THE BECKER-DÖRING CLUSTER EQUATIONS

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Abstract

The Becker-Döring equations provide a model of the dynamics of a system consisting of a large number of identical particles. The particles can coagulate to form clusters, which in turn can fragment into smaller clusters. This thesis discusses various aspects of the mathematical theory of these equations and a generalisation of the equations to two types of particles.

In Chapter 1, we describe previous work on the Becker-Döring equations and outline the extension to the two component case. We provide some physical background to the concept of metastability and discuss some of the problems associated with finding numerical results about metastable systems.

In Chapter 2 we state the equations that model the two component system. Basic results are proved for these equations including existence, density conservation and the structure of the equilibrium solutions. Under certain conditions, we prove that as \( t \to \infty \), solutions converge (weak\(^*\)) to an equilibrium.

In Chapter 3, we prove that there exists a class of metastable solutions to a finite system of Becker-Döring equations. These result provide theoretical backing to previously published numerical work on these equations.

In Chapter 4, we report on numerical approximations to the finite Becker-Döring equations. These results are used to gain a better understanding of the metastable solutions studied in Chapter 3.
Chapter 1

Introduction

1.1 General background

The Becker-Döring equations model the behaviour of clusters of particles, when these coagulate and fragment in a prescribed way: Only one particle may leave or join a cluster at a time. The rate at which clusters containing $r$ particles (referred to as $r$-clusters) coalesce with single particles (or monomers) is assumed to be proportional to the product of the monomer concentration ($c_1$) and the concentration of $r$-clusters ($c_r$). The constant of proportionality is denoted $a_r$ and is a non-negative constant. The rate at which $r$-clusters fragment into $(r-1)$-clusters and monomers is assumed to be directly proportional to $c_r$, and the constant of proportionality is denoted $b_r$ ($b_r \geq 0$). This means that the net rate at which $r$-clusters become $(r+1)$-clusters is $a_r c_1 c_r - b_{r+1} c_{r+1}$; this quantity is denoted by $J_r(c)$ or just $J_r$. This can all be represented schematically by the sketch shown in Figure 1.1.1.

![Figure 1.1.1: Schematic view of the Becker-Döring equations](image)

In their original 1935 paper, [1], R. Becker and W. Döring assumed that $c_1$ remained constant and derived a linear set of equations. These are:

\[
\begin{align*}
\dot{c}_1(t) &= 0 \\
\dot{c}_r(t) &= J_{r-1}(c(t)) - J_r(c(t)) \quad \text{for } r \geq 2.
\end{align*}
\]

J. M. Ball et al in 1986, [2], studied a modified form of these equations, where the system is not assumed to be connected to an external monomer source. The equations are:

\[
\begin{align*}
\dot{c}_1 &= -J_1(c) - \sum_{r=1}^{\infty} J_r(c) \\
\dot{c}_r &= J_{r-1}(c) - J_r(c) \quad \text{for } r \geq 2.
\end{align*}
\]

This form of the Becker-Döring equations was originally described by O. Penrose and J. L. Lebowitz in [3]. The treatment of the Becker-Döring equations given in [2] has proved to be a suitable basis on which to consider more general cluster equations, see [4], [5], [6], [7], [8] and [9]. Chapter 2 of this thesis contains a study of another form of the Becker-Döring equations. The study considers the
extent to which the existence and asymptotic results of [2] apply to the solution of these equations. The precise form of the equations will be given on page 4, after a formal summary of the contents of [2].

Ball et al prove that the equations (1.1.1) have a solution by showing that solutions of a truncated form of (1.1.1) tend to solutions of the full system as the truncated system increases in size. It is then shown that the system’s density, $\sum_{r=1}^{\infty} r c_r(t)$, is a conserved quantity, for finite values of $t$. This can be easily verified formally by the calculation:

$$\sum_{r=2}^{\infty} r c_r(t) = \sum_{r=2}^{\infty} r(J_r - 1) = 2J_1 + \sum_{r=2}^{\infty} J_r = -\dot{c}_1.$$ 

The cancellation of the $J_r$’s in the above, while algebraically trivial, is a key factor in many calculations and the general identities

$$\sum_{r=n}^{\infty} g_r(c_r(t) - c_r(0)) = \int_0^t g_n J_{n-1}(c(s)) + \sum_{r=n}^{\infty} (g_{r+1} - g_r) J_r(c(s)) \, ds$$

are used frequently. Equation (1.1.2) may be regarded as a weak form of equations (1.1.1).

The uniqueness of the solutions of (1.1.1) is established in [2] for a smaller set of cases than that for which existence is proved. This means that later theorems must either assume uniqueness or prove the result for all possible solutions.

The set of all equilibrium solutions is:

$$\left\{(Q,z') : z \geq 0, \sum_{r=1}^{\infty} rQ_r z^r < \infty \right\},$$

where $Q_r = \frac{a_{r-1} \cdot a_{r-2} \cdots a_1}{b_r \cdot b_{r-1} \cdots b_2}$.

In [2] and here, $F(z)$ is used to denote $\sum_{r=1}^{\infty} rQ_r z^r$. The radius of convergence of $F(z)$ is denoted by $z_s$ and $\rho_s$ is defined as $F(z_s)$. There are four distinct classes of behaviour for $F$ these classes are best illustrated by the sketches given below in Figure 1.1.2.

Since a solution’s density is conserved, one’s first guess at the asymptotic behaviour of $c$, is that it will converge to an equilibrium solution that has the same density as $c$, i.e. $c(t) \to (Q,z')$ as $t \to \infty$, where $F(z) = \sum_{r=1}^{\infty} r c_r(0) =: \rho_0$. For cases represented by I and III in Figure 1.1.2, however, this cannot happen when $\rho_0 > \rho_s$, since all equilibrium solutions have densities strictly less than that of the solution. This fact does not, as it might first seem, contradict the idea that $c(t)$ tends to an equilibrium solution, since convergence may be non-uniform. There are in fact two natural topologies on the solution space. One is generated by the norm $\|c\| = \sum_{r=1}^{\infty} r |c_r|$ and the other by $\|c\|^* = \sum_{r=1}^{\infty} |c_r|$; convergence in the latter is equivalent to term-wise convergence and forms a topology equivalent to the weak* topology of the former. So solutions may converge to equilibrium solutions in all circumstances but the convergence might be only weak* rather than strong/uniform. Put more loosely, it is possible that some density is lost in the limit, by the excess density going to form larger and larger clusters as $t \to \infty$. This is, in fact, the process that the Becker-Döring equations were originally formulated to model, namely condensation. By considering some facts from basic chemistry it is possible to see what the asymptotic behaviour of the system ‘ought’ to be. There is an upper limit on the equilibrium concentration of a solute dissolved in a solvent. When a solute is at this concentration the solution is said to be saturated. It is possible to have a chemical solution, not in equilibrium, where the solute’s concentration is above the saturated value, such a solution is called super-saturated. Starting with a super-saturated solution, what is observed is that the excess,
1.2 Two component Becker-Döring equations

When formulating the Becker-Döring equations three physically significant assumptions are made. The first is that clusters may grow or shrink by only one particle at a time. If this assumption is not made the equations one obtains are the coagulation-fragmentation equations, studies of which may be found in [4], [5] and [6]. The second assumption is that the system is spatially uniform. This assumption may be relaxed by adding a diffusion term to the equations, work on this is in [8] and [9]. The third assumption is that the clusters are composed of only one type of particle. Chapter 2 of this thesis considers the equations obtained if the clusters are made up of two types of particle, referred to as type I and type II particles. The concentration of clusters containing \( r \) type I particles and \( s \) type II particles at time \( t \) is denoted by \( c_{r,s}(t) \). Hence \( c_{0,1}(t) \) is the concentration of type I monomers and \( c_{0,1}(t) \) is that of type II monomers. The rates at which \( (r,s) \)-clusters coalesce with type I and type II monomers is assumed to be \( \alpha_{r,s}c_{0,1}c_{r,s} \) and \( \alpha_{r,s}c_{1,1}c_{r,s} \) respectively. Similarly, the rates at
which type I and type II monomers fragment from \((r,s)\)-clusters is assumed to be \(b_{r,s,c_{r,s}}\) and \(b'_{r,s,c_{r,s}}\) respectively. All four coefficients, \(a_{r,s}, a'_{r,s}, b_{r,s},\) and \(b'_{r,s}\) are non-negative constants. This can be represented by a schema equivalent to that in Figure 1.1.1 and this is shown in Figure 1.2.1 below. The diagrams for \(c_{r,0}\) and \(c_{0,s}\) are a little different from that shown in Figure 1.2.1, the drawing in Figure 1.2.2 shows representations of all the different interactions.

