem 2.1.16 implies that virtual sources do not need to be considered. Theorem 2.1.17 below is the basis behind several relevant numerical methods in Section 2.1.3 for determining if a flux system (or a reaction network) is equivalent to complex-balanced.

Theorem 2.1.17. *Let $(G, \boldsymbol{J})$ be a flux system, and $V_{G,s}$ its set of source vertices. Then $(G, \boldsymbol{J})$ is flux equivalent to some complex-balanced flux system if and only if $(G, \boldsymbol{J})$ is flux equivalent to some complex-balanced flux system $(G', \boldsymbol{J}')$ where $V_{G'} \subseteq V_{G,s}$.*

Proof. One direction is trivial. To prove the other direction, suppose $(G, \boldsymbol{J})$ is a flux system that is flux equivalent to some complex-balanced flux system $(\widetilde{G}, \widetilde{\boldsymbol{J}})$. If $\boldsymbol{y}^* \in V_{\widetilde{G}} \setminus V_{G,s}$, the set $\{\boldsymbol{y}^* \to \boldsymbol{y} \in G\}$ is empty; flux equivalent demands that

$$\boldsymbol{0} = \sum_{\boldsymbol{y}^* \to \boldsymbol{y} \in \widetilde{G}} \widetilde{J}_{\boldsymbol{y}^* \to \boldsymbol{y}}(\boldsymbol{y} - \boldsymbol{y}^*).$$

Theorem 2.1.16 implies we can maintain flux equivalence and complex balance even after dropping the vertex $\boldsymbol{y}^*$ from $V_{\widetilde{G}}$. Repeating this process for all vertices not in $V_{G,s}$ ultimately implies that there is a complex-balanced flux system $(G', \boldsymbol{J}')$ such that $(G', \boldsymbol{J}') \sim (G, \boldsymbol{J})$ and in addition $V_{G'} \subseteq V_{G,s}$. □

Theorem 2.1.18. *Let G be a reaction network, and $V_{G,s}$ its set of source vertices. Then the following are equivalent:*

(i) There exists a flux vector $\boldsymbol{J}$ such that $(G, \boldsymbol{J})$ is flux equivalent to some complex-balanced flux system.

(ii) There exists a flux vector $\boldsymbol{J}$ such that $(G, \boldsymbol{J})$ is flux equivalent to some complex-balanced flux system $(G', \boldsymbol{J}')$, where $V_{G'} \subseteq V_{G,s}$.

Proof. The proof follows immediately from Theorem 2.1.17. □

Theorem 2.1.19. *A mass-action system $G_{\boldsymbol{k}}$ is dynamically equivalent to some complex-balanced system if and only if it is dynamically equivalent to a complex-balanced system $G'_{\boldsymbol{k}'}$ that only uses the source vertices, i.e., $V_{G'} \subseteq V_{G,s}$.*

Proof. This theorem follows from Proposition 2.1.8 and Theorem 2.1.17. Suppose $G_{\boldsymbol{k}}$ is dynamically equivalent to some complex-balanced mass-action system $\widetilde{G}_{\widetilde{\boldsymbol{k}}}$. Define the appropriate fluxes $\boldsymbol{J}$ on G and $\widetilde{\boldsymbol{J}}$ on $\widetilde{G}$; by Proposition 2.1.8, the two flux systems are flux equivalent. Theorem 2.1.17 holds if and only if $(G, \boldsymbol{J})$ is flux equivalent to some complex-balanced flux system $(G', \boldsymbol{J}')$ where $V_{G'} \subseteq V_{G,s}$. Define the appropriate mass-action system $G'_{\boldsymbol{k}'}$ (see Proposition 2.1.10); we have one direction of this theorem. The other direction is trivially true. □

All of our theorems thus far have been concerned with flux systems; in the case of mass-action systems, implicit in everything is the existence of a complex-balanced steady state. However, the idea of redirecting fluxes can be adapted to show the surprising result that weak reversibility can be accomplished (if at all) with no extra vertices.

Theorem 2.1.20. *A mass-action system $G_{\boldsymbol{k}}$ is dynamically equivalent to some weakly reversible mass-action system if and only if it is dynamically equivalent to a weakly reversible mass-action system $G'_{\boldsymbol{k}'}$ that only uses its source vertices, i.e., $V_{G'} \subseteq V_{G,s}$.*

Proof. Without loss of generality, we may suppose that $G_{\boldsymbol{k}}$ is a weakly reversible mass-action system for which there exists a virtual source $\boldsymbol{y}^*$. As in Theorem 2.1.16, we remove the vertex $\boldsymbol{y}^*$ by redirecting the reactions flowing through it. Since G is weakly reversible, there exists some vertex $\boldsymbol{z}$ such that $\boldsymbol{z} \to \boldsymbol{y}^* \in G$. As before, we will try to replace pairs of reactions $\boldsymbol{z} \to \boldsymbol{y}^*$ and $\boldsymbol{y}^* \to \boldsymbol{y}$ with $\boldsymbol{z} \to \boldsymbol{y}$.

Enumerate the set $\{\boldsymbol{y}^* \to \boldsymbol{y} \in G\}$ as $\{\boldsymbol{y}^* \to \boldsymbol{y}_i\}_{i=1}^M$, and enumerate the set $\{\boldsymbol{z} \to \boldsymbol{y}^* \in G\}$ as $\{\boldsymbol{z}_j \to \boldsymbol{y}^*\}_{j=1}^N$. For simplicity, let $\alpha_j = k_{\boldsymbol{z}_j \to \boldsymbol{y}^*}$, and let $\beta_i = k_{\boldsymbol{y}^* \to \boldsymbol{y}_i}$. Informally speaking, in place of the reactions $\boldsymbol{z}_j \to \boldsymbol{y}^*$ and $\boldsymbol{y}^* \to \boldsymbol{y}_i$, we shall have the reaction $\boldsymbol{z}_j \to \boldsymbol{y}_i$ with rate constant $k'_{\boldsymbol{z}_j \to \boldsymbol{y}_i} = \alpha_j \frac{\beta_i}{\sum \beta_s}$. More precisely, let G' be the graph after deleting the vertex $\boldsymbol{y}^*$ and its adjacent edges from G, and (if needed) the edges $\boldsymbol{z}_j \to \boldsymbol{y}_i$ added for all $i = 1, 2, \ldots, M$ and $j = 1, 2, \ldots, N$. On G', take the rate constants to be $k'_{\boldsymbol{z}_j \to \boldsymbol{y}^*} = k'_{\boldsymbol{y}^* \to \boldsymbol{y}_i} = 0$ and

$$k'_{\boldsymbol{z}_j \to \boldsymbol{y}_i} = k_{\boldsymbol{z}_j \to \boldsymbol{y}_i} + \alpha_j \frac{\beta_i}{\sum \beta_s},$$

and all other rate constants same as in $G_{\boldsymbol{k}}$.

The assumption that $\boldsymbol{y}^*$ is a virtual source can be written as

$$\sum_{i=1}^{M} \beta_i \boldsymbol{y}_i = \sum_{i=1}^{M} \beta_i \boldsymbol{y}^*.$$

Now to check for dynamical equivalence at $\boldsymbol{z}_1$, we consider the differences due to the reactions

$\boldsymbol{z}_1 \to \boldsymbol{y}_i$:

$$
\begin{aligned}
\sum_{i=1}^{M}(k'_{\boldsymbol{z}_1\to\boldsymbol{y}_i} - k_{\boldsymbol{z}_1\to\boldsymbol{y}_i})(\boldsymbol{y}_i - \boldsymbol{z}_1) &= \sum_{i=1}^{M}\alpha_1\frac{\beta_i}{\sum\beta_s}(\boldsymbol{y}_i - \boldsymbol{z}_1) \\
&= \frac{\alpha_1}{\sum\beta_s}\left(\sum_{i=1}^{M}\beta_i\boldsymbol{y}^* - \sum_{i=1}^{M}\beta_i\boldsymbol{z}_1\right) \\
&= \alpha_1(\boldsymbol{y}^* - \boldsymbol{z}_1),
\end{aligned}
$$

which is the contribution from the reaction $\boldsymbol{z}_1 \to \boldsymbol{y}^*$. Since other reactions were untouched, we have dynamical equivalence at $\boldsymbol{z}_1$. There is nothing special about $j = 1$; the same holds for all source vertices $\boldsymbol{z}_2, \boldsymbol{z}_3, \ldots, \boldsymbol{z}_N$.

Finally, given any cycle $\boldsymbol{v}_1 \to \boldsymbol{v}_2 \to \cdots \to \boldsymbol{v}_\ell \to \boldsymbol{v}_1$ in G', whenever an edge $\boldsymbol{z}_j \to \boldsymbol{y}_i$ appears in the cycle, replace it with two edges $\boldsymbol{z}_j \to \boldsymbol{y}^* \to \boldsymbol{y}_i$, and obtain a cycle in G. Therefore, G' is still weakly reversible. □

We extend the above results (Theorems 2.1.16-2.1.20) to detailed-balanced fluxes and/or reversible networks. We summarize these results in the following theorems.

Theorem 2.1.21. *Let $(G, \boldsymbol{J})$ be a detailed-balanced flux system on a reaction network $G = (V, E)$. Suppose that $\boldsymbol{y}^* \in V$ is a virtual source. Then there exists an equivalent detailed-balanced flux system $(G', \boldsymbol{J}')$ with $V_{G'} = V \setminus \{\boldsymbol{y}^*\}$. Moreover,*

$$
J'_{\boldsymbol{y}_i\to\boldsymbol{y}_k} = J_{\boldsymbol{y}_i\to\boldsymbol{y}_k} + J_{\boldsymbol{y}^*\to\boldsymbol{y}_k}\frac{J_{\boldsymbol{y}_i\to\boldsymbol{y}^*}}{\sum_{\boldsymbol{y}_j\to\boldsymbol{y}^*\in G} J_{\boldsymbol{y}_j\to\boldsymbol{y}^*}} \tag{2.8}
$$

for any $\boldsymbol{y}_i, \boldsymbol{y}_k$ connected to $\boldsymbol{y}^*$ in $(G, \boldsymbol{J})$. Let other fluxes remain unchanged from $(G, \boldsymbol{J})$. In particular, $(G, \boldsymbol{J})$ is flux equivalent to some detailed-balanced flux system if and only if $(G, \boldsymbol{J})$ is flux equivalent to some detailed-balanced flux system $(G', \boldsymbol{J}')$ where $V_{G'} \subseteq V_{G,s}$.

Proof. As in Theorem 2.1.16, we divert fluxes away from $\boldsymbol{y}^*$. We only need to check detail balancing. Consider any two vertices $\boldsymbol{y}_i \neq \boldsymbol{y}_k$ where $\boldsymbol{y}_i \rightleftharpoons \boldsymbol{y}^*, \boldsymbol{y}_k \rightleftharpoons \boldsymbol{y}^* \in G$. Using the fact that the flux system was originally detailed-balanced, i.e., $J_{\boldsymbol{y}\to\boldsymbol{y}'} = J_{\boldsymbol{y}'\to\boldsymbol{y}}$, we obtain

$$\begin{aligned} J'_{\boldsymbol{y}_i\to\boldsymbol{y}_k} &= J_{\boldsymbol{y}_i\to\boldsymbol{y}_k} + J_{\boldsymbol{y}^*\to\boldsymbol{y}_k} \frac{J_{\boldsymbol{y}_i\to\boldsymbol{y}^*}}{\sum_{\boldsymbol{y}_j\to\boldsymbol{y}^*\in G} J_{\boldsymbol{y}_j\to\boldsymbol{y}^*}} \\ &= J_{\boldsymbol{y}_k\to\boldsymbol{y}_i} + J_{\boldsymbol{y}^*\to\boldsymbol{y}_i} \frac{J_{\boldsymbol{y}_k\to\boldsymbol{y}^*}}{\sum_{\boldsymbol{y}_j\to\boldsymbol{y}^*\in G} J_{\boldsymbol{y}_j\to\boldsymbol{y}^*}} \\ &= J'_{\boldsymbol{y}_k\to\boldsymbol{y}_i}. \end{aligned}$$

For any other pairs of reversible reaction, detail balancing is inherited from $(G, \boldsymbol{J})$. In other words, $(G', \boldsymbol{J}')$ is detailed-balanced. □

Theorem 2.1.22. *A mass-action system $G_{\boldsymbol{k}}$ is dynamically equivalent to some reversible system if and only if it is dynamically equivalent to a reversible system $G'_{\boldsymbol{k}'}$ that only uses its source vertices, i.e., $V_{G'} \subseteq V_{G,s}$.*

Proof. We assume that $G_{\boldsymbol{k}}$ is reversible and has a virtual source $\boldsymbol{y}^* \in V_G$. We will replace the reactions $\{\boldsymbol{y}^* \rightleftharpoons \boldsymbol{y}_i \in G\}$ by modifying/adding the reactions $\{\boldsymbol{y}_i \rightleftharpoons \boldsymbol{y}_k \colon \boldsymbol{y}_i \rightleftharpoons \boldsymbol{y}^*, \boldsymbol{y}_k \rightleftharpoons \boldsymbol{y}^* \in G\}$. For any $\boldsymbol{y}_i$, $\boldsymbol{y}_j$ such that $\boldsymbol{y}_i \rightleftharpoons \boldsymbol{y}^*$, $\boldsymbol{y}_k \rightleftharpoons \boldsymbol{y}^* \in G$, let $k'_{\boldsymbol{y}_i\to\boldsymbol{y}^*} = k'_{\boldsymbol{y}^*\to\boldsymbol{y}_i} = 0$ and

$$k'_{\boldsymbol{y}_i\to\boldsymbol{y}_j} = k_{\boldsymbol{y}_i\to\boldsymbol{y}_j} + k_{\boldsymbol{y}_i\to\boldsymbol{y}^*} \left(\frac{k_{\boldsymbol{y}^*\to\boldsymbol{y}_j}}{\sum k_{\boldsymbol{y}^*\to\boldsymbol{y}_s}} \right).$$

Similar to Theorem 2.1.20, it can be shown that $G_{\boldsymbol{k}}$ and $G'_{\boldsymbol{k}'}$ are dynamically equivalent. Moreover, by symmetry of construction, G' is reversible. □

Note that related results have been obtained recently for the problem of kinetic feedback design involving complex-balanced and weakly reversible systems [71]. Here, for the problem of dynamical equivalence, we show that a given system admits a dynamically equivalent system that is complex-balanced (or weakly reversible, or detailed-balanced, or reversible) if and only if such a system exists using *only* the complexes that are already present in the original system.

2.1.2.1 Connection to deficiency theory

Within the reaction network theory literature, *deficiency* is a well-known quantity defined for a network G. Equipped with mass-action kinetics, networks with low deficiency are known to enjoy special dynamical properties under mass-action kinetics. For example, the famous deficiency zero theorem says that a weakly reversible deficiency zero network is complex-balanced for any choices of rate constants [40, 56]. As we have introduced, complex-balanced systems enjoy properties such as uniqueness and stability of steady states, existence of a Lyapunov function, and the steady states admit a monomial parametrization [39, 42, 49, 56, 110]. Despite the strong implications, deficiency has a relatively simple definition.

Definition 2.1.23. Let $G = (V_G, E_G)$ be a reaction network with ℓ_G connected components. Suppose the dimension of the stoichiometric subspace S is $s = \dim S$; then the ***deficiency*** of the network G is the nonnegative integer

$$\delta_G = |V_G| - \ell_G - s. \tag{2.9}$$

It can be shown that $\delta_G = \dim(\ker Y \cap \operatorname{im} I_G)$, where Y is the stoichiometric matrix, with the vertices as its columns, and I_G the incidence matrix of G [60]. It follows that δ_G is a nonnegative integer. When the network is weakly reversible, we also have $\delta_G = \dim(\ker Y \cap \operatorname{im} A_{\boldsymbol{k}})$, where $-A_{\boldsymbol{k}}^T$ is the Laplacian of the weighted graph $G_{\boldsymbol{k}}$ [39, 49].

Deficiency continues to play an important role in the analysis of reaction networks and mass-action systems. In our procedure for removing virtual vertices, deficiency always decreases. This is similar to a result obtained in [71], where the removal of additional monomials that function as controls in a feedback system also leads to a decrease in deficiency.

Theorem 2.1.24. *Let $G_{\boldsymbol{k}}$ be a weakly reversible mass-action system with deficiency δ_G. Suppose it has a virtual source $\boldsymbol{y}^*$. Let $G'_{\boldsymbol{k}'}$ be the weakly reversible mass-action system as produced in Theorem 2.1.20, dynamically equivalent to $G_{\boldsymbol{k}}$ with $V_{G'} = V_G \setminus \{\boldsymbol{y}^*\}$. Then the deficiency of $G'_{\boldsymbol{k}'}$ is $\delta_{G'} = \delta_G - 1$.*

Proof. In the proof of Theorem 2.1.20, we replaced the reactions $\boldsymbol{z} \to \boldsymbol{y}^*$ and $\boldsymbol{y}^* \to \boldsymbol{y}$ with the reaction $\boldsymbol{z} \to \boldsymbol{y}$ by choosing appropriate rate constants. It is clear that $|V_{G'}| = |V_G| - 1$, and the number of linkage classes stays the same. We claim that the stoichiometric subspace S remains unchanged. Thus, the drop in deficiency is due to the removal of the vertex $\boldsymbol{y}^*$, and $\delta_{G'} = \delta_G - 1$.

First enumerate the reactions coming out of $\boldsymbol{y}^*$ as $\boldsymbol{y}^* \to \boldsymbol{y}_j$, and enumerate the reactions going into $\boldsymbol{y}^*$ as $\boldsymbol{z}_i \to \boldsymbol{y}^*$. Let S_0 be the span of the reaction vectors "untouched" by our procedure, more precisely,

$$S_0 = \text{span}_{\mathbb{R}}\{\boldsymbol{y} \to \boldsymbol{y}' \in G \colon \boldsymbol{y} \neq \boldsymbol{y}^* \text{ or } \boldsymbol{y}' \neq \boldsymbol{y}^*\}.$$

Let S_G be the stoichiometric subspace of G, in particular,

$$S_G = \text{span}_{\mathbb{R}}\{S_0,\, \boldsymbol{y}_j - \boldsymbol{y}^*,\, \boldsymbol{y}^* - \boldsymbol{z}_i\}_{i,j},$$

and $S_{G'}$ be the stoichiometric subspace of G', where

$$S_{G'} = \text{span}_{\mathbb{R}}\{S_0,\, \boldsymbol{y}_j - \boldsymbol{z}_i\}_{i,j}.$$

Clearly, $S_{G'} \subseteq S_G$, since $\boldsymbol{y}_j - \boldsymbol{z}_i = (\boldsymbol{y}_j - \boldsymbol{y}^*) + (\boldsymbol{y}^* - \boldsymbol{z}_i) \in S_G$. Moreover, because G is weakly reversible, the edge $\boldsymbol{y}^* \to \boldsymbol{y}_j$ is a part of a cycle; therefore, $S_G = \text{span}_{\mathbb{R}}\{S_0,\, \boldsymbol{y}^* - \boldsymbol{z}_i\}_i$. Finally, we note that $\boldsymbol{y}^*$ is in the convex hull of the vertices $\boldsymbol{y}_j$, and thus $\boldsymbol{y}^* - \boldsymbol{z}_i \in \text{span}_{\mathbb{R}}\{\boldsymbol{y}_j - \boldsymbol{z}_i\}_j$, which implies $S_G \subseteq S_{G'}$. In other words, $S_G = S_{G'}$ and $\delta_{G'} = \delta_G - 1$. □

2.1.3 Numerical methods

In this section, we characterize when a flux system or a mass-action system is equivalent to a complex-balanced system. We also describe a method to determine when a mass-action system is dynamically equivalent to a complex-balanced or weakly reversible system.

2.1.3.1 Flux equivalence to complex-balancing

Is a steady state flux system $(G, \boldsymbol{J})$ flux equivalent to a complex-balanced one? The answer lies in the following linear feasibility problem for an unknown vector $\boldsymbol{J}'$. Enumerate the set of source vertices in G as $\{\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_N\}$. Search for $\boldsymbol{J}' = (J'_{\boldsymbol{y}_i \to \boldsymbol{y}_j})_{i \neq j} \in \mathbb{R}^{N^2 - N}$ satisfying

$$\sum_{j \neq i} J'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} (\boldsymbol{y}_j - \boldsymbol{y}_i) = \sum_{\boldsymbol{y}_i \to \boldsymbol{y} \in G} J_{\boldsymbol{y}_i \to \boldsymbol{y}} (\boldsymbol{y} - \boldsymbol{y}_i) \qquad \text{for } i = 1, 2, \ldots, N, \tag{2.10}$$

$$\sum_{j \neq i} J'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} = \sum_{j \neq i} J'_{\boldsymbol{y}_j \to \boldsymbol{y}_i} \qquad \text{for } i = 1, 2, \ldots, N, \tag{18a}$$

$$\boldsymbol{J}' \geq 0. \tag{2.12}$$

If such a flux vector $\boldsymbol{J}'$ exists, then $(G, \boldsymbol{J})$ is flux equivalent to a complex-balanced system. If no such flux vector $\boldsymbol{J}'$ exists, then $(G, \boldsymbol{J})$ is not flux equivalent to a complex-balanced system.

Equation (2.10) is the flux equivalence condition, while (18a) ensures that the new flux system is complex-balanced. Equation (2.10) alone checks for flux equivalence between any two given systems $(G, \boldsymbol{J})$ and $(G', \boldsymbol{J}')$.

Example 2.1.25. We return to the network G in Figure 1.2(a) and Example 1.2.10. The network has 6 vertices, 4 of which are sources, and 4 reactions. At the moment, we consider a flux system on the graph G and ask, for what flux $\boldsymbol{J}$ is the flux system $(G, \boldsymbol{J})$ equivalent to a complex-balanced one? One can show that (2.10)-(2.12) hold if and only if

$$J_1 = J_3, \quad J_2 = J_4, \quad \text{and} \quad \frac{1}{5} < \frac{J_1}{J_2} < 5. \tag{2.13}$$

A chosen flux $\boldsymbol{J}$ that satisfies (2.13) is flux equivalent to a complex-balanced system, whose network is a subgraph of G' of Figure 1.2(b). The details of this characterization will be in an upcoming paper [47].

Remark 2.1.26. The setup for the detailed-balanced case is defined analogously. We keep

(2.10) and (2.12) and include the equation

$$J'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} = J'_{\boldsymbol{y}_j \to \boldsymbol{y}_i} \qquad \text{for } 1 \leq i \neq j \leq N. \tag{18b}$$

2.1.3.2 Dynamical equivalence to complex balancing

We considered above a set of equalities and inequalities necessary and sufficient for a flux system to be equivalent to a complex-balanced one. If the flux system arises from mass-action kinetics, we can write down an analogous system of equalities and inequalities necessary and sufficient for dynamical equivalence to a complex-balanced system.

Consider a mass-action system $G_{\boldsymbol{k}}$, whose vertices are points in $\mathbb{R}^n$, and enumerate the set of source vertices in G as $\{\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_N\}$. We set up a nonlinear feasibility problem for unknowns $\boldsymbol{k}'$ and $\boldsymbol{x}$. Search for vectors $\boldsymbol{k}' = (k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j})_{i \neq j} \in \mathbb{R}^{N^2 - N}$ and $\boldsymbol{x} \in \mathbb{R}^n$ satisfying

$$\sum_{j \neq i} k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} (\boldsymbol{y}_j - \boldsymbol{y}_i) = \sum_{\boldsymbol{y}_i \to \boldsymbol{y} \in G} k_{\boldsymbol{y}_i \to \boldsymbol{y}} (\boldsymbol{y} - \boldsymbol{y}_i) \qquad \text{for } i = 1, 2, \ldots, N, \tag{2.14}$$

$$\sum_{j \neq i} k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} \boldsymbol{x}^{\boldsymbol{y}_i} = \sum_{j \neq i} k'_{\boldsymbol{y}_j \to \boldsymbol{y}_i} \boldsymbol{x}^{\boldsymbol{y}_j} \qquad \text{for } i = 1, 2, \ldots, N, \tag{2.15}$$

$$\boldsymbol{k}' \geq 0, \tag{2.16}$$

$$\boldsymbol{x} > 0. \tag{2.17}$$

If such $\boldsymbol{k}'$ and $\boldsymbol{x}$ exist, then $G_{\boldsymbol{k}}$ is dynamically equivalent to a complex-balanced system with $\boldsymbol{x}$ a complex-balanced steady state. If no such rate constants and steady state exist, then $G_{\boldsymbol{k}}$ is not dynamically equivalent to a complex-balanced system.

Equation (2.14) enforces dynamical equivalence. Equations (2.15) and (2.17) imply that $\boldsymbol{x}$ is a positive complex-balanced steady state for an equivalent mass-action system; hence $\boldsymbol{x}$ is a positive steady state of $G_{\boldsymbol{k}}$. Note that in the inequality (2.16), some $k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j}$ can be zero, which implies that $\boldsymbol{y}_i \to \boldsymbol{y}_j$ is not a reaction in the equivalent network.

Equations (2.14)-(2.17) generally form a nonlinear problem. Despite that, for networks with additional structure, one may be able to extract more information about the rate constants. One such example is the network G in Figure 1.2(a). For this network we can completely characterize the parameter values for which the associated mass-action system has a complex-balanced realization.

Example 2.1.27. Consider a mass-action system on the network G of Figure 1.2(a) and Example 1.2.10, with rate constants

$$k_{\boldsymbol{y}_1 \to \boldsymbol{y}_5} = k_1, \quad k_{\boldsymbol{y}_2 \to \boldsymbol{y}_5} = k_2, \quad k_{\boldsymbol{y}_3 \to \boldsymbol{y}_6} = k_3, \quad \text{and} \quad k_{\boldsymbol{y}_4 \to \boldsymbol{y}_6} = k_4.$$

By a calculation, (2.14)-(2.17) hold if and only if

$$\frac{1}{25} < \frac{k_1 k_3}{k_2 k_4} < 25. \tag{2.18}$$

Again, a complex-balanced realization is a subgraph of G' in Figure 1.2(b). More precisely, it is the reversible square with one pair of reversible diagonal (either $\boldsymbol{y}_1 \rightleftharpoons \boldsymbol{y}_3$ or $\boldsymbol{y}_2 \rightleftharpoons \boldsymbol{y}_4$); which diagonal is needed depends on the magnitudes of $k_1 k_3$ and $k_2 k_4$. The details of this characterization can be found in an upcoming paper [47].

The complex-balanced realization described (the subgraph of G' in Figure 1.2(b)) has deficiency $\delta_{G'} = 1$. It is known that if its eight rate constants lie in a toric ideal of codimension $\delta_{G'} = 1$, then the mass-action system is complex-balanced [22]. While these eight rate constants are related to k_1, k_2, k_3, and k_4 by several linear equations, we found one explicit condition (2.18) for when the mass-action system $G_{\boldsymbol{k}}$ of Figure 1.2(a) is dynamically equivalent to a complex-balanced system.

Finally, note that the network of Example 2.1.27 gives rise to systems that are equivalent to complex-balanced for certain choices of rate constants, but *not* for other choices of rate constants. In a follow-up paper we will show that an entire class of networks give rise to systems that are equivalent to complex-balanced *for all choice of rate constants*. More precisely, we will prove that systems generated by single-target networks that have their (unique) target vertex in the strict relative interior of the convex hull of its source vertices are dynamically equivalent to detailed-balanced mass-action systems for any choice of rate constants [47].

2.1.3.3 Existence of a weakly reversible realization for a mass-action system

While complex-balanced mass-action systems are weakly reversible, not all weakly reversible mass-action systems are complex-balanced. There has been much work on determining when a weakly reversible mass-action system is complex-balanced or not. Nonetheless, weakly reversible mass-action systems always have at least one positive steady state within each stoichiometric compatibility class [17] and are conjectured to be persistent, and even permanent [27].

We present a simple nonlinear feasibility problem to determine when a mass-action system is dynamically equivalent to a weakly reversible one. Recall that a mass-action system is weakly reversible if and only if it is complex-balanced for *some* choice of rate constants. We introduce a scaling factor $\alpha_{\boldsymbol{y}_i \to \boldsymbol{y}_j}$ in order to decouple the dynamical equivalence condition from the complex-balanced condition.

Consider a mass-action system $G_{\boldsymbol{k}}$, whose vertices are points in $\mathbb{R}^n$, and enumerate the set of source vertices in G as $\{\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_N\}$. We set up a nonlinear feasibility problem for unknown rate constants $\boldsymbol{k}'$ and a scaling factor $\boldsymbol{\alpha}$. Search for vectors $\boldsymbol{k}' = (k_{\boldsymbol{y}_i \to \boldsymbol{y}_j})_{i \neq j}$ and $\boldsymbol{\alpha} = (\alpha_{\boldsymbol{y}_i \to \boldsymbol{y}_j})_{i \neq j} \in \mathbb{R}^{N^2 - N}$ satisfying.

$$\sum_{j \neq i} k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} (\boldsymbol{y}_j - \boldsymbol{y}_i) = \sum_{\boldsymbol{y}_i \to \boldsymbol{y} \in G} k_{\boldsymbol{y}_i \to \boldsymbol{y}} (\boldsymbol{y} - \boldsymbol{y}_i) \qquad \text{for } i = 1, 2, \ldots, N, \tag{2.19}$$

$$\sum_{j \neq i} \alpha_{\boldsymbol{y}_i \to \boldsymbol{y}_j} k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} = \sum_{j \neq i} \alpha_{\boldsymbol{y}_j \to \boldsymbol{y}_i} k'_{\boldsymbol{y}_j \to \boldsymbol{y}_i} \qquad \text{for } i = 1, 2, \ldots, N, \tag{2.20}$$

$$\boldsymbol{k}' \geq 0, \tag{2.21}$$

$$\boldsymbol{\alpha} > 0. \tag{2.22}$$

If such $\boldsymbol{k}'$ and $\boldsymbol{\alpha}$ exist, then $G_{\boldsymbol{k}}$ is dynamically equivalent to a weakly reversible mass-action system. If no solution exists, then $G_{\boldsymbol{k}}$ is *not* dynamically equivalent to a weakly reversible system.

Equation (2.19) enforces dynamical equivalence. Equation (2.20) can be regarded as a complex balancing condition that uses a different set of rate constants $\alpha_{\boldsymbol{y}_i \to \boldsymbol{y}_j} k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j}$. Since $\alpha_{\boldsymbol{y}_i \to \boldsymbol{y}_j} k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} \neq 0$ if and only if $k'_{\boldsymbol{y}_i \to \boldsymbol{y}_j} \neq 0$, we preserve the graph structure of $G'_{\boldsymbol{k}'}$. It is well-known that a reaction network is weakly reversible if and only if it is complex-balanced for some choice of rate constants [22]. The scaling factor $\boldsymbol{\alpha}$ frees the rate constants from the dynamical equivalence constraint.

Note that while (2.19))-(2.22)) are simple to describe, more sophisticated, computationally efficient methods have been developed [93, 103]. Weak reversibility is a condition of the underlying directed graph. Ultimately one is imposing conditions on the incidence matrix or the Kirchhoff matrix of the network. Algorithms to find weakly reversible realization for a fixed vertex set have been proposed initially using mixed-integer linear programming [61, 103] and later by a *polynomial time* algorithm based on linear programming [93]. However, as with previous work on complex-balanced realizations, one must fix the set of vertices to be used in the computation. According to Theorem 2.1.20, it suffices to find an equivalent network using the existing source vertices. Therefore, the mixed-integer linear programming algorithms proposed in [61, 103] and the polynomial time algorithm in [93] can be used in conjunction with Theorem 2.1.20 to completely characterize whether or not a mass-action system $G_{\boldsymbol{k}}$ is dynamically equivalent to a weakly reversible one.

2.1.4 Conclusion

If we are looking for a complex-balanced realization of a given polynomial (or power-law) dynamical system, there exists no a priori limit on the number of vertices in the objective network. Moreover, there are no a priori choices for the locations of the vertices. Here we prove that a solution exists if and only if the objective network can be constructed by using only the vertices that are already present in the original system (i.e., the exponents of the monomial terms present in the original system). We also prove that the same is true for detailed-balanced, reversible and weakly reversible systems.

2.2 Single-Target Networks

2.2.1 Target vertex and Detailed-balancing

In this section, we concerns the class of *single-target networks*. Let me recall some concepts and notation at first. Here, for any $\boldsymbol{x}$, $\boldsymbol{y} \in \mathbb{R}^n$, define the vector operations

$$\begin{aligned}
\boldsymbol{x}^{\boldsymbol{y}} &= x_1^{y_1} x_2^{y_2} \cdots x_n^{y_n} \quad \text{ whenever } \boldsymbol{x} \in \mathbb{R}^n_{>0}, \\
\log(\boldsymbol{x}) &= (\log x_1, \log x_2, \ldots, \log x_n)^\top \quad \text{ whenever } \boldsymbol{x} \in \mathbb{R}^n_{>0}, \\
\exp(\boldsymbol{x}) &= (e^{x_1}, e^{x_2}, \ldots, e^{x_n})^\top, \\
\boldsymbol{x} \circ \boldsymbol{y} &= (x_1 y_1, x_2 y_2, \ldots, x_n y_n)^\top,
\end{aligned}$$

and let $\langle \boldsymbol{x}, \boldsymbol{y} \rangle$ denote the standard scalar product of $\mathbb{R}^n$. If a set $X \subseteq \mathbb{R}^n$ is contained in some affine subspace of $\mathbb{R}^n$, we denote by X^{o} the *relative interior* of X with respect to the usual topology of $\mathbb{R}^n$. A vertex $\boldsymbol{y}' \in V$ is a ***target vertex*** if $\boldsymbol{y} \to \boldsymbol{y}' \in E$ for some $\boldsymbol{y} \in V$.

We will construct a dynamical system using the graph G and the data stored in the vertices. The coordinates of a source vertex are exponents of a monomial. In algebra, the Newton polytope of a polynomial is the convex hull of the exponents of the monomials. Here, we define the Newton polytope using all the monomials appearing in the right-hand side of the dynamical system. In [48], the Newton polytope of a reaction network is also called a *reactant polytope*.

Definition 2.2.1. The ***Newton polytope*** of a reaction network $G = (V, E)$ is the convex hull of the source vertices, i.e.,

$$\mathrm{Newt}(G) = \left\{ \sum_{\boldsymbol{y} \in V_s} \alpha_{\boldsymbol{y}} \boldsymbol{y} : \ \alpha_{\boldsymbol{y}} \geq 0 \text{ and } \sum_{\boldsymbol{y} \in V_s} \alpha_{\boldsymbol{y}} = 1 \right\}.$$

The more important object is the relative interior of the Newton polytope

$$\mathrm{Newt}(G)^{\mathrm{o}} = \left\{ \sum_{\boldsymbol{y} \in V_s} \alpha_{\boldsymbol{y}} \boldsymbol{y} :\ \alpha_{\boldsymbol{y}} > 0 \text{ and } \sum_{\boldsymbol{y} \in V_s} \alpha_{\boldsymbol{y}} = 1 \right\}.$$

Note that in $\mathrm{Newt}(G)^{\mathrm{o}}$, all the coefficients in the sum must be positive.

Now we revisit the mass-action system to understand the stoichiometric matrix,

Definition 2.2.2. Let $G = (V, E)$ be a reaction network in $\mathbb{R}^n$ with edge set $E = \{\boldsymbol{y}_i \to \boldsymbol{y}_i'\}_{i=1}^R$. Let $\boldsymbol{\kappa} = (\kappa_i)_{i=1}^R$ be the vector of ***rate constants***. Its ***associated dynamical system*** is the system of differential equations on $\mathbb{R}^n_{>0}$ given by

$$\frac{d\boldsymbol{x}}{dt} = \sum_{i=1}^{R} \kappa_i \boldsymbol{x}^{\boldsymbol{y}_i} (\boldsymbol{y}_i' - \boldsymbol{y}_i). \tag{2.23}$$

The system of differential equations (2.23) can be written as

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{\Gamma} \begin{pmatrix} \kappa_1 \boldsymbol{x}^{\boldsymbol{y}_1} \\ \kappa_2 \boldsymbol{x}^{\boldsymbol{y}_2} \\ \vdots \\ \kappa_R \boldsymbol{x}^{\boldsymbol{y}_R} \end{pmatrix},$$

where the ***stoichiometric matrix*** $\boldsymbol{\Gamma}$ has as its ith column the reaction vector $\boldsymbol{y}_i' - \boldsymbol{y}_i$. Since $\frac{d\boldsymbol{x}}{dt}$ lies in the ***stoichiometric subspace*** $S = \mathrm{Im}\, \boldsymbol{\Gamma}$, the solution to the system (2.23), with initial value $\boldsymbol{x}_0 \in \mathbb{R}^n_{>0}$, lies in the affine space $\boldsymbol{x}_0 + S$. The ***positive stoichiometric compatibility class*** is the set $(\boldsymbol{x}_0 + S)_{>} = (\boldsymbol{x}_0 + S) \cap \mathbb{R}^n_{>0}$.

In general, a weakly reversible mass-action system may not have a complex-balanced steady state — similarly for reversible systems and detailed-balanced steady states — unless the rate constants satisfy additional algebraic constraints [22, 35, 41, 82, 96, 108].

Detailed-balancing, being more restrictive than complex-balancing, requires that the rate constants satisfy the algebraic conditions for complex-balancing, in addition to the *circuit conditions*: for every cycle in the reversible network, the product of rate constants in one direction equals that of the other direction [35]. In other words, suppose in one orientation of a cycle, the rate constants are k_{1+}, $k_{2+}, \dots, k_{r+}$, and in the other orientation, the rate constants are k_{1-}, $k_{2-}, \dots, k_{r-}$; then the circuit condition along this cycle is

$$\prod_{i=1}^{r} k_{i+} = \prod_{i=1}^{r} k_{i-}. \tag{2.24}$$

For a reversible system, the algebraic conditions for detailed-balance are also not difficult to state [35]. Choose a forward direction for each reversible pair and let k_{i+} be its rate constant; let k_{i-} be the rate constant of the backward direction. Suppose the network has p reversible pairs of edges. Let $\Gamma' \in \mathbb{R}^{n \times p}$ be the matrix whose columns are the reaction vectors of the forward directions.

Theorem 2.2.3. *The reversible mass-action system $G_{\boldsymbol{k}}$ is detailed-balanced if and only if every $\boldsymbol{J} \in \ker \Gamma' \subseteq \mathbb{R}^p$ satisfies the Wegscheider condition:*

$$\prod_{i=1}^{p} (k_{i+})^{J_i} = \prod_{i=1}^{p} (k_{i-})^{J_i}.$$

2.2.2 Single-target networks

In this part, we classify all single-target networks under mass-action kinetics: those that have a globally attracting positive steady state for all choices of positive rate constants, and those that have no positive steady state for any choice of rate constants. The former occurs if and only if the target is in the relative interior of the Newton polytope, the convex hull of the source vertices.

It is not difficult to show that if every reaction vector points to the relative interior of the Newton polytope (i.e., "inward pointing"), then the mass-action system is always dynamically equivalent to a weakly reversible system. It follows immediately that the system has a positive steady state [17] and is conjectured to be *permanent* [27]. In the case of a single-target network with "inward pointing" reaction vectors (to be made precise below), we show that the dynamics is essentially that of a detailed-balanced system.

Definition 2.2.4. A reaction network $G = (V, E)$ is a ***single-target network*** if there exists a vertex $\boldsymbol{y}^*$ such that $V \setminus \{\boldsymbol{y}^*\}$ is the set of source vertices, and $E = \{\boldsymbol{y} \to \boldsymbol{y}^* : \boldsymbol{y} \in V \setminus \{\boldsymbol{y}^*\}\}$. We call $\boldsymbol{y}^*$ the ***target vertex***, while the remaining vertices are ***source vertices***.

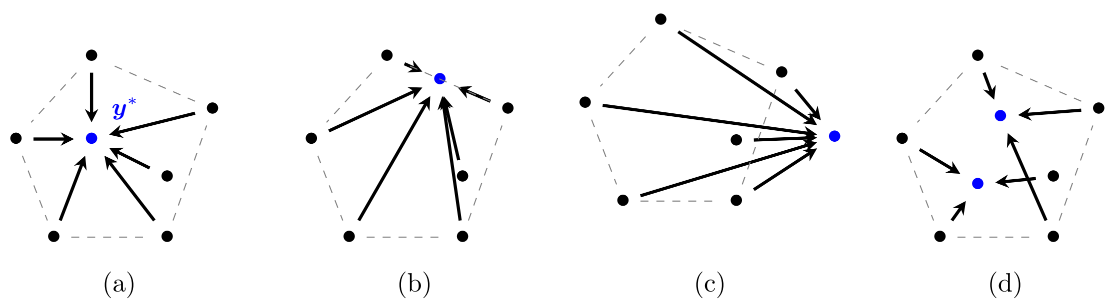


Figure 2.3: (a) A single-target network that is globally stable under mass-action kinetics. (b)–(c) Single-target networks with no positive steady states. (d) Not a single-target network.

Example 2.2.5. The reaction networks (a)–(c) in Figure 2.3 are single-target networks, while (d) is not a single-target network. The target vertex of (a) is in the relative interior of its Newton polytope. We will show that network (a) is typical of single-target networks that have exactly one globally stable steady state within each stoichiometric compatibility class, while the networks (b) and (c) have no positive steady state, regardless of the choice of kinetics. The deficiencies of the networks (a)–(c) are $\delta = 6 - \dim S$, while that of (d) is $\delta = 7 - \dim S$, where S is the stoichiometric subspace.

The geometry of a single-target network, i.e., whether the target is in the relative interior of the Newton polytope, determines whether the network admits a steady state flux, which is necessary for the existence a positive steady state under reasonable kinetics. In particular, the geometry can rule out the existence of positive steady states.

Lemma 2.2.6. *Let G be a single-target network. There exists a steady state flux on G if and only if the target vertex is in the relative interior of its Newton polytope.*

Proof. Let $\boldsymbol{y}^*$ be the target vertex of G, and enumerate the source vertices as $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_m$. The vector $\boldsymbol{J} = (J_i)_{\boldsymbol{y}_i \to \boldsymbol{y}^* \in E} \in \mathbb{R}^E_{>0}$ is a steady state flux if and only if

$$\sum_{i=1}^{m} J_i(\boldsymbol{y}^* - \boldsymbol{y}_i) = \boldsymbol{0}.$$

Rearranging, we see that $\boldsymbol{y}^* = \sum_i \frac{J_i}{J_T} \boldsymbol{y}_i$, where $J_T = \sum_i J_i$, and each $J_i > 0$. By definition, $\boldsymbol{y}^* \in \text{Newt}(G)^{\text{o}}$. □

Remark 2.2.7. At first glance, Lemma 2.2.6 is a result about fluxes, with no reference to any underlying kinetics. However, suppose the flux vector arises from any reasonable kinetics, such as mass-action or Michaelis–Menten kinetics — indeed the argument holds if each reaction rate function is differentiable (or Lipschitz) function mapping a state in $\mathbb{R}^n_{>0}$ to a positive number. Then for a single-target network whose target vertex is outside the relative interior of the Newton polytope, we can show that the trajectory, starting from any positive initial condition, will simply converge to the boundary of the positive orthant or to infinity. Indeed, there exists a Lyapunov function for such a dynamical system. When the target vertex is not in the relative interior of the convex hull of the sources, i.e., $\boldsymbol{y}^* \notin \text{Newt}(G)^{\text{o}}$, geometrically there is a hyperplane H (within the stoichiometric subspace) such that all the reaction vectors $\{\boldsymbol{y}^* - \boldsymbol{y}\}$ lie in a halfspace defined by H. (See Figures 2.3(b) and 2.3(c) for examples of such networks.) Let $\boldsymbol{w}$ be orthogonal to H such that $\langle \boldsymbol{w}, \boldsymbol{y}^* - \boldsymbol{y} \rangle \leq 0$ for all reactions $\boldsymbol{y} \to \boldsymbol{y}^*$. Then $V(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{w} \rangle$ defines a linear Lyapunov function for the single-target system, and all trajectories must converge to the boundary of the positive orthant or to infinity.

Even with the target vertex in $\text{Newt}(G)^{\text{o}}$, to deduce a positive steady state from a steady state flux $\boldsymbol{J}$ involves finding a positive solution $\boldsymbol{x}$ to the non-linear equations $J_{\boldsymbol{y} \to \boldsymbol{y}'} = k_{\boldsymbol{y} \to \boldsymbol{y}'} \boldsymbol{x}^{\boldsymbol{y}}$ for every reaction $\boldsymbol{y} \to \boldsymbol{y}'$. We will prove the existence of steady state for such single-target mass-action systems in Theorem 2.2.11. The result also applies to systems that are dynamically equivalent to a single-target network; for example see Examples 2.2.15 and 2.2.16. Our proof of the existence and global stability of a positive state will make use of the following theorems.

Theorem 2.2.8 ([14, 56, 84]). *Let $S \subseteq \mathbb{R}^n$ be a vector subspace, and let $\boldsymbol{x}_0$, $\boldsymbol{x}^* \in \mathbb{R}^n_{>0}$ be two arbitrary positive vectors. The intersection $(\boldsymbol{x}_0 + S) \cap (\boldsymbol{x}^* \circ \exp S^\perp)$ consists of exactly one point, where $\boldsymbol{x}^* \circ \exp S^\perp = \{\boldsymbol{x}^* \circ \exp(\boldsymbol{s}) \colon \boldsymbol{s} \in S^\perp\}$.*

Theorem 2.2.9 ([6, 18]). *Let $G_{\boldsymbol{\kappa}}$ be a complex-balanced system with one connected component. Any positive steady state is a global attractor within its stoichiometric compatibility class.*

We now give a necessary and sufficient condition for a single-target network to be dynamically equivalent to a detailed-balanced system under mass-action kinetics. This result is related to the theory of *star-like networks* [43], which have been shown to have a unique asymptotically stable steady state within each stoichiometric compatibility class. In what follows, $\mathbb{R}^E_{>0}$ denote the set of vectors of rate constants, indexed by E.