The equations can be written down as:

\[
\begin{align*}
\dot{c}_{r,s} &= J_{r-1,s} - J_{r,s} + J'_{r,s-1} - J'_{r,s} \quad \text{if } r \geq 1, s \geq 1 \\
\dot{c}_{r,0} &= J_{r-1,0} - J_{r,0} - J'_{r,0} \quad \text{if } r \geq 2 \\
\dot{c}_{0,s} &= -J_{0,s} + J'_{0,s-1} - J'_{0,s} \quad \text{if } s \geq 2 \\
\dot{c}_{1,0} &= -J_{1,0} - J'_{1,0} - \sum_{m=1}^{\infty} \sum_{r=0}^{m} J_{r,m-r} \\
\dot{c}_{0,1} &= -J_{0,1} - J'_{0,1} - \sum_{m=1}^{\infty} \sum_{r=0}^{m} J'_{r,m-r}
\end{align*}
\] (1.2.1)

where \(J_{r,s}(c) = a_{r,s}c_{1,0}c_{r,s} - b_{r+1,s}c_{r+1,s}\) and \(J'_{r,s}(c) = a'_{r,s}c_{0,1}c_{r,s} - b'_{r,s+1}c_{r,s+1}\). The equations (1.2.1) will be referred to as the two component Becker-Döring equations; when comparing the systems (1.1.1) and (1.2.1), equations (1.1.1) will be called the one component Becker-Döring equations.

The two component system has many of the properties of the one component system. Most important of these is density conservation. In the two component system there are two densities, and \((1.2.1)\) equations (1.1.1) will be called the one component Becker-Döring equations.

The two component system has many of the properties of the one component system. Most important of these is density conservation. In the two component system there are two densities, \(\sum_{r=1}^{\infty} \sum_{s=1}^{\infty} r c_{r,m-r}(t)\) and \(\sum_{r=1}^{\infty} \sum_{s=1}^{\infty} s c_{m-s,s}(t)\), both of which are conserved. The equivalent of equation (1.1.2) would be

\[
\sum_{m=1}^{\infty} \sum_{r=0}^{m} g_{r,m-r}(c_{r,m-r}(t) - c_{r,m-r}(0)) = \\
\int_{0}^{t} \sum_{m=1}^{\infty} \sum_{r=0}^{m} (g_{r+1,m-r} - g_{r,m-r} - g_{0,1}) J_{r,m-r}(c(\tau)) d\tau
\]
\[
+ \int_{0}^{t} \sum_{m=1}^{\infty} \sum_{s=0}^{m} (g_{m-s,s+1} - g_{m-s,s} - g_{0,1}) J'_{m-s,s}(c(\tau)) d\tau
\] (1.2.2)

but unfortunately it has only been possible to prove that it holds when the sequence \(g_{r,s}\) has certain properties (see Section 2.1.4 for more details); properties which both \(g_{r,s} = r\) and \(g_{r,s} = s\) satisfy. Problems arise because the extra degree of freedom in the two component system means that it is harder to find estimates that control the tails of the series \(\sum_{m=1}^{\infty} \sum_{r=0}^{m} g_{r,m-r} c_{r,m-r}\). Another consequence of the extra degree of freedom is that the set of all equilibrium points is more complicated than in the one component system. Examples of the different forms this set can take are given on pages 38–39. Since the equilibrium solutions take the expected form of \((Q_{r,s}w^{r}z^{s})^{*}\) there is a one to one correspondence between the set of all equilibrium solutions and the set, \(\Gamma\), of points \((w, z)\) for which \((Q_{r,s}w^{r}z^{s})^{*}\) has finite densities. The shape of \(\Gamma\) is determined by \(Q_{r,s}\) and so the way \(Q_{r,s}\) depends on \(r\) and \(s\) has a vital role to play in the asymptotic behaviour of the solutions. It is important, therefore, to have a physically realistic formula for \(Q_{r,s}\). Now \(Q_{r,s}\) may be identified as the statistical mechanics partition function for a \((r,s)\)-cluster. It is possible to use thermodynamic arguments\(^1\) to say that

\[
kT \ln(Q_{r,s}) = r \lambda_1^0 + s \lambda_2^0 + \sigma_0 (36\pi)^{1/3} (rV_1 + sV_2)^{2/3} + kT r \ln \left( \frac{r}{r+s} \right) + kT s \ln \left( \frac{s}{r+s} \right),
\] (1.2.3)

where \(k\) is Boltzmann’s constant and \(T\) is temperature. The constants \(\lambda_1^0, \lambda_2^0, \sigma_0, V_1\) and \(V_2\) depend on the physical/chemical properties of type I and type II particles. All the results in Chapter 2 apply

\(^{1}\)A private communication from J. A. D. Wattis.

\(^{2}\)the precise definition of \(Q_{r,s}\) may be found on page 35
1.2. TWO COMPONENT BECKER-DÖRING EQUATIONS

Figure 1.2.1: Schematic view of the interaction of $c_{r,s}$ with its nearest neighbours

Figure 1.2.2: Schematic for the full two component system
The solution showing all the quantities and sequences described so far and how these are related to one another is
would remain ‘very close’ to its initial data for a ‘long’ time but would eventually move away from
that (\( \gamma > \gamma_s \) we can see that if \( z = z_s \) and has a single minima if \( z > z_s \). The value at which \( (Q_\gamma z^\gamma) \) attains its minimum is denoted by \( \ell(z) \) here, but by \( \ell^* \) in [12]. Since for every \( \gamma \geq 2 \),
\[
\dot{c}_r = J_{\gamma-1}(c) - J_{\gamma}(c),
\]
we can see that if \( c \) had initial data \( (f_r) \) such that \( J_{\gamma}(f) = J_{\gamma-1}(f) \), for \( \gamma \geq 2 \), then \( \dot{c}_r(0) = 0 \) for every \( \gamma \geq 2 \). So distributions of this type are a good first guess for metastable states but, unfortunately, \( \sum_{\gamma=1}^{\infty} rf_r \) diverges for all such \( (f_r) \). One particular distribution with constant flux, however, is an upper bound to all solutions that have their initial data bounded by it. From this it is possible to construct metastable solutions.

To be more precise, Penrose showed that for each value of \( z > \gamma_s \), there is a unique distribution \( (f_r(z)) \) for which: (a) \( f_r(z) = z; \) (b) \( f_r(z) > 0 \), for \( r \geq 1; \) (c) \( J_{r}(f(z)) = J_{r-1}(f(z)) \), for \( r \geq 2 \) and (d) \( f_r(z) \) is bounded as \( r \to \infty \). Two important facts are that, if \( z > \gamma_s \) then \( f_r(z) > Q_r z^\gamma_s \) for \( r \geq 1 \) and that \( (f_r(z)) \) is a non-increasing sequence in \( r \). It is then proved that a solution of \( (1.1.1) \) with initial conditions
\[
c_r(0) = \begin{cases} f_r(z) & \text{for } 1 \leq r \leq \ell(z) \\ Q_r z^\gamma_s & \text{for } \ell(z) \leq r \end{cases}
\]
would remain ‘very close’ to its initial data for a ‘long’ time but would eventually move away from it.\(^1\) The first stage to proving this result is to show that \( (f_r(z)) \) is the upper bound just mentioned, i.e. if \( 0 \leq c_r(0) \leq f_r(z) \) for all \( r \geq 1 \) then \( 0 < c_r(t) \leq f_r(z) \) for all \( r \geq 1 \) and all \( t \geq 0 \). A sketch showing all the quantities and sequences described so far and how these are related to one another is given in Figure 1.3.1.