Theorem 2.2.10. *Let $G = (V, E)$ be a single-target network whose target vertex is in the relative interior of the Newton polytope. Then for any vector of rate constants $\boldsymbol{\kappa} \in \mathbb{R}^E_{>0}$, the mass-action system $G_{\boldsymbol{\kappa}}$ is dynamically equivalent to a detailed-balanced system that has a single connected component.*

Proof. Let $\boldsymbol{y}^*$ denote the target vertex, and enumerate the source vertices $\boldsymbol{y}_1, \boldsymbol{y}_2, \ldots, \boldsymbol{y}_m$. Let $\boldsymbol{\Gamma} \in \mathbb{R}^{n \times m}$ be the stoichiometric matrix, whose jth column is the reaction vector $\boldsymbol{y}^* - \boldsymbol{y}_j$. Let $\kappa_j > 0$ be an arbitrary rate constant for the edge $\boldsymbol{y}_j \to \boldsymbol{y}^*$, and let $\boldsymbol{\kappa} = (\kappa_j)_{j=1}^m$. Recall that the relative interior of the Newton polytope is

$$\operatorname{Newt}(G)^{\mathrm{o}} = \left\{ \sum_{j=1}^m \alpha_j \boldsymbol{y}_j : \alpha_j > 0 \text{ and } \sum_{j=1}^m \alpha_j = 1 \right\}.$$

We want to prove that $G_{\boldsymbol{\kappa}}$ is dynamically equivalent to a detailed-balanced system with vertex set $V_{G'} = V_G$ and edge set $E_{G'} = E_G \cup \{\boldsymbol{y}^* \to \boldsymbol{y}_j\}_{j=1}^m$. Moreover, for the original edges $\boldsymbol{y}_j \to \boldsymbol{y}^*$, we keep the same rate constants κ_j. Let κ'_j denote the rate constant of the reversible edge $\boldsymbol{y}^* \to \boldsymbol{y}_j$, whose value is to be determined. Consider the following conditions with unknowns $\kappa'_j > 0$ and $\boldsymbol{x} \in \mathbb{R}^n_{>0}$:

$$\sum_{j=1}^{m} \kappa'_j (\boldsymbol{y}_j - \boldsymbol{y}^*) = \boldsymbol{0}, \tag{2.25}$$

$$\kappa_j \boldsymbol{x}^{\boldsymbol{y}_j} = \kappa'_j \boldsymbol{x}^{\boldsymbol{y}^*} \qquad \text{for all } 1 \leq j \leq m. \tag{2.26}$$

The condition (2.25) ensures that the resulting system is dynamically equivalent to the original since the only difference between the two networks are the edges with source $\boldsymbol{y}^*$. The condition (2.26) ensures that resulting system is a detailed-balanced system with positive steady state $\boldsymbol{x}$. Condition (2.25) can be replaced with $\boldsymbol{\kappa}' = (\kappa'_j)_{j=1}^m \in \ker \boldsymbol{\Gamma}$. Isolating κ'_j in condition (2.26), we obtain

$$\kappa'_j = \kappa_j \boldsymbol{x}^{\boldsymbol{y}_j - \boldsymbol{y}^*} = \kappa_j e^{\langle \boldsymbol{y}_j - \boldsymbol{y}^*, \, \log \boldsymbol{x} \rangle}.$$

So (2.26) is equivalent to $\boldsymbol{\kappa}' \in \boldsymbol{\kappa} \circ \exp(\operatorname{Im} \boldsymbol{\Gamma}^\top)$. Therefore, that $G_{\boldsymbol{k}}$ is dynamically equivalent to a detailed-balanced system follows from the existence of $\boldsymbol{\kappa}'$ in the intersection $\ker \boldsymbol{\Gamma} \cap (\boldsymbol{\kappa} \circ \exp(\operatorname{Im} \boldsymbol{\Gamma}^\top)) \subseteq \mathbb{R}^m_{>0}$.

By Lemma 2.2.6, there exists a steady state flux $\boldsymbol{J}$ on G, i.e., $\boldsymbol{J} \in \ker \boldsymbol{\Gamma} \cap \mathbb{R}^m_{>0}$. Hence,

$$\ker \boldsymbol{\Gamma} \cap (\boldsymbol{\kappa} \circ \exp(\operatorname{Im} \boldsymbol{\Gamma}^\top)) = (\boldsymbol{J} + \ker \boldsymbol{\Gamma}) \cap (\boldsymbol{\kappa} \circ \exp(\ker \boldsymbol{\Gamma}^\perp)),$$

which is guaranteed to be non-empty for any positive $\boldsymbol{J}$, $\boldsymbol{\kappa}$ by Theorem 2.2.8 [14, 56]. Let $\boldsymbol{\kappa}' = (\kappa'_j)_{j=1}^m$ be in the intersection. Therefore, there exist positive solutions $\boldsymbol{x} \in \mathbb{R}^n_{>0}$ and $\kappa_j > 0$ satisfying conditions (2.25)–(2.26). The graph G' consists of the original edges $\boldsymbol{y}_j \to \boldsymbol{y}^*$ with the original rate constants $\kappa_j > 0$ and the edges $\boldsymbol{y}^* \to \boldsymbol{y}_j$ with rate constants $\kappa'_j > 0$. In other words, $G_{\boldsymbol{\kappa}}$ is dynamically equivalent to a detailed-balanced system $G'_{\widetilde{\boldsymbol{\kappa}}}$, where G' is strongly connected and $\widetilde{\boldsymbol{\kappa}} \in \mathbb{R}^{E'}_{>0}$ has coordinates given by $\boldsymbol{\kappa}$ and $\boldsymbol{\kappa}'$. $\square$

Theorem 2.2.11. *Let $G = (V, E)$ be a single-target network. For any vector of rate constants $\boldsymbol{\kappa} \in \mathbb{R}^E_{>0}$, let $G_{\boldsymbol{\kappa}}$ denote the corresponding mass-action system. Then exactly one of the following is true.*

1. *For any $\boldsymbol{\kappa}$, the mass-action system $G_{\boldsymbol{\kappa}}$ has no positive steady states and all trajectories must converge to the boundary of the positive orthant or to infinity.*

2. *For any $\boldsymbol{\kappa}$, the mass-action system $G_{\boldsymbol{\kappa}}$ has exactly one positive steady state within each of its stoichiometric compatibility class. Furthermore, this steady state is globally stable within its class.*

The latter occurs if and only if the target vertex of G is in the relative interior of the Newton polytope.

Proof. If $\boldsymbol{y}^* \notin \mathrm{Newt}(G)^{\mathrm{o}}$, by Lemma 2.2.6 and Remark 2.2.7 the network G admits no positive flux vector, i.e., $\ker \boldsymbol{\Gamma} \cap \mathbb{R}^E_{>0} = \varnothing$; therefore, any mass-action system generated by G cannot have a positive steady state and all trajectories must converge to the boundary of the positive orthant or to infinity. However, if $\boldsymbol{y}^* \in \mathrm{Newt}(G)^{\mathrm{o}}$, then by Theorem 2.2.10 the mass-action system is dynamically equivalent to a detailed-balanced system with one connected component regardless of the choice of rate constants. Since detailed-balanced systems are complex-balanced, this system, with one connected component, has within each of its stoichiometric compatibility class exactly one positive steady state, which is globally stable, as stated in Theorem 2.2.9 [6, 18]. □

Example 2.2.12. Consider the single-target networks in Figures 1(a)–(c). Mass-action systems generated by networks (b) and (c) can never have positive steady states, while systems generated by the network (a) have exactly one positive steady state within every stoichiometric compatibility class and it is globally stable.

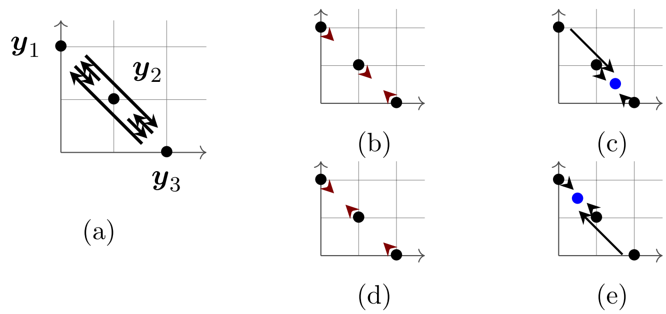


Figure 2.4: Consider (a) under mass-action kinetics, whose associated dynamics is given by (2.27). If the coefficient of $\boldsymbol{x}^{\boldsymbol{y}_1}$ in $\dot{x}$ is positive and the coefficient of $\boldsymbol{x}^{\boldsymbol{y}_3}$ in $\dot{x}$ is negative, then the system (2.27) can be realized by a single-target network, determined by the sign of $\boldsymbol{x}^{\boldsymbol{y}_2}$ in $\dot{x}$. If the net directions are as shown in (b), then (2.27) can be realized by the single-target network in (c). Similarly, if the net directions appear as in (d), then (2.27) can be realized by the network in (e).

Example 2.2.13. Consider the complete graph on the vertices

$$\boldsymbol{y}_1 = \begin{pmatrix} 0 \\ 2 \end{pmatrix}, \quad \boldsymbol{y}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \boldsymbol{y}_3 = \begin{pmatrix} 2 \\ 0 \end{pmatrix},$$

as shown in Figure 2.4(a). In [19], this network under mass-action kinetics, was shown to be dynamically equivalent to a complex-balanced system for any vector of positive rate constants. We claim that under mass-action kinetics, any subnetwork for which $\boldsymbol{y}_1 = (0,2)^\top$ and $\boldsymbol{y}_3 = (2,0)^\top$ are sources, can be realized by a single-target network, and is dynamically equivalent to a detailed-balanced system.

Let $\kappa_{ij} \geq 0$ be the rate constant (if non-zero) of the edge $\boldsymbol{y}_i \to \boldsymbol{y}_j$. The associated dynamical system

$$\begin{aligned} \frac{dx}{dt} &= y^2(\kappa_{12} + 2\kappa_{13}) + xy(-\kappa_{21} + \kappa_{23}) + x^2(-\kappa_{32} - 2\kappa_{31}) \\ \frac{dy}{dt} &= -y^2(\kappa_{12} + 2\kappa_{13}) - xy(-\kappa_{21} + \kappa_{23}) - x^2(-\kappa_{32} - 2\kappa_{31}) \end{aligned} \tag{2.27}$$

is a homogeneous degree two polynomial system, where we assume $\kappa_{12}+\kappa_{13} > 0$ and $\kappa_{32}+\kappa_{31} >$

0. The sign of $-\kappa_{12}+\kappa_{23}$ determines the structure of the single-target network that the mass-action system is dynamically equivalent to. Consider the net direction from each vertex, given by the weighted sum of reaction vectors originating from that vertex with weights given by the rate constants. If $-\kappa_{12}+\kappa_{23}\geq 0$, the net direction from each vertex is shown in Figure 2.4(b) (with possibly nothing from $\boldsymbol{y}_2$). Then the system can be realized by the single-target network in Figure 2.4(c). Denote by κ_i' the rate constant from $\boldsymbol{y}_i$ to the target $(1.5, 0.5)^\top$; the rate constants for the system on Figure 2.4(c) are

$$\kappa_1' = \frac{2}{3}(\kappa_{12}+2\kappa_{13}), \quad \kappa_2' = 2(-\kappa_{12}+\kappa_{23}), \quad \kappa_3' = 2(\kappa_{32}+2\kappa_{31}).$$

A similar argument shows that if $-\kappa_{12}+\kappa_{23}<0$, the net direction from each vertex is shown in Figure 2.4(d). The system can be realized by the single-target network in Figure 2.4(e), with rate constants

$$\kappa_1' = 2(\kappa_{12}+2\kappa_{13}), \quad \kappa_2' = 2(\kappa_{12}-\kappa_{23}), \quad \kappa_3' = \frac{2}{3}(\kappa_{32}+2\kappa_{31}).$$

This follows by considering linear equations coming from each of the three source vertices. For example, at $\boldsymbol{y}_1$, dynamical equivalence dictates that

$$\kappa_{12}\begin{pmatrix}1\\-1\end{pmatrix} + \kappa_{13}\begin{pmatrix}2\\-2\end{pmatrix} = \kappa_1'\begin{pmatrix}3/2\\-3/2\end{pmatrix},$$

from which one can easily solve for κ_1'. Similar considerations at the other source vertices provide the remaining rate constants.

This example can be extended to homogeneous polynomials of two variables. Order the terms of such a polynomial $p(x,y)$ by ascending degree of x. If the coefficient of the first term is positive, coefficient for the last term is negative, and there is exactly one sign change between consecutive terms, then for any positive initial condition, the system

$$\frac{dx}{dt} = p(x,y) \quad \text{and} \quad \frac{dy}{dt} = -p(x,y)$$

has exactly one positive steady state, which is globally stable. Indeed, the system can be realized by a single-target network, and is dynamically equivalent to a detailed-balanced system.

Example 2.2.14. In this example, we consider non-linear dynamical systems on $\mathbb{R}^n_{>0}$ of the form

$$\frac{d\boldsymbol{x}}{dt} = \sum_{i=1}^{m} -\kappa_i \boldsymbol{x}^{\boldsymbol{y}_i} \boldsymbol{y}_i, \tag{2.28}$$

where $\kappa_i > 0$ and $\boldsymbol{y}_i \in \mathbb{R}^n$ such that the origin is a positive convex combination of $\{\boldsymbol{y}_i \colon i = 1, 2, \ldots, m\}$. For example,

$$\frac{d}{dt}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \kappa_1 x^{-1} y^{-2} \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} + \kappa_2 y^{-3} z^{-1} \begin{pmatrix} 0 \\ 3 \\ 1 \end{pmatrix} + \kappa_3 x^{-2} y^3 z^2 \begin{pmatrix} 2 \\ -3 \\ -2 \end{pmatrix} + \kappa_4 x y^2 z \begin{pmatrix} -1 \\ -2 \\ -1 \end{pmatrix} + \kappa_5 x^4 y^{-2} z^{\frac{3}{2}} \begin{pmatrix} -4 \\ 2 \\ -3/2 \end{pmatrix}$$

belongs to this class. At first sight of the differential equations, there may be very little reason to believe that this system has a unique positive steady state, which is globally stable, within the affine space parallel to span$\{\boldsymbol{y}_i \colon i = 1, 2, \ldots, m\}$. However, with the tools developed in this paper, uniqueness of steady states and global stability immediately follow from Theorem 2.2.10. The reaction network that generates (2.28) under mass-action kinetics consists of the reactions $\boldsymbol{y}_i \to \boldsymbol{0}$ with rate constant $\kappa_i > 0$. By definition, the unique target $\boldsymbol{0}$ is in the relative interior of $\{\boldsymbol{y}_i \colon i = 1, 2, \ldots, m\}$. Therefore by Theorem 2.2.11, for any positive initial condition, there is exactly one positive steady state which is globally attracting.

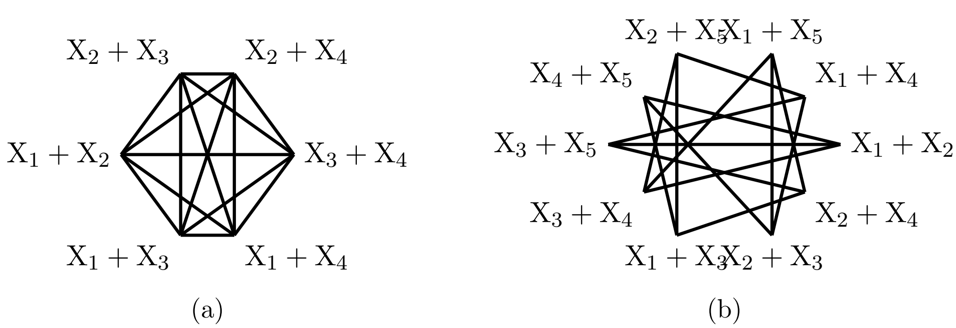


Figure 2.5: Reversible systems in (a) Example 2.2.15 and (b) Example 2.2.16 that are dynamically equivalent to detailed-balanced systems. Each undirected edge represents a pair of reversible edges.

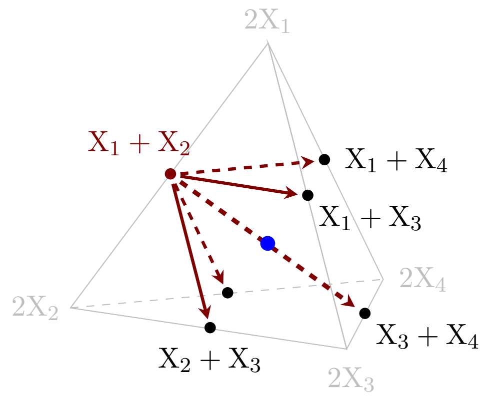


Figure 2.6: Geometric argument for dynamically equivalence to single-target network in Example 2.2.15. Shown are the edges with $X_1 + X_2$ as their source. The centre $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)^\top$ of the tetrahedron is marked in blue. With rate constants given in the example, the weighted sum of reaction vectors points from the source to the centre.

Example 2.2.15. Consider the reaction network shown in Figure 2.5(a), where each edge represents a reversible pair of reactions. Then in the language of the standard basis $\{\widehat{\mathbf{e}}_i \colon i = 1, \ldots 4\}$ of $\mathbb{R}^4$, the six vertices are $\{\boldsymbol{y}_{ij} = \widehat{\mathbf{e}}_i + \widehat{\mathbf{e}}_j \colon 1 \leq i < j \leq 4\}$. Edges take the form $\boldsymbol{y}_{ij} \rightleftharpoons \boldsymbol{y}_{pq}$ where $(i,j) \neq (p,q)$, with the network G being a complete graph.

A given vertex $\boldsymbol{y}_{ij}$ is source to two kinds of edges: an edge whose target has disjoint support from the source (i.e., $\boldsymbol{y}_{ij} \to \boldsymbol{y}_{pq}$ where i, j, p, q are distinct integers), and those whose targets share an index with the source (i.e., $\boldsymbol{y}_{ij} \to \boldsymbol{y}_{iq}$ or $\boldsymbol{y}_{ij} \to \boldsymbol{y}_{pj}$). The latter represents a chemical reaction with the common species acting as a catalyst.

Rate constant of an edge is assigned based on the source vertex and which type of edge it is. For example, consider the source vertex $\boldsymbol{y}_{12} = \widehat{\mathbf{e}}_1 + \widehat{\mathbf{e}}_2$. The edge $\boldsymbol{y}_{12} \to \boldsymbol{y}_{34}$ is assigned an arbitrary rate constant $\kappa_{12a} > 0$, while the catalytic reactions

$$\boldsymbol{y}_{12} \to \boldsymbol{y}_{13}, \quad \boldsymbol{y}_{12} \to \boldsymbol{y}_{14}, \quad \boldsymbol{y}_{12} \to \boldsymbol{y}_{23}, \quad \boldsymbol{y}_{12} \to \boldsymbol{y}_{24}$$

are assigned rate constants $\kappa_{12b} > 0$. The rate constant for $\boldsymbol{y}_{13} \to \boldsymbol{y}_{24}$ is $\kappa_{13a} > 0$, while other edges originating from $\boldsymbol{y}_{13}$ have rate constants $\kappa_{13b} > 0$. The remaining edges are assigned rate constants in a similar manner.

The mass-action system $G_{\boldsymbol{k}}$ is not detailed-balanced in general since the circuit condition (2.24) is generically violated along some cycles, e.g., the cycle with vertices $\boldsymbol{y}_{12}$, $\boldsymbol{y}_{24}$ and $\boldsymbol{y}_{34}$ is associated to the condition

$$\kappa_{12b}\kappa_{24a}\kappa_{34a} = \kappa_{12a}\kappa_{34b}\kappa_{24b}.$$

Moreover, this reversible network has deficiency $\delta = 2$; therefore, the mass-action system is not complex-balanced in general as well.

Nonetheless, the system can be realized by a single-target network and is dynamically equivalent to a detailed-balanced system. The weighted sum of reaction vectors coming out of the vertex $\boldsymbol{y}_{12}$ is

$$\begin{aligned}
&\kappa_{12a}\left(\boldsymbol{y}_{34}-\boldsymbol{y}_{12}\right)+\kappa_{12b}\left(\boldsymbol{y}_{13}-\boldsymbol{y}_{12}\right)+\kappa_{12b}\left(\boldsymbol{y}_{14}-\boldsymbol{y}_{12}\right)+\kappa_{12b}\left(\boldsymbol{y}_{23}-\boldsymbol{y}_{12}\right)+\kappa_{12b}\left(\boldsymbol{y}_{24}-\boldsymbol{y}_{12}\right)\\
&=\kappa_{12a}\begin{pmatrix}-1\\-1\\1\\1\end{pmatrix}+\kappa_{12b}\begin{pmatrix}-2\\-2\\2\\2\end{pmatrix}=2\left(\kappa_{12a}+2\kappa_{12b}\right)\begin{pmatrix}1/2-1\\1/2-1\\1/2\\1/2\end{pmatrix},
\end{aligned}$$

which is also the weighted reaction vector of $\boldsymbol{y}_{12} \to \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)^\top$ with rate constant given by $2\left(\kappa_{12a} + 2\kappa_{12b}\right)$. See Figure 2.6 for the geometry of this calculation. By symmetry, the weighted sum of reaction vectors out of any vertex of G can be written as an edge to $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)^\top$. Therefore, the mass-action system generated by the network in Figure 2.5(a) is dynamically equivalent to a single-target network with target vertex $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)^\top$, which is in the relative interior of the Newton polytope. By Theorem 2.2.11, the mass-action system is dynamically equivalent to a globally stable detailed-balanced system.

Example 2.2.16. Consider the reversible reaction network in Figure 2.5(b) in $\mathbb{R}^5$. This network is similar to that of Example 2.2.15 except it has *no* catalytic reaction. The ten vertices are $X_i + X_j$ with $1 \leq i < j \leq 5$. Edges take the form $X_i + X_j \rightleftharpoons X_p + X_q$ where i, j, p, q are all distinct. Further assume the rate constants depend only on the source vertices, i.e., all reactions originating from the vertex $X_i + X_j$ have the same rate constant.

This reversible network has deficiency $\delta = 5$. This system is in general neither complex-balanced nor detailed-balanced. For example, the Wegscheider's condition involves the equation $\kappa_{13}\kappa_{24}\kappa_{35} = \kappa_{12}\kappa_{34}$ among many others. Nonetheless, the system can be realized by a single-target network, whose target vertex $\frac{2}{5}X_1 + \frac{2}{5}X_2 + \frac{2}{5}X_3 + \frac{2}{5}X_4 + \frac{2}{5}X_5$ lies in the relative interior of the Newton polytope. Therefore, the mass-action system is dynamically equivalent to a globally stable detailed-balanced system.

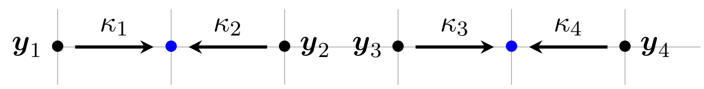
2.2.3 Networks with two targets

In the previous section, we have characterized the dynamics of all single-target networks under mass-action kinetics. In particular, we have seen that if the target vertex is in the relative interior of the Newton polytope, then any mass-action system generated by that network is dynamically equivalent to a detailed-balanced system, which has a globally attracting positive steady state within each stoichiometric compatibility class.

One may wonder if a similar result holds for networks with multiple targets, each in the relative interior of the Newton polytope. Networks with such "inward pointing" reaction vectors, or *endotatic networks* [27], are conjectured to be *persistent*, i.e., trajectories are bounded away from the boundary, and even *permanent*, i.e., admit a globally attracting compact set within each stoichiometric compatibility class. These conjectures have been proved for certain classes of networks: weakly reversible networks with one connected component [6, 18], strongly endotactic networks [48], and two-dimensional networks [27, 85].

Even with just *two* target vertices, there exist strongly endotactic networks with multiple positive steady states (within the same stoichiometric compatibility class), and thus cannot be globally stable. In the following examples, we relax the requirement, instead searching for a dynamically equivalent *complex-balanced* system. Because vertices that do not appear explicitly as monomials in the differential equations are not necessary when searching for a dynamically equivalent complex-balanced system [25], we restrict our attention to subnetworks on the complete graph defined by the source vertices.

Example 2.2.17. For example, consider the mass-action system



where the source vertices are $\boldsymbol{y}_1 = 0$, $\boldsymbol{y}_2 = 2$, $\boldsymbol{y}_3 = 3$ and $\boldsymbol{y}_4 = 5$, and the target vertices are $\boldsymbol{y}_5 = 1$ and $\boldsymbol{y}_6 = 4$. The associated dynamical system

$$\frac{dx}{dt} = \kappa_1 - \kappa_2 x^2 + \kappa_3 x^3 - \kappa_4 x^5$$

has *multiple* positive steady states for some choice of $\kappa_i > 0$ by Descartes' rule of signs. In particular, for these choices of $\kappa_i > 0$, it cannot be dynamically equivalent to a detailed-balanced (or complex-balanced) system, which necessarily has a *unique* positive steady state.

We claim that this system $G_{\boldsymbol{k}}$ is dynamically equivalent to a complex-balanced system if and only if $\kappa_1\kappa_4 \geq \kappa_2\kappa_3$. Let G' be the complete graph on the source vertices and let $\kappa'_{ij} \geq 0$ be the label on $\boldsymbol{y}_i \to \boldsymbol{y}_j$. The objective is a subgraph of G'.

Since there are four sources in G, which are also sources in G', there are four non-trivial linear relations on the edge labels of G and those of G', and two trivial equations ($0 = 0$) coming from the vertices $\boldsymbol{y}_5$ and $\boldsymbol{y}_6$. For example, the dynamical equivalence relation at $\boldsymbol{y}_2$ is

$$-\kappa_2 = -2\kappa_{21} + \kappa_{23} + 3\kappa_{24}.$$

Note that the dynamical equivalence relation can be transformed to that of the fluxes, by multiplying both sides of the linear equation by the source vertex's monomial. Fix a state $x > 0$, the value yet to be determined. Let $J_i = \kappa_i x^{\boldsymbol{y}_i}$ be the flux across the edge originating from $\boldsymbol{y}_i$. Similarly, on G' let $Q_{ij} = \kappa'_{ij} x^{\boldsymbol{y}_i}$ be the flux across the edge $\boldsymbol{y}_i \to \boldsymbol{y}_j$. Then the dynamical equivalence relation at $\boldsymbol{y}_2$ can be written as

$$-J_2 = -2Q_{21} + Q_{23} + 3Q_{24}.$$

The switch from rate constants to fluxes is convenient when considering dynamical equivalence and complex-balancing simultaneously. For example, in the objective system $G'_{\boldsymbol{\kappa}'}$, the state x is complex-balanced if and only if

$$(\kappa'_{21} + \kappa'_{23} + \kappa'_{24})x^{\boldsymbol{y}_2} = \kappa'_{12}x^{\boldsymbol{y}_1} + \kappa'_{32}x^{\boldsymbol{y}_3} + \kappa'_{42}x^{\boldsymbol{y}_4}.$$

In the language of flux, this reads $Q_{21} + Q_{23} + Q_{24} = Q_{12} + Q_{32} + Q_{42}$.

Hence, the four dynamical equivalence relations, in terms of fluxes, are

$$\begin{aligned} J_1 &= 2Q_{12} + 3Q_{13} + 5Q_{14}, \\ -J_2 &= -2Q_{21} + Q_{23} + 3Q_{24}, \\ J_3 &= -3Q_{31} - Q_{32} + 2Q_{34}, \\ -J_4 &= -5Q_{41} - 3Q_{42} - 2Q_{43}, \end{aligned}$$

while the complex-balanced conditions on G' are

$$\begin{aligned} Q_{12} + Q_{13} + Q_{14} &= Q_{21} + Q_{31} + Q_{41}, \qquad (2.29) \\ Q_{21} + Q_{23} + Q_{24} &= Q_{12} + Q_{32} + Q_{42}, \\ Q_{31} + Q_{32} + Q_{34} &= Q_{13} + Q_{23} + Q_{43}, \\ Q_{41} + Q_{42} + Q_{43} &= Q_{14} + Q_{24} + Q_{34}. \end{aligned}$$

It is not difficult to see from (2.29) that the left-hand side of the complex-balanced condition at $\boldsymbol{y}_1$ can be rewritten as

$$Q_{12} + Q_{13} + Q_{14} = \left(\frac{1}{2}J_1 - \frac{3}{2}Q_{13} - \frac{5}{2}Q_{14}\right) + Q_{13} + Q_{14} \leq \frac{1}{2}J_1,$$

while the right-hand side is

$$Q_{21} + Q_{31} + Q_{41} = \left(\frac{1}{2}J_2 + \frac{1}{2}Q_{23} + \frac{3}{2}Q_{24}\right) + Q_{31} + Q_{41} \geq \frac{1}{2}J_2.$$

In other words, $J_1 \geq J_2$. Similarly, from the last complex-balanced condition, we obtain $J_4 \geq J_3$. Therefore, $G_{\boldsymbol{k}}$ being dynamically equivalent to a complex-balanced system implies $J_1 J_4 \geq J_2 J_3$; equivalently, $\kappa_1\kappa_4 \geq \kappa_2\kappa_3$.

Conversely, suppose $\kappa_1\kappa_4 \geq \kappa_2\kappa_3$ or $J_1 J_4 \geq J_2 J_3$. Clearly the system of differential equations admits at least one positive steady state $x > 0$. At x, the fluxes are balanced, i.e., $J_1 + J_3 = J_2 + J_4$. Substituting the inequality into $\kappa_1 + \kappa_3 x^3 = \kappa_2 x^2 + \kappa_4 x^5$, we see that $J_1 \geq J_2$ and $J_4 \geq J_3$. The choice

$$Q_{12} = Q_{21} = \frac{J_2}{2}, \qquad Q_{34} = Q_{43} = \frac{J_3}{2}, \qquad Q_{14} = \frac{J_1 - J_2}{5} \qquad \text{and} \qquad Q_{41} = \frac{J_4 - J_3}{5}$$

satisfies the dynamical equivalence and complex-balanced conditions. Choose rate constants on the new network to be

$$\widetilde{\kappa}_{12} = \frac{\kappa_2}{2}, \qquad \widetilde{\kappa}_{34} = \frac{\kappa_3 x^3}{2}, \qquad \widetilde{\kappa}_{12} = \frac{\kappa_2 x^2}{2}, \qquad \widetilde{\kappa}_{43} = \frac{\kappa_3 x^3}{2},$$
$$\widetilde{\kappa}_{14} = \frac{1}{5}\left(\kappa_1 - \frac{\kappa_2 x^2}{2}\right) \qquad \text{and} \qquad \widetilde{\kappa}_{41} = \frac{1}{5}\left(\kappa_4 - \frac{\kappa_3 x^{-2}}{2}\right).$$

Note that $\widetilde{\kappa}_{14} = \frac{1}{10}(2J_1 - J_2) > 0$, and $\widetilde{\kappa}_{41} = \frac{1}{10x^5}(2J_4 - J_3) > 0$. With this choice of rate constants $\widetilde{\boldsymbol{\kappa}}$, the mass-action system is dynamically equivalent to a complex-balanced system with steady state x, which is the unique positive steady state of the system.

Example 2.2.18. Consider the network under mass-action kinetics in Figure 2.7(a) with four source vertices and two target vertices in $\mathbb{R}^2$. The source vertices correspond to the monomials

1, x^3, x^3y^2 and y^2. We will show that this system is dynamically equivalent to a complex-balanced system if and only if

$$\frac{1}{25} \leq \frac{\kappa_1\kappa_3}{\kappa_2\kappa_4} \leq 25.$$

Being dynamically equivalent to a complex-balanced system, if it can be done at all, can be achieved using only the source vertices [25]; thus we look for a subnetwork of the *complete graph* shown in Figure 2.7(b).

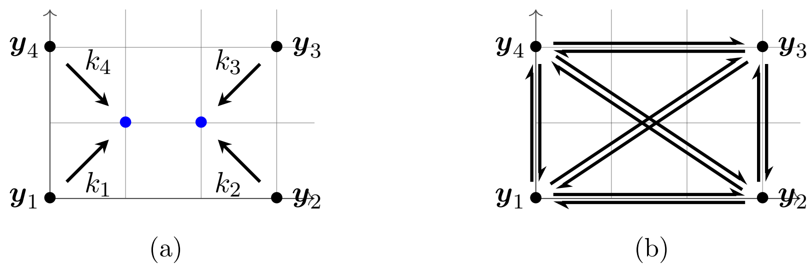


Figure 2.7: (a) The mass-action system with two target vertices from Example 2.2.18, which is dynamically equivalent to a complex-balanced system using a subnetwork of (b) if and only if $\frac{1}{25} \leq \frac{\kappa_1\kappa_3}{\kappa_2\kappa_4} \leq 25$.

Suppose $\boldsymbol{x} > \boldsymbol{0}$ is a steady state for which the system in Figure 2.7(a) is dynamically equivalent to a complex-balanced system. Note that $\boldsymbol{x}$ is a positive steady state for the system. Let $J_i = \kappa_i \boldsymbol{x}^{\boldsymbol{y}_i} > 0$ define a flux on the network. The steady state flux $\boldsymbol{J}$ thus satisfies $J_1 = J_3$ and $J_2 = J_4$. Let $\boldsymbol{Q}$, where $Q_{ij} \geq 0$ is to be determined, denote the flux across the edge $\boldsymbol{y}_i \to \boldsymbol{y}_j$ in Figure 2.7(b). Dynamical equivalence is obtained if and only if

$$J_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 3Q_{12} + 3Q_{13} \\ 2Q_{14} + 2Q_{13} \end{pmatrix}, \qquad J_3 \begin{pmatrix} -1 \\ -1 \end{pmatrix} = \begin{pmatrix} -3Q_{31} - 3Q_{34} \\ -2Q_{31} - 2Q_{32} \end{pmatrix},$$
$$J_2 \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -3Q_{21} - 3Q_{24} \\ 2Q_{23} + 2Q_{24} \end{pmatrix}, \qquad J_4 \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 3Q_{42} + 3Q_{43} \\ -2Q_{42} - 2Q_{41} \end{pmatrix}.$$

Meanwhile, complex-balancing is obtained on a subnetwork of that in Figure 2.7(b) if and only if

$$Q_{12} + Q_{13} + Q_{14} = Q_{21} + Q_{31} + Q_{41}, \tag{2.30}$$

$$Q_{21} + Q_{23} + Q_{24} = Q_{12} + Q_{32} + Q_{42}, \tag{2.31}$$

$$Q_{31} + Q_{32} + Q_{34} = Q_{13} + Q_{23} + Q_{43},$$

$$Q_{41} + Q_{42} + Q_{43} = Q_{14} + Q_{24} + Q_{34}.$$

Consider (2.30). The left-hand side satisfies the inequality

$$Q_{12} + Q_{13} + Q_{14} = (Q_{12} + Q_{13}) + (Q_{14} + Q_{13}) - Q_{13} = \frac{1}{3}J_1 + \frac{1}{2}J_1 - Q_{13} \leq \frac{5}{6}J_1.$$

By substituting the dynamical equivalence equation $J_4 = 2Q_{42} + 2Q_{41}$, we see that the right-hand side is

$$Q_{21} + Q_{31} + Q_{41} \geq Q_{41} = \frac{1}{2}J_4 - Q_{42} = \frac{1}{6}J_4 + \frac{1}{3}J_4 - Q_{42} = \frac{1}{6}J_4 + Q_{43} \geq \frac{1}{6}J_2.$$

Hence for the system in Figure 2.7(a) to be dynamically equivalent to a complex-balanced one, we have $J_2 \leq 5J_1$. Similarly, from (2.31), it can be shown that $J_1 \leq 5J_2$. Therefore, complex-balancing on a subnetwork of Figure 2.7(b) implies $\frac{1}{5} \leq \frac{J_1}{J_2} \leq 5$. Since $J_1 = J_3$ and $J_2 = J_4$ at steady state, i.e., $\kappa_1 = \kappa_3 x^3 y^2$ and $\kappa_2 x^3 = \kappa_4 y^2$ by definition, so

$$\frac{1}{25} \leq \frac{J_1 J_3}{J_2 J_4} = \frac{(\kappa_1)(\kappa_3 x^3 y^2)}{(\kappa_2 x^3)(\kappa_4 y^2)} \leq 25. \tag{2.32}$$

It follows that

$$\frac{1}{25} \leq \frac{\kappa_1 \kappa_3}{\kappa_2 \kappa_4} \leq 25$$

is a necessary condition for dynamical equivalence to complex-balancing.

Next we show that the inequality $\frac{1}{25} \leq \frac{\kappa_1\kappa_3}{\kappa_2\kappa_4} \leq 25$ is sufficient for the system in Figure 2.7(a) to be dynamically equivalent to a complex-balanced system on a subnetwork of Figure 2.7(b). We first deduce from (2.32) that a positive steady state exists, i.e., that there exist x^3 and $y^2 > 0$ such that $\kappa_1 = \kappa_3 x^3 y^2$ and $\kappa_2 x^3 = \kappa_4 y^2$. It is not difficult to see that

$$x^3 = \sqrt{\frac{\kappa_1\kappa_4}{\kappa_2\kappa_3}} \quad \text{and} \quad y^2 = \sqrt{\frac{\kappa_1\kappa_2}{\kappa_3\kappa_4}}$$

is a solution. Defining the fluxes to be $J_1 = \kappa_1$, $J_3 = \kappa_3 x^3 y^2$, $J_2 = \kappa_2 x^3$ and $J_4 = \kappa_4 y^2$, we obtain the inequality $\frac{1}{5} \leq \frac{J_1}{J_2} \leq 5$. Moreover, $J_1 = J_3$ and $J_2 = J_4$.

When $J_1 = 5J_2$, a solution $\boldsymbol{Q} \geq \boldsymbol{0}$ to the dynamical equivalence and complex-balanced conditions above is

$$\begin{aligned} Q_{14} &= Q_{32} = \frac{J_1}{6}, \qquad & Q_{13} &= Q_{31} = \frac{J_1}{3}, \\ Q_{41} &= Q_{23} = \frac{J_2}{2}, \qquad & Q_{21} &= Q_{43} = \frac{J_2}{3}, \end{aligned}$$

and the remaining $Q_{ij} = 0$. When $5J_1 = J_2$, a solution $\boldsymbol{Q} \geq \boldsymbol{0}$ to the dynamical equivalence and complex-balanced conditions above is

$$\begin{aligned} Q_{41} &= Q_{23} = \frac{J_2}{6}, \qquad & Q_{24} &= Q_{42} = \frac{J_2}{3}, \\ Q_{14} &= Q_{32} = \frac{J_1}{2}, \qquad & Q_{12} &= Q_{34} = \frac{J_1}{3}, \end{aligned}$$

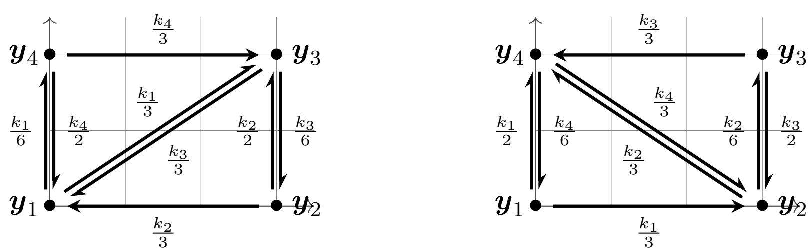
and the remaining $Q_{ij} = 0$. Whenever $\frac{1}{5} < \frac{J_1}{J_2} < 5$, the system is a convex combination of the two extremal cases, with a solution given by the appropriate convex combination of the two systems in Figure 2.8. Therefore, when $\frac{1}{5} \leq \frac{J_1}{J_2} \leq 5$, there exists $\boldsymbol{Q} \geq \boldsymbol{0}$ satisfying the dynamical equivalence and complex-balanced conditions.

The vector $\boldsymbol{Q}$, which depends on J_1, J_2 and hence a function of $\boldsymbol{x}$, can be used to generate rate constants for the new network. We first illustrate the process using the case $J_1 = 5J_2$, i.e., when $\kappa_2\kappa_4 = 25\kappa_1\kappa_3$, before we comment on the general case. Let $\kappa'_{ij} \geq 0$, the value to be determined, denote the rate constant of the reaction $\boldsymbol{y}_i \to \boldsymbol{y}_j$. Consider $Q_{21} = \frac{J_2}{3}$ and $Q_{23} = \frac{J_2}{6}$. By definition $J_2 = \kappa_2 x^3$ and $Q_{2j} = \kappa'_{2j} x^3$. Looking at the equation

$$\kappa'_{21} x^3 = Q_{21} = \frac{J_2}{3} = \frac{\kappa_2 x^3}{3},$$

it is clear we should choose $\kappa'_{21} = \frac{\kappa_2}{3}$. A similar argument forces $\kappa'_{23} = \frac{\kappa_2}{2}$. Noting that $J_3 = J_1$ and $J_4 = J_2$, we conclude $\kappa'_{32} = \frac{\kappa_3}{6}$, $\kappa'_{31} = \frac{\kappa_3}{3}$, $\kappa'_{41} = \frac{\kappa_4}{2}$, and $\kappa'_{43} = \frac{\kappa_4}{3}$. The mass-action system is shown in Figure 2.8(a).

In the general case $\frac{1}{25} \leq \frac{\kappa_1 \kappa_3}{\kappa_2 \kappa_4} \leq 25$, as noted earlier a solution $\boldsymbol{Q} \geq \boldsymbol{0}$ exists satisfying the dynamical equivalence and complex-balancing conditions. Such $\boldsymbol{Q}$ is a convex combination of the extremal cases; as a result, for any j, it is always the case that Q_{1j} and Q_{3j} are fractions of $J_1 = J_3$, and Q_{2j} and Q_{4j} are fractions of $J_2 = J_4$. Since Q_{ij} and J_i are both scalar multiples of $\boldsymbol{x}^{\boldsymbol{y}_i}$, the monomial gets cancelled from the equation and one can solve for κ'_{ij} as a fraction of κ_{ij}.



(a) (b)

Figure 2.8: The system in Figure 2.7(a) is dynamically equivalent to a complex-balanced system if and only if $\frac{1}{25} \leq \frac{\kappa_1 \kappa_3}{\kappa_2 \kappa_4} \leq 25$. The system is equivalent to (a) when $\kappa_2 \kappa_4 = 25 \kappa_1 \kappa_3$ and (b) when $25 \kappa_2 \kappa_4 = \kappa_1 \kappa_3$. For $\frac{1}{25} \leq \frac{\kappa_1 \kappa_3}{\kappa_2 \kappa_4} \leq 25$, the dynamically equivalent system is an appropriate convex combination of (a) and (b).

Remark 2.2.19. Example 2.2.18 has $(1,1)^\top$ and $(2,1)^\top$ as target vertices, with a distance of $d = 1$ between them. If we consider the two-target network with targets $(a_i, 1)$ distance $d > 0$ apart and has midpoint $(1.5, 1)^\top$, a similar analysis gives a necessary and sufficient condition for dynamical equivalence to complex-balancing:

$$\left(\frac{6-d}{d}\right)^2 \geq \frac{\kappa_1\kappa_3}{\kappa_2\kappa_4} \geq \left(\frac{d}{6-d}\right)^2.$$

As $d \to 0$, we recover a stable single-target system. As $d \to 3$, the condition becomes $\kappa_2\kappa_4 = \kappa_1\kappa_3$, which is necessary and sufficient for the system $\boldsymbol{y}_1 \rightleftharpoons \boldsymbol{y}_4$, $\boldsymbol{y}_2 \rightleftharpoons \boldsymbol{y}_3$ to be detailed-balanced [41].

Much work has been done to derive algebraic conditions on the rate constants that are necessary and sufficient for complex-balancing [19, 22, 35, 41]. In Examples 2.2.17 and 2.2.18 above, we are able to derive semi-algebraic conditions on the rate constants that are necessary and sufficient for dynamical equivalence to complex-balancing — at least for networks with special structure. To learn about stability properties of a mass-action system, dynamical equivalence to complex-balancing is extremely informative [110].

2.2.4 Conclusions

In this section, we introduced *single-target networks*, and classified the mass-action systems generated by them as either *(i) globally stable* (and actually dynamically equivalent to detailed balanced systems with a single connected component) or *(ii) having no positive steady states* (and moreover having all trajectories converge to the boundary of the positive orthant or to infinity). We showed that these two cases can be differentiated by a very simple geometric criterion: a single-target mass-action system is globally stable if and only if the target vertex is in the relative interior of the network's Newton polytope.

In general, the single-target condition is quite restrictive, and few networks of interest will satisfy it at the outset. On the other hand, it is a very simple geometric condition, which makes is easy to characterize the set in parameter space where networks that fail to be single-target give rise to systems that *can be realized by* single-target networks via dynamical equivalence. Using this idea, we have exhibited several examples where our results can be useful for analyzing networks that exhibit a high degree of symmetry or geometric structure, even if they are *not* single-target networks.

Finally, recognizing that single-target networks are related to (strongly) endotactic networks, we explored some networks with similar geometry but having multiple targets. For these examples we showed that the corresponding mass-action systems are dynamically equivalent to complex-balanced systems if and only if the rate constants satisfy some semi-algebraic conditions. While our examples have relatively simple structures that allow us to derive explicit inequalities on the rate constants, a natural question and future research direction is whether such semi-algebraic conditions on the rate constants can be obtained for more general classes of reaction networks.

Chapter 3

Reaction-diffusion systems

In this chapter, we study the long time behaviour for some chemical reaction-diffusion systems. In Section 3.1, we first analyze a three-species system with boundary equilibria in some stoichiometric classes, and whose right hand side is bounded above by a quadratic nonlinearity in the positive orthant. We prove similar results on a fairly general two-species reversible reaction-diffusion network as well. In Section 3.2, we work on on the similar systems but focus on local instability on the boundary equilibria.

3.1 Convergence to the complex balanced equilibrium for some chemical reaction-diffusion systems

3.1.1 Two reversible reaction-diffusion systems

3.1.1.1 The three-species system.

A case not covered so far in the literature is $A + 2B \rightleftharpoons B + C$; this has accessible boundary equilibria in some (not all) stoichiometric classes, translates to a 3×3 system (2×2 being, in general, easier to treat via the standard maximum principle for the heat equation), and the right hand side is not bounded above (in the positive orthant) by a linear term. More precisely, the PDE system we are looking at is

$$\begin{cases} a_t - d_a\Delta a = -k_1ab^2 + k_2bc & \\ b_t - d_b\Delta b = -k_1ab^2 + k_2bc & \text{in } \Omega\times(0,\infty) \\ c_t - d_c\Delta c = k_1ab^2 - k_2bc & \\ \nabla a\cdot\nu = \nabla b\cdot\nu = \nabla c\cdot\nu = 0 & \text{on } \partial\Omega\times(0,\infty) \\ a(\cdot,0)=a_0,\ b(\cdot,0)=b_0,\ c(\cdot,0)=c_0 & \text{in } \Omega, \end{cases} \tag{3.1}$$

where ν is the (outward) normal vector to $\partial\Omega$. We can, without loss of generality, assume that $k_1 = k_2 = 1$. Indeed, note that upon changing to $\widetilde{a}(x,t) = \alpha a(x,\tau t)$, $\widetilde{b}(x,t) = \alpha b(x,\tau t)$, $\widetilde{c}(x,t) = \alpha c(x,\tau t)$ for $\alpha = k_1k_2^{-1}$ and $\tau = k_1k_2^{-2}$ we end up with (3.1) satisfied by $\widetilde{a}$, $\widetilde{b}$, $\widetilde{c}$ with $k_1 = k_2 = 1$, $d_{\widetilde{a}} = \tau d_a$, $d_{\widetilde{b}} = \tau d_b$, $d_{\widetilde{c}} = \tau d_c$ and initial conditions αa_0, αb_0, αc_0. After an affine spatial transformation we can (and do) also assume the volume of Ω to be 1. The only important restriction we impose is the choice of spatial dimension $d = 1$; let us also fix $\Omega := (0,1)$ (could be any bounded interval). The restriction $d = 1$ is sufficient to obtain the uniform L^∞ bound on the solution, which is crucial to our analysis. We can (for the time being) only justify this uniform bound in the $d = 1$ case; note that only the estimates in subsection 3.1.2.1 are predicated on this restriction. The conserved (in time) quantities here are $\bar{a}+\bar{c}$ and $\bar{b}+\bar{c}$, where $\bar{f}$ denotes the average of the function f over Ω. If $b_\infty > 0$ we obviously can only have a boundary equilibrium at $(0, b_\infty, 0)$ (i.e. $a_\infty = c_\infty = 0$). The conservation of $\bar{a}+\bar{c}$ forces $a \equiv c \equiv 0$, the second equation of the system decouples into $b_t - d_b b_{xx} = 0$, and $b_\infty = \bar{b}_0$. This steady state cannot be approached from any initial state for which $\bar{a}_0 + \bar{c}_0 > 0$, so $(0, b_\infty, 0)$ is not an accessible boundary equilibrium. The other nontrivial type of steady states is given by $b_\infty = 0$ and $a_\infty + c_\infty = \bar{a}_0 + \bar{c}_0 > 0$. If $c_\infty = 0$, we get $b \equiv c \equiv 0$ (from the conservation of $\bar{b}+\bar{c}$); this is not an accessible boundary equilibrium either, and no initial data in the positive orthant will yield solutions which asymptotically converge to it. If, on the other hand, the initial data is on the b-axis (i.e. $a_0 \equiv c_0 \equiv 0$), then it is easy to see that (a, b, c) will converge exponentially to $(0, b_\infty, 0)$, where $b_\infty = \bar{b}_0$.