The solution \( c(t) \) is shown to evolve slowly by a rigorous version of the following argument. Since \( f(z) \) is an upper bound on \( c \) then \( c_r(t) \leq c_r(0) \) for \( 1 \leq r \leq \ell(z) \). Density, however, is conserved

\(^1\)Definitions of ‘very close’ and ‘long’ are explained in ‘Definition of metastability’.

1.3 Metastability

Metastability is a phenomenon exhibited by many thermodynamic systems as they undergo phase transitions. The one component Becker-Döring equations model physical systems that undergo condensation, and so it is reasonable to ask if there are any metastable solutions. This question was addressed by O. Penrose in [12], where he constructed sets of metastable solutions for both the linear and nonlinear Becker-Döring equations. In Chapter 3 of this thesis a class of metastable solutions for a finite truncation of equations (1.1.1) is given. The construction of this class and the proof of its metastability follow along the same lines as those used in [12].

A system must satisfy several conditions before it can be described as metastable. The full definition of metastability will be discussed in the sub-section headed ‘Definition of metastability’, on page 8. The most distinctive characteristic of metastable solution, however, is that it must be evolving very slowly while being bounded away from its equilibrium state(s), so this is considered first.

1.3.1 Slowly evolving solutions of the Becker-Döring equations

A summary will be given of how, in [12], the class of metastable solutions for the nonlinear Becker-Döring equations is constructed and of how these are shown to be slowly evolving. This is followed by some comments on how this result has been adapted to the finite system of equations.

A set of assumptions about the coefficients \( (a_r) \) and \( (b_r) \) are made (see page 60), the first major consequence of which, is that the sequence \( (Q_r z^\gamma) \) is non-increasing if \( z \leq z_s \) and has a single minima if \( z > z_s \). The value at which \( (Q_r z^\gamma) \) attains its minimum is denoted by \( \ell(z) \) here, but by \( \ell^* \) in [12]. Since for every \( \gamma \geq 2 \),
so any decrease in $\sum_{r=\ell(z)+1}^{\infty} r c_r(t)$ must be balanced by an increase in $\sum_{r=\ell(z)+1}^{\infty} r c_r(t)$. Changes in $\sum_{r=\ell(z)+1}^{\infty} r c_r(t)$ are closely related to changes in $\sum_{r=\ell(z)+1}^{\infty} c_r(t)$ and

$$
\sum_{r=\ell(z)+1}^{\infty} c_r(t) - \sum_{r=\ell(z)+1}^{\infty} c_r(0) = \int_{0}^{t} J_{\ell(z)}(c(s)) \, ds \\
\leq \int_{0}^{t} a_{\ell(z)} c_{1}(s)c_{\ell(z)}(s) \, ds \\
\leq a_{\ell(z)} Q_{\ell(z)} z^{\ell(z)+1} t = J^{*} t.
$$

Hence the result is then proved once $J^{*}$ is shown to be ‘very small’; this follows from the assumptions that are made about the coefficients.

Chapter 3 contains a similar construction and proof for the solutions of the truncated Becker-Döring equations:

$$
\begin{align*}
\dot{c}_1 &= -J_1(c) - \sum_{r=1}^{N} J_r(c) \\
\dot{c}_r &= J_{r-1}(c) - J_r(c) \\
\dot{c}_N &= J_{N-1}(c)
\end{align*}
$$

The reason for attempting such a task is to provide theoretical backing to the numerical results contained in [13]; this will be discussed in more detail under the section headed ‘Numerical comparisons’ on page 9. At first sight, adapting the proofs in [12] to the finite case seems easy. It is not. The idea is straightforward enough: Find an upper bound to the solutions of the system that restricts the growth of larger clusters. Then any solution with initial data that is below this bound and that has significantly more smaller clusters than its equilibrium state, will take a long time to change because to approach equilibrium means forming larger clusters and the upper bound limits this. However, the monotonicity of $(f_r(z))$ in $r$, is a vital ingredient of the proof that it was an upper bound to the solutions of (1.1.1) and it is here that the greater simplicity of the finite system conspires against us. Since there are only finitely many cluster sizes, there can be no loss of density in the limit, so $c(t) \to (Q_r z_r^*)_{r=1}^{N}$ as $t \to \infty$, where $z$ is the unique soliton of $\sum_{r=1}^{N} r Q_r z^r = \rho_0$. The values of $\rho_0$ that are of interest are precisely those values that result in $(Q_r z_r^*)_{r=1}^{N}$ being non-monotonic in $r$. So any
upper bound, \((U^t_r)^N\) of the solutions to (1.3.1) that restricts the growth of larger clusters cannot be monotonic in \(r\). The chronological order of proving the finite equivalent of Penrose’s results, was first to find alternative sufficient conditions for \(U\) being a restrictive upper bound and then proving that there existed sequences \((U^t_r)\) which satisfied these conditions. Proving the existence of \(U\) is technically the most complex part of the whole exercise, but once it is established it is comparatively simple to apply Penrose’s strategy.

1.3.2 Definition of metastability

Several rigorous definitions of metastability have been formulated, see for example [14], [15] and [3]. The definition used in Chapter 3 is equivalent to the one used by Penrose in [12]. This definition was originally formulated by Lebowitz and Penrose in [16]. To give an intuitive idea of what these definitions are trying to describe and to give some justification to the definition that will be used here, the earlier example of a super-saturated solution is discussed in more detail. The historical facts are taken from the very readable account written by W. J. Dunning in [17]. In the second half of the nineteenth century experiments were carried out on super-saturated solutions that were free from infection by contaminants such as atmospheric dust. It appeared that there were two types of super-saturated solution, metastable and liable. Metastable solutions had a lower concentration of solute than liable solutions and would only produce a precipitate if induced to do so, whereas liable solutions crystallised almost instantaneously. If the concentration of a metastable solution was increased past the “metastable limit” then it became a liable solution. While the two types of solution seem quite distinct, no sharp change is seen in the bulk properties of a solution when its concentration crosses the metastable limit. This anomaly was resolved by M. Volmer and A. Webber in [19], where they explained that metastability was essentially a kinetic phenomenon and that a metastable solution would produce a precipitate if only it were given enough time to do so. In 1875 de Coppet had carried out experiments measuring the time-lag, \(T_p\), before the onset of crystallisation for various concentrations, \(\rho\), of solute. He found that \(T_p\) did increase slightly as \(\rho\) was set at lower and lower liable values but as \(\rho\) approached the “metastable limit”, \(T_p\) suddenly became unmeasurable. This apparent discontinuity could be observed even if \(T_p\) is, as Volmer and Webber claimed, a continuous function of \(\rho\) for all \(\rho > \rho_s\), if \(T_p \sim \exp[\mathcal{E}(\rho - \rho_s)^{-\mu}]\) as \(\rho \searrow \rho_s\), for some positive constants \(\mathcal{E}\) and \(\mu\). In Figure 1.3.2, below, the graphs of \(T_p = 10(\rho - 1)^{-4}\) and \(T_p = \exp(\rho - 1)^{-4}\) are contrasted to demonstrate how a metastable limit is unlikely to be observed experimentally if \(T_p\) is algebraically large but would be seen if \(T_p\) was exponentially large.\(^4\)

In order to make rigorous the idea that, metastable solutions are those with an exponentially large time-lag, it is necessary to define ‘time-lag’ in a precise way. From an experimental point of view it is clear enough, the time-lag is how long it takes a solution to produce a measurable number of crystals. To form the mathematical equivalent of this, definitions of ‘a crystal’ and ‘measurable’ are needed. It is possible, by balancing surface and volume terms in the energy formulae for clusters, to show that there is a critical cluster size. If a cluster contains fewer particles than the critical value, then its energy is lowered by it shrinking in size, and if it has more than the critical value, its energy is lowered by an increase in its size. This means that a sub-critical cluster is most likely to shrink, while a super-critical cluster will probably grow to a measurable size. Hence it is natural to define ‘crystals’ as super-critical clusters. In situations modelled by the Becker-Döring equations, the critical cluster size is \(\ell(z)\) – the size that has the lowest equilibrium concentration. Given that a ‘very long time’ is going to be defined as a value that becomes greater than \(\exp[\mathcal{E}(\rho - \rho_s)^{-\mu}]\) as \(\rho \searrow \rho_s\), it is reasonable to define a measurable quantity as one that is at least algebraically small, i.e. is greater than some function \(\mathcal{E}(\rho - \rho_s)^{\mu}\) as \(\rho \searrow \rho_s\). It is now possible to define a metastable solution as one:

(a) where the total concentration of super-critical clusters is at most exponentially small but will eventually become algebraically small, and

(b) where it will take at least an exponentially long time for this to happen.