We are left with the accessible boundary equilibrium $(a_\infty, 0, c_\infty)$ for $a_\infty c_\infty > 0$. We do not know how to prove that $\bar{a}_0\bar{b}_0\bar{c}_0 > 0$ prevents convergence to such a steady state, but in this paper we will prove a slightly weaker statement, namely:

Theorem 3.1.1. *If $a_0,\ b_0, c_0 \in L^\infty(0,1)$ are a.e. positive and such that $b_0 \geq \delta$ a.e. in $(0,1)$ for some $\delta > 0$, then the (unique) global classical solution to (3.1) converges asymptotically exponentially fast (at an explicit rate) to the unique positive equilibrium in its stoichiometric class.*

The above theorem will be proved in Section 3.1.2.

3.1.1.2 The two-species system

Finally, in Section 3.1.3 we prove similar results on the convergence to the positive equilibrium for a two-species reversible reaction-diffusion network with accessible boundary equilibria:

$$m_1A + n_1B \rightleftharpoons m_2A + n_2B.$$

Assume $m_1,\ m_2,\ n_1,\ n_2$ are nonnegative integers and let $\bar{m} := m_1 - m_2$, $\bar{n} := n_2 - n_1$. The 2×2 reaction-diffusion system is

$$\begin{cases} a_t - d_a\Delta a = \bar{m}(k_2a^{m_2}b^{n_2} - k_1a^{m_1}b^{n_1}) & \text{in } \Omega \times (0,\infty) \\ b_t - d_b\Delta b = \bar{n}(k_1a^{m_1}b^{n_1} - k_2a^{m_2}b^{n_2}) & \text{in } \Omega \times (0,\infty) \\ \nabla a \cdot \nu = \nabla b \cdot \nu = 0 & \text{on } \partial\Omega \times (0,\infty) \\ a(\cdot,0) = a_0,\ b(\cdot,0) = b_0 & \text{in } \Omega. \end{cases} \tag{3.2}$$

If $\bar{m} \neq \bar{n}$ we can, as in the three species system, change to $\widetilde{a}(x,t) = \lambda a(x,\tau t)$, $\widetilde{b}(x,t) = \lambda b(x,\tau t)$ for $\lambda = (k_1/k_2)^{1/(\bar{m}-\bar{n})}$ and $\tau = k_1\lambda^{m_1+n_1-1}$. We end up with (3.2) satisfied by $\widetilde{a}$, $\widetilde{b}$ with $k_1 = k_2 = 1$ (d_a and d_b get multiplied by positive constants). If $\bar{m} = \bar{n} = 0$ no rescaling is necessary, while for $\bar{m} = \bar{n} \neq 0$ we only rescale $\widetilde{a}(x,t) = \lambda a(x,t)$ with $\lambda = (k_1/k_2)^{1/\bar{m}}$ to get the system (3.2) with $k_1 = k_2 = 1$, but where $\bar{m}$ and $\bar{n}$ are multiplied by two positive constants.

Thus, it is enough to study the more general (than mass-action) system

$$\begin{cases} a_t - d_a\Delta a = \lambda_a \bar{m}(a^{m_2}b^{n_2} - a^{m_1}b^{n_1}) & \text{in } \Omega\times(0,\infty) \\ b_t - d_b\Delta b = \lambda_b \bar{n}(a^{m_1}b^{n_1} - a^{m_2}b^{n_2}) & \text{in } \Omega\times(0,\infty) \\ \nabla a\cdot\nu = \nabla b\cdot\nu = 0 & \text{on } \partial\Omega\times(0,\infty) \\ a(\cdot,0) = a_0,\ b(\cdot,0) = b_0 & \text{in } \Omega, \end{cases} \tag{3.3}$$

where $\lambda_a,\ \lambda_b$ are positive constants.

Theorem 3.1.2. *Let Ω be a bounded domain of $\mathbb{R}^d$ with a smooth boundary, for some integer $d \geq 1$. If $\bar{m}\bar{n} \geq 0$ and $0 < \alpha \leq a_0(x), b_0(x) \leq \beta < +\infty$ for a.e. x in Ω, then the (unique) global classical solution to* (3.3) *converges asymptotically exponentially (at an explicit rate) to the unique positive equilibrium in its stoichiometric class.*

Remarks: (1) The reason for the restriction $\bar{m}\bar{n} \geq 0$ is technical, as the estimates that follow after the conservation law (3.39) in subsection 3.2 only hold under this restriction.

(2) If initial data is on the b-axis (or, respectively, the a-axis), then the solution (a, b) will converge exponentially to $(0, b_\infty)$ (or, respectively, to $(a_\infty, 0)$). These are the only two types of boundary equilibria in this case, and are both accessible. Theorem 3.1.2 shows that if the initial condition is bounded away from zero and infinity componentwise, then the solution will not decay to any such boundary equilibrium.

3.1.2 Asymptotic decay for the three-species system

We consider the entropy functional $E(a, b, c)$ and the corresponding entropy dissipation (when computed along solutions) $D(a, b, c) = -\frac{d}{dt}E(a, b, c)$ associated to the system:

$$E(a,b,c) = \int_0^1 a(\ln a - 1)dx + \int_0^1 b(\ln b - 1)dx + \int_0^1 c(\ln c - 1)dx \tag{3.4}$$

and

$$D(a,b,c) = 4d_a \int_0^1 |\partial_x \sqrt{a}|^2 dx + 4d_b \int_0^1 |\partial_x \sqrt{b}|^2 dx + 4d_c \int_0^1 |\partial_x \sqrt{c}|^2 dx \\ + \int_0^1 (ab^2 - bc) \ln(\frac{ab^2}{bc}) dx. \tag{3.5}$$

We would also like to record (for later use) the following *conservation laws*

$$\int_0^1 a(x,t)dx + \int_0^1 c(x,t)dx = \int_0^1 a_0(x)dx + \int_0^1 c_0(x)dx =: M_1, \\ \int_0^1 b(x,t)dx + \int_0^1 c(x,t)dx = \int_0^1 b_0(x)dx + \int_0^1 c_0(x)dx =: M_2, \tag{3.6}$$

for all $t \geq 0$. Note that these are simply obtained by adding equations 1 and 3 (respectively, 2 and 3) and integrating in space over $[0,1]$ by taking into account the boundary conditions. Note also that M_1 and M_2 are finite as long as $a_0, b_0, c_0 \in L^1(0,1)$.

3.1.2.1 Local L^2 estimate (a priori estimate)

Proposition 3.1.3. *Let (a,b,c) be a solution for (3.1) with initial condition (a_0,b_0,c_0) such that $a_0 > 0,\ b_0 > 0,\ c_0 > 0$ a.e. in $[0,1]$ and $a_0 \ln a_0, b_0 \ln b_0, c_0 \ln c_0 \in L^1(0,1)$. Then there exists a real constant C such that*

$$\|a\|_{L^2([0,1]\times[\tau,\tau+1])},\ \|b\|_{L^2([0,1]\times[\tau,\tau+1])},\ \|c\|_{L^2([0,1]\times[\tau,\tau+1])} \leq C$$

for any $\tau > 0$.

Proof. We start with the obvious inequality (which holds for all $x \in [0,1],\ t > 0$)

$$\left| \sqrt{a(x,t)} - \int_0^1 \sqrt{a(y,t)} dy \right| \leq \int_0^1 \left| \partial_y \sqrt{a(y,t)} \right| dy,$$

then use Hölder's inequality to get

$$\begin{aligned} a(x,t) &\leq \left(\int_0^1 \sqrt{a(y,t)}dy + \int_0^1 \left|\partial_y \sqrt{a(y,t)}\right|dy\right)^2 \\ &\leq 2\left(\int_0^1 \sqrt{a(y,t)}dy\right)^2 + 2\left(\int_0^1 \left|\partial_y \sqrt{a(y,t)}\right|dy\right)^2 \\ &\leq 2\int_0^1 a(y,t)dy + 2\int_0^1 \left|\partial_y \sqrt{a(y,t)}\right|^2 dy. \end{aligned} \tag{3.7}$$

Obviously, the above inequalities also hold for b and c. Next we integrate the entropy dissipation in time to obtain

$$E(a(t), b(t), c(t)) + \int_0^t D(a(s), b(s), c(s))ds = E(a_0, b_0, c_0),$$

where we have only displayed the dependence on time of the components of the solution vector. Since the last integrand in right hand side of (3.5) is nonnegative, we conclude

$$\begin{aligned} &E(a(t), b(t), c(t)) + 4d_a \int_0^t \int_0^1 |\partial_x \sqrt{a}|^2 dxdt + 4d_b \int_0^t \int_0^1 |\partial_x \sqrt{b}|^2 dxdt + \\ &4d_c \int_0^t \int_0^1 |\partial_x \sqrt{c}|^2 dxdt \leq E(a_0, b_0, c_0). \end{aligned} \tag{3.8}$$

Since $x(\ln x - 1) \geq -1$ for all $x \geq 0$ (at $x = 0$ this holds in the limiting sense), we get

$$\begin{aligned} &4d_a \int_0^t \int_0^1 |\partial_x \sqrt{a}|^2 dxdt + 4d_b \int_0^t \int_0^1 |\partial_x \sqrt{b}|^2 dxdt + 4d_c \int_0^t \int_0^1 |\partial_x \sqrt{c}|^2 dxdt \\ &\leq E(a_0, b_0, c_0) + 3, \end{aligned}$$

which implies

$$\begin{aligned}&\|\partial_x\sqrt{a}\|^2_{L^2([0,1]\times[0,t])}+\|\partial_x\sqrt{b}\|^2_{L^2([0,1]\times[0,t])}+\|\partial_x\sqrt{c}\|^2_{L^2([0,1]\times[0,t])}\\&\le\frac{E(a_0,b_0,c_0)+3}{4d}:=C_1\end{aligned}$$

for any $t\ge 0$, where $d:=\min\{d_a,d_b,d_c\}$. Finally, we take into account (3.6) and (3.7) to estimate

$$\begin{aligned}&\int_\tau^{\tau+1}\int_0^1 a^2dxdt\le\int_\tau^{\tau+1}\|a(t)\|_{L^\infty[0,1]}\left(\int_0^1 a(x,t)dx\right)dt\\&\le 2M_1\int_\tau^{\tau+1}\left(\int_0^1 a(x,t)dx+\int_0^1|\partial_x\sqrt{a(x,t)}|^2dx\right)dt\\&\le 2M_1\int_\tau^{\tau+1}\left(M_1+\int_0^1|\partial_x\sqrt{a(x,t)}|^2dx\right)dt\le 2{M_1}^2+2M_1C_1=:C\end{aligned}$$

Similar inequalities hold for b and c, therefore we have finished the proof. □

3.1.2.2 Uniform L^∞ estimate

In this section we shall prove that a classical solution to (3.1) is bounded uniformly in time (and therefore, it also exists for all time). To achieve this, our goal is to place ourselves in the setting of Theorem 4.1 [45]. We shall refrain from transcribing the assumptions (H1)–(H3) from [45] here, as they are universally satisfied by CRDN systems with nonnegative and essentially bounded initial conditions. On the other hand, assumption (H4') is both specific to our case and nontrivial to verify. We state it below, as it refers to a general semilinear parabolic $m\times m$ system

$$u_{i,t}-\kappa_i\Delta u_i=f_i(x,t,u),\ i=1,...,m, \tag{3.9}$$

where $x\in\Omega$, $t>0$, $u=(u_1,...,u_m)$. It reads:

There exist $K_1,\ K_2>0,\ 1\le p<\infty,\ 1\le r<1+\left[1-\frac{d}{p(d+2)}\right]\frac{2p}{d+2}$ such that

for each $1\le j\le m$ there exist $\alpha_{j,k},\ 1\le j\le k$ with $\alpha_{j,j}=1$ such that (3.10)

$$\sum_{k=1}^{j} \alpha_{j,k} f_j(x,t,v) \leq K_1|v|^r + K_2 \text{ for all } v \text{ in the positive orthant of } \mathbb{R}^m.$$

The following result is a version of Theorem 4.1 [45] (see a sketch of proof in Appendix).

Theorem 3.1.4. *Suppose the initial data $u_{j,0} \in L^\infty(\Omega)$, $j = 1, ..., m$, the generic assumptions (H1)–(H3) from* [45] *hold. Further assume* (3.10) *holds for some* $1 \leq p < \infty$ *and*

$$\|u\|_{L^p(\Omega\times(\tau,\tau+1);\mathbb{R}^m)} \leq M < \infty \text{ for all } \tau \geq 0. \tag{3.11}$$

Then

$$u \in L^\infty(\Omega \times [0,\infty); \mathbb{R}^m). \tag{3.12}$$

If we go back to (3.1) and denote by

$$u := (a,b,c),\ \ f := (-ab^2 + bc, -ab^2 + bc, ab^2 - bc)$$

we see that (3.10) is satisfied with $\alpha_{1,1} = 1, \alpha_{2,1} = -1,\ \alpha_{2,2} = 1,\ \alpha_{3,1} = 0,\ \alpha_{3,2} = -1,\ \alpha_{3,3} = 1$, $r = 2,\ K_1 = k_2/2,\ K_2 = 0$. Thus, if we can find $1 \leq p < \infty$ such that (3.11) and the first inequality in (3.10) (the one bounding r in terms of p) are satisfied, we can apply Theorem 3.1.4 in order to obtain the uniform L^∞ bound. But Proposition 3.1.3 shows that $p = 2$ does the job.

The same reference [45], Theorem 3.1 (checked, along with the preceding Lemma 3.1, to apply to bounded domains and Neumann BC) guarantees that the solution is classical, unique and nonnegative. Therefore, we have proved:

Theorem 3.1.5. *Let $a_0,\ b_0,\ c_0 \in L^\infty(0,1)$ such that $a_0 > 0,\ b_0 > 0,\ c_0 > 0$ a.e. in $(0,1)$ and $a_0 \ln a_0, b_0 \ln b_0, c_0 \ln c_0 \in L^1(0,1)$. Then a unique classical solution to the system* (3.1) *exists for all time. Furthermore, the solution is uniformly (with respect to time) bounded in $L^\infty(0,1)$, with bounds depending in a bounded way on the L^∞ norms of the initial data.*

Remark 3.1.6. If we approximate the initial data in $L^2(0,1)$ by BC compatible initial $a_{0,n},\ b_{0,n},\ c_{0,n}$ which are uniformly bounded in $L^\infty(0,1)$ by, say, $\eta := 2[\|a_0\|_\infty + \|b_0\|_\infty + \|c_0\|_\infty]$, then we can easily get the bound

$$\begin{aligned}&\|a_n(\cdot,t)-a(\cdot,t)\|_2^2+\|b_n(\cdot,t)-b(\cdot,t)\|_2^2+\|c_n(\cdot,t)-c(\cdot,t)\|_2^2\\&\le e^{Ct}\left[\|a_{0,n}-a_0\|_2^2+\|b_{0,n}-b_0\|_2^2+\|c_{0,n}-c_0\|_2^2\right]\end{aligned}$$

for all $t \geq 0$, where $C = C(\eta) > 0$ is a finite constant. It follows that for any $t \geq 0$, $a_n(t,\cdot)$ converges in $L^2(0,1)$ to $a(t,\cdot)$ (and likewise for b and c). Furthermore, note that if b_0 is bounded below by $2\delta > 0$, then the approximations $b_{0,n}$ above may also be chosen to satisfy the extra condition $b_{0,n} \geq \delta$ for all n. Via L^1 renormalization the approximations may also be chosen such that the approximating problem has the same complex-balanced equilibrium as the original one.

In the next subsection we use the Log-Sobolev and the Csizar-Kullback-Pinsker inequalities to first prove an entropy-entropy dissipation inequality which guarantees that the solution to (3.1) decays asymptotically to the complex balanced equilibrium at an explicit algebraic rate.

3.1.2.3 L^1 convergence

In view of Remark 3.1.6 we may assume $a_0,\ b_0,\ c_0$ to be smooth, positive on $[0,1]$ and to satisfy the compatibility conditions (i.e. they have zero derivatives at the boundary). Indeed, if we replace the initial data with approximations as in Remark 3.1.6, then all the decay constants appearing below may be chosen independent of n. Further assume $\beta = \|\frac{1}{b_0}\|_{L^\infty[0,1]} < \infty$; because the classical solution is continuous on the cylinder $[0,\infty) \times [0,1]$, there exists $t_1 > 0$ such that $\|\frac{1}{b(\cdot,t)}\|_{L^\infty[0,1]} < 10\beta$ for all $t \in [0,t_1]$. We next divide the second equation in (3.1) by $-b^2$ and use the uniform (in time) L^∞ boundedness of a to get

$$\partial_t\left(\frac{1}{b}\right) - d_b\Delta\left(\frac{1}{b}\right) = \frac{ab^2}{b^2} - \frac{bc}{b^2} - 2d_b\frac{|\nabla b|^2}{b^3} \leq a \leq k.$$

Using the maximum principle for the heat equation, we have that, for all $t \in [0, t_1]$,

$$\left\|\frac{1}{b(\cdot,t)}\right\|_{L^\infty[0,1]} \leq \left\|\frac{1}{b_0}\right\|_{L^\infty[0,1]} + kt = \beta + kt.$$

We can iterate this inequality in time to get

$$\widetilde{b}(t) := \inf_{x\in[0,1]} b(x,t) \geq (\beta + kt)^{-1} \tag{3.13}$$

for all $t > 0$. Therefore, we now have an estimate on how fast b can decay to zero.

There exists a unique equilibrium with all positive components for (3.1) and by (3.1) and (3.6) we see that it is given by $v_\infty := (a_\infty, b_\infty, c_\infty)$, where its components are uniquely determined by

$$a_\infty b_\infty = c_\infty,\ a_\infty + c_\infty = M_1,\ b_\infty + c_\infty = M_2. \tag{3.14}$$

Now we introduce the *relative entropy*

$$\begin{aligned} E(a,b,c|a_\infty,b_\infty,c_\infty) &= \int\limits_{[0,1]} \left(a \ln\frac{a}{a_\infty} - a + a_\infty\right)dx + \int\limits_{[0,1]} \left(b\ln\frac{b}{b_\infty} - b + b_\infty\right)dx \\ &+ \int\limits_{[0,1]} \left(c\ln\frac{c}{c_\infty} - c + c_\infty\right)dx \end{aligned} \tag{3.15}$$

and its corresponding *entropy dissipation*

$$\begin{aligned} D(a,b,c|a_\infty,b_\infty,c_\infty) &= d_a \int\limits_{[0,1]} \frac{|\nabla a|^2}{a}dx + d_b \int\limits_{[0,1]} \frac{|\nabla b|^2}{b}dx + d_c \int\limits_{[0,1]} \frac{|\nabla c|^2}{c}dx \\ &+ a_\infty b_\infty^2 \int\limits_{[0,1]} \Psi\left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty}\right)dx + b_\infty c_\infty \int\limits_{[0,1]} \Psi\left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2}\right)dx, \end{aligned} \tag{3.16}$$

where

$$\Psi(x;y) = x\ln\left(\frac{x}{y}\right) - x + y. \tag{3.17}$$

At this point we introduce the notation

$$\bar{f} := \int\limits_{[0,1]} f(x)dx \text{ for all essentially non-negative } f \in L^1(0,1).$$

On the basis of the following identity

$$\int\limits_{[0,1]} \left(a \ln \frac{a}{a_\infty} - a + a_\infty\right)dx = \int\limits_{[0,1]} \left(a \ln \frac{a}{\overline{a}} - a + \overline{a}\right)dx + \int\limits_{[0,1]} \left(\overline{a} \ln \frac{\overline{a}}{a_\infty} - \overline{a} + a_\infty\right)dx,$$

we get

$$E(a, b, c|a_\infty, b_\infty, c_\infty) = E(a, b, c|\overline{a}, \overline{b}, \overline{c}) + E(\overline{a}, \overline{b}, \overline{c}|a_\infty, b_\infty, c_\infty). \tag{3.18}$$

The Logarithmic Sobolev Inequality

$$\int\limits_{[0,1]} \frac{|\nabla f|^2}{f}dx \geq C_{LSI} \int\limits_{[0,1]} f \ln \frac{f}{\overline{f}}dx, \tag{3.19}$$

(where C_{LSI} only depends on the domain $[0, 1]$) yields

$$d_a \int\limits_{[0,1]} \frac{|\nabla a|^2}{a}dx + d_b \int\limits_{[0,1]} \frac{|\nabla b|^2}{b}dx + d_c \int\limits_{[0,1]} \frac{|\nabla c|^2}{c}dx \geq C_2 E(a, b, c|\overline{a}, \overline{b}, \overline{c}) \tag{3.20}$$

for an explicit constant $C_2 = \min\{d_a, d_b, d_c\} \cdot C_{LSI}$. Next, we define two integrand functions:

$$S_1(a, b, c) := \left(a \ln \frac{a}{a_\infty} - a + a_\infty\right) + \left(b \ln \frac{b}{b_\infty} - b + b_\infty\right) + \left(c \ln \frac{c}{c_\infty} - c + c_\infty\right),$$

$$S_2(a, b, c) := \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{c_\infty}\right) + \Psi\left(\frac{c}{c_\infty}; \frac{ab}{a_\infty b_\infty}\right)$$

and set $S(a,b,c) := S_1(a,b,c) + S_2(a,b,c)$. From (3.16), (3.18), (3.20) and (3.13) we get

$$
\begin{aligned}
&D(a,b,c|a_\infty,b_\infty,c_\infty) \geq C_2 E(a,b,c|\overline{a},\overline{b},\overline{c})\\
&+ a_\infty b_\infty^2 \int\limits_{[0,1]} \Psi\left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty}\right)dx + b_\infty c_\infty \int\limits_{[0,1]} \Psi\left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2}\right)dx\\
&\geq C_2\big[E(a,b,c|a_\infty,b_\infty,c_\infty) - E(\overline{a},\overline{b},\overline{c}|a_\infty,b_\infty,c_\infty)\big]\\
&+ a_\infty b_\infty \widetilde{b}(t) \int\limits_{[0,1]} \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{c_\infty}\right)dx + c_\infty \widetilde{b}(t) \int\limits_{[0,1]} \Psi\left(\frac{c}{c_\infty}; \frac{ab}{a_\infty b_\infty}\right)dx\\
&\geq C_2 \int\limits_{[0,1]} S_1(a,b,c)dx - C_2 \int\limits_{[0,1]} S_1(\overline{a},\overline{b},\overline{c})dx\\
&+ (\beta+kt)^{-1}\left[a_\infty b_\infty \int\limits_{[0,1]} \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{c_\infty}\right)dx + c_\infty \int\limits_{[0,1]} \Psi\left(\frac{c}{c_\infty}; \frac{ab}{a_\infty b_\infty}\right)dx\right]\\
&\geq C_3(t)\left\{\int\limits_{[0,1]} \big[S_1(a,b,c) + S_2(a,b,c)\big]dx - S_1(\overline{a},\overline{b},\overline{c})\right\}\\
&\geq C_3(t)\big[\widehat{S}(\overline{a},\overline{b},\overline{c}) - S_1(\overline{a},\overline{b},\overline{c})\big],
\end{aligned}
\tag{3.21}
$$

where

$$C_3(t) := (\beta+kt)^{-1}\min\{\beta C_2, a_\infty b_\infty, c_\infty\}$$

and $\widehat{S}$ is the *convexification* of S, i.e. the supremum of all affine functions below S. The last inequality above holds due to Jensen's inequality and the unit volume of the spatial domain.

We next define the compatible class:

$$
\begin{aligned}
C_{M_1,M_2} := \big\{&v = (x,y,z) \in \mathbb{R}^3_{\geq 0} : x+z = M_1,\ y+z = M_2,\\
&E(x,y,z|a_\infty,b_\infty,c_\infty) \leq E(a_0,b_0,c_0|a_\infty,b_\infty,c_\infty)\big\}.
\end{aligned}
$$

In this class, the first two conditions are related to the conservation laws (3.6) while the last one follows from the decreasing relative entropy. Since we know $\widehat{S} = \widehat{S_1 + S_2} \geq \widehat{S_1} + \widehat{S_2}$, S_1 is convex and S_2 is non-negative, we have

$$(\widehat{S} - S_1)(v) \geq (\widehat{S_1} + \widehat{S_2} - S_1)(v) \geq \widehat{S_2}(v) \geq 0. \tag{3.22}$$

Furthermore, it is not hard to verify that

$$v \in C_{M_1,M_2} \;\;\&\;\; S_2(v) = 0 \text{ if and only if } v = (a_\infty, b_\infty, c_\infty). \tag{3.23}$$

It follows

$$\widehat{S_2}(v) = 0 \text{ if and only if } v = (a_\infty, b_\infty, c_\infty).$$

Let

$$C_4 := \inf_{v \in C_{M_1,M_2}} \frac{(\widehat{S} - S_1)(v)}{E(v|a_\infty, b_\infty, c_\infty)}.$$

By (3.22) and (3.23) we get C_4 can only be zero if there exists a sequence $\{v_n\}_n \subset C_{M_1,M_2}$ such that $v_n \to (a_\infty, b_\infty, c_\infty)$ as $n \to \infty$. This means

$$\liminf_{v \in C_{M_1,M_2}, v \to v_\infty} \frac{(\widehat{S} - S_1)(v)}{E(v|a_\infty, b_\infty, c_\infty)} > 0 \;\text{ implies } C_4 > 0.$$

In order to show that the above limit inferior is positive we use the following lemma [75]:

Lemma 3.1.7. *There exists $\delta > 0$ such that for all $v \in B(v_\infty, \delta)$ (ball centered at v_∞ and of radius delta) $S(v)$ is locally convex in this ball.*

In particular, we get that $\widehat{S} \equiv S$ in the ball centered at $(a_\infty, b_\infty, c_\infty)$ with radius δ. Let us now define

$$D_2(v) := a_\infty b_\infty^2 \Psi\left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty}\right) + b_\infty c_\infty \Psi\left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2}\right)$$

and consider the Taylor expansion of

$$\frac{D_2(v)}{E(v|a_\infty, b_\infty, c_\infty)}$$

around the unique positive equilibrium $(a_\infty, b_\infty, c_\infty)$.

Since $a_\infty b_\infty = c_\infty$, we have $D_2(a_\infty, b_\infty, c_\infty) = \nabla D_2(a_\infty, b_\infty, c_\infty) = 0$ and quadratic term in the expansion is

$$D_2(v) = 2\left[\frac{-(v_1 - a_\infty)}{a_\infty} + \frac{-(v_2 - b_\infty)}{b_\infty} + \frac{(v_3 - c_\infty)}{c_\infty}\right]^2.$$

Thus,

$$\liminf_{v \in C_{M_1,M_2}, v \to v_\infty} \frac{D_2(v)}{E(v|a_\infty, b_\infty, c_\infty)} = \inf_{v \in C_{M_1,M_2}} \frac{2\left[\frac{-(x-a_\infty)}{a_\infty} + \frac{-(y-b_\infty)}{b_\infty} + \frac{(z-c_\infty)}{c_\infty}\right]^2}{\frac{(x-a_\infty)^2}{a_\infty} + \frac{(y-b_\infty)^2}{b_\infty} + \frac{(z-c_\infty)^2}{c_\infty}}$$

Since $v \in C_{M_1,M_2}$ (which means $x + z = a_\infty + c_\infty, y + z = b_\infty + c_\infty$), we get

$$-(x - a_\infty) = -(y - b_\infty) = z - c_\infty,$$

Then

$$\inf_{v \in C_{M_1,M_2}} \frac{2\left[\frac{-(x-a_\infty)}{a_\infty} + \frac{-(y-b_\infty)}{b_\infty} + \frac{(z-c_\infty)}{c_\infty}\right]^2}{\frac{(x-a_\infty)^2}{a_\infty} + \frac{(y-b_\infty)^2}{b_\infty} + \frac{(z-c_\infty)^2}{c_\infty}} = 2\left(\frac{1}{a_\infty} + \frac{1}{b_\infty} + \frac{1}{c_\infty}\right) > 0.$$

Also notice (by direct computation and using that $c_\infty = a_\infty b_\infty$) the identity $D_2(v) = bc_\infty S_2(v)$, which implies (in view of the above inequality)

$$\liminf_{v \in C_{M_1,M_2}, v \to v_\infty} \frac{S_2(v)}{E(v|a_\infty, b_\infty, c_\infty)} > 0.$$

Combining the above two steps, we have

$$\liminf_{v\in C_{M_1,M_2}, v\to v_\infty} \frac{(\widehat{S}-S_1)(v)}{E(v|a_\infty,b_\infty,c_\infty)}$$
$$= \liminf_{v\in C_{M_1,M_2}, v\to v_\infty} \frac{S_2(v)}{E(v|a_\infty,b_\infty,c_\infty)} > 0.$$

Therefore, in light of (3.21), we obtain

$$D(a,b,c|a_\infty,b_\infty,c_\infty) \geq C_3(t)C_4E(a,b,c|a_\infty,b_\infty,c_\infty)$$

so,

$$D(a,b,c|a_\infty,b_\infty,c_\infty) \geq C_5(\beta+kt)^{-1}E(a,b,c|a_\infty,b_\infty,c_\infty),$$

where $C_5 = \min\{1, C_4\} \times \min\{\beta C_2, a_\infty b_\infty^2, b_\infty c_\infty\}$. Then Gronwall's lemma yields

$$E(a,b,c|a_\infty,b_\infty,c_\infty) \leq E(a_0,b_0,c_0|a_\infty,b_\infty,c_\infty)(\beta+kt)^{\frac{-C_5}{k}}$$

for all $t > 0$.

Now we need the following lemma [9]:

Lemma 3.1.8. *For all non-negative and measurable functions $a, b, c : [0,1] \to \mathbb{R}$ and $\int_0^1(a+c) = M_1$, $\int_0^1(b+c) = M_2$. Then there exists a constant $C_K > 0$ depending boundedly only on M_1, M_2 such that:*

$$E(a,b,c|a_\infty,b_\infty,c_\infty) \geq C_K(\|a-a_\infty\|_1^2 + \|b-b_\infty\|_1^2 + \|c-c_\infty\|_1^2)$$

Therefore, we get

$$\|a(\cdot,t)-a_\infty\|_1^2 + \|b(\cdot,t)-b_\infty\|_1^2 + \|c(\cdot,t)-c_\infty\|_1^2 \leq C_6(\beta+kt)^{\frac{-C_5}{k}} \text{ for all } t \geq 0,$$

where $C_6 = \frac{E(a_0,b_0,c_0|a_\infty,b_\infty,c_\infty)}{C_K}$.

The above inequality shows that the solution stays away from the boundary equilibrium; in fact, its converges to the unique positive equilibrium in the L^1 norm. In order to show that the convergence rate is, in fact, exponential, we use the above inequality to conclude that there exists a time

$$T_\varepsilon := \max\left\{1, \frac{1}{k}\left(\frac{2}{\min\{a_\infty, b_\infty, c_\infty\}}\right)^{2k/C_5} - \frac{\beta}{k}\right\}$$

such that

$$|a(t)\|_1, \|b(t)\|_1, \|c(t)\|_1 > \varepsilon^2 := \min\{a_\infty, b_\infty, c_\infty\}/2 > 0 \text{ for all } t > T_\varepsilon. \tag{3.24}$$

We pause here briefly to comment on the fact that T_ε can also be taken independent of n if the initial data is as in Theorem 3.1.5 and is approximated as indicated in Remark 3.1.6. Thus, in view of Remark 3.1.6, we drop here the extra assumptions we made on the initial data in the beginning of this subsection.

3.1.2.4 Entropy entropy-dissipation estimate

In what follows we use the lower bound on the total mass of each species for $t \geq T_\varepsilon$ to improve the algebraic rate to an explicit exponential decay rate. The Poincaré inequality for the square roots of the densities minus their averages, along with a few important algebraic inequalities proved in the Appendix and (3.24) help us obtain an EEDI of the type $D(t) \geq cE(t)$, where c is a positive real number (independent of time). Most of the algebraic intricacies involved are due to the special algebraic coupling of the equations of the system.

By computation, we obtain

$$
\begin{aligned}
D(a,b,c|a_\infty,b_\infty,c_\infty) &= d_a \int\limits_{[0,1]} \frac{|\nabla a|^2}{a} dx + d_b \int\limits_{[0,1]} \frac{|\nabla b|^2}{b} dx + d_c \int\limits_{[0,1]} \frac{|\nabla c|^2}{c} dx \\
&+ a_\infty b_\infty^2 \int\limits_{[0,1]} \Psi\left(\frac{ab^2}{a_\infty b_\infty^2}; \frac{bc}{b_\infty c_\infty}\right) dx + b_\infty c_\infty \int\limits_{[0,1]} \Psi\left(\frac{bc}{b_\infty c_\infty}; \frac{ab^2}{a_\infty b_\infty^2}\right) dx \\
&\geq 4d_a \|\nabla\sqrt{a}\|_2^2 + 4d_b\|\nabla\sqrt{b}\|_2^2 + 4d_c\|\nabla\sqrt{c}\|_2^2 \\
&+ a_\infty b_\infty^2 \left\|\sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}}\right\|_2^2 + b_\infty c_\infty \left\|\sqrt{\frac{bc}{b_\infty c_\infty}} - \sqrt{\frac{ab^2}{a_\infty b_\infty^2}}\right\|_2^2 \\
&\geq C_7\left(\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 + \left\|\sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}}\right\|_2^2\right),
\end{aligned} \tag{3.25}
$$

where $C_7 := \min(4d_a, 4d_b, 4d_c, a_\infty b_\infty^2 + b_\infty c_\infty)$. Due to (3.6), we have $M := \max(M_1, M_2)$ such that $\overline{a(t)}, \overline{b(t)}, \overline{c(t)} < M$ for all $t \geq 0$. In what follows we drop the dependence on t from the notation; each time we write $\overline{a}$ or the likes we mean the spatial average of $a(t) = a(\cdot, t)$. Thus, we see that

$$
\Psi(x,y) \leq \frac{\Psi(M,y)}{(\sqrt{M}-\sqrt{y})^2}(\sqrt{x}-\sqrt{y})^2 \text{ for all } x \leq M.
$$

Since $0 < a_\infty, b_\infty, c_\infty < M$, we have

$$
\begin{aligned}
E(\overline{a},\overline{b},\overline{c}|a_\infty,b_\infty,c_\infty) &= \left(\overline{a}\ln\frac{\overline{a}}{a_\infty} - \overline{a} + a_\infty\right) + \left(\overline{b}\ln\frac{\overline{b}}{b_\infty} - \overline{b} + b_\infty\right) \\
&+ \left(\overline{c}\ln\frac{\overline{c}}{c_\infty} - \overline{c} + c_\infty\right) < \frac{\Psi(M,a_\infty)}{(\sqrt{M}-\sqrt{a_\infty})^2}(\sqrt{\overline{a}}-\sqrt{a_\infty})^2 \\
&+ \frac{\Psi(M,b_\infty)}{(\sqrt{M}-\sqrt{b_\infty})^2}(\sqrt{\overline{b}}-\sqrt{b_\infty})^2 + \frac{\Psi(M,c_\infty)}{(\sqrt{M}-\sqrt{c_\infty})^2}(\sqrt{\overline{c}}-\sqrt{c_\infty})^2 \\
&\leq C_8\left[(\sqrt{\overline{a}}-\sqrt{a_\infty})^2 + (\sqrt{\overline{b}}-\sqrt{b_\infty})^2 + (\sqrt{\overline{c}}-\sqrt{c_\infty})^2\right],
\end{aligned} \tag{3.26}
$$

where

$$
C_8 := \max\left\{\frac{\Psi(M,a_\infty)}{(\sqrt{M}-\sqrt{a_\infty})^2}, \frac{\Psi(M,b_\infty)}{(\sqrt{M}-\sqrt{b_\infty})^2}, \frac{\Psi(M,c_\infty)}{(\sqrt{M}-\sqrt{c_\infty})^2}\right\}.
$$

Next we claim that there exists a real constant C_9 such that

$$\begin{aligned} &\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 + \left\|\sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}}\right\|_2^2 \\ &> C_9\left[\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 + \left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2\right]. \end{aligned} \tag{3.27}$$

In order to get the above estimate, we introduce the deviations from the mean, i.e. $\delta_a = \sqrt{a} - \overline{\sqrt{a}}, \delta_b = \sqrt{b} - \overline{\sqrt{b}}, \delta_c = \sqrt{c} - \overline{\sqrt{c}}$. Now we make the decomposition

$$[0,1] = D_L \cup D_L^{\complement},$$

where $D_L = \{x \in [0,1] : |\delta_a|, |\delta_b|, |\delta_c| \le L\}$ for a fixed constant L. We expand

$$\sqrt{ab^2} = \left(\overline{\sqrt{a}} + \delta_a\right)\left(\overline{\sqrt{b}} + \delta_b\right)^2 = \overline{\sqrt{a}}\,\overline{\sqrt{b}}^2 + \left[\delta_a\left(\overline{\sqrt{b}} + \delta_b\right)^2 + \overline{\sqrt{a}}\left(2\overline{\sqrt{b}}\delta_b + \delta_b^2\right)\right]$$

and

$$\sqrt{bc} = \left(\overline{\sqrt{b}} + \delta_b\right)\left(\overline{\sqrt{c}} + \delta_c\right) = \overline{\sqrt{b}}\,\overline{\sqrt{c}} + \left[\delta_b\overline{\sqrt{c}} + \delta_c\left(\overline{\sqrt{b}} + \delta_b\right)\right]$$

to see that on the set D_L one has

$$\begin{aligned} &\delta_a\left(\overline{\sqrt{b}} + \delta_b\right)^2 + \overline{\sqrt{a}}\left(2\overline{\sqrt{b}}\delta_b + \delta_b^2\right) \\ &\le (|\delta_a| + |\delta_b|)\left[\left(\sqrt{M_2} + L\right)^2 + \sqrt{M_1}\left(2\sqrt{M_2} + L\right)\right] = (|\delta_a| + |\delta_b|)R_1 \end{aligned}$$

and

$$\begin{aligned} &\delta_b\overline{\sqrt{c}} + \delta_c\left(\overline{\sqrt{b}} + \delta_b\right) \\ &\le (|\delta_b| + |\delta_c|)\left[\sqrt{M_2} + (\sqrt{M_2} + L)\right] = (|\delta_b| + |\delta_c|)R_2, \end{aligned}$$

where $R_1 := \big(\sqrt{M_2}+L\big)^2 + \sqrt{M_1}\big(2\sqrt{M_2}+L\big)$ and $R_2 := \sqrt{M_2} + \big(\sqrt{M_2}+L\big)$. Thus,

$$\begin{aligned}
&\left\|\sqrt{\frac{ab^2}{a_\infty b_\infty^2}} - \sqrt{\frac{bc}{b_\infty c_\infty}}\right\|^2_{L^2(D_L)} = \left\|\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right.\\
&\left.+ \frac{[\delta_a(\overline{\sqrt{b}}+\delta_b)^2 + \overline{\sqrt{a}}(2\overline{\sqrt{b}}\delta_b+\delta_b^2)]}{\sqrt{a_\infty b_\infty^2}} - \frac{[\delta_b\overline{\sqrt{c}} + \delta_c(\overline{\sqrt{b}}+\delta_b)]}{\sqrt{b_\infty c_\infty}}\right\|^2_{L^2(D_L)}\\
&\geq \frac{1}{2}\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2 |D_L| - 2\big\||\delta_a|+|\delta_b|\big\|^2_{L^2(D_L)}\frac{R_1^2}{a_\infty b_\infty^2} \qquad (3.28)\\
&- 2\big\||\delta_b|+|\delta_c|\big\|^2_{L^2(D_L)}\frac{R_2^2}{b_\infty c_\infty}\\
&\geq \frac{1}{2}\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2 |D_L| - R(M_1,M_2,L)\big[\|\delta_a\|^2_{L^2(D_L)}+\\
&\|\delta_b\|^2_{L^2(D_L)} + \|\delta_c\|^2_{L^2(D_L)}\big],
\end{aligned}$$

where $R(M_1,M_2,L) := \frac{4R_1^2}{a_\infty b_\infty^2} + \frac{4R_2^2}{b_\infty c_\infty}$.

On the set $D_L^{\complement}$, by using Poincaré's inequality, we get

$$\begin{aligned}
&\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2\\
&\geq C_P(\|\delta_a\|^2_{L^2(D_L^{\complement})} + \|\delta_b\|^2_{L^2(D_L^{\complement})} + \|\delta_c\|^2_{L^2(D_L^{\complement})})\\
&\geq C_P L^2 |D_L^{\complement}|.
\end{aligned}$$

Since

$$\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2 \leq \left(\frac{\sqrt{M_1}\sqrt{M_2}^2}{\sqrt{a_\infty b_\infty^2}} + \frac{\sqrt{M_2}\sqrt{M_2}}{\sqrt{b_\infty c_\infty}}\right)^2,$$

we infer

$$\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 \geq \widetilde{R}\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2 |D_L^{\complement}|, \qquad (3.29)$$

where

$$\widetilde{R} := \frac{C_P L^2}{\left(\frac{\sqrt{M_1}\sqrt{M_2}^2}{\sqrt{a_\infty b_\infty^2}} + \frac{\sqrt{M_2}\sqrt{M_2}}{\sqrt{b_\infty c_\infty}}\right)^2}.$$

Pick $K > \frac{R+1}{\min\{1,C_P\}}$ and combine (3.28) and (3.29) to conclude

$$
\begin{aligned}
&3K\big(\|\nabla\sqrt{a}\|_2^2+\|\nabla\sqrt{b}\|_2^2+\|\nabla\sqrt{c}\|_2^2\big)+\left\|\sqrt{\frac{ab^2}{a_\infty b_\infty^2}}-\sqrt{\frac{bc}{b_\infty c_\infty}}\right\|_2^2\\
&\geq K\big(\|\nabla\sqrt{a}\|_2^2+\|\nabla\sqrt{b}\|_2^2+\|\nabla\sqrt{c}\|_2^2\big)+\min\left\{K\widetilde{R},\frac{1}{2}\right\}\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}}-\frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2\\
&+(KC_P-R)\big(\|\delta_a\|_{L^2(D_L)}^2+\|\delta_b\|_{L^2(D_L)}^2+\|\delta_c\|_{L^2(D_L)}^2\big)\\
&\geq C_{K,R}\left[\|\nabla\sqrt{a}\|_2^2+\|\nabla\sqrt{b}\|_2^2+\|\nabla\sqrt{c}\|_2^2+\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}}-\frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2\right].
\end{aligned}
$$

where $C_{K,R}=\min\big\{K,K\widetilde{R},\frac{1}{2},KC_P-R\big\}=\min\big\{K\widetilde{R},\frac{1}{2}\big\}$ (because $K-R>1$). Therefore, (3.27) is proved with $C_9=\frac{C_{K,R}}{3K}$.