\(^3\)For a physically rigorous derivation of the definition see [3] or [16]. For a fuller account of nucleation theory see [17] or [18].

\(^4\)Since condensation is a first order phase transition and \(\rho_s\) is the critical value of \(\rho\), then it is expected that \(T_p \rightarrow \infty\) as \(\rho \searrow \rho_s\).
1.4. NUMERICAL COMPARISONS

This definition does not, however, fully capture the kinetic/non-reversible nature of a metastable state, to do this one further condition must be added. Using the same language as above this could be phrased as:

(c) It is highly unlikely that the concentration of super-critical clusters will ever decrease by an algebraically small amount.

The actual definition used in Chapter 3 is a little different from this. The changes made to (a) and (b) are only in the wording but the third condition has had to be weakened. As Penrose explained in [12] commenting on the probability of events is beyond the scope of the existing Becker-Döring theory but it is possible to prove a statement that gives a strong indication that the full condition is satisfied.

1.4 Numerical comparisons

Finding experimental data about physical systems in a metastable state that can be compared with theoretical predictions is very difficult. In the example considered above, classical nucleation theory can be used to obtain an explicit expression for $T_\rho$ but experiments such as de Coppet’s do not provide reliable data for sufficiently low values of $\rho$. The situation is barely improved when computer simulations are used instead of real experiments. In [20], Kalos et al describe the results of simulations of the time evolution of a binary alloy on a cubic lattice (a situation that can be modelled by the Becker-Döring equations, see [21], [3] and [2]). In only one simulation was the system seen to ‘leave’ a metastable state, so experiment and theory could only be compared at one data point. In all the other simulations the predicted value of $T_\rho$ was greater than the life time of the simulation. That simulations run into the same problems as experiments is only to be expected. A simulation may be able to speed up the rate at which microscopic interactions take place but this will only be a ‘linear improvement’. To keep track of an exponentially varying quantity, such as $T_\rho$, it is necessary to make ‘exponential improvements’. When finding the numerical solutions of systems of ODEs, however, it is possible to vary the step sizes and so be able to pass quickly through whatever period of slow dynamics there may be. This strategy was adopted by C. H. Walshaw in [22]. Solutions of (1.3.1) were found for a range of initial data and system sizes. The density of the initial data was always set above $\rho_s$. 

Figure 1.3.2: Illustration of how an exponential $T_\rho$ gives an apparent metastable limit. The graphs are of $T_\rho = 10(\rho - 1)^{-4}$ and $T_\rho = \exp(\rho - 1)^{-4}$. The crosses mark possible experimental data points.
The coefficients were assigned the values:

\[ a_r = 1 \quad \text{and} \quad b_{r+1} = \exp \left( r^{2/3} - (r - 1)^{2/3} \right), \]

for \( r \geq 1 \). The graphs shown in Figure 1.4.1 are typical of the results presented in [22] and in [13]. It shows the numerical solution of \( c_1(t) \) plotted against \( \log_{10}(t) \). The initial data used is

\[ c_r(0) = \begin{cases} 
\rho & \text{for } r = 1 \\
0 & \text{for } 2 \leq r \leq 2,000
\end{cases} \]

where \( \rho \) takes the values 7.5, 8.0, \ldots, 11.0. The graphs, for \( \rho \geq 8.0 \), clearly show the solution going through: an initial period of rapid evolution; followed by a period of very slow change and then the decay to the equilibrium state – the final plateau is at the height of, within numerical error, the equilibrium value of \( c_1 \). To show that the ‘metastable phase’ would be observed on a macroscopic scale we could plot some macroscopic measure of the system, such as the Lyapunov function, against time. Plots of this type are shown in [23] and they display similar features to the above Figure. This is to be expected since \( c_1 \) is involved in every equation of the system and hence ‘sees the whole system’.

Numerical schemes of this type give the researcher a valuable tool for the investigation of metastable phenomenon. It is important, therefore, to know that the observed ‘metastable plateaux’ are not an artifact of the finite system. It is comparatively easy to find compelling, though circumstantial, evidence that this is not the case. In [24], M. Kreer proved that the solutions to the infinite system with initial data:

\[ c_r(0) = \begin{cases} 
Q_rz^r & \text{for } 1 \leq r \leq \ell(z) \\
0 & \text{for } \ell(z) + 1 \leq r
\end{cases} \]

were metastable – these states are exponentially close to those considered in [12]. Figure 1.4.2 shows the numerical solutions of the finite system \( (n = 2,000) \) with initial data the same as above, except with only \( n - \ell(z) \) zeros. The value of \( z \) was found for each value of \( \rho \), by solving \( \rho = \sum_{k=1}^{\ell(z)} rQ_rz^r \). The
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graphs from Figure 1.4.1 are super-imposed for comparison. The work in Chapter 3 proves that the exact solutions of the finite system have metastable states; in particular for the initial data considered above, the solution is metastable. Chapter 4 contains further verification that the states proved to be metastable in Chapter 3 generate metastable plateaux in the numerical solutions of the system. It also contains a comparison of an analytic lower bound on $T_{\rho}$ with the numerical approximation of its value.

It is therefore reasonable to argue that the numerical solutions of the finite system (1.3.1) give information about physical systems that is as reliable as the original model. This is not to say that there are no ‘finite effects’. There are. The most serious of these is that the closer $\rho$ is to $\rho_m (\approx 4.8$ in the example above) the larger $n$ must be. For example a system size of 2,000 is insufficient to see the metastable behaviour of solutions with a density of 7.5, but if $n = 3,000$ then a plateau can be observed – see Figure 1.4.3. The work in Section 3.4 shows how $n$ must depend on $\rho$ in order to avoid this problem. Unfortunately if $n$ is varied in this way, the routine becomes too costly, in cpu time, to run for lower values of $\rho$. As an example, it took 2 minutes to complete the run for $\rho = 7.5$, $n = 2,000$ but just increasing $n$ to 3,000 increased the running time to 107 minutes. In [23], Soheili studies various ways of approximating the Becker-Döring model which involve solving fewer equations. The methods were sufficiently successful to be used to investigate metastability in the two-component system, where problems of running cost are even more acute.
Figure 1.4.2: Comparison of numerical solutions of $c_1(t)$ for different initial data. The graphs show that the ‘metastable plateaux’ coincide with the truncation of metastable states of the infinite system.

Figure 1.4.3: Comparison of numerical solutions of $c_1(t)$ for different system sizes.
Chapter 2

Two Component Becker-Döring Equations

The two component Becker-Döring equations model the behaviour of clusters of two types of particle. In this chapter we investigate which properties of the one component system apply to the two component system.

2.1 Existence and Density Conservation

2.1.1 Notation

By establishing a few conventions for the notation, it is possible to simplify the two component equations and hence simplify many calculations. The conventions used throughout this chapter, unless stated otherwise, are:

(a) All terms that have a subscript 0; 0 are equal to zero.

(b) All terms that have a negative number in their subscript are equal to zero.

(c) For all \(n \geq 1\) \(b_{0,n} = b'_{n,0} := 0\).

Expressions can also be written in a more concise way if \(N_X^r + s = M\) is used to represent the sum of all \(X_{r,s}\) lying on all the diagonals from \(r + s = M\) up to and including \(r + s = N\), i.e. the sum \(\sum_{m=M}^{N} \sum_{r=0}^{m} X_{r,m-r}\). We also use \(\sum_{r,s=0}^{\infty} X_{r,s}\) to represent \(\sum_{r=0}^{\infty} \sum_{s=0}^{\infty} X_{r,s}\).