It remains to show that there exists a constant C_{10} such that

$$
\begin{aligned}
&\|\nabla\sqrt{a}\|_2^2+\|\nabla\sqrt{b}\|_2^2+\|\nabla\sqrt{c}\|_2^2+\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}}-\frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2\\
&\geq C_{10}\big[\big(\sqrt{\overline{a}}-\sqrt{a_\infty}\big)^2+\big(\sqrt{\overline{b}}-\sqrt{b_\infty}\big)^2+\big(\sqrt{\overline{c}}-\sqrt{c_\infty}\big)^2\big].
\end{aligned}
\tag{3.30}
$$

To this end, we introduce μ_a,μ_b,μ_c to parameterize $\sqrt{\overline{a}},\sqrt{\overline{b}},\sqrt{\overline{c}}$ with $\sqrt{\overline{a}}=\sqrt{a_\infty}(1+\mu_a)$, $\sqrt{\overline{b}}=\sqrt{b_\infty}(1+\mu_b)$, $\sqrt{\overline{c}}=\sqrt{c_\infty}(1+\mu_c)$, where $-1\leq\mu_a,\mu_b,\mu_c<\mu_k$ for $\mu_k=\frac{\sqrt{k}}{\min\{\sqrt{a_\infty},\sqrt{b_\infty},\sqrt{c_\infty}\}}-1$. Since $\delta_a=\sqrt{a}-\overline{\sqrt{a}}$, we have

$$
\begin{aligned}
&\|\delta_a\|_2^2=\overline{a}-(\overline{\sqrt{a}})^2=(\sqrt{\overline{a}}-\overline{\sqrt{a}})(\sqrt{\overline{a}}+\overline{\sqrt{a}})\\
&\implies\overline{\sqrt{a}}=-\frac{\|\delta_a\|_2^2}{\sqrt{\overline{a}}+\overline{\sqrt{a}}}+\sqrt{\overline{a}}=\sqrt{\overline{a}}-T(a)\|\delta_a\|_2^2,
\end{aligned}
$$

where $T(a)=\frac{1}{\sqrt{\overline{a}}+\overline{\sqrt{a}}}\leq\frac{1}{\varepsilon}$; this inequality follows from $\overline{a}=\|a\|_1>\varepsilon^2>0$. Similarly,

$$
\overline{\sqrt{b}}=\sqrt{\overline{b}}-T(b)\|\delta_b\|_2^2\ \ \&\ \ \overline{\sqrt{c}}=\sqrt{\overline{c}}-T(c)\|\delta_c\|_2^2,
$$

where $T(b) = \frac{1}{\sqrt{\bar{b}}+\overline{\sqrt{b}}}, T(c) = \frac{1}{\sqrt{\bar{c}}+\overline{\sqrt{c}}} \leq \frac{1}{\varepsilon}$. And since

$$\varepsilon^2 < \|b\|_1 \leq \|\sqrt{b}\|_\infty \|\sqrt{b}\|_1 \leq \sqrt{k}\|\sqrt{b}\|_1 \implies \overline{\sqrt{b}} \geq \frac{\varepsilon^2}{\sqrt{k}},$$

due to this lower bound on $\overline{\sqrt{b}}$, we can factor out $(\frac{\overline{\sqrt{b}}}{\sqrt{b_\infty}})^2$ and reduce (3.1) to the system associated with the reversible reaction $A + B \rightleftharpoons C$ (which does not have accessible boundary equilibria). More precisely, we have

$$\begin{aligned}
&\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}}\,\overline{\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2 = \frac{\left(\overline{\sqrt{b}}\right)^2}{b_\infty}\left(\frac{\overline{\sqrt{a}}\,\overline{\sqrt{b}}}{\sqrt{a_\infty b_\infty}} - \frac{\overline{\sqrt{c}}}{\sqrt{c_\infty}}\right)^2 \\
&\geq \frac{\varepsilon^4}{b_\infty k}\left\{\frac{(\sqrt{\bar{a}} - T(a)\|\delta_a\|_2^2)(\sqrt{\bar{b}} - T(b)\|\delta_b\|_2^2)}{\sqrt{a_\infty b_\infty}} - \frac{\sqrt{\bar{c}} - T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}}\right\}^2 \qquad (3.31) \\
&= \frac{\varepsilon^4}{b_\infty k}\left\{[1 + \mu_a - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}][1 + \mu_b - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}] - [1 + \mu_c - \frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}}]\right\}^2
\end{aligned}$$

$$\begin{aligned}
&= \frac{\varepsilon^4}{b_\infty k}\left\{[(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)] + \frac{T(a)\|\delta_a\|_2^2 T(b)\|\delta_b\|_2^2}{\sqrt{a_\infty}} + \frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}}\right. \\
&\left. - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}(1 + \mu_b) - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}(1 + \mu_a)\right\}^2 \\
&\geq \frac{\varepsilon^4}{b_\infty k}\left\{\frac{1}{2}[(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)]^2 - \left[\frac{T(a)\|\delta_a\|_2^2 T(b)\|\delta_b\|_2^2}{\sqrt{a_\infty}} + \frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}}\right.\right. \\
&\left.\left. - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}(1 + \mu_b) - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}(1 + \mu_a)\right]^2\right\} \\
&\geq \frac{\varepsilon^4}{b_\infty k}\left\{\frac{1}{2}\big[(1 + \mu_a)(1 + \mu_b) - (1 + \mu_c)\big]^2 - 4\left[\frac{T(a)\|\delta_a\|_2^2 T(b)\|\delta_b\|_2^2}{\sqrt{a_\infty}}\right]^2\right. \\
&\left. - 4\left[\frac{T(c)\|\delta_c\|_2^2}{\sqrt{c_\infty}}\right]^2 - 4\left[\frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}(1 + \mu_b)\right]^2 - 4\left[\frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}(1 + \mu_a)\right]^2\right\}.
\end{aligned}$$

Since $\|\delta_a\|_2^2 = \bar{a} - \left(\overline{\sqrt{a}}\right)^2$, we get $\|\delta_a\|_2^2 \leq k$; similarly, $\|\delta_b\|_2^2, \|\delta_c\|_2^2 \leq k$. Combined with

$T(a), T(b), T(c) \leq \frac{1}{\varepsilon}$ and $0 \leq 1+\mu_a,\ 1+\mu_b,\ 1+\mu_c \leq 1+\mu_k$, (3.31) gives

$$\begin{aligned}
&\left(\frac{\overline{\sqrt{a}\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2 \geq \frac{\varepsilon^4}{b_\infty k}\Big\{\frac{1}{2}\big[(1+\mu_a)(1+\mu_b)-(1+\mu_c)\big]^2 \\
&- \frac{4k^3}{\varepsilon^4 a_\infty}\|\delta_a\|_2^2 - \frac{4k}{\varepsilon^2 c_\infty}\|\delta_c\|_2^2 - \frac{4k(1+\mu_k)^2}{\varepsilon^2 a_\infty}\|\delta_a\|_2^2 - \frac{4k(1+\mu_k)^2}{\varepsilon^2 b_\infty}\|\delta_b\|_2^2\Big\} \\
&\geq \frac{\varepsilon^4}{2b_\infty k}\big[(1+\mu_a)(1+\mu_b)-(1+\mu_c)\big]^2 - C_{11}\big(\|\delta_a\|_2^2 + \|\delta_b\|_2^2 + \|\delta_c\|_2^2\big),
\end{aligned}$$

where

$$C_{11} := \max\left\{\frac{4k^2+4(1+\mu_k)^2}{a_\infty b_\infty}, \frac{4(1+\mu_k)^2}{b_\infty^2}, \frac{4(1+\mu_k)^2}{b_\infty c_\infty}\right\}.$$

Poincaré's inequality reveals

$$\begin{aligned}
&\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 + \left(\frac{\overline{\sqrt{a}\sqrt{b}}^2}{\sqrt{a_\infty b_\infty^2}} - \frac{\overline{\sqrt{b}\sqrt{c}}}{\sqrt{b_\infty c_\infty}}\right)^2 \\
&\geq C_{12}\big[(1+\mu_a)(1+\mu_b)-(1+\mu_c)\big]^2,
\end{aligned}$$

for $C_{12} := \frac{C_P \varepsilon^4}{2b_\infty k C_{11}}$. On the other hand,

$$(\sqrt{\overline{a}} - \sqrt{a_\infty})^2 + (\sqrt{\overline{b}} - \sqrt{b_\infty})^2 + (\sqrt{\overline{c}} - \sqrt{c_\infty})^2 = a_\infty \mu_a^2 + b_\infty \mu_b^2 + c_\infty \mu_c^2,$$

so we would like to compare $[(1+\mu_a)(1+\mu_b)-(1+\mu_c)]^2$ and $\mu_a^2+\mu_b^2+\mu_c^2$. The conservation laws (3.6) (applied to $\overline{a}$, $\overline{b}$, $\overline{c}$ and a_∞, b_∞, c_∞) yield

$$\begin{aligned}
&\frac{\overline{a}}{a_\infty} = (1+\mu_a),\ \frac{\overline{b}}{b_\infty} = (1+\mu_b),\ \frac{\overline{c}}{c_\infty} = (1+\mu_c), \\
&\overline{a} + \overline{c} = a_\infty + c_\infty = M_1,\ \overline{b} + \overline{c} = b_\infty + c_\infty = M_2,
\end{aligned}$$

and so, $a_\infty\mu_a + c_\infty\mu_c = b_\infty\mu_b + c_\infty\mu_c = 0$. Thus, unless μ_a, μ_b, μ_c are all zero (trivial case!), we get $\mu_a\mu_c < 0$ and $\mu_b\mu_c < 0$. If $\mu_a, \mu_b > 0$ and $0 > \mu_c$, then

$$\begin{aligned}
&[(1+\mu_a)(1+\mu_b)-(1+\mu_c)]^2 = (\mu_a\mu_b + \mu_a + \mu_b - \mu_c)^2 \\
&\geq (\mu_a\mu_b + \mu_a + \mu_b)^2 + (\mu_c)^2 > \mu_a^2 + \mu_b^2 + \mu_c^2.
\end{aligned}$$

Otherwise, if $\mu_a, \mu_b < 0$ and $0 < \mu_c$, then

$$\begin{aligned}&[(1+\mu_a)(1+\mu_b)-(1+\mu_c)]^2 = (\mu_a\mu_b+\mu_a+\mu_b-\mu_c)^2\\ &\geq (\mu_a+\mu_b-\mu_c)^2+(\mu_a\mu_b)^2 > \mu_a^2+\mu_b^2+\mu_c^2.\end{aligned}$$

Therefore, in both cases we have

$$[(1+\mu_a)(1+\mu_b)-(1+\mu_c)]^2 \geq \mu_a^2+\mu_b^2+\mu_c^2.$$

(Notice that when $\mu_a = \mu_b = \mu_c = 0$, both sides of the inequality are equal to zero.) Set

$$C_{10} := \frac{C_{12}}{\max(a_\infty, b_\infty, c_\infty)}$$

to conclude the proof of (3.30).

Proof of Theorem 3.1.1:

Proof. Finally, by (3.25), (3.26), (3.27) and (3.30), we obtain

$$\begin{aligned}&D(a,b,c|a_\infty,b_\infty,c_\infty)\\ &\geq C_7C_9C_{10}\left[\left(\sqrt{\overline{a}}-\sqrt{a_\infty}\right)^2+\left(\sqrt{\overline{b}}-\sqrt{b_\infty}\right)^2+\left(\sqrt{\overline{c}}-\sqrt{c_\infty}\right)^2\right]\\ &\geq \frac{C_7C_9C_{10}}{C_8}E(\overline{a},\overline{b},\overline{c}|a_\infty,b_\infty,c_\infty).\end{aligned}$$

In view of the above inequality and (3.20), we discover

$$D(a,b,c|a_\infty,b_\infty,c_\infty) \geq C_{13}E(a,b,c|a_\infty,b_\infty,c_\infty),$$

where

$$C_{13} := \min\left(\frac{C_7C_9C_{10}}{C_8}, C_2\right).$$

In conclusion, we have proved that the solution decays exponentially to the positive equilibrium (with explicit rate). $\square$

3.1.3 Asymptotic decay for the two-species system

In this section we prove Theorem 3.1.2.

3.1.3.1 Uniform boundedness and global existence for the two-species system

To show the uniform boundedness for classical solutions to (3.3) we employ an invariant region approach. Note that here we do not need the assumptions from Theorem 3.1.2 on the signs of $\bar{m}$ and $\bar{n}$.

Theorem 3.1.9. *Let f denote the two-dimensional mass-action vector field generated by the single reversible reaction $m_1A+n_1B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} m_2A+n_2B$, where $\bar{m}=m_1-m_2$ and $\bar{n}=n_2-n_1$ are nonzero. Then, for any compact set $K\subset\mathbb{R}^2_{>0}$ there exists a rectangle $R=[\alpha_1,\alpha_2]\times[\beta_1,\beta_2]\subset\mathbb{R}^2_{>0}$ such that $K\subset R$ and such that f points into the interior of R on ∂R.*

Proof. With the notation we have already introduced, $a,\ b$ denote the concentrations of A and B, and $\bar{m}=m_1-m_2,\ \bar{n}=n_2-n_1$. The corresponding ODE system reads

$$\begin{pmatrix} \dot{a} \\ \dot{b} \end{pmatrix} = (k_1a^{m_1}b^{n_1}-k_2a^{m_2}b^{n_2})\begin{pmatrix} -\lambda_a\bar{m} \\ \lambda_b\bar{n} \end{pmatrix},$$

so positive trajectories are confined to *stoichiometric classes* $(p+\operatorname{span}(-\lambda_a\bar{m},\lambda_b\bar{n})^t)\cap\mathbb{R}^2_{>0}$ (see Figure 3.1). The positive steady state manifold is the curve $a^{-\bar{m}}b^{\bar{n}}=k_1/k_2$, and it is easily checked that it intersects each stoichiometric class intersects at precisely one point. It is also easy to see that the unique steady state in each stoichiometric class is globally asymptotically stable on that class. It follows that a rectangular region $R\subset\mathbb{R}^2_{>0}$ is invariant if and only if it contains the steady state on each stoichiometric class that intersects R. If $\bar{m}\bar{n}\neq 0$ this can be achieved by choosing opposite vertices of R on the steady state curve (Figure 3.1**a, b.**). $\square$

Now we use a less general (tailored to our needs) version of **Corollary 14.8** from [97].

Figure 3.1: Construction of a rectangular invariant region for the reversible reaction $m_1A + n_1B \rightleftharpoons m_2A + n_2B$ for the cases **a.** $\bar{m} = m_1 - m_2$, $\bar{n} = n_2 - n_1$ nonzero and of the same sign; **b.** $\bar{m}, \bar{n}$ nonzero and of different signs.

Theorem 3.1.10. *Suppose that D is a $k \times k$ nonnegative definite diagonal matrix. Then any region of the form (invariant rectangle)*

$$\Sigma = \bigcap_{i=1}^{k} \{u : a_i \leq u_i \leq b_i\}$$

is invariant for the $k \times k$ reaction-diffusion system

$$v_t = Dv_{xx} + f(v, t)$$

provided that f points strictly into Σ on $\partial\Sigma$.

(1) By using the above two theorems we immediately conclude that if $\bar{m}\bar{n} \neq 0$, then the reaction-diffusion system (3.3) shares the same invariant regions with the corresponding reaction system. Thus, under the restrictions on a_0 and b_0 from the statement of Theorem 3.1.2, we get a uniform upper bound $0 < \omega < \infty$ for a and b; this also implies the existence of a unique global classical solution.

(2) If $\bar{m} = \bar{n} = 0$, then we are dealing with two decoupled homogeneous Neumann heat problems on the same domain. It is known that the lower and upper bounds on a_0, b_0 are preserved for all time. Both densities converge exponentially to the averages of the initial data.

(3) If only one of $\bar{m}$, $\bar{n}$ is zero, say $\bar{m} = 0$, then the equation for a decouples and,

as above, we have that a stays bounded globally in time between $\inf a_0$ and $\sup a_0$, and it converges exponentially to the average of a_0. The equation for b becomes

$$b_t - d_b \Delta b = \lambda_b |\bar{n}| a^{m_1} b^p \big(1 - b^{|\bar{n}|}\big),$$

where $p := \min\{n_1, n_2\}$. The positive equilibrium is $b_\infty \equiv 1$. Now we use Theorem 3.1.10 with $k = 1$ and $f(b,t) := \lambda_b |\bar{n}| a^{m_1} b^p \big(1 - b^{|\bar{n}|}\big)$; since a is bounded uniformly away from zero and infinity, we conclude that at the boundary of any interval $[\delta, M]$, (where $0 < \delta < 1 < M < \infty$) f does, indeed, point strictly inside said interval.

In conclusion, if $a_0,\ b_0$ are bounded away from zero by α and from infinity by β (as in the statement of Theorem 3.1.2) we get explicit (depending only on α and β) global bounds (and global existence and uniqueness) on $a,\ b$ in all cases.Let these bounds be $\varepsilon^2,\ \omega$, so that

$$0 < \varepsilon^2 \le \min\{a(x,t), b(x,t)\} \le \max\{a(x,t), b(x,t)\} \le \omega < \infty \text{ for all } (x,t) \in \Omega \times [0,\infty). \tag{3.32}$$

3.1.3.2 Convergence for the two-species system

We use the same entropy entropy dissipation method to obtain an explicit exponential convergence rate for the two species system in any dimension. Once again, the Log-Sobolev inequality, the Poincaré inequality for the square roots of the densities minus their averages, along with a few important algebraic inequalities proved in the Appendix help us obtain an EEDI of the type $D(t) \ge cE(t)$, where c is a positive real number (independent of time). Again we introduce the relative entropy

$$E(a,b|a_\infty,b_\infty) = \int_\Omega \left(a \ln \frac{a}{a_\infty} - a + a_\infty\right) dx + \int_\Omega \left(b \ln \frac{b}{b_\infty} - b + b_\infty\right) dx$$

and its corresponding entropy dissipation

$$D(a,b|a_\infty,b_\infty) = d_a\int_\Omega \frac{|\nabla a|^2}{a}dx + d_b\int_\Omega \frac{|\nabla b|^2}{b}dx$$
$$+ a_\infty^{m_1}b_\infty^{n_1}\int_\Omega \Psi\left(\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}};\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}\right)dx + a_\infty^{m_2}b_\infty^{n_2}\int_\Omega \Psi\left(\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}};\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}\right)dx.$$

Due to the following identity

$$E(a,b|a_\infty,b_\infty) = E(a,b|\overline{a},\overline{b}) + E(\overline{a},\overline{b}|a_\infty,b_\infty)$$

and the Logarithmic Sobolev Inequality (3.19) we have

$$d_a\int_\Omega \frac{|\nabla a|^2}{a}dx + d_b\int_\Omega \frac{|\nabla b|^2}{b}dx \geq D_1 E(a,b|\overline{a},\overline{b}), \tag{3.33}$$

where $D_1 = \min(d_a,d_b)\cdot C_{LSI}$.

From computation, we get the following estimate

$$\begin{aligned}
&D(a,b|a_\infty,b_\infty) = d_a\int_\Omega \frac{|\nabla a|^2}{a}dx + d_b\int_\Omega \frac{|\nabla b|^2}{b}dx\\
&+ a_\infty^{m_1}b_\infty^{n_1}\int_\Omega \Psi\left(\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}};\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}\right)dx + a_\infty^{m_2}b_\infty^{n_2}\int_\Omega \Psi\left(\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}};\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}\right)dx\\
&\geq 4d_a\|\nabla\sqrt{a}\|_2^2 + 4d_b\|\nabla\sqrt{b}\|_2^2 + 4d_c\|\nabla\sqrt{c}\|_2^2\\
&+ a_\infty^{m_1}b_\infty^{n_1}\left\|\sqrt{\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}}\right\|_2^2 + a_\infty^{m_2}b_\infty^{n_2}\left\|\sqrt{\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}} - \sqrt{\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}}\right\|_2^2\\
&\geq D_2\left(\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \|\nabla\sqrt{c}\|_2^2 + \left\|\sqrt{\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}}\right\|_2^2\right),
\end{aligned} \tag{3.34}$$

where $D_2 = \min(4d_a, 4d_b, 4d_c, a_\infty^{m_1}b_\infty^{n_1} + a_\infty^{m_2}b_\infty^{n_2})$.

The global L^∞ bounds on a and b ensure that there exists N such that $\overline{a},\overline{b} < N$. Thus, we get

$$\Psi(x,y) \leq \frac{\Psi(N,y)}{(\sqrt{N}-\sqrt{y})^2}(\sqrt{x}-\sqrt{y})^2 \text{ for all } x \leq N.$$

Since $0 < a_\infty, b_\infty < N$,

$$
\begin{aligned}
E(\bar{a},\bar{b}|a_\infty,b_\infty) &= \left(\bar{a}\ln\frac{\bar{a}}{a_\infty} - \bar{a} + a_\infty\right) + \left(\bar{b}\ln\frac{\bar{b}}{b_\infty} - \bar{b} + b_\infty\right) \\
&< \frac{\Psi(N,a_\infty)}{(\sqrt{N}-\sqrt{a_\infty})^2}(\sqrt{\bar{a}}-\sqrt{a_\infty})^2 + \frac{\Psi(N,b_\infty)}{(\sqrt{N}-\sqrt{b_\infty})^2}(\sqrt{\bar{b}}-\sqrt{b_\infty})^2 \\
&\le D_3\big[\big(\sqrt{\bar{a}}-\sqrt{a_\infty}\big)^2 + \big(\sqrt{\bar{b}}-\sqrt{b_\infty}\big)^2\big],
\end{aligned}
\tag{3.35}
$$

where

$$
D_3 = \max\left\{\frac{\Psi(N,a_\infty)}{(\sqrt{N}-\sqrt{a_\infty})^2}, \frac{\Psi(N,b_\infty)}{(\sqrt{N}-\sqrt{b_\infty})^2}\right\}.
$$

Now we claim there exists a constant $D_4 > 0$ such that

$$
\begin{aligned}
&\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \left\|\sqrt{\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}}\right\|_2^2 \\
&> D_4\left\{\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \left(\frac{\overline{\sqrt{a}}^{m_1}\,\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\,\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2\right\}.
\end{aligned}
\tag{3.36}
$$

Now we again introduce the deviations $\delta_a = \sqrt{a} - \overline{\sqrt{a}}, \delta_b = \sqrt{b} - \overline{\sqrt{b}}$ and make the decomposition

$$
\Omega = D_L \cup D_L^{\complement},
$$

where $D_L := \{x \in \Omega : |\delta_a|, |\delta_b| \le L\}$ with a fixed constant L. On the set D_L we get

$$
\begin{aligned}
\sqrt{a^{m_1}b^{n_1}} &= (\overline{\sqrt{a}} + \delta_a)^{m_1}(\overline{\sqrt{b}} + \delta_b)^{n_1} \\
&\le \overline{\sqrt{a}}^{m_1} \cdot \overline{\sqrt{b}}^{n_1} + (|\delta_a| + |\delta_b|)R_1(|\delta_a|, |\delta_b|, \overline{\sqrt{a}}, \overline{\sqrt{b}}),
\end{aligned}
$$

$$
\begin{aligned}
\sqrt{a^{m_2}b^{n_2}} &= (\overline{\sqrt{a}} + \delta_a)^{m_2}(\overline{\sqrt{b}} + \delta_b)^{n_2} \\
&\le \overline{\sqrt{a}}^{m_2} \cdot \overline{\sqrt{b}}^{n_2} + (|\delta_a| + |\delta_b|)R_2(|\delta_a|, |\delta_b|, \overline{\sqrt{a}}, \overline{\sqrt{b}}),
\end{aligned}
$$

where R_1 and R_2 are finite due to the boundedness of $|\delta_a|, |\delta_b|, \overline{\sqrt{a}}, \overline{\sqrt{b}}$. Then we get

$$\begin{aligned}
&\left\|\sqrt{\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}}-\sqrt{\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}}\right\|_{L^2(D_L)}^2 \\
&\geq \frac{1}{2}\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}}-\frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2|D_L| - 2\|(|\delta_a|+|\delta_b|)\|_{L^2(D_L)}^2\frac{R_1^2}{a_\infty^{m_1}b_\infty^{n_1}} \\
&- 2\|(|\delta_a|+|\delta_b|)\|_{L^2(D_L)}^2\frac{R_2^2}{a_\infty^{m_2}b_\infty^{n_2}} \\
&\geq \frac{1}{2}\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}}-\frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2|D_L| - R(|\delta_a|,|\delta_b|,\overline{\sqrt{a}},\overline{\sqrt{b}})[\|\delta_a\|_{L^2(D_L)}^2+ \\
&\|\delta_b\|_{L^2(D_L)}^2],
\end{aligned}$$

where $R(|\delta_a|,|\delta_b|,\overline{\sqrt{a}},\overline{\sqrt{b}}) = \frac{4R_1^2}{a_\infty^{m_1}b_\infty^{n_1}} + \frac{4R_2^2}{a_\infty^{m_2}b_\infty^{n_2}}$ is finite (depends on the choice of L and N).

On the set $D_L^\complement$, by using Poincaré's inequality, we get

$$\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 \geq C_P\big(\|\delta_a\|_{L^2(D_L^\complement)}^2 + \|\delta_b\|_{L^2(D_L^\complement)}^2\big) \geq C_P L^2|D_L^\complement|.$$

Since

$$\left|\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}}-\frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right| \leq \frac{\sqrt{N}^{m_1+n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} + \frac{\sqrt{N}^{m_2+n_2}}{a_\infty^{m_2}b_\infty^{n_2}},$$

we infer

$$\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 \geq \widetilde{R}\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}}-\frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2|D_L^\complement|,$$

where

$$\widetilde{R} = C_P L^2\left(\frac{\sqrt{N}^{m_1+n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} + \frac{\sqrt{N}^{m_2+n_2}}{a_\infty^{m_2}b_\infty^{n_2}}\right)^{-2}.$$

We combine the above two parts, pick $K > \frac{R+1}{\min\{1, C_P\}}$ and have the following

$$
\begin{aligned}
&3K(\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2) + \left\|\sqrt{\frac{a^{m_1}b^{n_1}}{a_\infty^{m_1}b_\infty^{n_1}}} - \sqrt{\frac{a^{m_2}b^{n_2}}{a_\infty^{m_2}b_\infty^{n_2}}}\right\|_2^2 \\
&\geq K(\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2) + K\widetilde{R}\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2 |D_L^\complement| \\
&+ \left\{\frac{1}{2}\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2 |D_L| - R\big[\|\delta_a\|_{L^2(D_L)}^2 + \|\delta_b\|_{L^2(D_L)}^2\big]\right\} \\
&+ KC_P(\|\delta_a\|_{L^2(D_L)}^2 + \|\delta_b\|_{L^2(D_L)}^2) \\
&\geq C_{K,R}\left[\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2\right],
\end{aligned}
$$

where $C_{K,R} := \min\{K\widetilde{R}, \frac{1}{2}\}$. We can fix $L > 0$ and get the corresponding R, then pick sufficiently large K (e.g. $K > R + 1$) such that we obtain (3.36) with $D_4 = \frac{C_{K,R}}{3K}$.

It remains to show that there exists a constant D_5 such that

$$
\begin{aligned}
&\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2 \\
&> D_5\big[\big(\sqrt{\overline{a}} - \sqrt{a_\infty}\big)^2 + \big(\sqrt{\overline{b}} - \sqrt{b_\infty}\big)^2\big].
\end{aligned}
\tag{3.37}
$$

We again introduce μ_a, μ_b to parameterize $\sqrt{\overline{a}}, \sqrt{\overline{b}}$ with

$$
\sqrt{\overline{a}} = \sqrt{a_\infty}(1 + \mu_a), \;\; \sqrt{\overline{b}} = \sqrt{b_\infty}(1 + \mu_b), \tag{3.38}
$$

where, in view of (3.32), we have $\mu_\varepsilon \leq \mu_a, \mu_b < \mu_\omega$ with $\mu_\varepsilon = \frac{\varepsilon}{\max\{\sqrt{a_\infty}, \sqrt{b_\infty}\}} - 1$ and $\mu_\omega = \frac{\sqrt{\omega}}{\min\{\sqrt{a_\infty}, \sqrt{b_\infty}\}} - 1$. We have $\overline{\sqrt{a}} = -\frac{\|\delta_a\|_2^2}{\sqrt{\overline{a}} + \overline{\sqrt{a}}} + \sqrt{\overline{a}} = \sqrt{\overline{a}} - T(a)\|\delta_a\|_2^2$, where $T(a) = \frac{1}{\sqrt{\overline{a}} + \overline{\sqrt{a}}}$. Similarly, $\overline{\sqrt{b}} = \sqrt{\overline{b}} - T(b)\|\delta_b\|_2^2$, where $T(b) = \frac{1}{\sqrt{\overline{b}} + \overline{\sqrt{b}}}$. Both $T(a), T(b)$ have uniform (in time) upper and lower bounds. Given the symmetry of (3.3), it suffices to discuss the case $\bar{m}, \bar{n} \geq 0$, so we make this assumption in what follows; thus, we can factor out $\left(\frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty}^{m_2}\sqrt{b_\infty}^{n_1}}\right)^2$ from the squared term in the left hand side of (3.37) to see that

$$\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2 = \frac{(\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_1})^2}{a_\infty^{m_2}b_\infty^{n_1}} \cdot \left(\frac{\overline{\sqrt{a}}^{\bar{m}}}{\sqrt{a_\infty}^{\bar{m}}} - \frac{\overline{\sqrt{b}}^{\bar{n}}}{\sqrt{b_\infty}^{\bar{n}}}\right)^2$$
$$\geq \frac{\varepsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}}\left[\left(1+\mu_a - \frac{T(a)\|\delta_a\|_2^2}{\sqrt{a_\infty}}\right)^{\bar{m}} - \left(1+\mu_b - \frac{T(b)\|\delta_b\|_2^2}{\sqrt{b_\infty}}\right)^{\bar{n}}\right]^2 =: A.$$

Of course, if $\bar{m},\ \bar{n} \leq 0$ we would factor out $\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty}^{m_1}\sqrt{b_\infty}^{n_2}}\right)^2$ instead, which would replace the constant $\frac{\varepsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}}$ by $\frac{\varepsilon^{2(m_1+n_2)}}{a_\infty^{m_1}b_\infty^{n_2}}$ and the proof would continue otherwise unchanged. We evaluate

$$A = \frac{\varepsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}}\big\{[(1+\mu_a)^{\bar{m}} + \|\delta_a\|_2 S_1(\mu_a, \|\delta_a\|_2, T(a))] - [(1+\mu_b)^{\bar{n}}$$
$$+ \|\delta_b\|_2 S_2(\mu_b, \|\delta_b\|_2, T(b))]\big\}^2$$
$$\geq \frac{\varepsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}}\left\{\frac{1}{2}[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2 - 2[\|\delta_a\|_2 S_1 - \|\delta_b\|_2 S_2]^2\right\}$$
$$\geq \frac{\varepsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}}\left\{\frac{1}{2}[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2 - 4(\|\delta_a\|_2^2 + \|\delta_b\|_2^2)S\right\},$$

where $S = \max(|S_1|, |S_2|)$.

We have $\|\delta_a\|_2^2 = \overline{a} - (\overline{\sqrt{a}})^2 \leq \omega$, similarly $\|\delta_b\|_2^2 \leq \omega$ and $T(a), T(b) \leq \frac{1}{\varepsilon}$, $\mu_a, \mu_b < \mu_\omega$; so S is uniformly bounded and

$$\left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2$$
$$\geq \frac{\varepsilon^{2(m_2+n_1)}}{2a_\infty^{m_2}b_\infty^{n_1}}[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2 - D_6(\|\delta_a\|_2^2 + \|\delta_b\|_2^2),$$

where $D_6 = 4\frac{\varepsilon^{2(m_2+n_1)}}{a_\infty^{m_2}b_\infty^{n_1}}\|S\|_\infty$. Poincaré's inequality yields

$$\|\nabla\sqrt{a}\|_2^2 + \|\nabla\sqrt{b}\|_2^2 + \left(\frac{\overline{\sqrt{a}}^{m_1}\overline{\sqrt{b}}^{n_1}}{\sqrt{a_\infty^{m_1}b_\infty^{n_1}}} - \frac{\overline{\sqrt{a}}^{m_2}\overline{\sqrt{b}}^{n_2}}{\sqrt{a_\infty^{m_2}b_\infty^{n_2}}}\right)^2$$
$$> D_7[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2,$$

where $D_7 = \frac{\varepsilon^{2(m_2+n_1)}}{2a_\infty^{m_2} b_\infty^{n_1}} D_6^{-1}$. On the other hand,

$$(\sqrt{\bar{a}} - \sqrt{a_\infty})^2 + (\sqrt{\bar{b}} - \sqrt{b_\infty})^2 = a_\infty \mu_a^2 + b_\infty \mu_b^2,$$

so we need to compare $[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2$ with $\mu_a^2 + \mu_b^2$. First assume $\bar{m}\bar{n} > 0$, i.e. both $\bar{m}$, $\bar{n}$ are positive integers. The conservation law for (3.3) reads

$$\lambda_b \bar{n} \bar{a}(t) + \lambda_a \bar{m} \bar{b}(t) = \lambda_b \bar{n} a_\infty + \lambda_a \bar{m} b_\infty \text{ for all } t \geq 0, \tag{3.39}$$

so (3.38) together with the nonnegativity of λ_a, λ_b, $\bar{m}$, $\bar{n}$ implies that either $\mu_a = \mu_b = 0$ (trivial case) or $\mu_a \mu_b < 0$. Recall that $\mu_a > -1$, $\mu_b > -1$ for all time. If $\mu_a > 0 > \mu_b$, then

$$[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2 \geq [(1+\mu_a) - (1+\mu_b)]^2 > \mu_a^2 + \mu_b^2.$$

Otherwise, if $\mu_b > 0 > \mu_a$,

$$[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2 = [(1+\mu_b)^{\bar{n}} - (1+\mu_a)^{\bar{m}}]^2 > \mu_a^2 + \mu_b^2,$$

so in all three cases we have that for all time $t \geq 0$

$$[(1+\mu_a)^{\bar{m}} - (1+\mu_b)^{\bar{n}}]^2 \geq \mu_a^2 + \mu_b^2.$$

Now, if $\bar{m} = \bar{n} = 0$, we get the decoupled heat equations case where $\mu_a = \mu_b = 0$ for all time t, so the inequality above is trivially satisfied. If $\bar{m} = 0$ and $\bar{n} > 0$, we get $\mu_a = 0$ for all time and it is easy to see that the inequality still holds because we can use $1 - (1+\mu_b)^{\bar{n}} \geq -\mu_b$ if $\mu_b \leq 0$ and $(1+\mu_b)^{\bar{n}} - 1 > \bar{n}\mu_b > \mu_b$ if $\mu_b > 0$.

Proof of Theorem 3.1.2:

Proof. Set $D_5 = \frac{D_7}{\max(a_\infty, b_\infty)}$ to see that (3.37) holds, and then combine (3.34), (3.35), (3.36) and (3.37) to reveal

$$D(a,b|a_\infty,b_\infty) \geq \frac{D_2D_4D_5}{D_3}E(\overline{a},\overline{b}|a_\infty,b_\infty).$$

In view of (3.33), we get

$$D(a,b|a_\infty,b_\infty) \geq D_8E(a,b|a_\infty,b_\infty)$$

for $D_8 = \min(\frac{D_2D_4D_5}{D_3}, D_1)$, which finally proves that the solution decays exponentially to the positive equilibrium at an explicit rate. □

3.1.4 Remarks on generalized model

Here we indicate how to adapt the above analysis to get convergence to the complex-balanced equilibrium for the following model

$$A + (r+1)B \rightleftharpoons rB + C,$$

where $r > 0$. By the Gagliardo-Nirenberg interpolation inequality [105] (in spatial dimension 1), we know that

$$\|u\|^2_{L^\infty} \leq C_1\|\nabla u\|^2_{L^2} \cdot \|u\|^2_{L^2} + C_2\|u\|^2_{L^2},$$

where $u = \sqrt{a}, \sqrt{b}, \sqrt{c}$. The above inequality implies the following

$$\|a\|_{L^\infty} \lesssim \|\nabla a\|^2_{L^2} \cdot \|a\|^2_{L^1} + \|a\|^2_{L^1} \lesssim \|\nabla a\|^2_{L^2} + \|a\|^2_{L^1};$$

the last inequality holds since $\|a\|^2_{L^1}$ has a uniform upper bound (due to the conservation law $\bar{a(t)} + \bar{c(t)} = \bar{a_0} + \bar{c_0}$). Therefore, we have

$$\int_0^T \|a\|_{L^\infty} dt \lesssim \int_0^T \|\nabla a\|^2_{L^2} dt + \|a\|^2_{L^1} \cdot T \lesssim H_1 + \|a\|^2_{L^1} \cdot T,$$

since $\int_0^\infty \|\nabla a\|^2_{L^2} dt = H_1 < \infty$ (similarly as (3.8)). Thus, we get that $\int_0^T \|a\|_{L^\infty} dt$ has at most linear growth, and this estimate holds for $b,\ c$ as well.

Now let us also make the assumption $\beta = \|\frac{1}{b_0}\|_{L^\infty[0,1]} < \infty$; because the classical solution is continuous, there exists $t_1 > 0$ such that $\|\frac{1}{b(\cdot,t)}\|_{L^\infty[0,1]} < 10\beta$ for all $t \in [0, t_1]$. We have the following equation for b:

$$\partial_t b - d_b \Delta b = b^r c - ab^{(r+1)}.$$

We next divide the above equation by $-b^{(r+1)}$ and get the following:

$$\partial_t\left(\frac{1}{b^r}\right) - d_b\Delta\left(\frac{1}{b^r}\right) = \frac{ab^{(r+1)}}{b^{(r+1)}} - \frac{b^r c}{b^{(r+1)}} - 2d_b r(r+2)\frac{|\nabla b|^2}{b^(r+2)} \leq a.$$

Using the maximum principle for the heat equation, we have that, for all $t \in [0, t_1]$,

$$\left\|\frac{1}{b^r(\cdot,t)}\right\|_{L^\infty[0,1]} \leq \left\|\frac{1}{b_0^r}\right\|_{L^\infty[0,1]} + \int_0^T \|a\|_{L^\infty} dt \lesssim \beta + \|a\|_{L^1}^2 \cdot t,$$

where $\beta = \|\frac{1}{b_0^r}\|_{L^\infty[0,1]} + H_1$. We can iterate this inequality in time to get

$$\widetilde{b}(t) := \inf_{x\in[0,1]} b^r(x,t) \geq (\beta + \|a\|_{L^1}^2 t)^{-1} \tag{3.40}$$

for all $t > 0$. We conclude that b^r decays to zero at most linearly, and use the following inequality

$$\Psi\left(\frac{ab^{(r+1)}}{a_\infty b_\infty^{(r+1)}}; \frac{b^r c}{b_\infty^r c_\infty}\right) = \left(\frac{b}{b_\infty}\right)^r \Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{b_\infty c_\infty}\right) \geq \frac{\widetilde{b}(t)}{b_\infty^r}\Psi\left(\frac{ab}{a_\infty b_\infty}; \frac{c}{b_\infty c_\infty}\right)$$

to get the L^1 convergence to the positive equilibrium by the same method as in the previous sections.

3.2 Instability of boundary equilibrium for a complex-balanced Reaction-Diffusion system

In this section, we study the network $A + 2B \rightleftharpoons B + C$ but in three dimensional space by using the elliptic and energy estimate to show that the unique boundary equilibria is locally instable (Theorem 3.2.1). Then for the general case of one reversible pair of reaction

$\alpha_1 A_1 + ... + \alpha_n A_n \rightleftharpoons \beta_1 A_1 + ... + \beta_n A_n$, we use the same technique but are able to show the locally stability of the unique positive equilibria (Theorem 3.2.4). It is worth mentioning that the local stability around positive equilibrium in L^∞ norm for this system can be achieved by [31] and [87]. This paper provides a different method to show the local stability in H^2 norm. Moreover we use this method using elliptic and energy estimate to show local instability around boundary equilibrium.

3.2.1 Introduction and some results

Here we consider $0 < T \leq \infty$ and a semi-linear parabolic system

$$\mathbf{u}_t - \mathcal{D}\Delta\mathbf{u} = R(\mathbf{u}) \text{ in } \Omega \times (0,T),$$

with an initial data

$$\mathbf{u}(\cdot,0) = \mathbf{u}_0 \text{ in } \Omega,$$

where $\mathbf{u} : \Omega \times [0,T) \to \mathbb{R}^n$ is a vector of concentrations at spatial position $x \in \Omega$ (an open and bounded subset of $\mathbb{R}^3$) and time $t \in [0,\infty)$, $\mathcal{D}$ is a positive definite, diagonal $n \times n$ matrix and we consider Neumann boundary conditions throughout this work:

$$\frac{\partial u_i}{\partial \mathbf{n}} := \nabla u_i \cdot \mathbf{n} = 0 \text{ on } \partial\Omega \times (0,T),\ i = 1,...,n,$$

where $\mathbf{n}$ is the outer normal vector at the boundary and $R : \mathbb{R}^n \to \mathbb{R}^n$ is a vector field whose components are polynomials and it is determined by the chemical reactions under consideration.

3.2.1.1 Instability

The system we consider in this section is $A + 2B \rightleftharpoons B + C$. The choice of spatial dimension $d = 3$ and we assume Ω is connected and bounded domain in $\mathbb{R}^3$. In this paper, our method to prove both stability and instability seems confined to three-D or lower, as it uses the Sobolev embedding inequality where the H^2 norm of the solutions leads to the boundness of the L^∞ norm. Notice that by rescaling time t, space x and the concentrations (a,b,c), from [46] we can always assume that reaction rates and domain volume are 1.

The corresponding 3×3 reaction-diffusion system is

$$\begin{cases} \widetilde{a}_t - d_a \Delta \widetilde{a} = -\widetilde{a}\widetilde{b}^2 + \widetilde{b}\widetilde{c} & x \in \Omega, t > 0, \\ \widetilde{b}_t - d_b \Delta \widetilde{b} = -\widetilde{a}\widetilde{b}^2 + \widetilde{b}\widetilde{c} & x \in \Omega, t > 0, \\ \widetilde{c}_t - d_c \Delta \widetilde{c} = \widetilde{a}\widetilde{b}^2 - \widetilde{b}\widetilde{c} & x \in \Omega, t > 0, \\ \frac{\partial \widetilde{a}}{\partial \mathbf{n}} = \frac{\partial \widetilde{b}}{\partial \mathbf{n}} = \frac{\partial \widetilde{c}}{\partial \mathbf{n}} = 0 & x \in \partial\Omega, t > 0, \\ \widetilde{a}(x,0) = \widetilde{a}_0(x), \widetilde{b}(x,0) = \widetilde{b}_0(x), \widetilde{c}(x,0) = \widetilde{c}_0(x) & x \in \Omega, \end{cases} \tag{3.41}$$

where $\mathbf{u} = (\widetilde{a}, \widetilde{b}, \widetilde{c})$ stands for the concentration of (A, B, C). In this case $\mathcal{D} = \text{diag}\{d_a, d_b, d_c\} \in M_{3\times3}(\mathbb{R})$ denotes the diagonal matrix of diffusion constants.

Considering the reaction system, we have the following conservation laws;

$$\begin{aligned} \int_\Omega \widetilde{a}(t,x)\ dx + \int_\Omega \widetilde{c}(t,x)\ dx &= \int_\Omega \widetilde{a}_0(x)\ dx + \int_\Omega \widetilde{c}_0(x)\ dx := M_1, \\ \int_\Omega \widetilde{b}(t,x)\ dx + \int_\Omega \widetilde{c}(t,x)\ dx &= \int_\Omega \widetilde{b}_0(x)\ dx + \int_\Omega \widetilde{c}_0(x)\ dx := M_2. \end{aligned} \tag{3.42}$$

From [46], in the case $A + 2B \rightleftharpoons B + C$ as long as $M_1 > M_2$ there are two types of equilibrium $(a_\infty, b_\infty, c_\infty)$ and $(a_\infty, 0, c_\infty)$ following (3.42), and we name $(a_\infty, b_\infty, c_\infty)$ as unique positive equilibrium and $(a_\infty, 0, c_\infty)$ as unique accessible boundary equilibrium. We exclude the case when $\int_\Omega b_0 dx = 0$, since in this situation the system degenerates to the heat equation and the solution converges to $(a_\infty, 0, c_\infty)$ because of b being zero.

To show the instability of boundary equilibria, we define $y^\intercal = (u^\intercal, u_t^\intercal)$ with $u = (\widetilde{a} - a_\infty, b, \widetilde{c} - c_\infty)^\intercal$ and get the equation for y such that $y_t = Ly + N(y)$ where L is the linear operator. Also we introduce two norms

$$\|y\| \coloneqq \|u\|_2 + \|u_t\|_2 \text{ and } \|\!|\!| y |\!|\!\| \coloneqq \|u\|_{H^2} + \|u_t\|_2,$$

where $\|\cdot\|_2$ represents the L^2 norm and $\|\cdot\|_{H^2}$ represents the H^2 norm. Our method to prove local instability for $A+2B \rightleftharpoons B+C$, as it first shows that the eigenvalues for operator L is non-positive [101] and then uses the energy estimate, elliptic estimate [5], and the rest is based on the argument of [52][50]. It is an important result that we can deal with local stability and local instability in this quadratic case in higher dimension.

In this section, we will prove the instability statement for accessible boundary equilibria, namely:

Theorem 3.2.1. *Consider a family of initial data $y^\delta(0) = \delta y_0$ with $\|y_0\| = 1$, $\int_\Omega b_0 dx \neq 0$ ($b_0 \geq 0$) and $|||y_0||| < \infty$ and let θ_0 be a fixed sufficiently small number. Then there exists a constant C_P and $\lambda > 0$ such that*

$$\|e^{Lt} y_0\| \geq C_P e^{\lambda t},$$

where L is a linear operator such that $y_t = Ly + N(y)$ and if $0 \leq t \leq T^\delta = \frac{1}{\lambda}\log\frac{\theta_0}{\delta}$, then at the escape time

$$\|y(T^\delta)\| \geq \tau_0 > 0,$$

where τ_0 depends explicitly on y_0 and is independent of δ.

Remark 3.2.2. In the following section, we define $T^* = \sup_t\{|||y||| < \sigma\}$ where σ is bounded and defined in Lemma 3.2.10 and in the proof of this theorem we show that $T^* \geq T^\delta$. Under the Sobolev embedding inequality, this guarantees the existence of solution up to the escape time T^δ.

We can use the same technique to adapt $A_1 + ... + A_l + 2B \rightleftharpoons B + C_1 + ... + C_r$ which is more generalized and we define $y^\intercal = (u^\intercal, u_t^\intercal)$ and $u = (\widetilde{a_1} - a_{1,\infty}, ..., \widetilde{a_l} - a_{l,\infty}, b, \widetilde{c_1} - c_{1,\infty}, ..., \widetilde{c_r} - c_{r,\infty})^\intercal$, we can prove the similar instability statement for accessible boundary equilibria, namely:

Theorem 3.2.3. *Consider a family of initial data $y^\delta(0) = \delta y_0$ with $\|y_0\| = 1$, $\int_\Omega b_0 dx \neq 0$ ($b_0 \geq 0$) and $|||y_0||| < \infty$ and let θ_0 be a fixed sufficiently small number. Then there exists a* *constant* C_P *and* $\lambda > 0$ *such that*

$$\|e^{Lt}y_0\| \geq C_P e^{\lambda t},$$

where L *is a linear operator such that* $y_t = Ly + N(y)$ *and if* $0 \leq t \leq T^\delta = \frac{1}{\lambda}\log\frac{\theta_0}{\delta}$*, then at the escape time*

$$\|y(T^\delta)\| \geq \tau_0 > 0,$$

where τ_0 *depends explicitly on* y_0 *and is independent of* δ*.*

The above theorems will be proved in next section.

3.2.1.2 Stability

Initially we consider proving the local stability at positive equilibria for simple case $A + 2B \rightleftharpoons B + C$ by defining the small perturbation $a = \widetilde{a} - a_\infty$, $b = \widetilde{b} - b_\infty$, $c = \widetilde{c} - c_\infty$ where $(a_\infty, b_\infty, c_\infty)$ is the unique positive equilibrium with $a_\infty b_\infty = c_\infty$ and compatible with the conservation law.

Therefore we get the following equation for perturbation

$$\begin{aligned} a_t - d_a\Delta a &= -(b + b_\infty)(ab - (c - b_\infty a - a_\infty b)), \\ b_t - d_b\Delta b &= -(b + b_\infty)(ab - (c - b_\infty a - a_\infty b)), \\ c_t - d_c\Delta c &= (b + b_\infty)(ab - (c - b_\infty a - a_\infty b)). \end{aligned} \tag{3.43}$$

By multiplying $b_\infty a, a_\infty b, c$ on (3.43) respectively and integrating over Ω by parts, we get the first part of the energy estimate.

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}(b_\infty\|a\|_2^2 + a_\infty\|b\|_2^2 + \|c\|_2^2) + (d_a b_\infty\|\nabla a\|_2^2 + d_b a_\infty\|\nabla b\|_2^2 + d_c\|\nabla c\|_2^2) \\ &= \int_\Omega (b + b_\infty)(ab - (c - b_\infty a - a_\infty b))(c - b_\infty a - a_\infty b)dx. \end{aligned} \tag{3.44}$$

Next step is the most crucial. We try to absorb the right hand side by the energy-dissipation term $d_a b_\infty \|\nabla a\|_2^2 + d_b a_\infty \|\nabla b\|_2^2 + d_c \|\nabla c\|_2^2$. However we can't apply Poincaré inequality to compare $\|\nabla a\|_2$ and $\|a\|_2$ directly since $\int_\Omega a\ dx$, $\int_\Omega b\ dx$, $\int_\Omega c\ dx$ is unknown. Motivated from the conservation law (3.42), we introduce two new variables $d = a + c, e = b + c$ where $\int_\Omega d\ dx = \int_\Omega e\ dx = 0$. Now we can apply Poincaré inequality on d and e to get

$$\|d\|_2 \lesssim \|\nabla d\|_2,\ \ \|e\|_2 \lesssim \|\nabla e\|_2.$$

In this paper, the notation $X \lesssim Y$ means that $X \leq CY$ for some constant $C > 0$.

Then we analyse the sign status for d and e and use the structure of non linearity along with Poincaré inequality, here we let $f = c - b_\infty a - a_\infty b$ to simplify the notation.

If $f \geq 0, ab \leq 0$ or $f \leq 0, ab \geq 0$, the integrand on the right hand side is non-positive, thus

$$\int_\Omega (b + b_\infty)(ab - (c - b_\infty a - a_\infty b))(c - b_\infty a - a_\infty b)dx \leq 0.$$

If $f < 0, ab < 0$ which implies a and b have different signs, thus

$$\begin{aligned}&\int_\Omega (b + b_\infty)(ab - (c - b_\infty a - a_\infty b))(c - b_\infty a - a_\infty b)dx \\ \lesssim &\int_\Omega (b + b_\infty)(ab)^2 dx = \int_\Omega b \cdot (ab)^2 dx + \int_\Omega b_\infty (ab)^2 dx.\end{aligned}$$

If $b \leq 0$, since $|ab| \lesssim (a - b)^2 = (d - e)^2$,

$$\int_\Omega b \cdot (ab)^2 dx + \int_\Omega b_\infty (ab)^2 dx \lesssim \int_\Omega (d^4 + e^4) dx.$$

If $b > 0$ which implies $a < 0$, we have $b < b - a = e - d \lesssim e^2 + d^2 + 1$,

$$\int_\Omega b \cdot (ab)^2 dx + \int_\Omega b_\infty (ab)^2 dx \lesssim \int_\Omega (e^2 + d^2 + 1)(d^4 + e^4) dx.$$

If $f > 0, ab > 0$ and if $f \geq ab$, the integrand on the right hand side is non-positive, thus

$$\int_\Omega (b + b_\infty)(ab - (c - b_\infty a - a_\infty b))(c - b_\infty a - a_\infty b)dx \leq 0.$$

If $0 < f < ab$ and if $a > 0, b > 0$, then we can get $c > b_\infty a + a_\infty b > 0$ which implies $d > a$ and $e > b$ and $ab < |d \cdot e| \lesssim d^2 + e^2$, then we have

$$\begin{aligned}
&\int_\Omega (b + b_\infty)(ab - (c - b_\infty a - a_\infty b))(c - b_\infty a - a_\infty b)dx \\
&\lesssim \int_\Omega (b + b_\infty)(ab)^2 dx = \int_\Omega b(ab)^2 dx + \int_\Omega b_\infty (ab)^2 dx \\
&\lesssim \int_\Omega (e^2 + 1)(d^4 + e^4)dx.
\end{aligned}$$

If $0 < f < ab$ and if $a < 0, b < 0, c \leq 0$, then we can get $d < a < 0$ and $e < b < 0$ and $ab < |d \cdot e| \lesssim d^2 + e^2$, then we have

$$\begin{aligned}
&\int_\Omega (b + b_\infty)(ab - (c - b_\infty a - a_\infty b))(c - b_\infty a - a_\infty b)dx \\
&\lesssim \int_\Omega (b + b_\infty)(ab)^2 dx \lesssim \int_\Omega (d^4 + e^4)dx.
\end{aligned}$$

If $0 < f < ab$ and if $a < 0, b < 0, c > 0$, then we have

$$ab + (b_\infty a + a_\infty b) > c > 0,$$

but $ab + (b_\infty a + a_\infty b) = b \cdot (a + a_\infty) + ab_\infty < 0$, this is the impossible case.

After considering all above cases, we can get the following

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}(b_\infty \|a\|_2^2 + a_\infty \|b\|_2^2 + \|c\|_2^2) + (d_a b_\infty \|\nabla a\|_2^2 + d_b a_\infty \|\nabla b\|_2^2 + d_c \|\nabla c\|_2^2) \\
&\lesssim g(\|a, b, c\|_\infty)(\|\nabla d\|_2^2 + \|\nabla e\|_2^2),
\end{aligned} \tag{3.45}$$

where $g(\|a,b,c\|_\infty) = \|(e^2+d^2)(e^2+d^2+1)\|_\infty$ and provided that $\|a,b,c\|_{L^\infty}$ is small enough such that $g \le \min(d_a b_\infty, d_b a_\infty, d_c)$, we have

$$\frac{d}{dt}(b_\infty\|a\|_2^2 + a_\infty\|b\|_2^2 + \|c\|_2^2) + (d_a b_\infty\|\nabla a\|_2^2 + d_b a_\infty\|\nabla b\|_2^2 + d_c\|\nabla c\|_2^2) \le 0. \tag{3.46}$$

Then we apply ∂_t on (3.43) and multiply them by $b_\infty a_t, a_\infty b_t, c_t$ respectively, then integrating over Ω by parts and sum up all three terms, we get

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}(b_\infty\|a_t\|_2^2 + a_\infty\|b_t\|_2^2 + \|c_t\|_2^2) + (d_a b_\infty\|\nabla a_t\|_2^2 + d_b a_\infty\|\nabla b_t\|_2^2 + d_c\|\nabla c_t\|_2^2)\\ &= \int_\Omega (b_\infty a_t + a_\infty b_t - c_t) b_t (c - a_\infty b - b_\infty a - ab)dx + \int_\Omega (b_\infty a_t + a_\infty b_t - c_t)\widetilde{b}(c_t - a_t\widetilde{b} - b_t\widetilde{a})dx.\end{aligned} \tag{3.47}$$

Similarly we analyse the sign status for the following variables $d_t = a_t + c_t, e_t = b_t + c_t$ which is also motivated from the conservation law and we also get

$$\int_\Omega d_t\ dx = \int_\Omega e_t\ dx = 0, \|d_t\|_2 \lesssim \|\nabla d_t\|_2,\ \|e_t\|_2 \lesssim \|\nabla e_t\|_2.$$

Considering all possible cases, we are able to show that if $\|a,b,c\|_{L^\infty}$ is small enough, we have the following

$$\frac{d}{dt}(b_\infty\|a_t\|_2^2 + a_\infty\|b_t\|_2^2 + \|c_t\|_2^2) + (d_a b_\infty\|\nabla a_t\|_2^2 + d_b a_\infty\|\nabla b_t\|_2^2 + d_c\|\nabla c_t\|_2^2) \lesssim 0. \tag{3.48}$$

Combing energy estimate (3.46)(3.48) with the elliptic estimate (from Theorem 3.2.6 in Section 2)

$$\|v_i\|_{H_2} \lesssim \|bc - ab^2 - 2abb_\infty - b^2 a_\infty\|_2 + \sum_{i=1}^3 \|\partial_t(v_i)\|_2 + \sum_{i=1}^3 \|v_i\|_2,$$

where $v = (a,b,c)$. Then we have the local stability for a, b, c in H^2 sense.

In the section 3.2.3, we consider the generalized case for one reversible pair

$$\alpha_1 A_1 + ... + \alpha_n A_n \rightleftharpoons \beta_1 A_1 + ... + \beta_n A_n.$$

The corresponding $n \times n$ reaction-diffusion system is

$$\begin{cases} \partial_t \widetilde{u}_i - d_i \Delta \widetilde{u}_i = (\beta_i - \alpha_i)(\widetilde{u}^\alpha - \widetilde{u}^\beta) & x \in \Omega, t > 0, \\ \nabla \widetilde{u}_i \cdot n = 0 & x \in \partial\Omega, t > 0, \\ \widetilde{u}_i(x, 0) = \widetilde{u}_{i,0}(x) & x \in \Omega, \end{cases} \tag{3.49}$$

where $\alpha = (\alpha_1, ..., \alpha_n)$ and $\beta = (\beta_1, ..., \beta_n)$ and α_i, β_j are non-negative integers. In this case $\mathcal{D} = \text{diag}\{d_i\} \in M_{n\times n}(\mathbb{R})$ denotes the diagonal matrix of diffusion constants.

From [46], as long as $\int_\Omega \widetilde{u}_{i,0}(x)\ dx > 0$ there must exist the unique positive equilibria and we name it as $u_\infty = (u_{1_\infty}, u_{2_\infty}, ..., u_{n_\infty})$. Therefore we have the unique positive equilibrium u_∞ with $u_\infty^\alpha = u_\infty^\beta$ under the conservation law $\forall i \in L := \{i \in \{1, ..., n\} | \alpha_i > \beta_i\}$, $\forall j \in R := \{j \in \{1, ..., n\} | \alpha_j < \beta_j\}$.

$$(\alpha_j - \beta_j) \int_\Omega \widetilde{u}_i(t, x)\ dx + (\beta_i - \alpha_i) \int_\Omega \widetilde{u}_j(t, x)\ dx = (\alpha_i - \beta_i) u_{i_\infty} + (\beta_j - \alpha_j) u_{j_\infty} := M_{i,j}. \tag{3.50}$$

We exclude the case when $\int_\Omega \widetilde{u}_i(t, x)\ dx = 0$, since in this situation the system degenerates to the heat equation and the solution converges to the boundary.

The method to prove local stability for $\alpha_1 A_1 + ... + \alpha_n A_n \rightleftharpoons \beta_1 A_1 + ... + \beta_n A_n$ is similar as in $A + 2B \rightleftharpoons B + C$ case. We show the energy which consists of L^2 norm of u and L^2 norm of u_t is non-increasing by energy estimate and analysing the sign status for every u_i. Then the elliptic estimate can show the local stability for u_i in H^2 sense.

In this section, we prove the local stability for the unique positive equilibrium $u_\infty = (u_{1_\infty}, u_{2_\infty}, ..., u_{n_\infty})$, namely:

Theorem 3.2.4. *For system* (3.49)*, there exists small constant* θ *such that if the initial perturbation* $u(x,0)$ *satisfying*

$$\sum_{i=1}^{n}(\|\partial_t u_i(x,0)\|_2 + \|u_i(x,0)\|_\infty) \le \theta,$$

then we have

$$\sum_{i=1}^{n} \|u_i(x,t)\|_{H_2} \lesssim e^{-lt},$$

where l *depends explicitly on* α, β *and* θ*.*

The above theorem will be proved in the Section 3.2.3.

3.2.2 Instability of boundary equilibria

3.2.2.1 Instability for $A + 2B \rightleftharpoons B + C$

Since we want to show the instability at the boundary equilibrium $(a_\infty, 0, c_\infty)$, we introduce three new variables as perturbation around the boundary equilibria.

$$a = \widetilde{a} - a_\infty, b = b, c = \widetilde{c} - c_\infty, u = (a, b, c)^\intercal. \tag{3.51}$$

Thus we have the conservation law for (a, b, c),

$$\int_\Omega a(t,x)\ dx + \int_\Omega c(t,x)\ dx = 0, \int_\Omega b(t,x)\ dx + \int_\Omega c(t,x)\ dx = 0. \tag{3.52}$$

Note that

$$-\widetilde{a}\widetilde{b}^2 + \widetilde{b}\widetilde{c} = -(a + a_\infty)b^2 + b(c + c_\infty) = bc_\infty + (bc - (a + a_\infty)b^2).$$

Therefore we get the equations for u,

$$\begin{cases} a_t - d_a\Delta a = bc_\infty + (bc - (a+a_\infty)b^2) & x \in \Omega, t > 0, \\ b_t - d_b\Delta b = bc_\infty + (bc - (a+a_\infty)b^2) & x \in \Omega, t > 0, \\ c_t - d_c\Delta c = -bc_\infty - (bc - (a+a_\infty)b^2) & x \in \Omega, t > 0, \\ \frac{\partial a}{\partial \mathbf{n}} = \frac{\partial b}{\partial \mathbf{n}} = \frac{\partial c}{\partial \mathbf{n}} = 0 & x \in \partial\Omega, t > 0, \\ a(x,0) = a_0(x), b(x,0) = b_0(x), c(x,0) = c_0(x) & x \in \Omega. \end{cases} \tag{3.53}$$

It is convenient to express (3.53) as

$$u_t = L_1 u + N_1(u), \tag{3.54}$$

where $L_1 := \begin{pmatrix} d_a\Delta & c_\infty & 0 \\ 0 & d_b\Delta + c_\infty & 0 \\ 0 & -c_\infty & d_c\Delta \end{pmatrix}$ and $N_1(u) := \begin{pmatrix} bc - (a+a_\infty)b^2 \\ bc - (a+a_\infty)b^2 \\ -bc + (a+a_\infty)b^2 \end{pmatrix}$.

We cite Theorem 1.1 and Theorem 1.2 in Section 11.3 in [101]. For open and bounded the domain Ω with sufficient smooth boundary and the Neumann boundary condition, we denote the eigenvalues by λ_j and the eigenfunctions by $v_j(x)$. Thus

$$\begin{cases} -\Delta v_j(x) = \lambda_j v_j(x) & x \in \Omega, \\ \frac{\partial v_j(x)}{\partial \mathbf{n}} = 0 & x \in \partial\Omega. \end{cases}$$

Then we can number them in ascending order,

$$0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq ...$$

The first eigenfunction $v_1(x)$ is a constant and the eigenfunctions forming a basis are complete in the L_2 sense.

Therefore the largest eigenvalue for Laplace operator is zero with the corresponding eigen-function is the constant function.

Lemma 3.2.5. *For the linear partial differential equations*

$$\begin{cases} u_t = L_1 u & x \in \Omega, t > 0, \\ \frac{\partial u}{\partial \mathbf{n}} = 0 & x \in \partial\Omega, t > 0, \end{cases}$$

we have the following estimate

$$\|e^{tL_1} u_0\|_2 \leq 3e^{c_\infty t}\|u_0\|_2.$$

Proof. To get the eigenvalues λ for $(d_b\Delta + c_\infty)b$ such that

$$(d_b\Delta + c_\infty)b = \lambda b \implies d_b\Delta b = (\lambda - c_\infty)b.$$

Since the largest eigenvalue for Laplace operator is zero, we have $\lambda \leq c_\infty$. And because the eigenfunctions forming a basis are complete in the L_2 sense, we can write initial data $b_0 \in L^2$ as $b_0(x) = \sum\limits_j b_j v_j(x)$ in the L_2 sense and we get

$$b(t,x) = e^{tL_1} b_0 = \sum_j b_j e^{\lambda_j t} v_j(x),$$

also in the L_2 sense, therefore

$$\begin{aligned} \|b(t,x)\|_2 = \|\sum_j b_j e^{\lambda_j t} v_j(x)\|_2 &= \sum_j \|e^{\lambda_j t} b_j v_j(x)\|_2 \\ \leq \sum_j \|e^{c_\infty t} b_j v_j(x)\|_2 &= e^{c_\infty t}\|\sum_j b_j v_j(x)\|_2 = e^{c_\infty t}\|b_0\|_2. \end{aligned}$$

Then for $a_t = d_a\Delta a + c_\infty b$, $c_t = d_c\Delta c - c_\infty b$, we multiply a and c, integrate over domain Ω

respectively and we get

$$\frac{1}{2}\frac{d}{dt}\|a\|_2^2 = \int_\Omega d_a \Delta a \ a \ dx + \int_\Omega c_\infty ba \ dx$$
$$= -\int_\Omega d_a |\nabla a|^2 dx + \int_\Omega c_\infty ba \ dx \le c_\infty \|a\|_2 \|b\|_2,$$

$$\frac{1}{2}\frac{d}{dt}\|c\|_2^2 = \int_\Omega d_c \Delta c \ c \ dx - \int_\Omega c_\infty bc \ dx$$
$$= -\int_\Omega d_c |\nabla c|^2 dx - \int_\Omega c_\infty bc \ dx \le c_\infty \|c\|_2 \|b\|_2.$$

which implies

$$\frac{d}{dt}\|a\|_2 \le c_\infty \|b\|_2 \le c_\infty e^{c_\infty t}\|b_0\|_2, , \ \frac{d}{dt}\|c\|_2 \le c_\infty \|b\|_2 \le c_\infty e^{c_\infty t}\|b_0\|_2.$$

Therefore we have

$$\|a(t,x)\|_2 \le \|a_0\|_2 + e^{c_\infty t}\|b_0\|_2, \ \|c(t,x)\|_2 \le \|c_0\|_2 + e^{c_\infty t}\|b_0\|_2. \tag{3.55}$$

□

In order to use the elliptic estimate, we also need the following variables

$$a_t = \widetilde{a}_t, b_t = \widetilde{b}_t, c_t = \widetilde{c}_t, u_t = (a_t, b_t, c_t)^\intercal.$$

Taking the time derivative on (3.54), we get

$$u_{tt} = L_2 u_t + N_2(u, u_t), \tag{3.56}$$

where $N_2(u, u_t) := \partial_t[N_1(u)]$ and $L_2 = L_1$.

Now we define $y^\intercal = (u^\intercal, u_t^\intercal)$ and get the equation for y,

$$y_t = Ly + N(y), \tag{3.57}$$

where $L = \begin{pmatrix} L_1 & 0 \\ 0 & L_2 \end{pmatrix}$ and $N(y) = \begin{pmatrix} N_1(u) \\ N_2(u, u_t) \end{pmatrix}$.

Considering Lemma 3.2.5 and L is block diagonal matrix, we can get

$$\begin{aligned} \|e^{tL}y\| &= \|e^{tL_1}u\|_2 + \|e^{tL_2}u_t\|_2 \\ &\leq 3e^{c_\infty t}\|u\|_2 + 3e^{c_\infty t}\|u_t\|_2 = 3e^{c_\infty t}\|y\|. \end{aligned}$$

Therefore we have

$$\|e^{tL}\| = \sup_{\|y\|\leq 1} \frac{\|e^{tL}y\|}{\|y\|} \leq 3e^{c_\infty t}. \tag{3.58}$$

In order to get the elliptic estimate, we cite the Theorem 10.5 in [5].

Supplementary Condition on L**.** $L(P, \Xi)$ is of even degree $2m$ (with respect to Ξ). For every pair linearly independent real vectors Ξ, Ξ', the polynomial $L(P, \Xi + \tau\Xi')$ in the complex variable τ has exactly m roots with positive imaginary part.

In this condition, P represents the points on the boundary $\partial\Omega$ and Ξ represents the tangent vector and Ξ' represents the normal vector at P.

Complementing Boundary Condition. For any $P \in \partial\Omega$ and any real, non-zero vector Ξ tangent to $\partial\Omega$ at P, let us regard $M^+(P, \Xi, \tau) = \prod_{h=1}^{m=3} (\tau - \tau_h^+(P, \Xi))$ where $\tau_h^+(P, \Xi)$ with $h = 1, 2, 3$ are the m roots (in τ) with positive imaginary part of the characteristic equation $L(P, \Xi + \tau\vec{n}) = 0$. And the elements of the matrix

$$\sum_{j=1}^{N} B'_{hj}(P, \Xi + \tau\vec{n}) L^{jk}(P, \Xi + \tau\vec{n}),$$

as polynomials in the indeterminate τ where $L^{jk}(P, \Xi + \tau\vec{n})$ is the matrix adjoint to $(l'_{ij}(P, \Xi + \tau\vec{n}))$. The definition of l'_{ij} will be shown in the following Theorem. The rows of the latter matrix are required to be linearly independent modulo $M^+(P, \Xi, \tau)$, i.e.,

$$\sum_{h=1}^{m} C_h \sum_{j=1}^{N} B'_{hj} L^{jk} \equiv 0 \ (\mathrm{mod}\ M^+),$$

only if the constants C_h are all zero.

Theorem 3.2.6. *For the elliptic systems of partial differential equations*

$$\sum_{j=1}^{N} l_{ij}(P, \partial) u_j(P) = F_i(P), \ \ i = 1, ..., N,$$

where the $l_{ij}(P, \partial)$, linear differential operators, are polynomials in $\partial = \{\partial_{x_1}, ..., \partial_{x_{n+1}}\}$ with coefficients depending on P over some domain Ω in $x_1, ..., x_{n+1}$-space. The orders of these operators are assumed to depend on two systems of integer weights, $s_1, ..., s_N$ and $t_1, ..., t_N$, attached to the equations and to the unknowns, respectively, s_i corresponding to the i-th equation and t_j to the j-th dependent variable u_j. The manner of the dependence is expressed by the inequality

$$\deg l_{ij}(P, \Xi) \leq s_i + t_j, \ \ i, j = 1, ..., N,$$

"deg" referring of course to the degree in Ξ.

If $L = \det(l'_{ij}(P))$ where $l'_{ij}(P)$ consists of the terms in $l_{ij}(P)$ which are just of the order $s_i + t_j$ (the leading part with the highest order) satisfies the supplementary condition and the boundary conditions are complementing

$$\sum_{j=1}^{N} B_{hj}(P, \partial) u_j(P) = \varphi_h(P) \ \text{on} \ \partial\Omega, \ \ h = 1, ..., m,$$

in terms of given polynomials in Ξ, $B_{hj}(P, \Xi)$, with complex coefficients depending on P with $m = \frac{1}{2}\deg(L(P)) > 0$. The orders of the boundary operators depend on two systems of integer *weights, in this case the system* $t_1, ..., t_N$*, already attached to the dependent variables and a new system* $r_1, ..., r_m$ *of which* r_h *pertains to the h-th boundary condition. The exact dependence is that expressed by the inequality*

$$\deg B_{hj}(P, \Xi) \leq r_h + t_j, \ \ h = 1, ..., m, j = 1, ..., N,$$

A constant K exists such that, if $\|u_j\|_{l_1+t_j}$ *is finite for j=1,...,N, then for a given integer* $l \geq l_1$*,* $\|u_j\|_{l+t_j}$ *is also finite, and*

$$\|u_j\|_{l+t_j} \leq K(\sum_i \|F_i\|_{l-s_i} + \sum_h \|\varphi_h\|_{l-r_h-1/p} + \sum_j \|u_j\|_0),$$

where $\|\cdot\|_j = \|\cdot\|_{H_j}$ *and K is dependent on the domain and the modulus of continuity of the leading coefficients in the* l_{ij}*.*

From the above Theorem 3.2.6, we get the following lemma.

Lemma 3.2.7. *For the system* $u_t = L_1 u + N_1(u)$ *in* (3.54) *with Neumann boundary condition* $\frac{\partial u}{\partial \mathbf{n}}|_{\partial\Omega} = 0$*, we have the following elliptic estimate*

$$\|u_i\|_{H_2} \lesssim \|N_1(u)\|_2 + \|u\|_2 + \|u_t\|_2.$$

Proof. We first need to check whether the system satisfies the conditions in Theorem 3.2.6. Now we rewrite the system (3.54) by putting u_t to the right side.

We set $s_i = 0, t_j = 2$ with $1 \leq i, j \leq 3$. Therefore we get

$$L(P, \Xi) = \det(l'_{ij}(P, \Xi)) = d_a d_b d_c(\xi_1^2 + \xi_2^2 + \xi_3^2)^3,$$

where $\Xi = (\xi_1, \xi_2, \xi_3)$. It's obvious to see $L \neq 0$ for real $\Xi \neq 0$ which implies it is the elliptic system. Next we check the supplement condition on operator L. $L(P, \Xi)$ is of the even degree

$2m$ with $m = 3$. Then for every pair of linearly independent real vectors Ξ, Ξ', we have

$$L(P, \Xi + \tau\Xi') = d_a d_b d_c((\xi_1 + \tau\xi_1')^2 + (\xi_2 + \tau\xi_2')^2 + (\xi_3 + \tau\xi_3')^2)^3.$$

The above polynomial has exactly $m = 3$ roots with positive imaginary roots since any real number can't be the root because of the linear independence and symmetric of the polynomial. We can also pick sufficient large A such that

$$A^{-1}|\Xi|^{2m} \leq |L(P, \Xi)| \leq A|\Xi|^{2m},$$

to show the system is uniform elliptic.

Next we need to check whether Neumann boundary condition is complementing . Since we have Neumann boundary condition which means

$$(n_1 \cdot \partial_1 + n_2 \cdot \partial_2 + n_3 \cdot \partial_3)v_i = 0, \text{ for } i = 1, 2, 3.$$

Then we set $r_h = -1$ with $h = 1, 2, 3$.

Here we set Ξ be any tangent to $\partial\Omega$ and $P \in \partial\Omega$. Therefore $B'_{hj}(P, \Xi) = n_1 \cdot \xi_1 + n_2 \cdot \xi + n_3 \cdot \xi_3$ if $h = j$. Since we know $L(P, \Xi + \tau\vec{n}) = 0$ has three roots with positive imaginary part $\tau_h^+(P, \Xi)$ with $h = 1, 2, 3$. We set

$$M^+(P, \Xi, \tau) = \prod_{h=1}^{m=3} (\tau - \tau_h^+(P, \Xi)).$$

And let $(L^{jk}(P, \Xi+\tau\vec{n}))$ denote the matrix ad-joint to $(l'_{ij}(P, \Xi+\tau\vec{n}))$. Then we have $(L^{jk}(P, \Xi+$

$\tau\vec{n})) = \text{diag}\{d_b d_c, d_a d_c, d_a d_b\} \cdot (\xi_1^2 + \xi_2^2 + \xi_3^2)^2$ which is also a diagonal matrix. Thus we get

$$\begin{aligned}
&\sum_{h=1}^{m=3} C_h \sum_{j=1}^{N=3} B'_{hj} L^{jk}(P, \Xi + \tau\vec{n}) \\
&= \widetilde{C_k}(n_1 \cdot (\xi_1 + \tau n_1) + n_2 \cdot (\xi + \tau n_2) + n_3 \cdot (\xi_3 + \tau n_3)) \\
&\quad \times ((\xi_1 + \tau n_1)^2 + (\xi_2 + \tau n_2)^2 + (\xi_3 + \tau n_3)^2)^2 \equiv 0 \ (\text{mod } M^+),
\end{aligned}$$

for $k = 1, 2, 3$ only if $\vec{n} \parallel (\xi_1 + \tau n_1, \xi_2 + \tau n_2, \xi_3 + \tau n_3)$ or $\{C_k\}$ are all zero. It's obvious to see that Neumann boundary conditions satisfy the complementing boundary condition. Then Theorem 3.2.6 shows that with $l_1 = \max(0, r_h + 1) = 0$, if $\|u_i\|_{H_2}$ are all finite, pick $l = l_1$, then for $i = 1, 2, 3$, we have

$$\|u_i\|_{H_2} \leq K(\|N_1(u)\|_2 + \sum_{i=1}^{3} \|\partial_t u_i\|_2 + \sum_{i=1}^{3} \|u_i\|_2), \tag{3.59}$$

where K is a constant depends on origin equation and bounded domain. □

Now we we start proving our main theorem, Theorem 3.2.1. First we show the existence of y_0 and the corresponding constant C_P.

Lemma 3.2.8. *If $\|y_0\| = 1$, $\int_\Omega b_0 dx \neq 0$ ($b_0 \geq 0$) and $|||y_0||| < \infty$, there exists $C_p > 0$ such that , there exists $C_p > 0$ such that*

$$\|e^{tL} y_0\| \geq C_P e^{c_\infty t}.$$

Proof. In our case, the conservation law and $\int_\Omega b_0 dx \neq 0$ imply

$$\int_\Omega b_0(x) dx = \int_\Omega a_0(x) dx = -\int_\Omega c_0(x) dx > 0. \tag{3.60}$$

Taking the integration over the domain Ω on first linear part $u_t = L_1 u$, we get

$$\frac{d}{dt}\int_\Omega b(t,x)dx = c_\infty \int_\Omega b(t,x)dx, \tag{3.61}$$

which implies

$$\int_\Omega b(t,x)dx = e^{c_\infty t}\int_\Omega b_0(x)dx. \tag{3.62}$$

Similarly from $u_t = L_1 u$, we get equations for a and c

$$\frac{d}{dt}\int_\Omega a(t,x)dx = c_\infty \int_\Omega b(t,x)dx, \ \frac{d}{dt}\int_\Omega c(t,x)dx = -c_\infty \int_\Omega b(t,x)dx. \tag{3.63}$$

From (3.60) and (3.63), we have

$$\int_\Omega a(t,x)dx = e^{c_\infty t}\int_\Omega b_0(x)dx, \ \int_\Omega c(t,x)dx = -e^{c_\infty t}\int_\Omega b_0(x)dx, \tag{3.64}$$

which implies

$$\|e^{tL_1}u_0\|_2 \geq 3\bar{b_0}e^{c_\infty t}, \tag{3.65}$$

where $\bar{b_0} := \int_\Omega b_0 dx$. Again by the conservation law, the second part $u_{tt} = L_2 u_t$ shows

$$\int_\Omega b_t(t,x)dx = \frac{d}{dt}\int_\Omega b(t,x)dx = c_\infty e^{c_\infty t}\int_\Omega b_0(x)dx. \tag{3.66}$$

Also by the conservation law (3.52) and (3.63), we have

$$\begin{aligned} \int_\Omega a_t(t,x)dx &= \frac{d}{dt}\int_\Omega a(t,x)dx = c_\infty e^{c_\infty t}\int_\Omega b_0(x)dx, \\ \int_\Omega c_t(t,x)dx &= \frac{d}{dt}\int_\Omega c(t,x)dx = -c_\infty e^{c_\infty t}\int_\Omega b_0(x)dx, \end{aligned} \tag{3.67}$$

which again imply

$$\|e^{tL_2}u_t\|_2 \geq 3c_\infty \bar{b_0}e^{c_\infty t}. \tag{3.68}$$

From (3.65) and (3.68), we can have the following

$$\|e^{tL}y_0\| \geq C_P e^{c_\infty t},$$

where $C_P = 3(c_\infty + 1)\bar{b_0}$. □

Then we do the estimate on the non-linear part $N(y)$ in the norm of $\|\cdot\|$.

Lemma 3.2.9.

$$\|N(y)\| \lesssim \||y\||^2 + \|| y \||^3 .$$

Proof.

$$\begin{aligned} \|N(y)\| &= \|N_1(u)\|_2 + \|N_2(u,u_t)\|_2 \\ &= 3\|bc - (a+a_\infty)b^2\|_2 + 3\|(bc-(a+a_\infty)b^2)_t\|_2. \end{aligned} \tag{3.69}$$

By using Sobolev embedding inequality $\|y\|_\infty \leq C_{SI} \cdot \|y\|_{H_2}$, we can control the right hand side by norm $\||\cdot\||$. For the $N_1(u)$ part,

$$\begin{aligned} \|bc - (a+a_\infty)b^2\|_2 &\leq \|bc\|_2 + \|ab^2\|_2 + \|\widetilde{a}_\infty b^2\|_2 \\ &\leq \|b\|_\infty(\|c\|_2 + \|\widetilde{a}_\infty b\|_2 + \|b\|_\infty\|a\|_2) \\ &\leq C_{SI}(1+a_\infty) \|| y \||^2 + C_{SI}^2 \|| y \||^3 . \end{aligned}$$

For the $N_2(u,u_t)$ part,

$$\begin{aligned} &\|(bc-(a+a_\infty)b^2)_t\|_2 \leq \|(bc)_t\|_2 + \|(ab^2)_t\|_2 + \|(\widetilde{a}_\infty b^2)_t\|_2 \\ &\leq (\|b\|_\infty\|c_t\|_2 + \|c\|_\infty\|b_t\|_2) + (\|b\|_\infty^2\|a_t\|_2 + 2\|a\|_\infty\|b\|_\infty\|b_t\|_2) + 2\widetilde{a}_\infty\|b\|_\infty\|b_t\|_2 \\ &\leq 2C_{SI}(1+a_\infty) \|| y \||^2 + 3C_{SI}^2 \|| y \||^3 . \end{aligned}$$

Combining the above two parts, we get the following

$$\|N(y)\| \leq C_N(|||y\,|||^2 + |||\,y|||^3), \tag{3.70}$$

for all y and $|||y||| \leq \infty$ and constant $C_N = \max\{9C_{SI}(1+a_\infty), 12C_{SI}^2\}$.

□

Next we do the estimate on u and u_t in the norm of $|||\cdot|||$.

Lemma 3.2.10. *Suppose $|||y||| < \sigma$ and σ is sufficiently small with $\|a,b,c\|_\infty < C_{SI}\cdot\sigma$ such that $\|b\|_\infty(1+\|a\|_\infty+a_\infty) < \min(c_\infty, 1)$ and $\|b\|_\infty+\|b\|_\infty^2+\|c\|_\infty+2(\|a\|_\infty+a_\infty)\|b\|_\infty < \min(c_\infty, 1)$, we have the following estimate*

$$|||y|||^2 \lesssim \int_0^t \|y\|^2 \; ds + \|y_0\|^2.$$

Proof. Given $|||y||| < \sigma$ is sufficiently small, we have the smallness of $\|a,b,c\|_\infty < C_{SI}\cdot\sigma$ by Sobolev embedding inequality. Recall the equations (3.53), we multiply a, b, c respectively and do the integral over the domain Ω and get

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}(\|a\|_2^2 + \|b\|_2^2 + \|c\|_2^2) + (d_a\|\nabla a\|_2^2 + d_b\|\nabla b\|_2^2 + d_c\|\nabla c\|_2^2)\\
&= \int_\Omega (a+b-c)b\widetilde{c}_\infty + (a+b-c)(bc-(a+a_\infty)b^2)\; dx\\
&\leq c_\infty\|b\|_2(\|a\|_2+\|b\|_2+\|c\|_2) + \int_\Omega (a+b-c)(bc-(a+a_\infty)b^2)\; dx\\
&\leq c_\infty\|u\|_2^2 + \|b\|_\infty(1+\|a\|_\infty+a_\infty)\|u\|_2^2 \lesssim \|u\|_2^2.
\end{aligned} \tag{3.71}$$

Next on the equations (3.56), we multiply a_t, b_t, c_t respectively and do the integral over the domain Ω again and get

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}(\|a_t\|_2^2 + \|b_t\|_2^2 + \|c_t\|_2^2) + (d_a\|\nabla a_t\|_2^2 + d_b\|\nabla b_t\|_2^2 + d_c\|\nabla c_t\|_2^2) \\
&= \int_\Omega (a_t + b_t - c_t)b_t c_\infty + (a_t + b_t - c_t)(bc - (a + a_\infty)b^2)_t \; dx \\
&= \int_\Omega (a_t + b_t - c_t)b_t c_\infty + (a_t + b_t - c_t)(b_t c + bc_t - a_t b^2 - 2(a + a_\infty)bb_t) \; dx \\
&\le c_\infty\|b_t\|_2(\|a_t\|_2 + \|b_t\|_2 + \|c_t\|_2) + (\|a_t\|_2 + \|b_t\|_2 + \|c_t\|_2) \\
&\quad \times (\|b_t\|_2\|c\|_\infty + \|c_t\|_2\|b\|_\infty + \|a_t\|_2\|b\|_\infty^2 + 2(\|a\|_\infty + a_\infty)\|b\|_\infty\|b_t\|_2) \\
&\le C_{u_t}(\|a_t\|_2 + \|b_t\|_2 + \|c_t\|_2)^2,
\end{aligned}$$

where constant $C_{u_t} = 3[c_\infty + \|b\|_\infty + \|b\|_\infty^2 + \|c\|_\infty + 2(\|a\|_\infty + a_\infty)\|b\|_\infty]$.

Then we get

$$\frac{d}{dt}(\|a_t\|_2^2 + \|b_t\|_2^2 + \|c_t\|_2^2) \le 2C_{u_t}(\|a_t\|_2 + \|b_t\|_2 + \|c_t\|_2)^2. \tag{3.72}$$

Recall the elliptic estimate (3.59)

$$\|u_i\|_{H_2} \lesssim \|bc - (a + a_\infty)b^2\|_2 + \|u\|_2 + \|u_t\|_2 \text{ with } u = (a, b, c)^\intercal.$$

Combining this with (3.71), (3.72), we get the H_2 estimate for u which is the first part of $|||\cdot|||$ norm

$$\begin{aligned}
&\|u_i\|_{H_2}^2 \lesssim \|bc - (a + a_\infty)b^2\|_2^2 + \|u\|_2^2 + \|u_t\|_2^2 \\
&\le \|b\|_\infty^2(1 + \|a\|_\infty + a_\infty)^2\|u\|_2^2 + \|u\|_2^2 + \|u_t\|_2^2 \lesssim \|u\|_2^2 + \|u_t\|_2^2 \\
&\lesssim \int_0^t \|b\|_2(\|a\|_2 + \|b\|_2 + \|c\|_2) \; ds + \|a_0\|_2^2 + \|b_0\|_2^2 + \|c_0\|_2^2 \\
&\quad + \int_0^t (\|a_t\|_2 + \|b_t\|_2 + \|c_t\|_2)^2 \; ds + \|a_t(0)\|_2^2 + \|b_t(0)\|_2^2 + \|c_t(0)\|_2^2 \\
&\lesssim \int_0^t \|y\|^2 \; ds + \|y_0\|^2,
\end{aligned} \tag{3.73}$$

where the above inequalities hold because $|||y||| \le \sigma$. Again from (3.72), we get the L_2 estimate for u_t which is the second part of $|||\cdot|||$ norm

$$\begin{aligned}
&\|u_t\|_2^2 \lesssim \|a_t\|_2^2 + \|b_t\|_2^2 + \|c_t\|_2^2 \\
&\le \int_0^t (\|a_t\|_2 + \|b_t\|_2 + \|c_t\|_2)^2 \, ds + \|a_t(0)\|_2^2 + \|b_t(0)\|_2^2 + \|c_t(0)\|_2^2 \\
&\lesssim \int_0^t \|y\|^2 \, ds + \|y_0\|^2.
\end{aligned} \tag{3.74}$$

□

Finally, we proof Theorem 3.2.1 with all above lemma. The proof is based on the argument of [52].

Proof. Now we denote

$$\begin{aligned}
&T^\delta = \frac{1}{c_\infty} \log \frac{\theta_0}{\delta}, \\
&T^* = \sup_t \{|||y||| < \sigma\}, \\
&T^{**} = \sup_t \{\|y\| \le 2\delta e^{c_\infty t} \|y_0\|\}.
\end{aligned}$$

For $t \le \min\{T^\delta, T^*, T^{**}\}$, we can get from (3.73) and (3.74), and consider a family of initial data $y^\delta(0) = \delta y_0$ with $\|y_0\| = 1$ and $|||y_0||| < \infty$,

$$|||y|||^2 \lesssim \int_0^t \|y\|^2 \, ds + \delta^2 \|y_0\|^2 \lesssim \|y_0\|^2 (\delta^2 e^{2\tilde{c}_\infty t} + \delta^2),$$

which implies

$$|||\, y||| \lesssim \|y_0\| (\delta e^{c_\infty t} + \delta) \lesssim \delta e^{c_\infty t}. \tag{3.75}$$

Then there exists the constant C_1 such that

$$|||y||| \leq C_1 \delta e^{c_\infty t}.$$

Applying the Duhamel principle to $y_t = Ly + N(y)$, we have

$$\begin{aligned}
&\|y(t) - \delta e^{Lt} y_0\| = \| \int_0^t e^{L(t-\tau)} N(y(\tau))\ d\tau \| \\
&\lesssim \int_0^t e^{c_\infty (t-\tau)} \|N(y(\tau))\|\ d\tau \\
&\lesssim \int_0^t e^{c_\infty (t-\tau)} (|||y\ |||^2 + |||\ y|||^3)\ d\tau \\
&\lesssim \int_0^t e^{c_\infty (t-\tau)} (\delta^2 e^{2\widetilde{c}_\infty \tau} + \delta^3 e^{3\widetilde{c}_\infty \tau})\ d\tau \\
&\lesssim \delta^2 e^{2\widetilde{c}_\infty t} + \delta^3 e^{3\widetilde{c}_\infty t},
\end{aligned} \tag{3.76}$$

where the first inequality holds by (3.58), the second inequality holds by by Lemma 3.2.9 and the third inequality holds by (3.75).

Then there exists the constant C_2 such that

$$\|y(t) - \delta e^{Lt} y_0\| \leq C_2(\delta^2 e^{2\widetilde{c}_\infty t} + \delta^3 e^{3\widetilde{c}_\infty t}).$$

In order to find the escape time, it suffices to show that

$$\min \left\{ T^\delta, T^*, T^{**} \right\} = T^\delta,$$

by fixing θ_0 small enough. Set

$$\theta_0 = \min\{\frac{\sigma}{C_1}, \frac{1}{2C_2}, \frac{C_p}{4}, \sqrt{\frac{C_p}{4}}\}.$$

On the one hand, if $T^* < T^\delta$ is the smallest, then for $0 \leq t \leq T^*$,

$$|||y(T^*)||| \leq C_1 \delta e^{c_\infty T^*} < C_1 \delta e^{c_\infty T^\delta} = C_1 \theta_0 < \sigma,$$

which is a contradiction to the definition of T^*. On the other hand, if $T^{**} < T^\delta$ is the smallest, then we have

$$\begin{aligned}\|y(T^{**})\| &\leq \delta e^{c_\infty T^{**}}\|y_0\| + C_2(\delta^2 e^{2\widetilde{c}_\infty T^{**}} + \delta^3 e^{3\widetilde{c}_\infty T^{**}}) \\ &< \delta e^{c_\infty T^{**}} + C_2(\delta e^{c_\infty T^{**}}\theta_0 + \delta e^{c_\infty T^{**}}\theta_0^2) \\ &< 2\delta e^{c_\infty t},\end{aligned}$$

which is a contradiction to the definition of T^{**}.

Moreover, if there exists a constant C_p such that

$$\|e^{tL}y_0\| \geq C_p e^{c_\infty t},$$

then at the escape time $t = T^\delta$, we have the following estimate

$$\|\delta e^{LT^\delta}y_0\| \geq C_p \delta e^{c_\infty T^\delta} = C_p\theta_0,$$

where the non-linear term is

$$\delta^2 e^{2\widetilde{c}_\infty T^\delta} + \delta^3 e^{3\widetilde{c}_\infty T^\delta} = \theta_0^2 + \theta_0^3,$$

then

$$\|y(T^\delta)\| \geq \tau_0 = \frac{1}{2}C_p\theta_0 > 0,$$

which depends explicitly on σ, C_p, c_∞, y_0 and is independent of δ.

□

Therefore we conclude the local instability for δy_0 as long as $\|y_0\| = 1$, $\int_\Omega b_0 dx \neq 0$ and $|||y_0||| < \infty$ and sufficient small δ.

Remark 3.2.11. If the initial data $\int_\Omega b_0 dx = 0$, this means $b \equiv 0, \forall x \in \Omega, t > 0$ and

$R(u) \equiv 0, \forall x \in \Omega, t > 0$ which implies the equations for a and c coincide with the heat equation. Therefore, in this case the system will converge to the accessible boundary equilibria $(a_\infty, 0, c_\infty)$.

3.2.2.2 Instability in generalized case

Here we indicate how to adapt the above analysis to get instability result for the following generalized case

$$A_1 + ... + A_l + 2B \rightleftharpoons B + C_1 + ... + C_r.$$

The corresponding reaction-diffusion system is

$$\begin{cases} \partial_t \widetilde{a_i} - d_i \Delta \widetilde{a_i} = -\widetilde{b}^2 \prod \widetilde{a_i} + \widetilde{b} \prod \widetilde{c_j} & i = 1, ..., l, x \in \Omega, t > 0, \\ \partial_t \widetilde{b} - d_b \Delta \widetilde{b} = -\widetilde{b}^2 \prod \widetilde{a_i} + \widetilde{b} \prod \widetilde{c_j} & x \in \Omega, t > 0, \\ \partial_t \widetilde{c_j} - d_j \Delta \widetilde{c_j} = \widetilde{b}^2 \prod \widetilde{a_i} - \widetilde{b} \prod \widetilde{c_j} & j = 1, ..., r, x \in \Omega, t > 0, \\ \nabla \widetilde{a_i} \cdot n = \nabla \widetilde{b} \cdot n = \nabla \widetilde{c_j} \cdot n = 0 & x \in \partial\Omega, t > 0, \\ \widetilde{a_i}(x,0) = \widetilde{a}_{i,0}(x), \widetilde{b}(x,0) = \widetilde{b}_0(x), \widetilde{c_j}(x,0) = \widetilde{c}_{j,0}(x) & x \in \Omega. \end{cases} \tag{3.77}$$

For this reaction system, we have the following conservation laws;

$$\begin{aligned} \int_\Omega \widetilde{a_i}\ dx + \int_\Omega \widetilde{c_j}\ dx &= \int_\Omega \widetilde{a}_{i,0}(x)\ dx + \int_\Omega \widetilde{c}_{j,0}(x)\ dx := M_{1,ij}, \\ \int_\Omega \widetilde{b_i}\ dx + \int_\Omega \widetilde{c_j}\ dx &= \int_\Omega \widetilde{b}_{i,0}(x)\ dx + \int_\Omega \widetilde{c}_{i,0}(x)\ dx := M_{2,ij}. \end{aligned} \tag{3.78}$$

Again we are interested in the *accessible boundary equilibrium* of a reaction network, as long as $M_{1,ij} > M_{2,ij}$ $i = 1, ..., l, j = 1, ..., r$ there are two types of equilibria following the conservation laws and we name $(a_{i,\infty}, 0, c_{j,\infty})$ as unique accessible boundary equilibria which follows (3.78),

$$a_{i,\infty} + c_{j,\infty} = M_{1,ij},\ b_{i,\infty} + c_{j,\infty} = M_{2,ij}.$$

Similarly we introduce new variables as perturbation around the boundary equilibrium

$$a_i = \widetilde{a}_i - a_{i,\infty}, b = b, c_j = \widetilde{c}_j - c_{j,\infty}, u = (a_i, b, c_j)^\intercal.$$

Then we can get the equation for a_i, b and c_j with $i = 1, ..., l$, $j = 1, ..., r$

$$\begin{cases} \partial_t a_i - d_i \Delta a_i = b \prod c_{j,\infty} + N(a_i, b, c_j) & x \in \Omega, t > 0, \\ \partial_t b - d_b \Delta b = b \prod c_{j,\infty} + N(a_i, b, c_j) & x \in \Omega, t > 0, \\ \partial_t c_j - d_j \Delta c_j = -b \prod c_{j,\infty} - N(a_i, b, c_j) & x \in \Omega, t > 0, \\ \frac{\partial a}{\partial \mathbf{n}} = \frac{\partial b}{\partial \mathbf{n}} = \frac{\partial c}{\partial \mathbf{n}} = 0 & x \in \partial\Omega, t > 0, \\ a_i(x, 0) = a_{i,0}(x), b(x, 0) = b_0(x c_j(x, 0) = c_{j,0}(x) & x \in \Omega, \end{cases} \tag{3.79}$$

where $N(a_i, b, c_j) = -b^2 \prod(a_i + \widetilde{a}_{i,\infty}) + b \prod(c_j + c_{j,\infty}) - b \prod c_{j,\infty}$.

Again we can express (3.79) as

$$u_t = L_1 u + N_u(u),$$

where $L_1 := \begin{pmatrix} d_i \Delta & \prod c_{j,\infty} & 0 \\ 0 & d_b \Delta + \prod c_{j,\infty} & 0 \\ 0 & -\prod c_{j,\infty} & d_j \Delta \end{pmatrix}$ and $N_1(u) := \begin{pmatrix} N(a_i, b, c_j) \\ N(a_i, b, c_j) \\ -N(a_i, b, c_j) \end{pmatrix}$.