2.1.2 Definitions and identities

The two component Becker-Döring equations are:

\[
\begin{align*}
\dot{c}_{1,0} &= -J_{1,0} - J'_{1,0} - \sum_{r+s=1}^{\infty} J_{r,s} \\
\dot{c}_{0,1} &= -J_{0,1} - J'_{0,1} - \sum_{r+s=1}^{\infty} J'_{r,s} \\
\dot{c}_{r,s} &= J_{r-1,s} - J_{r,s} + J'_{r,s} - J'_{r,s-1} - J'_{r,s} \text{ if } r + s \geq 2
\end{align*}
\]

(2.1.1)

where \(J_{r,s} = \alpha_{r,s} c_{r,s} c_{1,0} - b_{r+1,s} c_{r+1,s}\) and \(J'_{r,s} = \alpha'_{r,s} c_{r,s} c_{0,1} - b'_{r,s+1} c_{r,s+1}\). In order to study the properties of solutions to (2.1.1) we introduce the Banach space

\[
X = \left\{ x = (x_{r,s}) : \|x\| := \sum_{r+s=1}^{\infty} (r + s)|x_{r,s}| < \infty \right\},
\]
and the subspace $X^+ = \{ x : \text{for each } (r,s), x_{r,s} \geq 0 \}$.

**Definition 2.1.1.** Let $0 < T \leq \infty$. A solution $c = (c_{r,s})$ of (2.1.1) on $[0,T)$ is a function $c : [0,T) \to X^+$ such that:

(i) each $c_{r,s} : [0,T) \to \mathbb{R}$ is continuous and $\sup_{t \in [0,T)} \|c(t)\| < \infty$;

(ii) $\int_0^t \sum_{r+s=1}^\infty a_{r,s} c_{r,s}(\tau) \, d\tau < \infty$, $\int_0^t \sum_{r+s=1}^\infty b_{r,s} c_{r,s}(\tau) \, d\tau < \infty$,

\[
\int_0^t \sum_{r+s=1}^\infty a'_{r,s} c_{r,s}(\tau) \, d\tau < \infty, \quad \int_0^t \sum_{r+s=1}^\infty b'_{r,s} c_{r,s}(\tau) \, d\tau < \infty, \text{ for all } t \in [0,T), \text{ and}
\]

(iii) $c_{1,0}(t) = c_{1,0}(0) - \int_0^t \left[ \sum_{r+s=1}^\infty J_{r,s}(c(\tau)) + J_{1,0}(c(\tau)) + J_{1,0}'(c(\tau)) \right] \, d\tau$,

\[
c_{0,1}(t) = c_{0,1}(0) - \int_0^t \left[ \sum_{r+s=1}^\infty J'_{r,s}(c(\tau)) + J_{0,1}(c(\tau)) + J_{0,1}'(c(\tau)) \right] \, d\tau,
\]

\[
c_{r,s}(t) = c_{r,s}(0) + \int_0^t \left[ J_{r-1,s}(c(\tau)) - J_{r,s}(c(\tau)) + J'_{r,s-1}(c(\tau)) - J'_{r,s}(c(\tau)) \right] \, d\tau,
\]

for all $(r,s)$ for which $r+s \geq 2$.

We will often have to take sums of $(g_{r,s} \hat{c}_{r,s})$, where $g_{r,s}$ is some function of $r$ and $s$. The following identities are of sums taken over two types of finite region of $\mathbb{N} \times \mathbb{N}$. In the first, the sum considered is over the region $n \leq r + s \leq N$, where $n \geq 2$. A schematic for this is shown in Figure 2.1.1, from which we can write down:

\[
\sum_{r+s=n}^N g_{r,s} \hat{c}_{r,s} = \sum_{r+s=n}^{N-1} \left[ g_{r+1,s} J_{r,s} + g_{r,s+1} J'_{r,s} \right]
\]

\[
+ \sum_{r+s=n}^{N-1} \left[ (g_{r+1,s} - g_{r,s}) J_{r,s} + (g_{r,s+1} - g_{r,s}) J'_{r,s} \right]
\]

\[
- \sum_{r+s=N}^N \left[ g_{r,s} (J_{r,s} + J'_{r,s}) \right]. \tag{2.1.3}
\]

For a rectangular region $\{ m \leq r \leq M \} \times \{ n \leq s \leq N \}$ there are two distinct cases. One where both $m \geq 1$ and $n \geq 1$ and the other where $m = 0$ and $n \geq 2$ (the case $n = 0$, $m \geq 2$ differs only in the expected way). Both these cases are illustrated in Figure 2.1.2.

For $m \geq 1$, $n \geq 1$:

\[
\sum_{r=m}^M \sum_{s=n}^N g_{r,s} \hat{c}_{r,s} = \sum_{s=n}^N \left[ g_{m,s} J_{m-1,s} \right] + \sum_{r=m}^M \left[ g_{r,N} J'_{r,N-1} \right]
\]

\[
+ \sum_{r=m}^M \sum_{s=n}^N \left[ (g_{r+1,s} - g_{r,s}) J_{r,s} \right] + \sum_{r=m}^M \sum_{s=n}^N \left[ (g_{r,s+1} - g_{r,s}) J'_{r,s} \right]
\]

\[
- \sum_{s=n}^N \left[ g_{M,s} J_{M,s} \right] - \sum_{r=m}^M \left[ g_{r,N} J'_{r,N} \right]. \tag{2.1.4}
\]
2.1. EXISTENCE AND DENSITY CONSERVATION

Figure 2.1.1: Schematic for sums of \((g_{r,s}, \hat{c}_{r,s})\) along finitely many diagonals.

Figure 2.1.2: Schematic for sums of \((g_{r,s}, \hat{c}_{r,s})\) within finite rectangles.
For \( m = 0, n \geq 2 \):

\[
\sum_{r=0}^{M} \sum_{s=n}^{N} g_{r,s} \dot{c}_{r,s} = \sum_{r=0}^{M} [g_{r,s} J'_{r,s-1}]
+ \sum_{r=0}^{M-1} \sum_{s=n}^{N} [(g_{r+1,s} - g_{r,s}) J_{r,s}]
+ \sum_{r=0}^{M} \sum_{s=n}^{N-1} [(g_{r,s+1} - g_{r,s}) J'_{r,s}]
- \sum_{s=n}^{N} [g_{M,s} J_{M,s}] - \sum_{r=0}^{M} [g_{r,N} J'_{r,N}].
\]

(2.1.5)

### 2.1.3 Existence of a solution

It is possible to prove the existence of solutions using the same method as that used by Ball et al in [2]. To this end, we first consider a finite-dimensional system (Figure 2.1.3 shows the schematic):

\[
\begin{aligned}
\dot{c}_{r,s} &= J_{r-1,s} - J_{r,s} + J'_{r,s-1} - J'_{r,s} & \text{if } 1 \leq r + s \leq n - 1, \\
\dot{c}_{1,0} &= -J_{1,0} - J'_{1,0} - \sum_{r+s=1}^{n-1} J_{r,s} \\
\dot{c}_{0,1} &= -J_{0,1} - J'_{0,1} - \sum_{r+s=1}^{n-1} J'_{r,s}
\end{aligned}
\]

(2.1.6)

![Figure 2.1.3: Schematic for the finite Becker-Döring equations](image)

**Lemma 2.1.2**

For any \( \{\hat{c}_{r,s}\}_{r+s=1}^{n} \) where each \( \hat{c}_{r,s} \geq 0 \), the system (2.1.6) has a unique solution \( \{c_{r,s}\}_{r+s=1}^{n} \), for which \( c_{r,s}(0) = \hat{c}_{r,s} \) and for all \( t \geq 0 \), \( c_{r,s}(t) \geq 0 \). Further, for all \( t \geq 0 \), \( \sum_{r+s=1}^{n} r c_{r,s}(t) = \sum_{r+s=1}^{n} r c_{r,s}(0) \) and \( \sum_{r+s=1}^{n} s c_{r,s}(t) = \sum_{r+s=1}^{n} s c_{r,s}(0) \).