Similarly we can get the largest eigenvalue for L_1 is $\prod c_{j,\infty} > 0$, then we can get

$$\|e^{tL_1} u_0\|_2 \leq e^{\prod c_{j,\infty} t} \|u_0\|_2,$$

which implies

$$\|e^{tL_1}\|_2 \leq e^{\prod c_{j,\infty} t}.$$

In order to use the elliptic estimate, we also need the following variables

$$a_t = \widetilde{a}_t, b_t = \widetilde{b}_t, c_t = \widetilde{c}_t, u_t = (a_t, b_t, c_t)^\intercal.$$

Taking the time derivative on (3.79), we get

$$u_{tt} = L_2 u_t + N_2(u, u_t), \tag{3.80}$$

where $N_2(u, u_t) \coloneqq \partial_t[N_1(u)]$ and $L_2 = L_1$. Recall $y^\intercal = (u^\intercal, u_t^\intercal)$ and get the equation for y,

$$y_t = Ly + N(y), \tag{3.81}$$

where $L = \begin{pmatrix} L_1 & 0 \\ 0 & L_2 \end{pmatrix}$ and $N(y) = \begin{pmatrix} N_1(u) \\ N_2(u, u_t) \end{pmatrix}$. Again considering Lemma 3.2.5 and L is block diagonal matrix, we can get

$$\|e^{tL}\| \leq e^{\prod c_{j,\infty} t}.$$

Since the linear term Ly dominates $N(y)$ term (or the right hand side) because of the smallness of $|||y|||$ and the assumption of $\|y_0\| = 1$, $\int_\Omega b_0 dx \neq 0$ ($b_0 \geq 0$) and $|||y_0||| < \infty$ and the conservation law (3.78) also implies the existence of the constant $C_p > 0$ such that $\|e^{tL} y_0\| \geq C_P e^{c_\infty t}$, we can use the similar analysis as above to get the local instability of the accessible boundary equilibria.

3.2.3 Local stability for $\alpha_1 A_1 + ... + \alpha_n A_n \rightleftharpoons \beta_1 A_1 + ... + \beta_n A_n$

To show the stability at the unique positive equilibria u_∞, we again introduce the small perturbation $u_i = \widetilde{u}_i - u_{i_\infty}$ around the boundary equilibria. Then we get the following equation for perturbation.

$$\begin{aligned}\partial_t u_i - d_i\Delta u_i &= (\beta_i-\alpha_i)(\prod_{i=1}^n (u_i+u_{i\infty})^{\alpha_i} - \prod_{i=1}^n (u_i+u_{i\infty})^{\beta_i}) \\ &= (\beta_i-\alpha_i)\prod_{i=1}^n (u_i+u_{i\infty})^{\gamma_i}(\prod_{i=1}^n (u_i+u_{i\infty})^{\alpha_i-\gamma_i} - \prod_{i=1}^n (u_i+u_{i\infty})^{\beta_i-\gamma_i}),\end{aligned} \tag{3.82}$$

where $\gamma = (\gamma_1, ..., \gamma_n)$ with $\gamma_i = \min\{\alpha_i, \beta_i\}$. We also donate

$$L := \{i \in \{1, ..., n\} | \alpha_i > \beta_i\}, R := \{j \in \{1, ..., n\} | \alpha_j < \beta_j\},$$

$$L_0 := \{i_0 \in \{1, ..., n\} | \alpha_{i_0} \neq 0\}, R_0 := \{j_0 \in \{1, ..., n\} | \beta_{j_0} \neq 0\}.$$

and we assume $L \neq \varnothing, R \neq \varnothing, L \cup R = \{1, 2, ..., n\}$ and $L_0 \cap R_0 \neq \varnothing$. The last assumption means we don't consider the case where the system only has positive equilibrium since [34] has already shown the global convergence without boundary equilibrium.

Now we we start proving the main theorem, Theorem 3.2.4 in this section. First we do the energy estimate on the system.

W.l.o.g we assume there exists m such that $0 < m < n$ and $L = \{1, ..., m\}$, $R = \{m+1, ..., n\}$. Then we write the perturbation in the following way

$$\begin{aligned}&\partial_t u_i - d_i\Delta u_i \\ &= (\beta_i-\alpha_i)\prod_{i=1}^n (u_i+u_{i\infty})^{\gamma_i}(\prod_{i=1}^n (u_i+u_{i\infty})^{\alpha_i-\gamma_i} - \prod_{i=1}^n (u_i+u_{i\infty})^{\beta_i-\gamma_i}) \\ &= (\beta_i-\alpha_i)\prod_{i=1}^n (u_i+u_{i\infty})^{\gamma_i}\{[u_\infty^{\alpha-\gamma} + \sum_{i=1}^m (\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}} + N_1(u,u_\infty)] \\ &\quad - [u_\infty^{\beta-\gamma} + \sum_{j=m+1}^n (\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}} + N_2(u,u_\infty)]\} \\ &= (\beta_i-\alpha_i)\prod_{i=1}^n (u_i+u_{i\infty})^{\gamma_i}[\sum_{i=1}^m (\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}} - \sum_{j=m+1}^n (\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}} \\ &\quad + N_1(u,u_\infty) - N_2(u,u_\infty)],\end{aligned} \tag{3.83}$$

where

$$N_1(u,u_\infty)=\prod_{i=1}^{n}(u_i+u_{i\infty})^{\alpha_i-\gamma_i}-u_\infty^{\alpha-\gamma}-\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}},$$

$$N_2(u,u_\infty)=\prod_{i=1}^{n}(u_i+u_{i\infty})^{\beta_i-\gamma_i}-u_\infty^{\beta-\gamma}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}.$$

Both N_1 and N_2 are non-linear term w.r.t. u_i and for simplicity we define $N:=N_1-N_2$.

Multiplying $\frac{(\alpha_i-\gamma_i)}{(\alpha_i-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}u_i$, $\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}u_j$ on (3.83) respectively, then integrating over Ω by parts, we get the following

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}(\sum_{i=1}^{m}(\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\|u_i\|_2^2+\sum_{j=m+1}^{n}\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\|u_j\|_2^2)\\
&+(\sum_{i=1}^{m}d_i\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\|\nabla u_i\|_2^2+\sum_{j=m+1}^{n}d_j\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\|\nabla u_j\|_2^2)\\
&=\int_\Omega\prod_{i=1}^{n}(u_i+u_{i\infty})^{\gamma_i}[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}+N(u,u_\infty)]\\
&\quad\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}+\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}})dx.
\end{aligned}\tag{3.84}$$

Now we do the estimate on the right hand side of (3.84).

Lemma 3.2.12. *If* $\forall t\geq 0$, $\sum_{i=1}^{n}\|u_i(x,t)\|_\infty\leq\theta$, *we have*

$$\begin{aligned}
&\int_\Omega\prod_{i=1}^{n}(u_i+u_{i\infty})^{\gamma_i}[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}+N(u,u_\infty)]\\
&\quad\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}u_i+\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}})dx\\
&\lesssim\sum_{i=1}^{m}d_i\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\|\nabla u_i\|_2^2+\sum_{j=m+1}^{n}d_j\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\|\nabla u_j\|_2^2.
\end{aligned}\tag{3.85}$$

Proof. Now we consider the sign situation for $\{u_i\}, i = 1, ..., n$ in following two cases.

1. The first case is when the sign for $\{u_i\}_{i\in L}$ is different from $\{u_j\}_{j\in R}$,

   (a) $\forall i \in L\ u_i \leq 0$, $\forall j \in R\ u_j \geq 0$.

   (b) $\forall i \in L\ u_i \geq 0$, $\forall j \in R\ u_j \leq 0$.

2. The rest situations belong to the second case and we divide this case into three following parts,

   (a) $\{u_j\}_{j\in R}$ has positive and negative members.

   (b) $\forall j \in R\ u_j \leq 0$, $\exists i \in L$ such that $u_i \leq 0$.

   (c) $\forall j \in R\ u_j \geq 0$, $\exists i \in L$ such that $u_i \geq 0$.

We first deal with $2(a)$ when $\{u_r\}_{r\in R}$ has positive and negative members. For each $l \in L$ with $u_l \leq 0$, we further assume that $u_N \leq 0$ for $N \in \{m+1, ..., o\}$ and $u_P \geq 0$ for $P \in \{o+1, ..., n\}$. Recall (3.50), we have the following conservation laws, $\forall l \in L$, $\forall k \in R$,

$$\frac{1}{\alpha_l - \beta_l}\int_\Omega u_l(t,x)\ dx + \frac{1}{\beta_k - \alpha_k}\int_\Omega u_k(t,x)\ dx = 0. \tag{3.86}$$

Here we define $\theta_{l,k} = \frac{1}{\alpha_l-\beta_l}u_l + \frac{1}{\beta_k-\alpha_k}u_k$. From (3.86), we get $\int_\Omega \theta_{l,k}(t,x)\ dx = 0$.

For $N \in \{m+1, ..., o\}$, since $u_l, u_N \leq 0$, we have

$$|u_l| = |(\alpha_l - \beta_l)\theta_{l,N} - \frac{\alpha_l - \beta_l}{\beta_N - \alpha_N}u_N| \leq (\alpha_l - \beta_l)|\theta_{l,N}|,$$

$$|u_N| = |(\beta_N - \alpha_N)\theta_{l,N} - \frac{\beta_N - \alpha_N}{\alpha_l - \beta_l}u_l| \leq (\beta_N - \alpha_N)|\theta_{l,N}|.$$

For $P \in \{o+1, ..., n\}$, since $u_P \geq 0, u_o \leq 0$, we have

$$\theta_{l,P} - \theta_{l,o} = \frac{1}{\beta_P - \alpha_P} u_P - \frac{1}{\beta_o - \alpha_o} u_o \geq 0,$$

which implies

$$0 \leq u_P = (\beta_P - \alpha_P)(\theta_{l,P} - \theta_{l,o}) + \frac{\beta_P - \alpha_P}{\beta_o - \alpha_o} u_o \leq (\beta_P - \alpha_P)(\theta_{l,P} - \theta_{l,o}).$$

Combining the above two parts, we have for each $r \in R$, $l \in L$ with $u_l \leq 0$,

$$u_r \leq \begin{cases} (\beta_r - \alpha_r)|\theta_{l,r}|, & r \in \{m+1, ..., o\}, \\ (\beta_r - \alpha_r)(\theta_{l,r} - \theta_{l,o}), & r \in \{o+1, ..., n\}, \end{cases} \tag{3.87}$$

$$|u_l| \leq (\alpha_l - \beta_l)|\theta_{l,k_l}|,$$

where $k_l \in R$ and u_{k_l}, u_l have the same sign.

For each $l \in L$ with $u_l \geq 0$, recall that $\{u_r\}_{r \in R}$ has positive and negative members and $u_N \leq 0$ for $N \in \{m+1, ..., o\}$ and $u_P \geq 0$ for $P \in \{o+1, ..., n\}$ and $\theta_{l,k} = \frac{1}{\alpha_l - \beta_l} u_l + \frac{1}{\beta_k - \alpha_k} u_k$ with $\int_\Omega \theta_{l,k}(t,x)\, dx = 0$, $\forall k \in R$.

For $P \in \{o+1, ..., n\}$, since $u_l, u_P \geq 0$, we have

$$0 \leq u_l = (\alpha_l - \beta_l)\theta_{l,P} - \frac{\alpha_l - \beta_l}{\beta_P - \alpha_P} u_P \leq (\alpha_l - \beta_l)\theta_{l,P},$$

$$0 \leq u_P = (\beta_P - \alpha_P)\theta_{l,P} - \frac{\beta_P - \alpha_P}{\alpha_l - \beta_l} u_l \leq (\beta_P - \alpha_P)\theta_{l,P}.$$

For $N \in \{m+1, ..., o\}$, since $u_N \leq 0, u_n \geq 0$, we have

$$\theta_{l,N} - \theta_{l,n} = \frac{1}{\beta_N - \alpha_N} u_N - \frac{1}{\beta_n - \alpha_n} u_n \leq 0,$$

which implies

$$|u_N| = |(\beta_N - \alpha_N)(\theta_{l,N} - \theta_{l,n}) + \frac{\beta_N - \alpha_N}{\beta_n - \alpha_n} u_n| \leq (\beta_N - \alpha_N)|\theta_{l,N} - \theta_{l,n}|.$$

Combining the above two parts, we have for each $r \in R$, $l \in L$ with $u_l \geq 0$,

$$u_r \leq \begin{cases} (\beta_r - \alpha_r)|\theta_{l,r} - \theta_{l,o}|, & r \in \{m+1, ..., o\}, \\ (\beta_r - \alpha_r)\theta_{l,r}, & r \in \{o+1, ..., n\}, \end{cases} \tag{3.88}$$

$$|u_l| \leq (\alpha_l - \beta_l)|\theta_{l,k_l}|,$$

where $k_l \in R$ and u_{k_l}, u_l have the same sign.

In $2(b)$ when $\forall j \in R$ $u_j \leq 0$, $\exists i \in L$ such that $u_i \leq 0$. Then we can assume that $u_N \leq 0$ for $N \in \{1, ..., q\}$ and $u_P \geq 0$ for $P \in \{q+1, ..., m\}$. Again we define $\theta_{l,k} = \frac{1}{\alpha_l - \beta_l} u_l + \frac{1}{\beta_k - \alpha_k} u_k$, $\forall l \in L$, $\forall k \in R$ with $\int_\Omega \theta_{l,k}(t, x)\, dx = 0$ and we do the similar estimate as (3.87).

For $N \in \{1, ..., q\}$, since $u_N \leq 0$, $\forall j \in R$ $u_j \leq 0$, we have

$$|u_N| = |(\alpha_N - \beta_N)\theta_{N,j} - \frac{\alpha_N - \beta_N}{\beta_j - \alpha_j} u_j| \leq (\alpha_N - \beta_N)|\theta_{N,j}|,$$

$$|u_j| = |(\beta_j - \alpha_j)\theta_{N,j} - \frac{\beta_j - \alpha_j}{\alpha_N - \beta_N} u_j| \leq (\beta_j - \alpha_j)|\theta_{N,j}|.$$

For $P \in \{q+1, ..., m\}$, since $u_P \geq 0, u_q \leq 0$, we have

$$\theta_{P,j} - \theta_{q,j} = \frac{1}{\alpha_P - \beta_P} u_P - \frac{1}{\alpha_q - \beta_q} u_q \geq 0,$$

which implies

$$0 \leq u_P = (\alpha_P - \beta_P)(\theta_{P,j} - \theta_{q,j}) + \frac{\alpha_P - \beta_P}{\alpha_q - \beta_q} u_q \leq (\alpha_P - \beta_P)(\theta_{P,j} - \theta_{q,j}).$$

Thus we have for each $j \in R$, $l \in L$,

$$u_l \leq \begin{cases} (\alpha_l - \beta_l)|\theta_{l,j}|, & l \in \{1, ..., q\}, \\ (\alpha_l - \beta_l)(\theta_{l,j} - \theta_{q,j}), & l \in \{q+1, ..., m\}, \end{cases} \tag{3.89}$$

$$|u_j| \leq (\beta_j - \alpha_j)|\theta_{k_j,j}|,$$

where $k_j \in L$ and u_{k_j}, u_j have the same sign.

In $2(c)$ when $\forall j \in R$ $u_j \geq 0$, $\exists i \in L$ such that $u_i \geq 0$. Then we can assume that $u_N \geq 0$ for $N \in \{1, ..., q\}$ and $u_P \leq 0$ for $P \in \{q+1, ..., m\}$. Again we define $\theta_{l,k} = \frac{1}{\alpha_l - \beta_l} u_l + \frac{1}{\beta_k - \alpha_k} u_k$, $\forall l \in L$, $\forall k \in R$ with $\int_\Omega \theta_{l,k}(t, x)\, dx = 0$ and we do the similar estimate as (3.88).

For $N \in \{1, ..., q\}$, since $u_N \geq 0$, $\forall j \in R$ $u_j \geq 0$, we have

$$|u_N| = |(\alpha_N - \beta_N)\theta_{N,j} - \frac{\alpha_N - \beta_N}{\beta_j - \alpha_j} u_j| \leq (\alpha_N - \beta_N)|\theta_{N,j}|,$$

$$|u_j| = |(\beta_j - \alpha_j)\theta_{N,j} - \frac{\beta_j - \alpha_j}{\alpha_N - \beta_N} u_j| \leq (\beta_j - \alpha_j)|\theta_{N,j}|.$$

For $P \in \{q+1, ..., m\}$, since $u_P \leq 0, u_q \geq 0$, we have

$$\theta_{P,j} - \theta_{q,j} = \frac{1}{\alpha_P - \beta_P} u_P - \frac{1}{\alpha_q - \beta_q} u_q \leq 0,$$

which implies

$$|u_P| = |(\alpha_P - \beta_P)(\theta_{P,j} - \theta_{q,j}) + \frac{\alpha_P - \beta_P}{\alpha_q - \beta_q} u_q| \leq (\alpha_P - \beta_P)|\theta_{P,j} - \theta_{q,j}|.$$

Thus we have for each $j \in R$, $l \in L$,

$$u_l \leq \begin{cases} (\alpha_l - \beta_l)|\theta_{l,j}|, & l \in \{1, ..., q\}, \\ (\alpha_l - \beta_l)|\theta_{l,j} - \theta_{q,j}|, & l \in \{q+1, ..., m\}, \end{cases} \tag{3.90}$$

$$|u_j| \le (\beta_j - \alpha_j)|\theta_{k_j,j}|$$

where $k_j \in L$ and u_{k_j}, u_j have the same sign.

Recall the right hand side of (3.84) and the following inequality,

$$\begin{aligned}
&[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} - \sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} + N(u,u_\infty)] \\
&\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} + \sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}}) \le \frac{1}{4}(N(u,u_\infty))^2,
\end{aligned}$$

which implies that

$$\begin{aligned}
&\int_\Omega \prod_{i=1}^{n}(u_i+u_{i_\infty})^{\gamma_i}[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} - \sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} + N(u,u_\infty)] \\
&\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} + \sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}})dx \qquad (3.91)\\
&\le \frac{1}{4}\int_\Omega \prod_{i=1}^{n}(u_i+u_{i_\infty})^{\gamma_i}(N(u,u_\infty))^2dx.
\end{aligned}$$

Since $N(u,u_\infty)$ is the non-linear part for $\prod_{i=1}^{n}(u_i+u_{i_\infty})^{\alpha_i-\gamma_i} - \prod_{i=1}^{n}(u_i+u_{i_\infty})^{\beta_i-\gamma_i}$, each component contains as least two of $\{u_i\}, i = 1,...,n$. So every non-linear component should be in the form of $f(u,u_\infty)u_iu_j$ where $f(u,u_\infty)$ is the polynomial for (u,u_∞) and we have the following estimate,

$$\begin{aligned}
(f(u,u_\infty)u_iu_j)^2 &\le \|f\cdot u_i\|_\infty^2 \cdot u_j^2 \\
&\lesssim \|u_i\|_\infty^2 \cdot \sum_{l\in L, r\in R}\theta_{l,r}^2. \qquad (3.92)
\end{aligned}$$

From (3.91), (3.92) and using Poincaré inequality motivated from $\int_\Omega \theta_{l,k}(t,x)\ dx = 0$, we get

$$\begin{aligned}
&\frac{1}{4}\int_\Omega \prod_{i=1}^{n}(u_i+u_{i\infty})^{\gamma_i}(f(u,u_\infty)u_iu_j)^2dx \\
&\lesssim \prod_{i=1}^{n}(\|u_i\|_\infty+u_{i\infty})^{\gamma_i}\|u_i\|_\infty^2\sum_{l\in L,r\in R}\int_\Omega \theta_{l,r}^2dx \\
&\lesssim \|u_1\|_\infty^2\sum_{l\in L,r\in R}\int_\Omega \nabla^2\theta_{l,r}dx \\
&\lesssim \|u_i\|_\infty^2\sum_{l\in L,r\in R}(\|\nabla u_l\|_2^2+\|\nabla u_r\|_2^2).
\end{aligned} \tag{3.93}$$

We can do the similar estimate on all non-linear components of $N(u,u_\infty)$ as above. Therefore as long as $\sum_{i=1}^{n}\|u_i\|_\infty \le \theta$ are sufficiently small such that $\forall i\in L$, $\forall j\in R$,

$$\frac{1}{4}\prod_{i=1}^{n}(\|u_i\|_\infty+u_{i\infty})^{\gamma_i}\|f(\theta,u_{i\infty})\|_\infty^2\theta^2 \le \min\{d_i\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}, d_j\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\},$$

we can get

$$\begin{aligned}
&\sum_{i=1}^{m}d_i\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\|\nabla u_i\|_2^2+\sum_{j=m+1}^{n}d_j\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\|\nabla u_j\|_2^2 \\
&\ge \int_\Omega \prod_{i=1}^{n}(u_i+u_{i\infty})^{\gamma_i}[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}+N(u,u_\infty)] \\
&\quad\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}+\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}})dx.
\end{aligned} \tag{3.94}$$

In the first case, we first consider $1(a)$ when $\forall i\in L\ u_i\le 0$, $\forall j\in R\ u_j\ge 0$. This implies

$$\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\le 0.$$

Recall $N(u,u_\infty)$ is the non-linear part and each component contains as least two of $\{u_i\}_{i=1,\dots,n}$, as long as $\|u_i\|_\infty$ are sufficiently small, we can get

$$\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}}+N(u,u_\infty)\le 0.$$

Also recall the right hand side of (3.84), we get

$$\begin{aligned}&\int_\Omega\prod_{i=1}^{n}(u_i+u_{i_\infty})^{\gamma_i}[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}}+N(u,u_\infty)]\\&\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}}+\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}})dx\le 0,\end{aligned}\tag{3.95}$$

the above estimate also works for $1(b)$ when $\forall i\in L, u_i\ge 0$ and $\forall j\in R, u_j\le 0$.

□

Combining (3.94) (3.95) and the equation (3.84), we get the first part of energy estimate

Lemma 3.2.13. *If* $\forall t\ge 0$, $\sum_{i=1}^{n}\|u_i(x,t)\|_\infty\le\theta$, *then we have*

$$\frac{d}{dt}(\sum_{i=1}^{m}(\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}}\|u_i\|_2^2+\sum_{j=m+1}^{n}\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}}\|u_j\|_2^2)\le 0,\tag{3.96}$$

this implies $\sum_{i=1}^{n}\|u_i(x,t)\|_2$ *decay w.r.t time.*

In order to use the elliptic estimate in Theorem 3.2.6, we need to do the energy estimate on $\|\partial_t u_i\|_2$. By taking time partial derivative on (3.83), multiplying $\frac{(\alpha_i-\gamma_i)}{(\alpha_i-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}}\partial_t u_i$, $\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}}\partial_t u_j$ respectively and integrating over Ω, we get the following

$$\frac{1}{2}\frac{d}{dt}(\sum_{i=1}^{m}(\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\|\partial_t u_i\|_2^2+\sum_{j=m+1}^{n}\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\|\partial_t u_j\|_2^2)$$
$$+(\sum_{i=1}^{m}d_i\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\|\nabla\partial_t u_i\|_2^2+\sum_{j=m+1}^{n}d_j\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\|\nabla\partial_t u_j\|_2^2) \tag{3.97}$$
$$:= I+II,$$

where

$$I=\int_\Omega\prod_{i=1}^{n}(u_i+u_{i\infty})^{\gamma_i}[\sum_{i=1}^{m}(\alpha_i-\gamma_i)\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\partial_t u_i-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\partial_t u_j+\partial_t N(u,u_\infty)]$$
$$\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\partial_t u_i+\sum_{j=m+1}^{n}(\beta_j-\gamma_j)\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\partial_t u_j)dx,$$

and

$$II=\int_\Omega\partial_t\{\prod_{i=1}^{n}(u_i+u_{i\infty})^{\gamma_i}\}[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}-\sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}+N(u,u_\infty)]$$
$$\times(-\sum_{i=1}^{m}(\alpha_i-\gamma_i)\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\partial_t u_i+\sum_{j=m+1}^{n}(\beta_j-\gamma_j)\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\partial_t u_j)dx.$$

The idea for the proof in the following Lemma is similar to the estimate in Lemma 3.2.12.

Lemma 3.2.14. *If* $\forall t\geq 0,\ \sum_{i=1}^{n}\|u_i(x,t)\|_\infty\leq\theta,$ *we have*

$$I+II\leq\sum_{i=1}^{m}d_i\frac{(\alpha_i-\gamma_i)}{(\alpha-\beta_i)}\frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}}\|\nabla\partial_t u_i\|_2^2+\sum_{j=m+1}^{n}d_j\frac{(\beta_j-\gamma_j)}{(\beta_j-\alpha_j)}\frac{u_\infty^{\beta-\gamma}}{u_{j\infty}}\|\nabla\partial_t u_j\|_2^2. \tag{3.98}$$

Proof. Again we consider the sign situation for $\{\partial_t u_i\}, i=1,...,n$ in two cases.

1. The first case is when the sign for $\{\partial_t u_i\}_{i\in L}$ is different from $\{\partial_t u_j\}_{j\in R}$,

   (a) $\forall i \in L\ \partial_t u_i \le 0$, $\forall j \in R\ \partial_t u_j \ge 0$.

   (b) $\forall i \in L\ \partial_t u_i \ge 0$, $\forall j \in R\ \partial_t u_j \le 0$.

2. The rest situations belong to the second case and we divide this case into three following parts,

   (a) $\{u_j\}_{j\in R}$ has positive and negative members.

   (b) $\forall j \in R$, $\partial_t u_j \le 0$, $\exists i \in L$ such that $\partial_t u_i \le 0$.

   (c) $\forall j \in R$, $\partial_t u_j \ge 0$, $\exists i \in L$ such that $\partial_t u_i \ge 0$.

We first deal with the second case, for each $l \in L$ with $\partial_t u_l \le 0$. The assumption implies either $\{\partial_t u_r\}_{r\in R}$ have different signs or $\forall j \in R$, $\partial_t u_j \le 0$. W.l.o.g. we assume $\partial_t u_N \le 0$ for $N \in \{m+1, ..., o\}$ and $\partial_t u_P \ge 0$ for $P \in \{o+1, ..., n\}$. Recall (3.86), we have the similar conservation laws for $\partial_t u_i$, $\forall k \in R$

$$\frac{1}{\alpha_l - \beta_l}\int_\Omega \partial_t u_l\ dx + \frac{1}{\beta_k - \alpha_k}\int_\Omega \partial_t u_k\ dx = 0. \tag{3.99}$$

Here we define $\theta^t_{l,k} = \frac{1}{\alpha_l - \beta_l}\partial_t u_l + \frac{1}{\beta_k - \alpha_k}\partial_t u_k$ and $\int_\Omega \theta^t_{l,k}\ dx = 0$.

For $N \in \{m+1, ..., o\}$, we have

$$|\partial_t u_l| \le (\alpha_l - \beta_l)|\theta^t_{l,N}|,\ \ |\partial_t u_N| \le (\beta_N - \alpha_N)|\theta^t_{l,N}|.$$

For $P \in \{o+1, ..., n\}$, we have

$$\theta^t_{l,P} - \theta^t_{l,o} = \frac{1}{\beta_P - \alpha_P}\partial_t u_P - \frac{1}{\beta_o - \alpha_o}\partial_t u_o,$$

which implies

$$0 \leq \partial_t u_P \leq (\beta_P - \alpha_P)(\theta_{l,P} - \theta_{l,o}).$$

Combining the above two parts, we have for each $r \in R$,

$$\partial_t u_r \leq \begin{cases} (\beta_r - \alpha_r)|\theta^t_{l,r}|, & r \in \{m+1, ..., o\}, \\ (\beta_r - \alpha_r)(\theta^t_{l,r} - \theta^t_{l,o}), & r \in \{o+1, ..., n\}. \end{cases} \tag{3.100}$$

Then for each $l \in L$ with $\partial_t u_l \geq 0$, the assumption again implies either $\{\partial_t u_r\}_{r \in R}$ have different signs or $\forall j \in R$, $\partial_t u_j \leq 0$. We can get the similar estimate, for each $l \in L$,

$$|\partial_t u_l| \leq (\alpha_l - \beta_l)|\theta^t_{l,k_l}|,$$

where $k_l \in R$ and $\partial_t u_{k_l}, \partial_t u_l$ have the same sign.

Recall (3.92), we can do the similar estimate on the right hand side of (3.97), since

$$\begin{aligned} I = &\int_\Omega \prod_{i=1}^n (u_i + u_{i\infty})^{\gamma_i} [\sum_{i=1}^m (\alpha_i - \gamma_i) \frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}} \partial_t u_i - \sum_{j=m+1}^n (\beta_j - \gamma_j) \frac{u_\infty^{\beta-\gamma}}{u_{j\infty}} \partial_t u_j \\ &+ \partial_t N(u, u_\infty)](-\sum_{i=1}^m (\alpha_i - \gamma_i) \frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}} \partial_t u_i + \sum_{j=m+1}^n (\beta_j - \gamma_j) \frac{u_\infty^{\beta-\gamma}}{u_{j\infty}} \partial_t u_j) dx \\ \leq &\frac{1}{4} \int_\Omega \prod_{i=1}^n (u_i + u_{i\infty})^{\gamma_i} (\partial_t N(u, u_\infty))^2 dx, \end{aligned}$$

and

$$II = \int_\Omega \partial_t\{\prod_{i=1}^n (u_i + u_{i_\infty})^{\gamma_i}\}[\sum_{i=1}^m (\alpha_i - \gamma_i) u_i \frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} - \sum_{j=m+1}^n (\beta_j - \gamma_j) u_j \frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} + N(u, u_\infty)]$$
$$\times (-\sum_{i=1}^m (\alpha_i - \gamma_i) \frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} \partial_t u_i + \sum_{j=m+1}^n (\beta_j - \gamma_j) \frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} \partial_t u_j) dx$$
$$\leq \| \sum_{i=1}^m (\alpha_i - \gamma_i) u_i \frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} - \sum_{j=m+1}^n (\beta_j - \gamma_j) u_j \frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} + N(u, u_\infty) \|_\infty$$
$$\times \int_\Omega |\partial_t\{\prod_{i=1}^n (u_i + u_{i_\infty})^{\gamma_i}\}(-\sum_{i=1}^m (\alpha_i - \gamma_i) \frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} \partial_t u_i + \sum_{j=m+1}^n (\beta_j - \gamma_j) \frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} \partial_t u_j)| dx,$$

where

$$\partial_t\{\prod_{i=1}^n (u_i + u_{i_\infty})^{\gamma_i}\} = \sum \gamma_i \frac{u_\infty^\gamma}{u_{i_\infty}} \partial_t u_i + N^\gamma(u, \partial_t u, u_\infty),$$

with N^γ is the non-linear part for $\partial_t\{\prod_{i=1}^n (u_i + u_{i_\infty})^{\gamma_i}\}$.

By using Poincaré inequality motivated from $\forall l \in L$, $\forall k \in R$, $\int_\Omega \theta_{l,k}^t(t,x)\ dx = 0$ and the smallness of $\|u_i\|_\infty$, we can get

$$\sum_{i=1}^m d_i \frac{(\alpha_i - \gamma_i)}{(\alpha - \beta_i)} \frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} \|\nabla \partial_t u_i\|_2^2 + \sum_{j=m+1}^n d_j \frac{(\beta_j - \gamma_j)}{(\beta_j - \alpha_j)} \frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} \|\nabla \partial_t u_j\|_2^2 \geq I + II. \tag{3.101}$$

In the first case, we first consider when $\forall i \in L, \partial_t u_i \leq 0$ and $\forall j \in R, \partial_t u_j \geq 0$. This implies

$$\sum_{i=1}^m (\alpha_i - \gamma_i) \frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} \partial_t u_i - \sum_{j=m+1}^n (\beta_j - \gamma_j) \frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} \partial_t u_j \leq 0.$$

Then we can write

$$I + II = \int_\Omega III \cdot (-\sum_{i=1}^m (\alpha_i - \gamma_i) \frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} \partial_t u_i + \sum_{j=m+1}^n (\beta_j - \gamma_j) \frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} \partial_t u_j) dx, \tag{3.102}$$

where

$$III = \prod_{i=1}^{n}(u_i + u_{i\infty})^{\gamma_i}[\sum_{i=1}^{m}(\alpha_i - \gamma_i)\frac{u_{\infty}^{\alpha-\gamma}}{u_{i\infty}}\partial_t u_i - \sum_{j=m+1}^{n}(\beta_j - \gamma_j)\frac{u_{\infty}^{\beta-\gamma}}{u_{j\infty}}\partial_t u_j + +\partial_t N(u, u_\infty)]$$
$$+ \partial_t\{\prod_{i=1}^{n}(u_i + u_{i\infty})^{\gamma_i}\}[\sum_{i=1}^{m}(\alpha_i - \gamma_i)\frac{u_{\infty}^{\alpha-\gamma}}{u_{i\infty}}u_i - \sum_{j=m+1}^{n}(\beta_j - \gamma_j)\frac{u_{\infty}^{\beta-\gamma}}{u_{j\infty}}u_j + N(u, u_\infty)].$$

And because of the smallness of $\|u_i\|_\infty$ the value (sign) of III is controlled by

$$u_{\infty}^{\gamma}[\sum_{i=1}^{m}(\alpha_i - \gamma_i)\frac{u_{\infty}^{\alpha-\gamma}}{u_{i\infty}}\partial_t u_i - \sum_{j=m+1}^{n}(\beta_j - \gamma_j)\frac{u_{\infty}^{\beta-\gamma}}{u_{j\infty}}\partial_t u_j] \leq 0.$$

Therefore (3.102) and the above inequality implies that in the first case

$$I + II \leq 0. \tag{3.103}$$

□

Combining (3.101) (3.103) and the equation (3.97), we get the second part of energy estimate

Lemma 3.2.15. *If* $\forall t \geq 0$, $\sum_{i=1}^{n}\|u_i(x,t)\|_\infty \leq \theta$, *then we have*

$$\frac{d}{dt}(\sum_{i=1}^{m}(\frac{(\alpha_i - \gamma_i)}{(\alpha - \beta_i)}\frac{u_{\infty}^{\alpha-\gamma}}{u_{i\infty}}\|\partial_t u_i\|_2^2 + \sum_{j=m+1}^{n}\frac{(\beta_j - \gamma_j)}{(\beta_j - \alpha_j)}\frac{u_{\infty}^{\beta-\gamma}}{u_{j\infty}}\|\partial_t u_j\|_2^2) \leq 0, \tag{3.104}$$

this implies $\sum_{i=1}^{n}\|\partial_t u_i(x,t)\|_2$ *decay w.r.t time.*

Finally, we proof Theorem 3.2.4 by Lemma 3.2.13 and Lemma 3.2.15.

Proof. We first do the elliptic estimate for the system (3.49). It's not hard to check that the system satisfies the Supplementary Condition and the Neumann boundary condition satisfies the Complementing Boundary Condition. By using Theorem 3.2.6, we have for $i = 1, ..., n$,

$$\begin{aligned}\|u_i\|_{H_2} \leq K\Big(\|((u+u_\infty)^\gamma - u_\infty^\gamma)[\sum_{i=1}^{m}(\alpha_i-\gamma_i)u_i\frac{u_\infty^{\alpha-\gamma}}{u_{i_\infty}} - \sum_{j=m+1}^{n}(\beta_j-\gamma_j)u_j\frac{u_\infty^{\beta-\gamma}}{u_{j_\infty}} \\ + N(u,u_\infty) + u_\infty^\gamma N(u,u_\infty)]\|_2 + \sum_{i=1}^{n}\|\partial_t u_i\|_2 + \sum_{i=1}^{n}\|u_i\|_2)\Big),\end{aligned} \tag{3.105}$$

where K is a constant depends on origin equation and bounded domain. By using Sobolev Embedding Inequality, we can have

$$\|v_i\|_{L^\infty} \lesssim \sum_{i=1}^{n}\|u_i\|_2 + \sum_{i=1}^{n}\|\partial_t u_i\|_2.$$

The above holds because $\|u_i\|_\infty$ is sufficiently small which guarantees $(u+u_\infty)^\gamma - u_\infty^\gamma$ and $N(u, u_\infty) \ll 1$.

The continuity argument implies L^∞ will be always small to follow Lemma 3.2.13 and Lemma 3.2.15. As long as the initial L^2 on $\{\partial_t u_i\}$ and L^∞ on $\{u_i\}$ are sufficiently small, L^∞ can keep being small along with the time t while L^2 is non-increasing from the estimate which implies the existence of weak solution around the positive equilibrium.

The *Remark 3.1* in [87] shows that for a reversible reaction with nonnegative initial data in $L^1 \cap L\log L$ if the solution is globally (in time) essentially bounded, the solution converges exponentially to the complex-balanced equilibrium in L^1 norm. By using the interpolation with L^1 and boundness of L^∞, we can get the exponential convergence in $L^p(1 < p < \infty)$ sense.

Now we return to the origin equation on $\{u_i\}_{i=1,...,n}$,

$$\partial_t u_i - d_i\Delta u_i = (\beta_i - \alpha_i)(\widetilde{u}^\alpha - \widetilde{u}^\beta).$$

Because of the Poincaré inequality, we have

$$\|\partial_t u - \bar{\partial_t u}\|_{L^2} \lesssim \|\nabla \partial_t u\|_{L^2},$$

which implies

$$\|\partial_t u_i\|_{L^2} \lesssim \|\nabla \partial_t u_i\|_{L^2} + |\int_\Omega \partial_t u_i dx|.$$

Since we know $\sum_{i=1}^{n}(\|\partial_t u_i(x,0)\|_2 + \|u_i(x,0)\|_\infty) \leq \theta \ll 1$, we have

$$\begin{aligned}
&|\int_\Omega \partial_t u_i dx| = |d_i \int_\Omega \Delta u_i dx + \int_\Omega (\beta_i - \alpha_i)(\widetilde{u}^\alpha - \widetilde{u}^\beta)dx| \\
&\lesssim u_\infty^\gamma \| \sum_{i=1}^{m} (\alpha_i - \gamma_i) u_i \frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}} - \sum_{j=m+1}^{n} (\beta_j - \gamma_j) u_j \frac{u_\infty^{\beta-\gamma}}{u_{j\infty}} \|_{L^1} \\
&\lesssim e^{-lt},
\end{aligned} \tag{3.106}$$

where exponential decaying rate l is determined from the interpolation. Recall the estimate in Lemma 3.2.15 where we get

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}(\sum_{i=1}^{m}(\frac{(\alpha_i - \gamma_i)}{(\alpha - \beta_i)} \frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}} \|\partial_t u_i\|_2^2 + \sum_{j=m+1}^{n} \frac{(\beta_j - \gamma_j)}{(\beta_j - \alpha_j)} \frac{u_\infty^{\beta-\gamma}}{u_{j\infty}} \|\partial_t u_j\|_2^2) \\
&+ (\sum_{i=1}^{m} d_i \frac{(\alpha_i - \gamma_i)}{(\alpha - \beta_i)} \frac{u_\infty^{\alpha-\gamma}}{u_{i\infty}} \|\nabla \partial_t u_i\|_2^2 + \sum_{j=m+1}^{n} d_j \frac{(\beta_j - \gamma_j)}{(\beta_j - \alpha_j)} \frac{u_\infty^{\beta-\gamma}}{u_{j\infty}} \|\nabla \partial_t u_j\|_2^2) \leq 0.
\end{aligned} \tag{3.107}$$

Then we can have the following

$$\frac{1}{2}\frac{d}{dt}(\sum_{i=1}^{n} \|\partial_t u_i\|_2^2) + (\sum_{i=1}^{n} \|\partial_t u_i\|_2^2) \lesssim \sum_{i=1}^{n} |\int_\Omega \partial_t u_i dx| \lesssim e^{-lt}.$$

The Gronwall's inequality implies that $\sum_{i=1}^{n} \|\partial_t u_i\|_2^2$ decays exponentially. Then the elliptic estimate (3.105) implies exponential convergence to positive equilibrium in H^2 sense.

□

Chapter 4

Kinetic Theory

In this chapter, we study the long time behaviour for some chemical reaction-diffusion systems.

In Section 4.1, we first analyze a three-species system with boundary equilibria in some stoichiometric classes, and whose right hand side is bounded above by a quadratic nonlinearity in the positive orthant. We prove similar results on a fairly general two-species reversible reaction-diffusion network as well.

4.1 Damping of kinetic transport equation with diffuse boundary condition

4.1.1 Introduction and the main result

Motivated by the recent progress in the Landau damping ([12, 51, 81]), we are mainly interested in the quantitative asymptotic behavior of the exponential moments of the fluctuation

$$\int_{\mathbb{R}^3} e^{\theta|v|^2}|f(t,x,v)|\mathrm{d}v \quad \text{in some } \textit{strong} \text{ space in } x \text{ without any differentiability assumption.}$$

We emphasize that the strong-in-x control of moments is a key step toward nonlinear problems such as the Vlasov-Poisson systems. The low regularity framework has a significant benefit in the nonlinear boundary problems. We refer to [36, 88] for the method of control the force field of the Vlasov-Poisson-Boltzmann systems interacting with the diffuse reflection boundary. In this paper, we contribute toward establishing a decay of *exponential moments* of the fluctuation in L^∞_x with *an almost optimal rate* $\frac{1}{t^{3-}}$ when the domain is a *general strictly convex domain* in 3D.

Theorem 4.1.1. *Let Ω be smooth and strictly convex. Assume* (1.12) *for any* $\mathfrak{M} \geq 0$. *Assume* $\|e^{\theta'|v|^2} f_0\|_{L^\infty_{x,v}} < \infty$ *for* $0 < \theta' < 1/2$, *and* $\|\varphi_4(t_{\mathbf{f}}) f_0\|_{L^1_{x,v}} < \infty$, *with* $\varphi_4(t_{\mathbf{f}})$ *defined in Definition 4.1.16. There exists a unique solution* $F(t,x,v) = \mathfrak{M}\mu(v) + f(t,x,v) \geq 0$ *to* (1.10) *and* (1.11), *such that* $\sup_{t\geq 0} \|e^{\theta'|v|^2} f(t)\|_{L^\infty_{x,v}} \leq C \|e^{\theta'|v|^2} f_0\|_{L^\infty_{x,v}}$, *and*

$$\iint_{\Omega\times\mathbb{R}^3} f(t,x,v)\mathrm{d}x\mathrm{d}v = \iint_{\Omega\times\mathbb{R}^3} f_0(x,v)\mathrm{d}x\mathrm{d}v = 0, \quad \textit{for all } t \geq 0. \tag{4.1}$$

Moreover, for any $\theta \in [0,\theta')$, *there exists* $C_\theta > 0$ *such that*

$$\sup_{x\in\bar{\Omega}} \int_{\mathbb{R}^3} e^{\theta|v|^2} |f(t,x,v)|\mathrm{d}v \leq C_\theta \langle t\rangle^{-3} (\ln\langle t\rangle)^2, \quad \textit{for all } t \geq 0. \tag{4.2}$$

Here, we have used a notation $\langle\cdot\rangle := e + |\cdot|$.

Remark 4.1.2. In contrast to [68], we do not need any symmetric condition on the domain.

Remark 4.1.3. Without loss of generality, we set $\mathfrak{M} = 1$ in the rest of the paper, for the sake of simplicity. Following the same proof of this paper, it is straightforward to prove the result to a D-dimension for any $D \in \mathbb{N}$ with different decay rates.

We record the equation, initial datum, and the boundary condition for the fluctuation f in (1.13):

$$\partial_t f + v\cdot\nabla_x f = 0, \ \text{ for } \ (t,x,v) \in \mathbb{R}_+ \times \Omega \times \mathbb{R}^3, \tag{4.3}$$

$$f(t,x,v)|_{t=0} = f_0(x,v) := F_0(x,v) - \mathfrak{M}\mu(v), \ \text{ for } \ (x,v) \in \Omega\times\mathbb{R}^3, \tag{4.4}$$

$$f(t,x,v) = c_\mu \mu(v) \int_{n(x)\cdot v_1 > 0} f(t,x,v_1)\{n(x)\cdot v_1\}\mathrm{d}v_1, \ \text{ for } \ (t,x,v) \in \mathbb{R}_+ \times \gamma_-. \tag{4.5}$$

Notations. We shall clarify some notations: $A \lesssim_\theta B$ if $A \leq CB$ for a constant $C = C(\theta) > 0$ which depends on θ but is independent on A, B; $A \sim B$ if $A \lesssim B$ and $B \lesssim A$; $A \leq O(B)$ if

$|A| \lesssim B$; $\|\cdot\|_{L^1_{x,v}}$ for the norm of $L^1(\Omega \times \mathbb{R}^3)$; $\|\cdot\|_{L^\infty_{x,v}}$ or $\|\cdot\|_\infty$ for the norm of $L^\infty(\bar{\Omega} \times \mathbb{R}^3)$; $|g|_{L^1_{\gamma_\pm}} = \int_{\gamma_\pm} |g(x,v)||n(x)\cdot v| \mathrm{d}S_x \mathrm{d}v$; in the time integration, the differential term is omitted, e.g. we let $\int_{t_*}^t \|f\|_{L^1_{x,v}}$ stand for $\int_{t_*}^t \|f\|_{L^1_{x,v}} \mathrm{d}s$.

4.1.1.1 Novel L^1-L^∞ framework via Stochastic Cycles

In a broad sense, our argument of the L^1-L^∞ framework to prove Theorem 4.1.1 bears some resemblance to the framework developed in the study of the Boltzmann equation [2, 36, 90]. A foundational idea of our novel L^1-L^∞ framework over the whole paper is to *transfer a velocity mixing from the diffusive reflection (4.5) to a spatial mixing through the transport operator*. This idea is realized via *the stochastic cycles*:

Definition 4.1.4. Define the backward exit time $t_{\mathbf{b}}$ and the forward exit time $t_{\mathbf{f}}$

$$\begin{aligned} &t_{\mathbf{b}}(x,v) := \sup\{s \geq 0 : x - \tau v \in \Omega,\ \forall \tau \in [0,s)\},\ x_{\mathbf{b}}(x,v) := x - t_{\mathbf{b}}(x,v)v, \\ &(t_{\mathbf{f}}, x_{\mathbf{f}})(x,v) := (t_{\mathbf{b}}, x_{\mathbf{b}})(x,-v). \end{aligned} \tag{4.6}$$

We define the stochastic cycles: $t_1(t,x,v) = t - t_{\mathbf{b}}(x,v)$, $x_1(x,v) = x_{\mathbf{b}}(x,v) := x - t_{\mathbf{b}}(x,v)v$,

$$\begin{aligned} &t_k(t,x,v,v_1,...,v_{k-1}) = t_{k-1} - t_{\mathbf{b}}(x_{k-1}, v_{k-1}), \\ &x_k(t,x,v,v_1,...,v_{k-1}) = x_{k-1} - t_{\mathbf{b}}(x_{k-1}, v_{k-1})v_{k-1}, \end{aligned} \tag{4.7}$$

where a free variable $v_j \in \mathcal{V}_j := \{v_j \in \mathbb{R}^3 : n(x_j)\cdot v_j > 0\}$.

Lemma 4.1.5. *Suppose f solve (4.3), (4.5) and $t_* \leq t$. For $g(t,x,v) := \varrho(t)w(v)f(t,x,v)$ with given $\varrho(t)$, $w(v)$,*

$$g(t,x,v) = \mathbf{1}_{t_1 \leq t_*} g(t_*, x - (t-t_*)v, v) \tag{4.8}$$

$$+ \int_{\max(t_*,t_1)}^t \varrho'(s)w(v)f(s, x-(t-s)v, v)\mathrm{d}s \tag{4.9}$$

$$+ c_\mu w\mu(v) \int_{\prod_{j=1}^k \mathcal{V}_j} \sum_{i=1}^{k-1} \Big\{ \mathbf{1}_{t_{i+1} < t_* \leq t_i} g(t_*, x_i - (t_i - t_*)v_i, v_i) \Big\} \mathrm{d}\Sigma_i^k \tag{4.10}$$

$$+ c_\mu w\mu(v)\int_{\prod_{j=1}^k \mathcal{V}_j}\sum_{i=1}^{k-1}\Big\{\mathbf{1}_{t_*\leq t_i}\int_{\max(t_*,t_{i+1})}^{t_i} w(v_i)\varrho'(s)f(s,x_i-(t_i-s)v_i,v_i)\mathrm{d}s\Big\}\mathrm{d}\Sigma_i^k \tag{4.11}$$

$$+ c_\mu w\mu(v)\int_{\prod_{j=1}^k \mathcal{V}_j}\mathbf{1}_{t_k\geq t_*}g(t_k,x_k,v_k)\mathrm{d}\Sigma_k^k, \tag{4.12}$$

where $\mathrm{d}\Sigma_i^k := \mathrm{d}\sigma_k\cdots\mathrm{d}\sigma_{i+1}\frac{\mathrm{d}\sigma_i}{c_\mu\mu(v_i)w(v_i)}\mathrm{d}\sigma_{i-1}\cdots\mathrm{d}\sigma_1$*, with* $\mathrm{d}\sigma_j = c_\mu\mu(v_j)\{n(x_j)\cdot v_j\}\mathrm{d}v_j$ *on* $\mathcal{V}_j$ *which is the probability measure.*

4.1.1.2 Weighted L^1-estimates

As the first part of our L^1-L^∞ framework, we prove an L^1-decay of the fluctuation f as $t\to\infty$ in Proposition 4.1.7, following the idea of aperiodic Ergodic theorem (e.g. [13,92]). We prove a key lower bound with a *unreachable defect*, crucially using the stochastic formulation in Lemma 4.1.5 (see the precise statement in Lemma 4.1.14): for $f_0\geq 0$, $t-t_*\gg 1$,

$$f(t,x,v)\geq \mathfrak{m}(x,v)\{\|f(t_*)\|_{L^1_{x,v}} - \|\mathbf{1}_{t_{\mathbf{f}}\gtrsim|t-t_*|}f(t_*)\|_{L^1_{x,v}}\} \ \text{ for some non-negative function } \mathfrak{m}. \tag{4.13}$$

This unreachable defect, which stems from small velocity particles in the outgoing flux of the diffuse reflection (1.11), is intrinsic unless the wall Maxwellian $c_\mu\mu(v)$ vanishes around $|v|=0$.

Next we control the unreachable defect using the weighted L^1-estimates. Due to the invariance of $x_{\mathbf{b}}$ and $x_{\mathbf{f}}$ under $v\cdot\nabla_x$, which has been crucially used in construction of the distance function invariant under Vlasov operator in [36], a weight $\varphi(t_{\mathbf{f}})$ provide an effective dissipation $v\cdot\nabla_x\varphi(t_{\mathbf{f}}) = -\varphi'(t_{\mathbf{f}})$ for $\varphi'\geq 0$, as long as a byproduct term on γ_- can be controlled. Inspired by the proof of an L^1-trace theorem of [66], we derive that

Lemma 4.1.6. *Suppose* $\varphi(\tau)\geq 0$, $\varphi'\geq 0$, *and*

$$\int_1^\infty \tau^{-5}\varphi(\tau)\mathrm{d}\tau<\infty. \tag{4.14}$$

Suppose f solve (4.3) and (4.5). Then there exists $C > 0$ such that for all $0 \le t_* \le t$,

$$\begin{aligned} &\|\varphi(t_{\mathbf{f}})f(t)\|_{L^1_{x,v}} + \int_{t_*}^t \|\varphi'(t_{\mathbf{f}})f\|_{L^1_{x,v}} + \int_{t_*}^t |\varphi(t_{\mathbf{f}})f|_{L^1_{\gamma_+}} - \frac{1}{4}\int_{t_*}^t |f|_{L^1_{\gamma_+}} \\ &\le \|\varphi(t_{\mathbf{f}})f(t_*)\|_{L^1_{x,v}} + C\|f(t_*)\|_{L^1_{x,v}}. \end{aligned} \tag{4.15}$$

It is worth informing beforehand that the exponent -5 in (4.14) will basically restrict the decay rate of Theorem 4.1.1. Some postulation on the wall Maxwellian such as $\mu(v)/\langle v\rangle^r < \infty$ for some $r > 0$ in (1.11) or a similar assumption on the inflow boundary condition would provide faster decay.

Employing a function φ with $\varphi' \to \infty$ as $\tau \to \infty$ (see φ_1 in (4.49)), an L^1-term majorizes the unreachable defect of the lower bound (4.13) with a large factor $\varphi(\frac{3T_0}{4})$. Adding (4.13) and (4.15) with the proper ratio, suggested by the large factor, we establish the uniform estimates of the following energies (see φ_i's in (4.49)), with $\|\mathfrak{m}\|_{L^1_{x,v}} \sim \delta_{\mathfrak{m},T_0}$ (see (4.44)),

$$|\!|\!| f |\!|\!|_i := \|f\|_{L^1_{x,v}} + \frac{4\delta_{\mathfrak{m},T_0}}{\varphi_{i-1}(\frac{3T_0}{4})}\|\varphi_{i-1}(t_{\mathbf{f}})f\|_{L^1_{x,v}} + \frac{4\delta_{\mathfrak{m},T_0}}{T_0\varphi_{i-1}(\frac{3T_0}{4})}\|\varphi_i(t_{\mathbf{f}})f\|_{L^1_{x,v}}, \quad \text{for} \quad i = 1, 4. \tag{4.16}$$

Finally we interpolate $\|\varphi_1(t_{\mathbf{f}})f\|_{L^1_{x,v}}$ by $\|\varphi_0(t_{\mathbf{f}})f\|_{L^1_{x,v}}$ and $\|\varphi_4(t_{\mathbf{f}})f\|_{L^1_{x,v}}$, and using the boundedness of $|\!|\!| f |\!|\!|_4$, we prove the L^1-decay result (see also the similar result in [13]):

Proposition 4.1.7. *Given the same assumptions of Theorem 4.1.1,*

$$\|f(t)\|_{L^1_{x,v}} \lesssim (\ln\langle t\rangle)^2\langle t\rangle^{-4}\{\|e^{\theta'|v|^2}f_0\|_{L^\infty_{x,v}} + \|\varphi_4(t_{\mathbf{f}})f_0\|_{L^1_{x,v}}\}. \tag{4.17}$$

4.1.1.3 An L^∞-estimate of Moments

We bootstrap the L^1-decay secured in Proposition 4.1.7 to the pointwise bound of the moments. Again, the crucial tool is the stochastic cycle representation in Lemma 4.1.5 for $t_* = 0$. In light of (4.17), we have a natural choice of ϱ so that $\varrho'(t) \lesssim (\ln\langle t\rangle)^{-2}\langle t\rangle^4$ (see (4.79)). We first establish the control of the time integration terms of (4.11) (we control (4.9) similarly, after applying the stochastic cycles twice):

Lemma 4.1.8. *For* $i = 2, \cdots, k-1$, $w(v) = e^{\theta|v|^2}$ *for* $\theta > 0$, *and a differentiable* $\varrho(t)$, *we have*

$$\Big| \int_{\prod_{j=1}^k \mathcal{V}_j} \mathbf{1}_{t_{i+1}<0\leq t_i} \int_0^{t_i} w(v_i)\varrho'(s) f(s, x_i - (t_i - s)v_i, v_i) \mathrm{d}s \mathrm{d}\Sigma_i^k \Big| \lesssim \int_0^t \|\varrho'(s) f(s)\|_{L^1_{x,v}} \mathrm{d}s. \quad (4.18)$$

Using the change of variables $v_{i-1} \mapsto (x_{\mathbf{b}}(x_{i-1}, v_{i-1}), t_{\mathbf{b}}(x_{i-1}, v_{i-1}))$ is the key idea of the proof, which has been crucially used in evaluating the boundary singularity in [36]. By this change of variables we are able to convert the velocity integral of $\mathrm{d}\sigma_{j-1}$ into an integration of the spatial variable $x_i - (t_i - s)v_i = x_{\mathbf{b}}(x_{i-1}, v_{i-1}) - (t_{i-1} - t_{\mathbf{b}}(x_{i-1}, v_{i-1}) - s)v_i$, while the singularity occurs from its Jacobian when $t_{\mathbf{b}}(x_{i-1}, v_{i-1}) = 0$ (see Lemma 4.1.10). We remedy such singularity by applying the change of variables twice for $j = i-1$ and $j = i-2$: among the free variables $\{x_{\mathbf{b}}(x_{i-1}, v_{i-1}), t_{\mathbf{b}}(x_{i-1}, v_{i-1}), x_{\mathbf{b}}(x_{i-2}, v_{i-2}), t_{\mathbf{b}}(x_{i-2}, v_{i-2})\}$ we utilize $x_{\mathbf{b}}(x_{i-1}, v_{i-1})$ and $t_{\mathbf{b}}(x_{i-2}, v_{i-2})$ for the spatial variables $x_i - (t_i - s)v_i = x_{\mathbf{b}}(x_{i-1}, v_{i-1}) - (t_{i-2} - t_{\mathbf{b}}(x_{i-2}, v_{i-2}) - t_{\mathbf{b}}(x_{i-1}, v_{i-1}) - s)v_i$, while we are able to appease singularity from the two change of variables using the integration of $x_{\mathbf{b}}(x_{i-2}, v_{i-2})$ and $t_{\mathbf{b}}(x_{i-1}, v_{i-1})$.

Next we control (4.12) by establishing the following estimate:

Lemma 4.1.9. *There exists* $\mathfrak{C} = \mathfrak{C}(\Omega) > 0$ *(see* (4.78) *for the precise choice) such that*

$$\text{if } k \geq \mathfrak{C}t \text{ then } \sup_{(x,v)\in\bar{\Omega}\times\mathbb{R}^3} \Big(\int_{\prod_{j=1}^{k-1} \mathcal{V}_j} \mathbf{1}_{t_k(t,x,v,v_1,\cdots,v_{k-1})\geq 0} \mathrm{d}\sigma_1 \cdots \mathrm{d}\sigma_{k-1} \Big) \lesssim e^{-t}. \quad (4.19)$$

Similar results have been used in [2, 36, 90] but in this paper, we improve the result (the choice of k, in particular) using a sharper bound for the summation of combination from Stirling's formula.

4.1.2 Preliminaries

In this section we state basic preliminaries mainly collected from [2, 36, 65, 66, 90].

Lemma 4.1.10 (Lemma 9 in [36]). *Suppose Ω is an open bounded subset of $\mathbb{R}^3$ and $\partial\Omega$ is smooth.*

- *For $x \in \partial\Omega$, consider a map*

$$v \in \{v \in \mathbb{R}^3 : n(x) \cdot v > 0\} \mapsto (x_{\mathbf{b}}, t_{\mathbf{b}}) := (x_{\mathbf{b}}(x,v), t_{\mathbf{b}}(x,v)) \in \partial\Omega \times \mathbb{R}_+. \tag{4.20}$$

Then the map (4.20) is bijective and has the change of variable formula as

$$\mathrm{d}v = |t_{\mathbf{b}}|^{-4} |n(x_{\mathbf{b}}) \cdot (x - x_{\mathbf{b}})| \mathrm{d}t_{\mathbf{b}} \mathrm{d}S_{x_{\mathbf{b}}}. \tag{4.21}$$

- *Similarly we have a bijective map*

$$v \in \{v \in \mathbb{R}^3 : n(x) \cdot v < 0\} \mapsto (x_{\mathbf{f}}, t_{\mathbf{f}}) := (x_{\mathbf{f}}(x,v), t_{\mathbf{f}}(x,v)) \in \partial\Omega \times \mathbb{R}_+, \tag{4.22}$$

$$\mathrm{d}v = |t_{\mathbf{f}}|^{-4} |n(x_{\mathbf{f}}) \cdot (x - x_{\mathbf{f}})| \mathrm{d}t_{\mathbf{f}} \mathrm{d}S_{x_{\mathbf{f}}}.$$

Lemma 4.1.11 (Lemma 3, Lemma 4 in [36]). *For any g,*

$$\int_{\gamma_\pm} \int_0^{t_\mp(x,v)} g(x \mp sv, v) |n(x) \cdot v| \mathrm{d}s \mathrm{d}v \mathrm{d}S_x = \iint_{\Omega \times \mathbb{R}^3} g(y,v) \mathrm{d}y \mathrm{d}v, \tag{4.23}$$

$$\int_{\gamma_\pm} g(x_\mp(x,v), v) |n(x) \cdot v| \mathrm{d}v \mathrm{d}S_x = \int_{\gamma_\mp} g(y,v) |n(y) \cdot v| \mathrm{d}v \mathrm{d}S_y. \tag{4.24}$$

Here, for the sake of simplicity, we have abused the notations temporarily: $t_- = t_{\mathbf{b}}, x_- = x_{\mathbf{b}}$ and $t_+ = t_{\mathbf{f}}, x_+ = x_{\mathbf{f}}$.

Lemma 4.1.12. *Suppose f solve (4.3) and (4.5). For $0 \leq t_* \leq t$,*

$$\|f(t)\|_{L^1_{x,v}} \leq \|f(t_*)\|_{L^1_{x,v}}, \tag{4.25}$$

$$\int_{t_*}^t |f(s)|_{L^1_{\gamma_+}} \leq \|f(t_*)\|_{L^1_{x,v}} + O(\delta^2) \int_{t_*}^t |f(s)|_{L^1_{\gamma_+}}. \tag{4.26}$$

Proof. The bound (4.25) is from $\|f(t)\|_{L^1_{x,v}} + \int_{t*}^t \iint_{\gamma_+} |f| - \int_{t*}^t \iint_{\gamma_-} |f| = \|f(t_*)\|_{L^1_{x,v}}$, and, due to the choice of c_μ in (1.11), we have

$$\int_{t*}^t \iint_{\gamma_+} |f| - \int_{t*}^t \iint_{\gamma_-} |f| = \int_{t*}^t \iint_{\gamma_+} |f| - \int_{t*}^t \Big| \iint_{\gamma_+} f \Big| \geq \int_{t*}^t \iint_{\gamma_+} |f| - \int_{t*}^t \iint_{\gamma_+} |f| = 0.$$

Next we work on (4.26) inspired by the proof of the L^1-trace theorem in [65]. Choose $\delta \in (0, t - t_*)$. For $(x, v) \in \gamma_+$,

$$\begin{aligned} |f(s,x,v)| \leq &\underbrace{\mathbf{1}_{0 \leq s-(t-\delta) < t_{\mathbf{b}}(x,v)} |f(t-\delta, x-(s-(t-\delta))v, v)|}_{(4.27)_1} \\ &+ \underbrace{\mathbf{1}_{s-(t-\delta) \geq t_{\mathbf{b}}(x,v)} |f(s - t_{\mathbf{b}}(x,v), x_{\mathbf{b}}(x,v), v)|}_{(4.27)_2}. \end{aligned} \tag{4.27}$$

From (4.23) and (4.25), we have $\int_{t_*}^t \int_{\gamma_+} (4.27)_1 \leq \|f(t-\delta)\|_{L^1_{x,v}} \leq \|f(t_*)\|_{L^1_{x,v}}$. Now we consider $(4.27)_2$. For $y = x_{\mathbf{b}}(x,v)$, we have $\mathbf{1}_{s-(t-\delta)\geq t_{\mathbf{b}}(x,v)} = \mathbf{1}_{s-(t-\delta)\geq t_{\mathbf{f}}(y,v)} \leq \mathbf{1}_{\delta \geq t_{\mathbf{f}}(y,v)}$ for $s \in [t_*, t]$. From the above inequality, further using the Fubini's theorem, (4.24), and (4.5) successively, we derive that

$$\begin{aligned} &\int_{t_*}^t \int_{\gamma_+} (4.27)_2 = \int_{\gamma_+} \int_{t-\delta+t_{\mathbf{b}}(x,v)}^t |f(s - t_{\mathbf{b}}(x,v), x_{\mathbf{b}}(x,v), v)| \mathrm{d}s \{n(x)\cdot v\} \mathrm{d}S_x \mathrm{d}v \\ &\leq \int_{\partial\Omega} \int_{n(y)\cdot v<0} \mathbf{1}_{\delta > t_{\mathbf{f}}(y,v)} \int_{t-\delta}^t |f(s,y,v)| \mathrm{d}s |n(y)\cdot v| \mathrm{d}S_y \mathrm{d}v \\ &\leq \int_{\partial\Omega} \underbrace{\Big(\int_{n(y)\cdot v<0} \mathbf{1}_{\delta > t_{\mathbf{f}}(y,v)} c_\mu \mu(v) |n(y)\cdot v| \mathrm{d}v \Big)}_{(4.28)_*} \int_{t-\delta}^t \int_{n(y)\cdot v_1 > 0} |f(s,y,v_1)| \{n(y)\cdot v_1\} \mathrm{d}v_1 \mathrm{d}s \mathrm{d}S_y. \end{aligned} \tag{4.28}$$

From $|n(y)\cdot v|/|v|^2 \lesssim t_{\mathbf{f}}(y,v)$, we note that $\mathbf{1}_{|n(y)\cdot v|\lesssim \delta |v|^2} \geq \mathbf{1}_{\delta > t_{\mathbf{f}}(y,v)}$. For ϑ being the angle between v and $n(y)$,

$$\begin{aligned}\int_{|n(y)\cdot v|\lesssim\delta|v|^2} \mu(v)\{n(y)\cdot v\}\mathrm{d}v &\leq \int_{|n(y)\cdot v|\lesssim\delta|v|^2}\mu(v)\delta|v|^2\mathrm{d}v, \quad \text{by setting } r=|v|,\\ &\leq C\int_0^\infty \delta r^2 e^{-\frac{r^2}{2}} r^2 \mathrm{d}r \int_{\cos\vartheta<\delta r}\sin\vartheta \mathrm{d}\vartheta \\ &\leq C\int_0^\infty \delta r^2 e^{-\frac{r^2}{2}} r^2\delta r \mathrm{d}r \leq C\delta^2.\end{aligned} \tag{4.29}$$

Then, from (4.28) and (4.29), we conclude $\int_{t_*}^t\int_{\gamma_+}(4.27)_2 \leq (4.28) \lesssim \delta^2\int_{t_*}^t\int_{\gamma_+}|f|$. □

Lemma 4.1.13. *For a strictly convex domain with a smooth boundary,*

$$\max\{|n(y)\cdot(y-z)|, |n(z)\cdot(y-z)|\} \lesssim |y-z|^2 \text{ for all } y,z\in\partial\Omega. \tag{4.30}$$

If we further assume that the domain is strictly convex then there exists $C_\Omega > 0$ such that

$$\min\big(|n(y)\cdot(y-z)|, |n(z)\cdot(y-z)|\big) \geq C_\Omega |y-z|^2 \text{ for all } y,z\in\partial\Omega. \tag{4.31}$$

4.1.3 Weighted L^1-Estimates

The main purpose of this section to prove Proposition 4.1.7, which happens at the end of this section. We shall start it by settling one of the key cornerstones, Lemma 4.1.14, the lower bound with the unreachable defect.

Lemma 4.1.14. *Suppose f solve (4.3) with (4.5). Assume $f_0(x,v)\geq 0$ (no need of (4.1)). For any $T_0 \gg 1$ and $N\in\mathbb{N}$ there exists $\mathfrak{m}(x,v)\geq 0$, which only depends on Ω and T_0 (see (4.42) for the precise form), such that*

$$f(NT_0,x,v) \geq \mathfrak{m}(x,v)\Big\{\iint_{\Omega\times\mathbb{R}^3} f((N-1)T_0,x,v)\mathrm{d}v\mathrm{d}x - \iint_{\Omega\times\mathbb{R}^3}\mathbf{1}_{t_{\mathbf{f}}(x,v)\geq\frac{3T_0}{4}} f((N-1)T_0,x,v)\mathrm{d}v\mathrm{d}x\Big\}. \tag{4.32}$$

Proof. **Step 1.** It is standard to derive $f(t,x,v)\geq 0$ from the assumption $f_0(x,v)\geq 0$. For the proof we refer to the standard sequence argument in the proof of Theorem 1 in [2]. Together with (4.8)-(4.12) for $t=NT_0$, $t_*=(N-1)T_0$, $k=3$, we can derive that

$$f(NT_0,x,v)\geq \mathbf{1}_{t_{\mathbf{b}}(x,v)\leq \frac{T_0}{4}}c_\mu\mu(v)\int_{\mathcal{V}_1}\int_{\mathcal{V}_2}\int_{\mathcal{V}_3}\mathbf{1}_{t_3\geq (N-1)T_0}f(t_3,x_3,v_3)\{n(x_3)\cdot v_3\}\mathrm{d}v_3\mathrm{d}\sigma_2\mathrm{d}\sigma_1. \tag{4.33}$$

Now applying Lemma 4.1.10 for $v_1\in\mathcal{V}_1$ and $v_2\in\mathcal{V}_2$ with (4.20) and (4.21), we derive that

$$\begin{aligned}(4.33)\geq{}& \mathbf{1}_{t_{\mathbf{b}}(x,v)\leq \frac{T_0}{4}}c_\mu\mu(v)\int_0^{t-t_{\mathbf{b}}(x,v)}\int_{\partial\Omega}\underbrace{\frac{|n(x_2)\cdot(x_1-x_2)|}{|t_{\mathbf{b},1}|^4}\frac{|n(x_1)\cdot(x_1-x_2)|}{t_{\mathbf{b},1}}c_\mu\mu\Big(\frac{|x_1-x_2|}{t_{\mathbf{b},1}}\Big)}_{(4.34)_1}\\ &\times\int_0^{t-t_{\mathbf{b}}(x,v)-t_{\mathbf{b},1}}\int_{\partial\Omega}\underbrace{\frac{|n(x_3)\cdot(x_2-x_3)|}{|t_{\mathbf{b},2}|^4}\frac{|n(x_2)\cdot(x_2-x_3)|}{t_{\mathbf{b},2}}c_\mu\mu\Big(\frac{|x_2-x_3|}{t_{\mathbf{b},2}}\Big)\mathbf{1}_{t_3\geq(N-1)T_0}}_{(4.34)_2}\\ &\times\int_{n(x_3)\cdot v_3>0}f(t_3,x_3,v_3)\{n(x_3)\cdot v_3\}\mathrm{d}v_3\mathrm{d}S_{x_3}\mathrm{d}t_{\mathbf{b},2}\mathrm{d}S_{x_2}\mathrm{d}t_{\mathbf{b},1},\end{aligned} \tag{4.34}$$

where $t_3=NT_0-t_{\mathbf{b}}(x,v)-t_{\mathbf{b},1}-t_{\mathbf{b},2}$.

Step 2. To have a positive pointwise lower bound of the integrands of the first two lines of (4.34) we will further restrict integration regimes. Note that $x_1=x_{\mathbf{b}}(x,v)$ is given, and x_2,x_3 are free variables. Now we restrict the range of x_2 as, for $\delta>0$,

$$\mathcal{X}_2^\delta:=\{x_2\in\partial\Omega:|x_1-x_2|>\delta\text{ and }|x_2-x_3|>\delta\}, \tag{4.35}$$

where we pick δ such that $0<\delta\ll|\partial\Omega|<\infty$, we can derive that $|\partial\Omega|/2\leq|\mathcal{X}_2^\delta|\leq|\partial\Omega|$.

For two free variables $t_{\mathbf{b},1}$ and $t_{\mathbf{b},2}$ we use, only inside the proof of Lemma 4.1.14, two free variables

$$\begin{aligned} t_+ &= t_{\mathbf{b},1} + t_{\mathbf{b},2} \in [0, T_0 - t_{\mathbf{b}}(x,v)], \\ t_- &= t_{\mathbf{b},1} - t_{\mathbf{b},2} \in [-(T_0 - t_{\mathbf{b}}(x,v)), T_0 - t_{\mathbf{b}}(x,v)]. \end{aligned} \tag{4.36}$$

Note that the ranges come from $t_3 \geq (N-1)T_0$. Now we restrict the integral regimes of the new variables as

$$\begin{aligned} \mathfrak{T}_+^{T_0} &:= \Big\{ t_+ \in [0,\infty) : T_0 - t_{\mathbf{b}}(x,v) - \min\Big(t_{\mathbf{b}}(x_3,v_3), \frac{T_0}{4}\Big) \leq t_+ \leq T_0 - t_{\mathbf{b}}(x,v) \Big\}, \\ \mathfrak{T}_-^{T_0} &:= \Big\{ t_- \in \mathbb{R} : |t_-| \leq T_0 - t_{\mathbf{b}}(x,v) - \min\Big(t_{\mathbf{b}}(x_3,v_3), \frac{T_0}{4}\Big) \Big\}. \end{aligned} \tag{4.37}$$

As a consequence of (4.37) we will derive (4.38) and (4.39). Firstly, from $t_{\mathbf{b}}(x,v) \leq \frac{T_0}{4}$ in (4.34) and (4.36)

$$\begin{aligned} \min\big(t_{\mathbf{b},1}, t_{\mathbf{b},2}\big) &= \min\Big(\frac{t_+ + t_-}{2}, \frac{t_+ - t_-}{2}\Big) \geq \frac{1}{2}\{T_0 - t_{\mathbf{b}}(x,v) - \frac{T_0}{4} - \frac{T_0}{4}\} \geq \frac{T_0}{8}, \\ \max\big(t_{\mathbf{b},1}, t_{\mathbf{b},2}\big) &= \max\Big(\frac{t_+ + t_-}{2}, \frac{t_+ - t_-}{2}\Big) \leq T_0. \end{aligned} \tag{4.38}$$

Therefore, from (4.35) we exclude the case when x_1, x_2, x_3 are too close and from (4.37) we exclude the case when either $t_{\mathbf{b},1}$ or $t_{\mathbf{b},2}$ is too small or too large.
Secondly, we prove (4.39). Note that if $t_+ \in \mathfrak{T}_+^{T_0}$ then $(N-1)T_0 \leq t_3 = NT_0 - t_{\mathbf{b}}(x,v) - t_+ \leq (N-1)T_0 + \min\{t_{\mathbf{b}}(x_3,v_3), \frac{3T_0}{4}\}$. This implies that,

$$\begin{aligned} &\text{if } \ t_{\mathbf{f}}(y,v_3) = t_3 - (N-1)T_0 = T_0 - t_{\mathbf{b}}(x,v) - t_+ \in \Big[0, \frac{3T_0}{4}\Big], \\ &\text{then } \ y = X((N-1)T_0; t_3, x_3, v_3), \end{aligned} \tag{4.39}$$

where we have use an observation $t_{\mathbf{f}}(y,v_3) \leq t_{\mathbf{b}}(x_3,v_3)$ since $x_3 = x_{\mathbf{f}}(y,v_3)$.

Step 3. For (4.34), we adopt the new variables (4.36), and apply the restriction of integral regimes in (4.35) and (4.37). Recall (4.31) from the convexity of the domain. From

(4.38) and (4.31), we derive that

$$(4.34)_i \geq \frac{C_\Omega|x_i - x_{i+1}|^2}{T_0^4}\frac{C_\Omega|x_i - x_{i+1}|^2}{T_0}\frac{1}{2\pi}e^{-\frac{|x_i-x_{i+1}|^2}{2(T_0/8)^2}} \geq \frac{C_\Omega^2\delta^4}{2\pi T_0^5}e^{-\frac{32\mathrm{diam}(\Omega)^2}{T_0^2}}, \quad \text{for } i = 1, 2.$$

Here $\mathrm{diam}(\Omega) = \sup_{x,y\in\bar{\Omega}}|x-y| < \infty$. Finally we get

$$\begin{aligned}(4.34) \geq \mathbf{1}_{t_{\mathbf{b}}(x,v)\leq\frac{T_0}{4}} & \frac{C_\Omega^4\delta^8}{(2\pi)^2T_0^{10}}e^{-\frac{64\mathrm{diam}(\Omega)^2}{T_0^2}}c_\mu\mu(v)\int_{\partial\Omega}\mathrm{d}S_{x_3}\int_{n(x_3)\cdot v_3>0}\mathrm{d}v_3\{n(x_3)\cdot v_3\}\int_{\mathfrak{T}_+^{T_0}}\mathrm{d}t_+ \\ & \times\int_{\mathcal{X}_2^\delta}\mathrm{d}S_{x_2}\int_{\mathfrak{T}_-^{T_0}}\mathrm{d}t_- f(NT_0 - t_{\mathbf{b}}(x,v) - t_+, x_3, v_3) \\ \geq \mathbf{1}_{t_{\mathbf{b}}(x,v)\leq\frac{T_0}{4}} & \frac{C_\Omega^4\delta^8}{(2\pi)^2T_0^{10}}e^{-\frac{64\mathrm{diam}(\Omega)^2}{T_0^2}}c_\mu\mu(v)|\mathcal{X}_2^\delta|T_0\int_{\partial\Omega}\mathrm{d}S_{x_3}\int_{n(x_3)\cdot v_3>0}\mathrm{d}v_3\{n(x_3)\cdot v_3\} \\ & \times\int_{T_0-t_{\mathbf{b}}(x,v)-\min\left(t_{\mathbf{b}}(x_3,v_3),\frac{T_0}{4}\right)}^{T_0-t_{\mathbf{b}}(x,v)}\mathrm{d}t_+ f(NT_0 - t_{\mathbf{b}}(x,v) - t_+, x_3, v_3).\end{aligned} \tag{4.40}$$

Now we focus on the integrand of (4.40). Note that $(NT_0 - t_{\mathbf{b}}(x,v) - t_+) - (N-1)T_0 = T_0 - t_{\mathbf{b}}(x,v) - t_+ \in \left[0, \min\left(t_{\mathbf{b}}(x_3,v_3), \frac{T_0}{4}\right)\right]$. Therefore

$$(4.40) = \int_{T_0-t_{\mathbf{b}}(x,v)-\min\{t_{\mathbf{b}}(x_3,v_3),\frac{T_0}{4}\}}^{T_0-t_{\mathbf{b}}(x,v)} f((N-1)T_0, x_3 - (T_0 - t_{\mathbf{b}}(x,v) - t_+)v_3, v_3)\mathrm{d}t_+. \tag{4.41}$$

Note that, from (4.39), $t_{\mathbf{f}}(x_3 - (T_0 - t_{\mathbf{b}}(x,v) - t_+)v_3, v_3) \in \left[0, \frac{3T_0}{4}\right]$. Now applying (4.23), we conclude that

$$(4.34) \geq \mathbf{1}_{t_{\mathbf{b}}(x,v)\leq\frac{T_0}{4}}\frac{C_\Omega^4\delta^8}{(2\pi)^2T_0^{10}}e^{-\frac{64\mathrm{diam}(\Omega)^2}{T_0^2}}c_\mu\mu(v)|\mathcal{X}_2^\delta|T_0\iint_{\Omega\times\mathbb{R}^3}\mathbf{1}_{t_{\mathbf{f}}(y,v)\in[0,\frac{3T_0}{4}]}f((N-1)T_0, y, v)\mathrm{d}v\mathrm{d}y.$$

We conclude (4.32) by setting

$$\mathfrak{m}(x,v) := \mathbf{1}_{t_{\mathbf{b}}(x,v)\leq\frac{T_0}{4}}(2\pi)^{-2}C_\Omega^4\delta^8T_0^{-9}\exp(-64\mathrm{diam}(\Omega)^2T_0^{-2})|\mathcal{X}_2^\delta|c_\mu\mu(v). \tag{4.42}$$

Recall that $\mathcal{X}_2^\delta$ and δ is defined in (4.35). $\square$

An immediate consequence of Lemma 4.1.14, as in [13], follows.

Proposition 4.1.15. *Suppose f solve* (4.3) *and (4.5), and satisfy (4.1). Then for all $T_0 \gg 1$, $0 < \delta \ll 1$, and $N \in \mathbb{N}$*

$$\|f(NT_0)\|_{L^1_{x,v}} \leq (1 - \|\mathfrak{m}\|_{L^1_{x,v}})\|f((N-1)T_0)\|_{L^1_{x,v}} + 2\|\mathfrak{m}\|_{L^1_{x,v}}\|\mathbf{1}_{t_{\mathbf{f}} \geq \frac{3T_0}{4}} f((N-1)T_0)\|_{L^1_{x,v}}. \quad (4.43)$$

Here, with $\mathcal{X}_2^\delta$ in (4.35),

$$\|\mathfrak{m}\|_{L^1_{x,v}} = \delta_{\mathfrak{m},T_0} \sim (2\pi)^{-2} C_\Omega^4 \delta^8 T_0^{-8} \exp(-64 diam(\Omega)^2 T_0^{-2}) |\mathcal{X}_2^\delta| |\partial\Omega|. \quad (4.44)$$

Proof. Decompose

$$\begin{aligned} f((N-1)T_0, x, v) &= f_{N-1,+}(x,v) - f_{N-1,-}(x,v) \\ &:= \mathbf{1}_{f((N-1)T_0,x,v) \geq 0} |f((N-1)T_0, x, v)| - \mathbf{1}_{f((N-1)T_0,x,v)<0} |f((N-1)T_0, x, v)|. \end{aligned}$$

Let $f_\pm(s, x, v)$ solve (4.3) for $s \in [(N-1)T_0, NT_0]$ with the initial data $f_{N-1,+}$ and $f_{N-1,-}$ at $s = (N-1)T_0$, respectively. Now we apply Lemma 4.1.14 to each $f_\pm(t, x, v)$ and conclude (4.32) for both $f = f_+$ and $f = f_-$ respectively. We also note that $\iint_{\Omega\times\mathbb{R}^3} f((N-1)T_0, x, v)\mathrm{d}x\mathrm{d}v = \iint_{\Omega\times\mathbb{R}^3} f_{N-1,+}(x,v)\mathrm{d}x\mathrm{d}v - \iint_{\Omega\times\mathbb{R}^3} f_{N-1,-}(x,v)\mathrm{d}x\mathrm{d}v = 0$ implies $\iint_{\Omega\times\mathbb{R}^3} f_{N-1,\pm}(x,v)\mathrm{d}x\mathrm{d}v = \frac{1}{2}\iint_{\Omega\times\mathbb{R}^3} |f((N-1)T_0, x, v)|\mathrm{d}x\mathrm{d}v$. Then we derive that

$$\begin{aligned} f_\pm(NT_0, x, v) &\geq \mathfrak{m}(x,v) \iint f_{N-1,\pm}(x,v)\mathrm{d}x\mathrm{d}v - \mathfrak{m}(x,v) \iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{t_{\mathbf{f}}(x,v) \geq \frac{3T_0}{4}} f_{N-1,\pm}(x,v)\mathrm{d}x\mathrm{d}v \\ &\geq \mathfrak{l}(x,v) := \frac{\mathfrak{m}(x,v)}{2} \iint_{\Omega\times\mathbb{R}^3} |f((N-1)T_0)| - \mathfrak{m}(x,v) \iint_{\Omega\times\mathbb{R}^3} \mathbf{1}_{t_{\mathbf{f}}(x,v) \geq \frac{3T_0}{4}} |f((N-1)T_0)|. \end{aligned} \quad (4.45)$$

Then we deduce that

$$\begin{aligned} |f(NT_0, x, v)| &= |f_+(NT_0, x, v) - \mathfrak{l}(x,v) - f_-(NT_0, x, v) + \mathfrak{l}(x,v)| \\ &\leq |f_+(NT_0, x, v) - \mathfrak{l}(x,v)| + |f_-(NT_0, x, v) - \mathfrak{l}(x,v)| \\ &\leq f_+(NT_0, x, v) + f_-(NT_0, x, v) - 2\mathfrak{l}(x,v). \end{aligned}$$

Note that $f_+(NT_0, x, v) + f_-(NT_0, x, v)$ solves (4.3) with the initial datum $f_{N-1,+} + f_{N-1,-} = |f((N-1)T_0, x, v)|$ at $(N-1)T_0$. Then using (4.1) and taking an integration to (4.45) over $\Omega \times \mathbb{R}^3$, we derive

(4.43).

For (4.44) it suffices to bound $\|\mathbf{1}_{t_{\mathbf{b}}(x,v)\leq\frac{T_0}{4}}c_\mu\mu(v)\|_{L^1_{x,v}}$. From (4.23) and $t_{\mathbf{b}}(x-sv,v)=t_{\mathbf{b}}(x,v)-s$,

$$\begin{aligned}
&\|\mathbf{1}_{t_{\mathbf{b}}(x,v)\leq\frac{T_0}{4}}c_\mu\mu(v)\|_{L^1_{x,v}}=\int_{\partial\Omega}\int_{n(x)\cdot v>0}\int_{\max\{0,t_{\mathbf{b}}(x,v)-\frac{T_0}{4}\}}^{t_{\mathbf{b}}(x,v)}c_\mu\mu(v)\{n(x)\cdot v\}\mathrm{d}s\mathrm{d}v\mathrm{d}S_x\\
&=\int_{\partial\Omega}\int_{n(x)\cdot v>0}\Big(\mathbf{1}_{t_{\mathbf{b}}(x,v)\leq\frac{T_0}{4}}\int_0^{t_{\mathbf{b}}(x,v)}\mathrm{d}s+\mathbf{1}_{t_{\mathbf{b}}(x,v)\geq\frac{T_0}{4}}\int_{t_{\mathbf{b}}(x,v)-\frac{T_0}{2}}^{t_{\mathbf{b}}(x,v)}\mathrm{d}s\Big)c_\mu\mu(v)\{n(x)\cdot v\}\mathrm{d}v\mathrm{d}S_x\sim T_0|\partial\Omega|.
\end{aligned}$$

Combining the above bound with (4.42), we conclude (4.44). □

Next, we prove an important result, Lemma 4.1.6, which will be used frequently in this paper.

Proof of Lemma 4.1.6. Note that in the sense of distribution $[\partial_t+v\cdot\nabla_x](\varphi(t_{\mathbf{f}})|f|)=\varphi'(t_{\mathbf{f}})v\cdot\nabla_x t_{\mathbf{f}}|f|=-\varphi'(t_{\mathbf{f}})|f|$. From this equation and (4.5), we derive that

$$\begin{aligned}
&\|\varphi(t_{\mathbf{f}})f(t)\|_{L^1_{x,v}}+\int_{t_*}^t\|\varphi'(t_{\mathbf{f}})f(s)\|_{L^1_{x,v}}+\int_{t_*}^t\int_{\gamma_+}\varphi(t_{\mathbf{f}})|f|\mathrm{d}v\mathrm{d}S_x\leq\ \|\varphi(t_{\mathbf{f}})f(t_*)\|_{L^1_{x,v}}\\
&+\int_{t_*}^t\int_{\partial\Omega}\int_{n(x)\cdot v<0}\varphi(t_{\mathbf{f}})c_\mu\mu(v)|n(x)\cdot v|\int_{n(x)\cdot v_1>0}|f(s,x,v_1)|\{n(x)\cdot v_1\}\mathrm{d}v_1\mathrm{d}v\mathrm{d}S_x\mathrm{d}s. \quad (4.46)
\end{aligned}$$

We only need to consider (4.46) with the corresponding $\varphi(t_{\mathbf{f}})$. We prove the following claim: If (4.14) holds then $\sup_{x\in\partial\Omega}\int_{n(x)\cdot v<0}\varphi(t_{\mathbf{f}})(x,v)c_\mu\mu(v)|n(x)\cdot v|\mathrm{d}v\lesssim 1$. From the claim (4.26), we conclude (4.15), through, for $C>1$,

$$\begin{aligned}
(4.46)&\leq C\int_{t_*}^t\int_{\gamma_+}|f(s,x,v_1)|\{n(x)\cdot v_1\}\mathrm{d}v_1\mathrm{d}S_x\mathrm{d}s\\
&\leq C\|f((N-1)T_0)\|_{L^1_{x,v}}+\frac{1}{4}\int_{(N-1)T_0}^{NT_0}|f(s)|_{L^1(\gamma_+)}.
\end{aligned}$$

For $0<\delta\ll 1$, we split $\int_{n(x)\cdot v<0}\varphi(t_{\mathbf{f}})(x,v)c_\mu\mu(v)|n(x)\cdot v|\mathrm{d}v$ into two parts: integration over the regimes of $t_{\mathbf{f}}\leq\delta$ and $t_{\mathbf{f}}>\delta$ respectively. When $t_{\mathbf{f}}\leq\delta$, from (4.30), we derive that

$|n(x)\cdot v|/|v|^2 \lesssim t_{\mathbf{f}} \leq \delta$. Then we bound

$$\int_{n(x)\cdot v<0} \mathbf{1}_{t_{\mathbf{f}}\leq\delta}\varphi(t_{\mathbf{f}})(x,v)c_\mu\mu(v)|n(x)\cdot v|\mathrm{d}v \lesssim \delta\varphi(\delta)\int_{\mathbb{R}^3}|v|^2\mu(v)\mathrm{d}v \lesssim 1. \tag{4.47}$$

Now we focus on the integration over the regimes of $t_{\mathbf{f}} > \delta$. From (4.22) we derive that $\int_{n\cdot v<0}\varphi(t_{\mathbf{f}})c_\mu\mu(v)|n\cdot v|\mathrm{d}v$ equals

$$c_\mu\int_{\partial\Omega}\int_\delta^\infty \varphi(t_{\mathbf{f}})\mu\Big(\frac{|x-x_{\mathbf{f}}|}{t_{\mathbf{f}}}\Big)\frac{|n(x)\cdot(x-x_{\mathbf{f}})|^2}{|t_{\mathbf{f}}|^5}\mathrm{d}t_{\mathbf{f}}\mathrm{d}S_{x_{\mathbf{f}}}. \tag{4.48}$$

From (4.30) and (4.14), we derive that (4.48) $\lesssim \int_\delta^\infty \frac{\varphi(t_{\mathbf{f}})}{|t_{\mathbf{f}}|^5}\int_{\partial\Omega}|x-x_{\mathbf{f}}|^4 e^{-\frac{|x-x_{\mathbf{f}}|^2}{2|t_{\mathbf{f}}|^2}}\mathrm{d}S_{x_{\mathbf{f}}}\mathrm{d}t_{\mathbf{f}} \lesssim \int_\delta^\infty \frac{\varphi(t_{\mathbf{f}})}{|t_{\mathbf{f}}|^5}\mathrm{d}t_{\mathbf{f}} \lesssim 1$. Together with above bound and (4.47) we prove our claim. □

We will use the following φ's inspired from [13].

Definition 4.1.16. For $\delta > 0$,

$$\begin{aligned}&\varphi_0(\tau) := (\ln(e+1))^{-1}\ln(e+\ln(e+\tau)),\quad \varphi_1(\tau) := (e\ln(e+1))^{-1}(e+\tau)\ln(e+\ln(e+\tau)),\\ &\varphi_3(\tau) := e^{-3}(\tau+e)^3\big(\ln(\tau+e)\big)^{-(1+\delta)},\quad \varphi_4(\tau) := e^{-4}(\tau+e)^4\big(\ln(\tau+e)\big)^{-(1+\delta)}.\end{aligned} \tag{4.49}$$

First, we check φ_i satisfies (4.14) for $i = 0,1,2,3,4$: for example, for $\delta > 0$

$\int_1^\infty \tau^{-5}e^{-4}(\tau+e)^4\big(\ln(\tau+e)\big)^{-(1+\delta)}\mathrm{d}\tau \lesssim 1+\int_{10}^\infty(\tau+e)^{-1}\big(\ln(\tau+e)\big)^{-(1+\delta)}\mathrm{d}\tau \lesssim \int_1^\infty \frac{1}{s^{1+\delta}}\mathrm{d}s$
, with $s = \ln(\tau+e)$.

Second, we notice that

$$\varphi_i(0) = 1 \quad \text{for } i = 0,1,3,4. \tag{4.50}$$

Finally, we check

$$\varphi_1'(\tau) = (e\ln(e+1))^{-1}\{\ln(e+\ln(e+\tau)) + (e+\ln(e+\tau))^{-1}\} \geq (e\ln(e+1))^{-1}\varphi_0(\tau), \quad \varphi_0'(\tau) \geq 0,$$
$$\varphi_4'(\tau) = \big(4 - \frac{1+\delta}{\ln(\tau+e)}\big)e^{-4}(\tau+e)^3\big(\ln(\tau+e)\big)^{-(1+\delta)} \geq \varphi_3(\tau), \quad \varphi_3'(\tau) \geq 0. \tag{4.51}$$

Proposition 4.1.17. *Choose $T_0 > 10$ such that*

$$4C(2+T_0)T_0^{-1}\Big(\varphi_i(\frac{3T_0}{4})\Big)^{-1} \leq \frac{1}{2} \quad \textit{for} \quad i = 0, 3. \tag{4.52}$$

For all $N \in \mathbb{N}$ and $i \in \{1, 4\}$,

$$\|f(NT_0)\|_{L^1_{x,v}} + \frac{4\delta_{\mathfrak{m},T_0}}{\varphi_{i-1}(\frac{3T_0}{4})}\Big\{\|\varphi_{i-1}(t_{\mathbf{f}})f(NT_0)\|_{L^1_{x,v}} + \frac{1}{T_0}\|\varphi_i(t_{\mathbf{f}})f(NT_0)\|_{L^1_{x,v}} + \frac{1}{2T_0}\int_{(N-1)T_0}^{NT_0}|f|_{L^1_{\gamma+}}\Big\}$$
$$\leq (4.53)_* \times \|f((N-1)T_0)\|_{L^1_{x,v}} + \frac{4\delta_{\mathfrak{m},T_0}}{\varphi_{i-1}(\frac{3T_0}{4})}\Big\{\frac{3}{4}\|\varphi_{i-1}(t_{\mathbf{f}})f((N-1)T_0)\|_{L^1_{x,v}} + \frac{1}{T_0}\|\varphi_i(t_{\mathbf{f}})f((N-1)T_0)\|_{L^1_{x,v}}\Big\}, \tag{4.53}$$

with $(4.53)_* := (1 - \delta_{\mathfrak{m},T_0}\{1 - \frac{4C(2+T_0)}{T_0\varphi_{i-1}(\frac{3T_0}{4})}\})$ *where* δ_{m,T_0} *is defined in* (4.44).