**Proof.**

First consider the solution \( c_{r,s}^{(\varepsilon)} \) of a system derived from (2.1.6) by adding \( \varepsilon > 0 \) onto each equation.
Standard results (see [25]) give us that these solutions exist uniquely and that as $\varepsilon \to 0$ they tend to
the unique solution of (2.1.6) defined on some interval $[0,t_0]$. Let $\tau \geq 0$ be any time at which all $c_{r,s}^{(c)}(\tau) \geq 0$ and at least one particular $c_{p,q}^{(c)}(\tau) = 0$, then $c_{p,q}^{(c)}(\tau) > 0$. Hence all $c_{r,s}^{(c)}$ are non-negative
and so for all $t \in [0,t_0]$, $c_{r,s}(t) \geq 0$.

Notice that equations (2.1.6) can be derived formally from equations (2.1.1) by setting $J_{r,s} = 0$
whenever $r + s \geq n$ and so we can use equation (2.1.3), with $g_{r,s} = r$, to write down:

$$\sum_{r+s=2}^{n} r c_{r,s}(t) = J_{0,1} + 2J_{1,0} + \sum_{r+s=2}^{n-1} J_{r,s} = -\dot{c}_{1,0}(t).$$

Hence $\sum_{r+s=1}^{n} r c_{r,s}(t)$ has a constant value for all $t \in [0,t_0]$. Similarly for $\sum_{r+s=1}^{n} sc_{r,s}(t)$. We can now conclude that $c$ is a global solution by observing that for every $(p,q)$,

$$0 \leq c_{p,q}(t) \leq (p + q)^{-1} \sum_{r+s=1}^{n} (r + s)c_{r,s}(0).$$

\[\square\]

**Theorem 2.1.3**

Suppose that there exists a positive sequence $(g_m)$ and a constant $\delta > 0$, for which
$g_{m+1} - g_m \geq \delta$, $m = 1, 2, \ldots$, and where

$$a_{r,s}(g_{r+s+1} - g_{r+s}) = O(g_{r+s})$$

(2.1.7)

$$a'_{r,s}(g_{r+s+1} - g_{r+s}) = O(g_{r+s}).$$

(2.1.8)

Let $\{\dot{c}_{r,s}\}_{r+s=1}^{\infty}$ satisfy $\sum_{r+s=1}^{\infty} [g_{r+s}\dot{c}_{r,s}] < \infty$. Then there exists a solution of (2.1.1) on $[0,\infty)$ with
c(0) = $\dot{c}$ and the additional properties that, for any $T > 0$:

$$\sup_{t \in [0,T]} \sum_{r+s=1}^{\infty} g_{r+s}c_{r,s}(t) < \infty, \quad \int_{0}^{T} \sum_{r+s=1}^{\infty} [(g_{r+s+1} - g_{r+s})b_{r,s}c_{r,s}(\tau)] d\tau < \infty$$

(2.1.9)

and

$$\int_{0}^{T} \sum_{r+s=1}^{\infty} [(g_{r+s+1} - g_{r+s})b'_{r,s}c_{r,s}(\tau)] d\tau < \infty$$

(2.1.10)

**Proof.**

First note that $g_{m+1} - g_m \geq \delta \implies g_m \geq \delta m$, so

$$\sum_{r+s=1}^{\infty} g_{r+s}c_{r,s} < \infty \implies \delta\|\dot{c}\| < \infty.$$

Let $c^{(n)}$ denote the solution of equations (2.1.6) for which $c^{(n)}(0) = \{\dot{c}_{r,s}\}_{r+s=1}^{n}$. Lemma 2.1.2

tells us that $\sum_{r+s=1}^{n} (r + s)c^{(n)}_{r,s}(t) = \sum_{r+s=1}^{n} (r + s)\dot{c}_{r,s}$ and so for each $(r, s)$, $0 \leq c^{(n)}_{r,s}(t) \leq \|\dot{c}\|/(r + s)$. Hence, for $r + s \geq 2$:

$$|c^{(n)}_{r,s}| \leq a_{r-1,s} \frac{\|\dot{c}\|^2}{r + s - 1} + a_{r,s} \frac{\|\dot{c}\|^2}{r + s} + b_{r,s} \frac{\|\dot{c}\|^2}{r + s} + b'_{r,s} \frac{\|\dot{c}\|^2}{r + s + 1} + a'_{r-1,s} \frac{\|\dot{c}\|^2}{r + s - 1} + a'_{r,s} \frac{\|\dot{c}\|^2}{r + s} + b'_{r,s} \frac{\|\dot{c}\|^2}{r + s} + b'_{r,s+1} \frac{\|\dot{c}\|^2}{r + s + 1} \leq M_{r,s} < \infty,$$

which implies that $\left\{c^{(n)}_{r,s}(\cdot)\right\}_{n=2}^{\infty}$ is equicontinuous on $[0,\infty)$, for every $(r, s)$ with $r + s \geq 2$. So the
Arzela-Ascoli theorem tells us that we can find a subsequence $n_k$, which becomes infinite as $k \to \infty$, and functions $c_{r,s} : [0,\infty) \to \mathbb{R}$, such that for every $(r, s)$ with $r + s \geq 2$, $c^{(n_k)}_{r,s} \to c_{r,s}$ uniformly on
compact intervals of \([0, \infty)\), as \(k \to \infty\). Since \(c^{n_k} \geq 0\) then \(c_{r,s} \geq 0\) and since \(\sum_{r+s=2}^{N} (r+s)c_{r,s}(t) = \lim_{k \to \infty} \sum_{r+s=2}^{N} (r+s)c^{n_k}_{r,s}(t) \leq \|\tilde{c}\|\), we know that

\[
\sum_{r+s=2}^{\infty} (r+s)c_{r,s}(t) \leq \|\tilde{c}\| \quad \text{for all } t \geq 0. \tag{2.1.11}
\]

Dealing with \(c_{1,0}\) and \(c_{0,1}\) is some what more complicated, since we have not assumed any knowledge of \(b_{r,s}\) or \(b'_{r,s}\), we cannot bound \(|c_{1,0}^{n_k}|\) and \(|c_{0,1}^{n_k}|\) easily. This can be done, though, by using the bounds on the growth of \(a_{r,s}\) and \(a'_{r,s}\). First we observe that since \(|c_{1,0}^{n_k}| \leq \|\tilde{c}\|\) and \(|c_{0,1}^{n_k}| \leq \|\tilde{c}\|\) there exist functions \(c_{1,0}, c_{0,1} \in L^{\infty}(0, \infty)\) such that for some subsequence of \(n_k\) (denoted \(n_k\), for simplicity)

\[
\begin{align*}
\int_{0}^{\infty} \left( c_{1,0}^{n_k}(\tau) - c_{1,0}(\tau) \right) \phi(\tau) d\tau & \to 0 \\
\int_{0}^{\infty} \left( c_{0,1}^{n_k}(\tau) - c_{0,1}(\tau) \right) \phi(\tau) d\tau & \to 0 \\
\end{align*}
\]

as \(k \to \infty\), for every \(\phi \in L^1(0, \infty)\)

Once we have shown that \(c_{1,0}^{n_k} \to c_{1,0}\) and \(c_{0,1}^{n_k} \to c_{0,1}\) uniformly on compact subintervals of \([0, \infty)\), it is easy to verify that \(c\) is a solution of (2.1.1). We show that the convergence is uniform by proving that both \(c_{1,0}^{n_k}\) and \(c_{0,1}^{n_k}\) are Cauchy sequences. This is done as follows (using \(c^k\) to denote \(c^{n_k}\)):

\[
|c_{1,0}^{k}(t) - c_{1,0}(t)| + |c_{0,1}^{k}(t) - c_{0,1}(t)|
\leq 2 \int_{0}^{t} \left| J_{1,0}(c^k(\tau)) - J_{1,0}(c(\tau)) \right| + \left| J'_{0,1}(c^k(\tau)) - J'_{0,1}(c(\tau)) \right| \ d\tau \\
+ 2 \int_{0}^{t} \left| J'_{1,0}(c^k(\tau)) - J'_{1,0}(c(\tau)) \right| + \left| J_{0,1}(c^k(\tau)) - J_{0,1}(c(\tau)) \right| \ d\tau \\
+ \int_{0}^{t} \left( \sum_{r+s=2}^{N-1} + \sum_{r+s=N}^{n_k-1} \right) \left| J_{r,s}(c^k(\tau)) - J_{r,s}(c(\tau)) \right| + \left| J_{r,s}(c^k(\tau)) - J_{r,s}(c(\tau)) \right| \ d\tau
\leq A + B + C + D + E + F, \tag{2.1.12}
\]

where \(A\) to \(F\) are defined below.

\[
A = 2 \int_{0}^{t} a_{1,0} \left| c_{1,0}^{k}(\tau) - c_{1,0}(\tau) \right| \left( c_{1,0}^{k}(\tau) + c_{1,0}(\tau) \right) \ d\tau
\]

\[
+ 2 \int_{0}^{t} a_{0,1} \left| c_{0,1}^{k}(\tau) - c_{0,1}(\tau) \right| \left( c_{0,1}^{k}(\tau) + c_{0,1}(\tau) \right) \ d\tau \\
+ 2 \int_{0}^{t} b_{2,0} \left| c_{2,0}^{k}(\tau) - c_{2,0}(\tau) \right| + b_{0,2} \left| c_{0,2}^{k}(\tau) - c_{0,2}(\tau) \right| \ d\tau \quad (a)
\]

\[
B = 2 \int_{0}^{t} \left( a_{0,1} c_{0,1}^{k} + a'_{1,0} c_{0,1}^{l} \right) \left| c_{1,0}^{k}(\tau) - c_{1,0}(\tau) \right| \ d\tau
\]

\[
+ 2 \int_{0}^{t} \left( b_{1,1} + b'_{1,1} \right) \left| c_{1,1}^{k}(\tau) - c_{1,1}(\tau) \right| \ d\tau. \quad (b)
\]
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To show that line (e) can be set arbitrarily small, we will show that if $\epsilon > 0$ is some constant, and $t \in [0, T]$. Applying Gronwall’s inequality to this gives:

$$|c_{1,0}^k(t) - c_{1,0}^l(t)| + |c_{0,1}^k(t) - c_{0,1}^l(t)| \leq K \left( \varepsilon + \int_0^t |c_{1,0}^l(\tau) - c_{1,0}^k(\tau)| + |c_{0,1}^l(\tau) - c_{0,1}^k(\tau)| d\tau \right),$$

where $K > 0$ is some constant, and $t \in [0, T]$. Applying Gronwall’s inequality to this gives:

$$|c_{1,0}^k(t) - c_{1,0}^l(t)| + |c_{0,1}^k(t) - c_{0,1}^l(t)| \leq \varepsilon e^{Kt}.$$  \hspace{1cm} (2.1.14)

To show that line (e) can be set arbitrarily small, we will show that if $N, n_k > N_\varepsilon$ then, for all $t \in [0, T]$:

$$\int_0^t \sum_{r+s=N} \left[ g_{r+s} c_{r,s}^{n_k}(\tau) \right] d\tau +$$

$$\int_0^t \sum_{r+s=N} \left[ (g_{r+s+1} - g_{r+s}) \left( b_{r+s+1} c_{r,s+1}^{n_k}(\tau) + b'_{r+s+1} c_{r,s+1}^{n_k}(\tau) \right) \right] d\tau < \varepsilon,$$  \hspace{1cm} (2.1.15)
where $T$ takes any given positive, finite value.

The closest thing we have to equation (2.1.15) is equation (2.1.3), which after replacing $g_{r,s}$ with $g_{r+s}$ and $J_{r,s}(c^{n_k}) = 0$ for all $(r,s)$ with $r + s \geq n_k$, can be rearranged to give:

$$\frac{d}{dt} \left( \sum_{r+s=N}^{n_k} g_{r+s} c_{r,s}^{n_k}(t) \right)$$

$$+ \sum_{r+s=N}^{n_k-1} \left[ (g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(t) + (g_{r+s+1} - g_{r+s}) b'_{r,s+1} c_{r,s+1}^{n_k}(t) \right]$$

$$= \sum_{r+s=N-1}^{N-1} \left[ g_{r+s+1} J_{r,s}(c^{n_k}(t)) + g_{r+s+1} J'_{r,s}(c^{n_k}(t)) \right]$$

$$+ \sum_{r+s=N}^{n_k-1} \left[ (g_{r+s+1} - g_{r+s}) a_{r,s} c_{r,0}^{n_k}(t) c_{r,s}^{n_k}(t) + (g_{r+s+1} - g_{r+s}) a_{r,s} c_{r,1}^{n_k}(t) c_{r,s}^{n_k}(t) \right]$$  (2.1.16)

where $N \geq 2$. Integrating both sides and using the bounds on $c_{1,0}^{n_k}$, $c_{0,1}^{n_k}$ and $\sum_{r+s=1}^{\infty} g_{r+s} c_{r,s}$ plus the inequalities (2.1.7) and (2.1.8), we can find constants $\alpha$, $\beta$ and $K$ independent of $k$ such that:

$$\sum_{r+s=N}^{n_k} g_{r+s} c_{r,s}^{n_k}(t)$$

$$+ \int_0^t \sum_{r+s=N}^{n_k-1} \left[ (g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(\tau) + (g_{r+s+1} - g_{r+s}) b'_{r,s+1} c_{r,s+1}^{n_k}(\tau) \right] d\tau$$

$$\leq \sum_{r+s=2}^{n_k} g_{r+s} c_{r,s}^{n_k}(t)$$

$$+ \int_0^t \sum_{r+s=2}^{n_k-1} \left[ (g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(\tau) + (g_{r+s+1} - g_{r+s}) b'_{r,s+1} c_{r,s+1}^{n_k}(\tau) \right] d\tau$$

$$\leq \alpha + \beta t + K \left( \int_0^t \sum_{r+s=2}^{n_k} g_{r+s} c_{r,s}^{n_k}(\tau) d\tau \right)$$  (2.1.17)

This is too crude an estimate to be of any direct use in showing that the left hand side is arbitrarily small, but with $N = 2$ (i.e. the second line) the expected limit of the left hand side is the sum of those terms which (2.1.9) and (2.1.10) claim are finite. So we continue with this line of reasoning by applying Gronwall’s inequality to get:

$$\sum_{r+s=2}^{n_k} g_{r+s} c_{r,s}^{n_k}(t) + \int_0^t \sum_{r+s=2}^{n_k-1} \left[ (g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(\tau) \right] d\tau$$

$$+ \int_0^t \sum_{r+s=2}^{n_k-1} \left[ (g_{r+s+1} - g_{r+s}) b'_{r,s+1} c_{r,s+1}^{n_k}(\tau) \right] d\tau \leq M e^{Kt},$$  (2.1.18)

for all $t \geq 0$, where $M$ is another constant independent of $k$. This inequality allows us to pass to the expected limit, by splitting the two sums up as $\left( \sum_{r+s=2}^{\ell-1} + \sum_{r+s=\ell}^{n_k} \right)$ and $\left( \sum_{r+s=2}^{\ell-1} + \sum_{r+s=\ell}^{n_k-1} \right)$ respectively, then letting $k \to \infty$ and then $\ell \to \infty$, the monotone convergence theorem then gives:

$$\sum_{r+s=2}^{\infty} g_{r+s} c_{r,s}(t) + \int_0^t \sum_{r+s=2}^{\infty} \left[ (g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}(\tau) \right] d\tau$$
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\[ + \int_0^t \sum_{r+s=2}^{\infty} [(g_{r+s+1} - g_{r+s})b_{r,s+1}c_{r,s+1}(\tau)] \, d\tau \leq M e^{KT}. \quad (2.1.19) \]

So for any \( T > 0 \), \( \sup_{t \in [0,T]} \sum_{r+s=1}^{\infty} g_{r+s}c_{r,s}(t) \), \( \int_0^T \sum_{r+s=1}^{\infty} [(g_{r+s+1} - g_{r+s})b_{r,s}c_{r,s}(\tau)] \, d\tau \) and \( \int_0^T \sum_{r+s=1}^{\infty} [(g_{r+s+1} - g_{r+s})b_{r,s}c_{r,s}(\tau)] \, d\tau \) are all less than \( M_1 \| \dot{c} \| + M e^{KT} \), where \( M_1 = \max\{g_1, g_2(b_1,0 + b_0,1), g_2(b_1,0 + b_0,1)\} \). This proves (2.1.9) and (2.1.10).