Proof. As key steps we will repeatedly apply Lemma 4.1.6 with φ_i's in (4.49). Applying Lemma 4.1.6 to $f(t,x,v)$, solving (4.3) and (4.5), with φ_i for $i = 0, 1, 4$ in (4.49), and using (4.50), we derive that, for $i = 1, 4$ and $(N-1)T_0 \leq t_* \leq NT_0$,

$$\|\varphi_{i-1}(t_{\mathbf{f}})f(NT_0)\|_{L^1_{x,v}} + \frac{3}{4}\int_{t_*}^{NT_0}|f|_{L^1_{\gamma+}} \leq \|\varphi_{i-1}(t_{\mathbf{f}})f(t_*)\|_{L^1_{x,v}} + C\|f(t_*)\|_{L^1_{x,v}}, \tag{4.54}$$
$$\|\varphi_i(t_{\mathbf{f}})f(NT_0)\|_{L^1_{x,v}} + \int_{(N-1)T_0}^{NT_0}\{\|\varphi_i'(t_{\mathbf{f}})f\|_{L^1_{x,v}} + \frac{3}{4}|f|_{L^1_{\gamma+}}\}$$
$$\leq \|\varphi_i(t_{\mathbf{f}})f((N-1)T_0)\|_{L^1_{x,v}} + C\|f((N-1)T_0)\|_{L^1_{x,v}}. \tag{4.55}$$

From (4.25), (4.51) and (4.54), we derive that, for $i = 1, 4$,

$$\int_{(N-1)T_0}^{NT_0}\|\varphi_i'(t_{\mathbf{f}})f\|_{L^1_{x,v}} \geq \int_{(N-1)T_0}^{NT_0}\|\varphi_{i-1}(t_{\mathbf{f}})f(t_*)\|_{L^1_{x,v}}\mathrm{d}t_*$$
$$\geq T_0\|\varphi_{i-1}(t_{\mathbf{f}})f(NT_0)\|_{L^1_{x,v}} - CT_0\|f((N-1)T_0)\|_{L^1_{x,v}}.$$

From the above bound and (4.55), we conclude that, for $i = 1, 4$,

$$\begin{aligned} &\|\varphi_i(t_{\mathbf{f}}) f(NT_0)\|_{L^1_{x,v}} + T_0 \|\varphi_{i-1}(t_{\mathbf{f}}) f(NT_0)\|_{L^1_{x,v}} + \frac{3}{4}\int_{(N-1)T_0}^{NT_0} |f|_{L^1_{\gamma_+}} \\ &\leq \|\varphi_i(t_{\mathbf{f}}) f((N-1)T_0)\|_{L^1_{x,v}} + C(1+T_0)\|f((N-1)T_0)\|_{L^1_{x,v}}. \end{aligned} \tag{4.56}$$

Now we combine (4.43) with (4.54)-(4.56). From (4.43) and

$$\mathbf{1}_{t_{\mathbf{f}} \geq \frac{3T_0}{4}} \leq \big(\varphi_{i-1}(\frac{3T_0}{4})\big)^{-1} \varphi_{i-1}(t_{\mathbf{f}}),$$

with $\delta_{\mathfrak{m},T_0}$ in (4.44),

$$\|f(NT_0)\|_{L^1_{x,v}} \leq (1-\delta_{\mathfrak{m},T_0})\|f((N-1)T_0)\|_{L^1_{x,v}} + 2\delta_{\mathfrak{m},T_0}\Big(\varphi_{i-1}(\frac{3T_0}{4})\Big)^{-1} \|\varphi_{i-1}(t_{\mathbf{f}}) f((N-1)T_0)\|_{L^1_{x,v}}. \tag{4.57}$$

For $i = 1, 4$, from (4.57) + $\frac{4\delta_{\mathfrak{m},T_0}}{T_0 \varphi_{i-1}(\frac{3T_0}{4})}\big\{(4.54)|_{t=NT_0} + (4.56)\big\}$, and $T_0 > 0$ in (4.52), we deduce (4.53). □

Now we are well equipped to prove Proposition 4.1.7.

Proof of Proposition 4.1.7. Fix T_0 in (4.52) and recall norms of $|||\cdot|||_1$ and $|||\cdot|||_4$ in (4.16). From (4.53), for $i = 1, 4$,

$$|||f(NT_0)|||_i \leq |||f((N-1)T_0)|||_i \leq \cdots \leq |||f(0)|||_i, \quad \text{for all } N \in \mathbb{N}. \tag{4.58}$$

Step 1. Since $\varphi_1(\tau)/\varphi_4(\tau)$ is a decreasing function of $\tau \gg 1$, for $M \gg 1$ $\big(M$ will be chosen large enough to satisfy (4.61) and (4.66)$\big)$, we have $\varphi_1(t_{\mathbf{f}}) = \mathbf{1}_{t_{\mathbf{f}} \geq M}\varphi_1(t_{\mathbf{f}}) + \mathbf{1}_{t_{\mathbf{f}}<M}\varphi_1(t_{\mathbf{f}}) = \mathbf{1}_{t_{\mathbf{f}} \geq M}\frac{\varphi_1(M)}{\varphi_4(M)}\varphi_4(t_{\mathbf{f}}) + \mathbf{1}_{t_{\mathbf{f}}<M} M\varphi_0(t_{\mathbf{f}})$. From the above bound and (4.58) for $i = 4$, for $M \gg 1$,

$N \in \mathbb{N}$,

$$\frac{1}{M}\|\varphi_1(t_{\mathbf{f}})f((N-1)T_0)\|_{L^1_{x,v}} \leq \frac{1}{M}\frac{\varphi_1(M)}{\varphi_4(M)}\frac{T_0\varphi_3(\frac{3T_0}{4})}{4\delta_{\mathfrak{m},T_0}}|||f(0)|||_4 + \|\varphi_0(t_{\mathbf{f}})f((N-1)T_0)\|_{L^1_{x,v}}. \tag{4.59}$$

From (4.53) and (4.59), with $(4.60)_* := \max\big\{(1-\delta_{\mathfrak{m},T_0}\{1-\frac{4C(2+T_0)}{T_0\varphi_0(\frac{3T_0}{4})}\}),(\frac{3}{4}+\frac{1}{T_0}),(1-\frac{1}{M})\big\}$,

$$|||f(NT_0)|||_1 \leq (4.60)_* \times |||f((N-1)T_0)|||_1 + \frac{1}{M}\frac{\varphi_1(M)}{\varphi_4(M)}\frac{\varphi_3(\frac{3T_0}{4})}{\varphi_0(\frac{3T_0}{4})}|||f(0)|||_4. \tag{4.60}$$

Step 2. Tentatively we make an assumption, which will be justified later behind (4.66),

$$\Big(1+\frac{1}{M}\Big)^{-1} \geq \max\Big\{\Big(1-\delta_{\mathfrak{m},T_0}\Big\{1-\frac{4C(2+T_0)}{T_0\varphi_0(\frac{3T_0}{4})}\Big\}\Big),\Big(\frac{3}{4}+\frac{1}{T_0}\Big),\Big(1-\frac{1}{M}\Big)\Big\}. \tag{4.61}$$

For $t \geq 0$, choose $N_* \in \mathbb{N}$ such that $t \in [N_*T_0,(N_*+1)T_0]$. From (4.60) and (4.61), we derive, for all $0 \leq N \leq N_*+1$,

$$|||f(NT_0)|||_1 \leq \Big(1+\frac{1}{M}\Big)^{-1}|||f((N-1)T_0)|||_1 + \mathfrak{R}, \quad \text{with } \mathfrak{R} := \frac{1}{M}\frac{\varphi_1(M)}{\varphi_4(M)}\frac{\varphi_3(\frac{3T_0}{4})}{\varphi_0(\frac{3T_0}{4})}|||f(0)|||_4. \tag{4.62}$$

From (4.15) and $N_*T_0 \leq t$, then there exists $C>0$ such that,

$$\|\varphi(t_{\mathbf{f}})f(t)\|_{L^1_{x,v}} \leq \|\varphi(t_{\mathbf{f}})f(N_*T_0)\|_{L^1_{x,v}} + C\|f(N_*T_0)\|_{L^1_{x,v}}. \tag{4.63}$$

Now applying (4.63) first and using (4.62) successively, we conclude that

$$\begin{aligned}|||f(t)|||_1 &\lesssim |||f(N_*T_0)|||_1 \leq \Big(1+\frac{1}{M}\Big)^{-1}|||f((N_*-1)T_0)|||_1 + \mathfrak{R}\\ &\leq \Big(1+\frac{1}{M}\Big)^{-2}|||f((N_*-2)T_0)|||_1 + \Big(1+\frac{1}{M}\Big)^{-1}\mathfrak{R} + \mathfrak{R} \leq \cdots\\ &\leq \Big(1+\frac{1}{M}\Big)^{-N_*}|||f(0)|||_1 + (1+M)\mathfrak{R}.\end{aligned} \tag{4.64}$$

From $\left(1+\frac{1}{M}\right)^{-N_*} = \left((1+\frac{1}{M})^{-M}\right)^{\frac{N_*}{M}} \leq e^{-\frac{N_*}{2M}} \leq e^{-\frac{t}{2T_0 M}}$, $(1+M)\mathfrak{R} \leq 2\frac{\varphi_1(M)}{\varphi_4(M)}\frac{\varphi_3(\frac{3T_0}{4})}{\varphi_0(\frac{3T_0}{4})}\|\!|f(0)|\!\|_4$, we have

$$\|\!|f(t)|\!\|_1 \leq (4.64) \lesssim \max\left\{e^{-\frac{t}{2T_0 M}}, \varphi_1(M)/\varphi_4(M)\right\}\left\{\|\!|f(0)|\!\|_1 + \|\!|f(0)|\!\|_4\right\}. \tag{4.65}$$

Following an optimization trick (making $|e^{-\frac{t}{2T_0 M}} - \varphi_1(M)/\varphi_4(M)| \ll 1$ as much as possible), choosing

$$M = t[2T_0 \ln(10+t)^3]^{-1}, \text{ so that } \max\left\{e^{-\frac{t}{2T_0 M}}, \varphi_1(M)/\varphi_4(M)\right\} \lesssim (\ln\langle t\rangle)^{2-\frac{\delta}{2}}\langle t\rangle^{-3}. \tag{4.66}$$

Clearly such a choice assures our precondition (4.61) for $t \gg 1$. On the other hand it is straightforward to check $\|\!|f(0)|\!\|_1 + \|\varphi_3(t_{\mathbf{f}})f_0\|_{L^1_{x,v}} \lesssim \|e^{\theta'|v|^2}f_0\|_{L^\infty_{x,v}}$ from (4.23) and (4.21), while $\|\varphi_4(t_{\mathbf{f}})f_0\|_{L^1_{x,v}} < \infty$ has been taken for grated from the postulation of Theorem 4.1.1. Setting $\varphi = \varphi_1, t_* = t/2$ and from (4.51), we have

$$\frac{t}{2}\|f(t)\|_{L^1_{x,v}} \lesssim \int_{\frac{t}{2}}^{t} \|\varphi_1'(t_{\mathbf{f}})f(s)\|_{L^1_{x,v}}\mathrm{d}s$$

Applying (4.15) and (4.25), we get

$$\int_{\frac{t}{2}}^{t} \|\varphi_1'(t_{\mathbf{f}})f(s)\|_{L^1_{x,v}}\mathrm{d}s \lesssim \left\|\!\left| f\left(\frac{t}{2}\right)\right|\!\right\|_1$$

From (4.65) and (4.66), we derive

$$\left\|\!\left| f\left(\frac{t}{2}\right)\right|\!\right\|_1 \lesssim (\ln\langle t\rangle)^{2-\frac{\delta}{2}}\langle t\rangle^{-3}\{\|e^{\theta'|v|^2}f_0\|_{L^\infty_{x,v}} + \|\varphi_4(t_{\mathbf{f}})f_0\|_{L^1_{x,v}}\}.$$

Therefore, we finally prove (4.17). □

4.1.4 L^∞-Estimates of Moments

We give proofs for Lemma 4.1.8 and Lemma 4.1.9.

Proof of Lemma 4.1.8. For (4.18) it suffices to prove this upper bound for

$$\int_{\mathcal{V}_1}\cdots\int_{\mathcal{V}_{i-1}}\int_0^{t_i}\int_{\mathcal{V}_i}\mathbf{1}_{t_{i+1}<0\leq t_i}\varrho'(s)|f(s,x_i-(t_i-s)v_i,v_i)|\{n(x_i)\cdot v_i\}\mathrm{d}v_i\mathrm{d}s\mathrm{d}\sigma_{i-1}\cdots\mathrm{d}\sigma_1. \tag{4.67}$$

Step 1. Applying Lemma 4.1.10, (4.20), (4.21) with $x=x_j$ and $v=v_j$, we derive the change of variables, for $j=i-1,i-2$,

$$v_j\in\mathcal{V}_j\mapsto(x_{j+1},t_{\mathbf{b},j}):=(x_{\mathbf{b}}(x_j,v_j),t_{\mathbf{b}}(x_j,v_j))\in\partial\Omega\times[0,t_j],$$

with $\mathrm{d}v_j=|t_{\mathbf{b},j}|^{-4}|n(x_{j+1})\cdot(x_j-x_{j+1})|\mathrm{d}t_{\mathbf{b},j}\mathrm{d}S_{x_i}$. Applying above change of variables twice, we derive that (4.67) equals

$$\begin{aligned}&\int_{\mathcal{V}_1}\mathrm{d}\sigma_1\cdots\int_{\mathcal{V}_{i-3}}\mathrm{d}\sigma_{i-3}\\&\times\int_0^{t_{i-2}}\mathrm{d}t_{\mathbf{b},i-2}\int_{\partial\Omega}\mathrm{d}S_{x_{i-1}}c_\mu\mu\Big(\frac{|x_{i-2}-x_{i-1}|}{|t_{\mathbf{b},i-2}|}\Big)\frac{|n(x_{i-1})\cdot(x_{i-2}-x_{i-1})||n(x_{i-2})\cdot(x_{i-2}-x_{i-1})|}{|t_{\mathbf{b},i-2}|^5}\\&\times\int_0^{t_{i-2}-t_{\mathbf{b},i-2}}\mathrm{d}t_{\mathbf{b},i-1}\int_{\partial\Omega}\mathrm{d}S_{x_i}c_\mu\mu\Big(\frac{|x_{i-1}-x_i|}{|t_{\mathbf{b},i-1}|}\Big)\frac{|n(x_i)\cdot(x_{i-1}-x_i)||n(x_{i-1})\cdot(x_{i-1}-x_i)|}{|t_{\mathbf{b},i-1}|^5}\\&\times\Big(\int_0^{t_{i-1}-t_{\mathbf{b},i-1}}\int_{\mathcal{V}_i}\mathbf{1}_{t_{i-1}-t_{\mathbf{b},i-1}-t_{\mathbf{b}}(x_i,v_i)<0}\varrho'(s)|f(s,x_i-(t_i-s)v_i,v_i)|\{n(x_i)\cdot v_i\}\mathrm{d}v_i\mathrm{d}s\Big),\end{aligned}\tag{4.68}$$

with t_{i-2}, x_{i-2} defined in (4.7), and $t_{i-1}=t_{i-2}-t_{\mathbf{b},i-2}$. Using (4.31), we bound the above integration as

$$\begin{aligned}&\int_{\mathcal{V}_1}\mathrm{d}\sigma_1\cdots\int_{\mathcal{V}_{i-3}}\mathrm{d}\sigma_{i-3}\int_0^{t_{i-2}}\mathrm{d}t_{\mathbf{b},i-1}\int_0^{t_{i-2}-t_{\mathbf{b},i-1}}\mathrm{d}t_{\mathbf{b},i-2}\int_{\partial\Omega}\mathrm{d}S_{x_i}\\&\times\underbrace{\Big(\int_{\partial\Omega}c_\mu\mu\Big(\frac{|x_{i-2}-x_{i-1}|}{|t_{\mathbf{b},i-2}|}\Big)\frac{|x_{i-2}-x_{i-1}|^4}{|t_{\mathbf{b},i-2}|^5}c_\mu\mu\Big(\frac{|x_{i-1}-x_i|}{|t_{\mathbf{b},i-1}|}\Big)\frac{|x_{i-1}-x_i|^4}{|t_{\mathbf{b},i-1}|^5}\mathrm{d}S_{x_{i-1}}\Big)}_{(4.69)_*}(4.68).\end{aligned}\tag{4.69}$$

Step 2. We claim that

$$(4.69)_* \lesssim \mathbf{1}_{t_{\mathbf{b},i-1}\le t_{\mathbf{b},i-2}} \langle t_{\mathbf{b},i-2}\rangle^{-5} + \mathbf{1}_{t_{\mathbf{b},i-1}\ge t_{\mathbf{b},i-2}} \langle t_{\mathbf{b},i-1}\rangle^{-5}. \tag{4.70}$$

We split the cases: *Case 1:* $t_{\mathbf{b},i-1} \le t_{\mathbf{b},i-2}$. Using $|x_{i-2}-x_{i-1}| \lesssim_\Omega 1$, we bound

$$c_\mu \mu\Big(\frac{|x_{i-2}-x_{i-1}|}{|t_{\mathbf{b},i-2}|}\Big)\frac{|x_{i-2}-x_{i-1}|^4}{|t_{\mathbf{b},i-2}|^5} \lesssim \mathbf{1}_{t_{\mathbf{b},i-2}\le 1}\frac{1}{|t_{\mathbf{b},i-2}|} + \mathbf{1}_{t_{\mathbf{b},i-2}\ge 1}\frac{1}{|t_{\mathbf{b},i-2}|^5}, \tag{4.71}$$

$$c_\mu \mu\Big(\frac{|x_{i-1}-x_{i}|}{|t_{\mathbf{b},i-1}|}\Big)\frac{|x_{i-1}-x_{i}|^4}{|t_{\mathbf{b},i-1}|^5} \lesssim \mu^{\frac{1}{2}}\Big(\frac{|x_{i-1}-x_{i}|}{|t_{\mathbf{b},i-1}|}\Big)\Big\{\mathbf{1}_{t_{\mathbf{b},i-1}\le 1}\frac{1}{|t_{\mathbf{b},i-1}|} + \mathbf{1}_{t_{\mathbf{b},i-1}\ge 1}\frac{1}{|t_{\mathbf{b},i-1}|^5}\Big\}. \tag{4.72}$$

We employ a change of variables, for $x_i \in \partial\Omega$ and $t_{\mathbf{b},i-1} \ge 0$, $x_{i-1} \in \partial\Omega \mapsto z := \frac{1}{t_{\mathbf{b},i-1}}(x_{i-1}-x_i) \in \mathfrak{S}_{x_i,t_{\mathbf{b},i-1}}$, where the image $\mathfrak{S}_{x_i,t_{\mathbf{b},i-1}}$ of the map is a two dimensional smooth hypersurface. Using the local chart of $\partial\Omega$ we have $\mathrm{d}S_{x_{i-1}} \lesssim |t_{\mathbf{b},i-1}|^2 \mathrm{d}S_z$. From this change of variables and (4.71), (4.72), we conclude that

$$\begin{aligned}
&\mathbf{1}_{t_{\mathbf{b},i-1}\le t_{\mathbf{b},i-2}}(4.69)_* \\
&\lesssim \mathbf{1}_{t_{\mathbf{b},i-1}\le t_{\mathbf{b},i-2}}(4.71)\int_{\mathfrak{S}_{x_i,t_{\mathbf{b},i-1}}} \mu^{\frac{1}{2}}(z)\Big\{\mathbf{1}_{t_{\mathbf{b},i-1}\le 1}|t_{\mathbf{b},i-1}| + \mathbf{1}_{t_{\mathbf{b},i-1}\ge 1}\frac{1}{|t_{\mathbf{b},i-1}|^3}\Big\}\mathrm{d}S_z \\
&\lesssim \mathbf{1}_{t_{\mathbf{b},i-1}\le t_{\mathbf{b},i-2}}\Big\{\mathbf{1}_{t_{\mathbf{b},i-2}\le 1}\frac{1}{|t_{\mathbf{b},i-2}|} + \mathbf{1}_{t_{\mathbf{b},i-2}\ge 1}\frac{1}{|t_{\mathbf{b},i-2}|^5}\Big\}\Big\{\mathbf{1}_{t_{\mathbf{b},i-1}\le 1}|t_{\mathbf{b},i-1}| + \mathbf{1}_{t_{\mathbf{b},i-1}\ge 1}\frac{1}{|t_{\mathbf{b},i-1}|^3}\Big\} \\
&\lesssim \mathbf{1}_{t_{\mathbf{b},i-1}\le t_{\mathbf{b},i-2}}\Big\{\mathbf{1}_{t_{\mathbf{b},i-2}\le 1}\frac{t_{\mathbf{b},i-1}}{t_{\mathbf{b},i-2}} + \mathbf{1}_{t_{\mathbf{b},i-2}\ge 1}\frac{1}{|t_{\mathbf{b},i-2}|^5}\Big\} \lesssim \mathbf{1}_{t_{\mathbf{b},i-2}\le 1} + \mathbf{1}_{t_{\mathbf{b},i-2}\ge 1}\frac{1}{|t_{\mathbf{b},i-2}|^5}.
\end{aligned} \tag{4.73}$$

Case 2: $t_{\mathbf{b},i-1} \ge t_{\mathbf{b},i-2}$. We change the role of $i-1$ and $i-2$ and follow the argument of the previous case. Using $|x_{i-1}-x_i| \lesssim_\Omega 1$, we bound

$$c_\mu \mu\Big(\frac{|x_{i-1}-x_{i}|}{|t_{\mathbf{b},i-1}|}\Big)\frac{|x_{i-1}-x_{i}|^4}{|t_{\mathbf{b},i-1}|^5} \lesssim \mathbf{1}_{t_{\mathbf{b},i-1}\le 1}\frac{1}{|t_{\mathbf{b},i-1}|} + \mathbf{1}_{t_{\mathbf{b},i-1}\ge 1}\frac{1}{|t_{\mathbf{b},i-1}|^5},$$

$$c_\mu \mu\Big(\frac{|x_{i-2}-x_{i-1}|}{|t_{\mathbf{b},i-2}|}\Big)\frac{|x_{i-2}-x_{i-1}|^4}{|t_{\mathbf{b},i-2}|^5} \lesssim \mu^{\frac{1}{2}}\Big(\frac{|x_{i-2}-x_{i-1}|}{|t_{\mathbf{b},i-2}|}\Big)\{\mathbf{1}_{t_{\mathbf{b},i-2}\le 1}\frac{1}{|t_{\mathbf{b},i-2}|} + \mathbf{1}_{t_{\mathbf{b},i-2}\ge 1}\frac{1}{|t_{\mathbf{b},i-2}|^5}\}.$$

We employ a change of variables, for $x_{i-1} \in \partial\Omega$ and $t_{\mathbf{b},i-2} \geq 0$, $x_{i-2} \in \partial\Omega \mapsto z := \frac{1}{t_{\mathbf{b},i-2}}(x_{i-2} - x_{i-1}) \in \mathfrak{S}_{x_2, t_{\mathbf{b},i-2}}$, with $\mathrm{d}S_{x_{i-2}} \lesssim |t_{\mathbf{b},i-2}|^2 \mathrm{d}S_z$. Then we can conclude that $\mathbf{1}_{t_{\mathbf{b},i-1} \geq t_{\mathbf{b},i-2}}(4.69)_* \lesssim \mathbf{1}_{t_{\mathbf{b},i-1} \leq 1} + \mathbf{1}_{t_{\mathbf{b},i-1} \geq 1} |t_{\mathbf{b},i-1}|^{-5}$. Clearly this bound and (4.73) imply (4.70).

Step 3. Now we use (4.70) to (4.69). Then we have

$$(4.67) \lesssim \int_{\mathcal{V}_1} \mathrm{d}\sigma_1 \cdots \int_{\mathcal{V}_{i-3}} \mathrm{d}\sigma_{i-3} \int_0^{t_{i-2}} \mathrm{d}t_{\mathbf{b},i-1} \langle t_{\mathbf{b},i-1} \rangle^{-5} \int_0^{\min\{t_{i-2} - t_{\mathbf{b},i-1}, t_{\mathbf{b},i-1}\}} \mathrm{d}t_{\mathbf{b},i-2} \int_{\partial\Omega} \mathrm{d}S_{x_i} (4.68) \tag{4.74}$$

$$+ \int_{\mathcal{V}_1} \mathrm{d}\sigma_1 \cdots \int_{\mathcal{V}_{i-3}} \mathrm{d}\sigma_{i-3} \int_0^{t_{i-2}} \mathrm{d}t_{\mathbf{b},i-2} \langle t_{\mathbf{b},i-2} \rangle^{-5} \int_0^{\max\{t_{i-2} - t_{\mathbf{b},i-2}, t_{\mathbf{b},i-2}\}} \mathrm{d}t_{\mathbf{b},i-1} \int_{\partial\Omega} \mathrm{d}S_{x_i} (4.68). \tag{4.75}$$

We first consider (4.74). We employ the following change of variables $(x_i, t_{\mathbf{b},i-2}) \mapsto y = x_i - (t_{i-2} - t_{\mathbf{b},i-2} - t_{\mathbf{b},i-1} - s) v_i \in \Omega$, with $|n(x_i) \cdot v_i| \mathrm{d}S_{x_i} \mathrm{d}t_{\mathbf{b},i-2} = \mathrm{d}y$. Applying this change of variables we derive that

$$\begin{aligned}(4.74) &\leq \int_{\mathcal{V}_1} \mathrm{d}\sigma_1 \cdots \int_{\mathcal{V}_{i-3}} \mathrm{d}\sigma_{i-3} \int_0^{t_{i-2}} \mathrm{d}t_{\mathbf{b},i-1} \langle t_{\mathbf{b},i-1} \rangle^{-5} \int_0^t \iint_{\Omega \times \mathbb{R}^3} \varrho'(s) |f(s, y, v_i)| \mathrm{d}v_i \mathrm{d}y \mathrm{d}s \\ &\lesssim \int_0^t \|\varrho' f(s)\|_{L^1_{x,v}} \mathrm{d}s.\end{aligned}$$

A bound of (4.75) can be derived exactly as the one for (4.74), using the change of variables $(x_i, t_{\mathbf{b},i-1}) \mapsto y = x_i - (t_{i-2} - t_{\mathbf{b},i-2} - t_{\mathbf{b},i-1} - s) v_i \in \Omega$ with $|n(x_i) \cdot v_i| \mathrm{d}S_{x_i} \mathrm{d}t_{\mathbf{b},i-1} = \mathrm{d}y$. □

***Proof of Lemma 4.1.9*.** **Step 1.** Define $\mathcal{V}_i^\delta := \{v_i \in \mathcal{V}_i : |n(x_i) \cdot v_i| / |v_i|^2 < \delta\}$. From (4.29), we have $\int_{\mathcal{V}_j^\delta} \mathrm{d}\sigma_j \leq C\delta^2$. On the other hand, from (4.31), we have $t_{\mathbf{b}}(x_i, v_i) \geq C_\Omega |n(x_i) \cdot v_i| / |v_i|^2$. Therefore if $v_i \in \mathcal{V}_i \backslash \mathcal{V}_i^\delta$, we have $t_{\mathbf{b}}(x_i, v_i) \geq C_\Omega \delta$.

If $t_k(t, x, v, v_1, \cdots, v_{k-1}) \geq 0$, we conclude such $v_i \in \mathcal{V}_i \backslash \mathcal{V}_i^\delta$ can exist at most $[\frac{t}{C_\Omega \delta}] + 1$

times. Denote the combination $\begin{pmatrix} M \\ N \end{pmatrix} = \frac{M(M-1)\cdots(M-N+1)}{N(N-1)\cdots 1} = \frac{M!}{N!(M-N)!}$ for $M, N \in \mathbb{N}$ and $M \geq N$. For $0 < \delta \ll 1$, we have

$$\begin{aligned} \int_{\prod_{j=1}^{k-1}\mathcal{V}_j} \mathbf{1}_{t_k(t,x,v,v_1,\cdots,v_{k-1})\geq 0} \mathrm{d}\sigma_{k-1}\cdots \mathrm{d}\sigma_1 &\leq \sum_{m=0}^{[\frac{t}{C_\Omega \delta}]+1} \begin{pmatrix} k \\ m \end{pmatrix} \Big(\int_{\mathcal{V}_i^\delta} \mathrm{d}\sigma_i \Big)^{k-m} \\ &\leq (C\delta^2)^{k-[\frac{t}{C_\Omega\delta}]} \underbrace{\sum_{m=0}^{[\frac{t}{C_\Omega \delta}]+1} \begin{pmatrix} k \\ m \end{pmatrix}}_{(4.76)_*} . \end{aligned} \tag{4.76}$$

Step 2. Recall the Stirling's formula $\sqrt{2\pi}k^{k+\frac{1}{2}}e^{-k} \leq k! \leq k^{k+\frac{1}{2}}e^{-k+1}$ (e.g. [86]). Using this bound and $(1+\frac{1}{\mathfrak{a}-1})^{\mathfrak{a}-1} \leq e$, we have, for $\mathfrak{a} \geq 2$ $\begin{pmatrix} k \\ \frac{k}{\mathfrak{a}} \end{pmatrix} = \frac{k!}{(k-\frac{k}{\mathfrak{a}})!\frac{k}{\mathfrak{a}}!} \leq (\frac{\mathfrak{a}}{\mathfrak{a}-1})^{\frac{\mathfrak{a}}{\mathfrak{a}-1}k}\mathfrak{a}^{\frac{k}{\mathfrak{a}}}\sqrt{\frac{\mathfrak{a}^2}{k(\mathfrak{a}-1)}} = \frac{1}{\sqrt{k}}\left(\mathfrak{a}^{\frac{1}{\mathfrak{a}}}(\frac{\mathfrak{a}}{\mathfrak{a}-1})^{\frac{\mathfrak{a}}{\mathfrak{a}-1}}\right)^k \sqrt{\frac{\mathfrak{a}^2}{\mathfrak{a}-1}} \leq \frac{1}{\sqrt{k}}(e\mathfrak{a})^{\frac{k}{\mathfrak{a}}}\sqrt{\frac{\mathfrak{a}^2}{\mathfrak{a}-1}}$. Hence,

$$\sum_{i=1}^{[\frac{k}{\mathfrak{a}}]} \begin{pmatrix} k \\ i \end{pmatrix} \leq \frac{k}{\mathfrak{a}} \begin{pmatrix} k \\ \frac{k}{\mathfrak{a}} \end{pmatrix} \leq \frac{e}{2\pi}\sqrt{\frac{k}{\mathfrak{a}}}(e\mathfrak{a})^{\frac{k}{\mathfrak{a}}}. \tag{4.77}$$

Step 3. Now we estimate $(4.76)_*$. For fix $0 < \delta \ll 1$ which is independent of t, choose

$$\mathfrak{a} \in \mathbb{N} \text{ such that } (\delta^{2\mathfrak{a}} e\mathfrak{a})^{\frac{1}{C_\Omega\delta}} \leq e^{-2}, \text{ and set } k := \mathfrak{a}\Big([\frac{t}{C_\Omega\delta}]+1\Big). \tag{4.78}$$

Using (4.77), we derive $(4.76)_* \lesssim \sqrt{[\frac{t}{C_\Omega\delta}]+1}\Big(e^{\frac{k}{[\frac{t}{C_\Omega\delta}]+1}}\Big)^{[\frac{t}{C_\Omega\delta}]+1} \lesssim \sqrt{[\frac{t}{C_\Omega\delta}]+1}(e\mathfrak{a})^{[\frac{t}{C_\Omega\delta}]+1}$ and hence (4.76) is bounded by $(\delta^{2\mathfrak{a}}e\mathfrak{a})^{[\frac{t}{C_\Omega\delta}]+1}\sqrt{[\frac{t}{C_\Omega\delta}]+1} \lesssim e^{-t}$. This completes the proof. □

Equipped with Proposition 4.1.7, and Lemma 4.1.8-4.1.9, we present a proof of the main theorem:

Proof of Theorem 4.1.1. Let $w(v) := e^{\theta|v|^2}, w'(v) := e^{\theta'|v|^2}$ for $0 < \theta < \theta' < 1/2$. It is standard ([2]) to construct a unique solution of f to (4.3)-(4.5) and prove its bound $\|w'f(t)\|_{L^\infty_{x,v}} \lesssim \|w'f(0)\|_{L^\infty_{x,v}}$. To utilize the L^1-decay of (4.17), we set

$$\varrho(t) := (\ln\langle t\rangle)^{-2}\langle t\rangle^5. \tag{4.79}$$

Clearly we have $\varrho'(t) \lesssim (\ln\langle t\rangle)^{-2}\langle t\rangle^4$ for $t \gg 1$.

From Lemma 4.1.5, we derive the form of $\int_{\mathbb{R}^3} w(v)|f|\mathrm{d}v$ (i.e. $\varrho = 1$). First we split $t_1 \le 3t/4$ case and get (4.80). Next, for $t_1 \ge 3t/4$ case, we follow along the stochastic cycles twice with $k = 2$ and $t_* = t/2$ and get (4.81), (4.82).

$$\begin{aligned}\int_{\mathbb{R}^3} w(v)|f(t,x,v)|\mathrm{d}v \le &\int_{\mathbb{R}^3} \mathbf{1}_{t_1\le 3t/4} w(v)|f(3t/4, x-(t-3t/4)v, v)|\mathrm{d}v \qquad (4.80)\\ &+\int_{\mathbb{R}^3} \mathbf{1}_{t_1\ge 3t/4} c_\mu w(v)\mu(v)\\ &\quad\times \int_{\prod_{j=1}^2 \mathcal{V}_j} \mathbf{1}_{t_2<t/2<t_1} w(v_1)|f(t/2, x_1-(t_1-t/2)v_1, v_1)|\mathrm{d}\Sigma_1^2\mathrm{d}v \qquad (4.81)\\ &+\int_{\mathbb{R}^3} \mathbf{1}_{t_1\ge 3t/4} c_\mu w(v)\mu(v)\Big|\int_{\prod_{j=1}^2 \mathcal{V}_j} \mathbf{1}_{t_2\ge t/2} w(v_2) f(t_2, x_2, v_2)\mathrm{d}\Sigma_2^2\Big|\mathrm{d}v.\end{aligned}$$
(4.82)

where $\mathrm{d}\Sigma_1^2 = \mathrm{d}\sigma_2 \frac{\mathrm{d}\sigma_1}{c_\mu\mu(v_1)w(v_1)}$ and $\mathrm{d}\Sigma_2^2 = \frac{\mathrm{d}\sigma_2}{c_\mu\mu(v_2)w(v_2)}\mathrm{d}\sigma_1$, with the probability measure $\mathrm{d}\sigma_j = c_\mu\mu(v_j)\{n(x_j)\cdot v_j\}\mathrm{d}v_j$ on $\mathcal{V}_j$ for $j = 1, 2$.

For (4.80), considering the change of variables $v \mapsto y = x - (t - 3t/4)v \in \Omega$ where we use $t - t_{\mathbf{b}}(x, v) = t_1 \le 3t/4$, thus we have $\mathrm{d}v \lesssim t^{-3}\mathrm{d}y$. Then, from the L^∞-boundedness, $t \gg 1$, $|\Omega| \lesssim 1$ and $0 < w < w'$, we deduce that

$$(4.80) \lesssim \int_\Omega w(v)|f(3t/4, y, v)|\langle t\rangle^{-3}\mathrm{d}y \lesssim \langle t\rangle^{-3}\|wf(0)\|_{L^\infty_{x,v}} \le \langle t\rangle^{-3}\|w'f(0)\|_{L^\infty_{x,v}}. \tag{4.83}$$

For (4.81), since $\int_{\mathbb{R}^3} w(v)\mu(v)\mathrm{d}v \lesssim 1$ and $\mathrm{d}\sigma_2$ is the probability measure in $\mathrm{d}\Sigma_1^2$, we have

$$(4.81) \lesssim \int_{\mathcal{V}_1} \mathbf{1}_{t_2<t/2<t_1} |f(t/2, x_1 - (t_1 - t/2)v_1, v_1)| \{n(x_1)\cdot v_1\} \mathrm{d}v_1 \tag{4.84}$$

Note that $t_1 \geq 3t/4$ implies $t/4 \leq t_1 - t/2 \leq t$. Considering the change of variables $v_1 \mapsto y = x - (t_1 - t/2)v_1 \in \Omega$ where we use $t_1 - t_{\mathbf{b}}(x_1, v_1) = t_2 \leq t/2$, clearly we get $\mathrm{d}v_1 \lesssim t^{-3}\mathrm{d}y$. Again, from the L^∞-boundedness, $t \gg 1$, $|\Omega| \lesssim 1$ and $0 < n(x_1)\cdot v_1 \lesssim w(v_1) < w'(v_1)$, we derive

$$(4.84) \lesssim \int_\Omega w(v_1)|f(t/2, y, v_1)| \langle t\rangle^{-3} \mathrm{d}y \lesssim \langle t\rangle^{-3} \|wf(0)\|_{L^\infty_{x,v}} \leq \langle t\rangle^{-3} \|w'f(0)\|_{L^\infty_{x,v}}. \tag{4.85}$$

Now we only need to bound (4.82). Since $\int_{\mathbb{R}^3} w(v)\mu(v)\mathrm{d}v \lesssim 1$ and $\mathrm{d}\sigma_1$ is the probability measure in $\mathrm{d}\Sigma_2^2$, it suffices to prove the decay of

$$\sup_{v\in\mathbb{R}^3, v_1\in\mathcal{V}_1} \Big| \int_{\mathcal{V}_2} \mathbf{1}_{t_2\geq t/2} f(t_2, x_2, v_2)\{n(x_2)\cdot v_2\}\mathrm{d}v_2 \Big|. \tag{4.86}$$

Now we define $g := \rho(t_2)w(v_2)f(t_2, x_2, v_2)$, and note that

$$\frac{1}{\rho(t_2)} \int_{\mathcal{V}_2} \frac{|n(x_2)\cdot v_2|}{w(v_2)} g(t_2, x_2, v_2)\mathrm{d}v_2 = \int_{\mathcal{V}_2} f(t_2, x_2, v_2)\{n(x_2)\cdot v_2\}\mathrm{d}v_2.$$

Therefore, it suffices to show the decay of $\left|\frac{1}{\rho(t_2)} \int_{\mathcal{V}_2} \mathbf{1}_{t_2\geq t/2} \frac{|n(x_2)\cdot v_2|}{w(v_2)} g(t_2, x_2, v_2)\mathrm{d}v_2\right|$.

Applying Lemma 4.1.5 with $w(v) = e^{\theta|v|^2}$, $\varrho(t)$ in (4.79), and choosing $t_* = 0$, $k \geq \mathfrak{C}t$ with $k \sim t$ as in Lemma 4.1.9, we obtain the corresponding expansion of $g(t_2, x_2, v_2) = \rho(t_2)w(v_2)f(t_2, x_2, v_2)$ as (4.87)-(4.91): for $3 \leq i \leq k$,

$$g(t_2, x_2, v_2) = \mathbf{1}_{t_3\leq 0}\ g(0, x_2 - t_2v_2, v_2) \tag{4.87}$$

$$+ \int_{\max(0,t_3)}^{t_2} \varrho'(s)w(v_2)f(s, x_2 - (t_2 - s)v_2, v_2)\mathrm{d}s \tag{4.88}$$

$$+ c_\mu w\mu(v_2) \int_{\prod_{j=3}^k \mathcal{V}_j} \sum_{i=3}^{k-1} \Big\{ \mathbf{1}_{t_{i+1}<0\leq t_i} g(0, x_i - t_iv_i, v_i) \Big\} \mathrm{d}\widetilde{\Sigma}_i^k \tag{4.89}$$

$$+ c_\mu w\mu(v_2) \int_{\prod_{j=3}^k \mathcal{V}_j} \sum_{i=3}^{k-1} \Big\{ \mathbf{1}_{0\le t_i} \int_{\max(0,t_{i+1})}^{t_i} w(v_i)\varrho'(s) f(s, x_i - (t_i - s)v_i, v_i) \mathrm{d}s \Big\} \mathrm{d}\widetilde{\Sigma}_i^k \tag{4.90}$$

$$+ c_\mu w\mu(v_2) \int_{\prod_{j=3}^k \mathcal{V}_j} \mathbf{1}_{t_k \ge 0}\; g(t_k, x_k, v_k) \mathrm{d}\widetilde{\Sigma}_k^k, \tag{4.91}$$

where $\mathrm{d}\widetilde{\Sigma}_i^k := \mathrm{d}\sigma_k \cdots \mathrm{d}\sigma_{i+1} \frac{\mathrm{d}\sigma_i}{c_\mu \mu(v_i) w(v_i)} \mathrm{d}\sigma_{i-1} \cdots \mathrm{d}\sigma_3$. Here, we regard t_2, x_2, v_2 as free parameters.

We will estimate the contribution of (4.87)-(4.91) in $\frac{1}{\rho(t_2)} \int_{\mathcal{V}_2} \frac{n(x_2)\cdot v_2}{w(v_2)} g(t_2, x_2, v_2) \mathrm{d}v_2$ term by term.

For the contribution of (4.87), we note $t \ge t_2 \ge t/2$ and consider the change of variables $v_2 \mapsto y = x_2 - t_2 v_2 \in \Omega$ where we use $t_3 \le 0$, clearly we have $\mathrm{d}v_2 \lesssim t^{-3}\mathrm{d}y$. From the L^∞-boundedness, $t_2 \ge t/2 \gg 1$, $|\Omega| \lesssim 1$ and $0 < n(x_2)\cdot v_2 \lesssim w(v_2) < w'(v_2)$, we deduce that

$$\begin{aligned} \frac{1}{\rho(t_2)} \int_{\mathcal{V}_2} \frac{|n(x_2)\cdot v_2|}{w(v_2)} |(4.87)| \mathrm{d}v_2 &\lesssim \frac{1}{\rho(t_2)} \int_\Omega \varrho(0) w(v_2) |f(0, y, v_2)| \langle t \rangle^{-3} \mathrm{d}y \\ &\lesssim \frac{1}{\rho(t)} \langle t\rangle^{-3} \varrho(0) \|wf(0)\|_{L^\infty_{x,v}} \lesssim \frac{1}{\rho(t)} \langle t\rangle^{-3} \|w' f(0)\|_{L^\infty_{x,v}}. \end{aligned} \tag{4.92}$$

Now we bound the contribution of (4.88). Recall Lemma 4.1.8 and Proposition 4.1.7 with $\varrho'(t) \lesssim (\ln\langle t\rangle)^{-2} \langle t\rangle^4$, we have

$$\begin{aligned} \frac{1}{\rho(t_2)} \int_{\mathcal{V}_2} \frac{|n(x_2)\cdot v_2|}{w(v_2)} |(4.88)| \mathrm{d}v_2 &\lesssim \frac{1}{\rho(t)} \int_0^t \|\rho'(s) f(s)\|_{L^1_{x,v}} \mathrm{d}s \\ &\lesssim \frac{1}{\rho(t)} \int_0^t \|(\ln\langle s\rangle)^{-2} \langle s\rangle^4 f(s)\|_{L^1_{x,v}} \mathrm{d}s \\ &\lesssim \frac{t}{\rho(t)} \times \{ \|w' f(0)\|_{L^\infty_{x,v}} + \|\varphi_4(t_{\mathbf{f}}) f(0)\|_{L^1_{x,v}} \}. \end{aligned} \tag{4.93}$$

Next, we bound the contribution of (4.89). From the L^∞-boundedness and $0 < n(x_2)\cdot$

$v_2 \lesssim w(v_2) < w'(v_2) < \mu^{-1}(v_2)$, we derive

$$\begin{aligned}\frac{1}{\rho(t_2)}\int_{\mathbb{R}^3}\frac{|n(x_2)\cdot v_2|}{w(v_2)}|(4.89)|\mathrm{d}v_2 &\lesssim \frac{k}{\rho(t)}\Big(\sup_i \int_{\prod_{j=1}^k \mathcal{V}_j} \mathbf{1}_{t_{i+1}<0\le t_i}\mathrm{d}\widetilde{\Sigma}_i^k\Big)\varrho(0)\|wf(0)\|_{L^\infty_{x,v}} \\ &\lesssim \frac{k}{\rho(t)}\Big(\int_{n(x_j)\cdot v_j>0}\frac{|n(x_j)\cdot v_j|}{w(v_j)}\mathrm{d}v_j\Big)\|wf(0)\|_{L^\infty_{x,v}} \\ &\lesssim \frac{k}{\rho(t)}\|w'f(0)\|_{L^\infty_{x,v}}.\end{aligned} \tag{4.94}$$

Again recall Lemma 4.1.8 and Proposition 4.1.7, we bound the contribution of (4.90). From $0 < n(x_2)\cdot v_2 \lesssim \mu^{-1}(v_2)$ and $\varrho'(t) \lesssim (\ln\langle t\rangle)^{-2}\langle t\rangle^4$, we have

$$\begin{aligned}&\frac{1}{\rho(t_2)}\int_{\mathbb{R}^3}\frac{|n(x_2)\cdot v_2|}{w(v_2)}|(4.90)|\mathrm{d}v_2 \\ &\lesssim \frac{k}{\rho(t)}\times\sup_i\int_{\prod_{j=3}^k\mathcal{V}_j}\mathbf{1}_{0\le t_i}\int_{\max(0,t_{i+1})}^{t_i} w(v_i)\varrho'(s)f(s,x_i-(t_i-s)v_i,v_i)\mathrm{d}s\mathrm{d}\widetilde{\Sigma}_i^k \\ &\lesssim \frac{1}{\rho(t)}\int_0^t\|\rho'(s)f(s)\|_{L^1_{x,v}}\mathrm{d}s \lesssim \frac{k}{\rho(t)}\int_0^t\|(\ln\langle s\rangle)^{-2}\langle s\rangle^4 f(s)\|_{L^1_{x,v}}\mathrm{d}s \\ &\lesssim \frac{kt}{\rho(t)}\times\{\|w'f(0)\|_{L^\infty_{x,v}}+\|\varphi_4(t_{\mathbf{f}})f(0)\|_{L^1_{x,v}}\}.\end{aligned} \tag{4.95}$$

Lastly we bound the contribution of (4.91). From Lemma 4.1.9 and $0 < n(x_2)\cdot v_2 \lesssim w(v_2) < w'(v_2)$, we get

$$\begin{aligned}&\frac{1}{\rho(t_2)}\int_{\mathbb{R}^3}\frac{|n(x_2)\cdot v_2|}{w(v_2)}|(4.91)|\mathrm{d}v_2 \\ &\lesssim \frac{1}{\rho(t)}\sup_{(x,v)\in\bar{\Omega}\times\mathbb{R}^3}\Big(\int_{\prod_{j=1}^{k-1}\mathcal{V}_j}\mathbf{1}_{t_k(t,x,v,v_1,\cdots,v_{k-1})\ge 0}\mathrm{d}\sigma_1\cdots\mathrm{d}\sigma_{k-1}\Big)\sup_{t_k\ge 0}\|wf(t_k)\|_{L^\infty_{x,v}} \\ &\lesssim \frac{1}{\rho(t)}e^{-t}\|wf(0)\|_{L^\infty_{x,v}} \lesssim e^{-t}\|w'f(0)\|_{L^\infty_{x,v}}.\end{aligned} \tag{4.96}$$

Collecting estimates from (4.92)-(4.96) and using $k\sim t$, we derive

$$\Big|\frac{1}{\rho(t_2)}\int_{\mathcal{V}_2}\mathbf{1}_{t_2\ge t/2}\frac{|n(x_2)\cdot v_2|}{w(v_2)}g(t_2,x_2,v_2)\mathrm{d}v_2\Big| \le \max\{\frac{1}{\rho(t)}\langle t\rangle^{-3},\frac{(k+1)t}{\rho(t)},e^{-t}\} \lesssim \frac{\langle t\rangle^2}{\rho(t)}. \tag{4.97}$$

For (4.82), using $\varrho(t) = (\ln\langle t\rangle)^{-2}\langle t\rangle^5$, $0 < w(v) < \mu^{-1}(v)$ and (4.97), we conclude

$$(4.82) \lesssim \langle t\rangle^{-3}(\ln\langle t\rangle)^2. \tag{4.98}$$

The above bound, together with (4.83) and (4.85), proves (4.2). $\square$

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