Returning to the establishment of (2.1.15), notice that we can rewrite equation (2.1.16) and integrate both sides to get:

\[
\int_0^t \sum_{r+s=N}^{n_k} g_{r+s}c_{r,s}^{n_k}(\tau) \, d\tau \\
+ \int_0^t \int_0^\tau \sum_{r+s=N}^{n_k} [(g_{r+s+1} - g_{r+s})b_{r,s+1}c_{r,s+1}(\eta) + (g_{r+s+1} - g_{r+s})b_{r,s}c_{r,s}(\eta)] \, d\eta \, d\tau \\
\leq g_N \int_0^t \int_0^\tau \sum_{r+s=N-1}^{N-1} [J_{r,s}(c^{n_k}(\eta)) + J'_{r,s}(c^{n_k}(\eta))] \, d\eta \, d\tau \\
+ \left( \sum_{r+s=N}^{n_k} g_{r+s}c_{r,s} \right) t + K \left( \int_0^t \int_0^\tau \sum_{r+s=N}^{n_k} [g_{r+s}c_{r,s}^{n_k}(\eta)] \, d\eta \, d\tau \right). \quad (2.1.20)
\]

Now the second term on the right hand side can be made arbitrarily small for all \( t \in [0,2T] \). If the same could be done for the first term on the right, we could use Gronwall’s inequality to replace the right hand side with \( \varepsilon^2 e^{2KT} \); which would bring us very close to what we want. To bound this first term, replace \( g_m \) by 1 in (2.1.16) and then integrate to obtain:

\[
\sum_{r+s=N}^{n_k} [c_{r,s}^{n_k}(t) - \dot{c}_{r,s}] = \int_0^t \sum_{r+s=N-1}^{N-1} [J_{r,s}(c^{n_k}(\tau)) + J'_{r,s}(c^{n_k}(\tau))] \, d\tau. \quad (2.1.21)
\]

We can pass to the expected limit as \( k \to \infty \) on the right using \( \{c_{1,0}^{n_k}\} \) and \( \{c_{0,1}^{n_k}\} \)'s weak convergence together with \( \{c_{r,s}^{n_k}\} \)'s uniform convergence. On the left we know that for any fixed \( \ell \),

\[
\lim_{k \to \infty} \sum_{r+s=N}^{n_k} [c_{r,s}^{n_k}(t) - c_{r,s}(t)] = 0, \text{ while } \lim_{k \to \infty} \sum_{r+s=\ell}^{n_k} [c_{r,s}^{n_k}(t) - \dot{c}_{r,s}] = \sum_{r+s=\ell}^{n_k} [c_{r,s}(t) - \dot{c}_{r,s}]
\]

which implies

\[
g_N \int_0^t \int_0^\tau \sum_{r+s=N-1}^{N-1} [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\eta \, d\tau \leq g_N \int_0^{2T} \sum_{r+s=N}^{\infty} [c_{r,s}(\tau) + \dot{c}_{r,s}] \, d\tau \\
\leq \int_0^{2T} \sum_{r+s=N}^{\infty} [g_{r,s}c_{r,s}(\tau) + g_{r,s}\dot{c}_{r,s}] \, d\tau.
\]
We now know that \( \sum_{r+s=1}^{\infty} g_{r,s} c_{r,s}(t) < \infty \) for all \( t \in [0, 2T] \) and so we can find an \( N_\varepsilon \) for which

\[
N > N_\varepsilon \implies g_N \int_0^t \int_0^\tau \sum_{r+s=N-1}^{N-1} [J_{r,s}(c(\eta)) + J_{r,s}'(c(\eta))] \, d\eta \, d\tau < \varepsilon, \quad \text{for all } t \in [0, 2T].
\]

The bounded convergence theorem then allows us to find a \( k_\varepsilon \) for which

\[
N > N_\varepsilon, k > k_\varepsilon \implies g_N \int_0^t \int_0^\tau \sum_{r+s=N}^{N-1} [J_{r,s}(c^{n_k}(\eta)) + J_{r,s}'(c^{n_k}(\eta))] \, d\eta \, d\tau < 2\varepsilon,
\]

for all \( t \in [0, 2T] \). Substituting this into (2.1.20) and applying Gronwall’s inequality gives

\[
\int_0^t \sum_{r+s=N}^{n_k} g_{r+s} c_{r,s}^{n_k}(\tau) \, d\tau + \int_0^\tau \sum_{r+s=N}^{n_k-1} [(g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(\eta) + (g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(\tau)] \, d\eta \, d\tau < 3\varepsilon e^{2KT}, \quad \text{for all } t \in [0, 2T]. \tag{2.1.23}
\]

We obtain (2.1.15), by:

\[
\int_0^{t/2} \sum_{r+s=N}^{n_k-1} [g_{r+s} c_{r,s}^{n_k}(\tau)] \, d\tau + \int_0^{t/2} \sum_{r+s=N}^{n_k-1} [(g_{r+s+1} - g_{r+s}) (b_{r+1,s} c_{r+1,s}^{n_k}(\tau) + b_{r+1,s} c_{r+1,s}^{n_k}(\tau))] \, d\tau < \frac{1}{\min\{1, t/2\}} \int_0^t \sum_{r+s=N}^{n_k-1} [g_{r+s} c_{r,s}^{n_k}(\tau)] \, d\tau
\]

\[
+ \frac{t/2}{\min\{1, t/2\}} \int_0^{t/2} \sum_{r+s=N}^{n_k-1} [(g_{r+s+1} - g_{r+s}) (b_{r+1,s} c_{r+1,s}^{n_k}(\tau) + b_{r+1,s} c_{r+1,s}^{n_k}(\tau))] \, d\tau < \text{con.} \int_0^t \sum_{r+s=N}^{n_k-1} [g_{r+s} c_{r,s}^{n_k}(\tau)] \, d\tau
\]

\[
+ \text{con.} \int_0^t (t - \tau) \sum_{r+s=N}^{n_k-1} [(g_{r+s+1} - g_{r+s}) (b_{r+1,s} c_{r+1,s}^{n_k}(\tau) + b_{r+1,s} c_{r+1,s}^{n_k}(\tau))] \, d\tau < \text{con.} \int_0^t \sum_{r+s=N}^{n_k-1} [g_{r+s} c_{r,s}^{n_k}(\tau)] \, d\tau
\]

\[
+ \text{con.} \int_0^\tau \sum_{r+s=N}^{n_k-1} [(g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(\eta) + (g_{r+s+1} - g_{r+s}) b_{r+1,s} c_{r+1,s}^{n_k}(\eta)] \, d\eta \, d\tau < \varepsilon, \quad \text{for all } t/2 \in [0, T].
\]

This, as earlier arguments explained, implies that all \( \{c_{r,s}^{n_k}(\cdot)\} \to \{c_{r,s}(\cdot)\} \) uniformly on compact intervals of \([0, \infty)\) as \( k \to \infty \), and we now have enough information about \( c \) to show that it is a solution of (2.1.1) on \([0, \infty)\).

We will consider each of the defining properties from Definition 2.1.1 in turn. For part (i), the uniform convergence on any interval \([0, T]\) together with the continuity of every \( c_{r,s}^{n_k} \) on \([0, \infty)\), implies
that the limit, \( c_{r_s} \), is continuous on \([0, \infty)\). Equation (2.1.11) combines with the bounds \( 0 \leq c_{1,0}^{L} \leq \| \hat{c} \| \) and \( 0 \leq c_{1,0}^{U} \leq \| \hat{c} \| \) to give that \( \sup_{t \in [0, \infty)} \| c(t) \| \leq 3 \| \hat{c} \| < \infty \).

All of the inequalities in part (ii) follow from (2.1.19), and the assumed properties of \( a_{r,s} \), \( a'_{r,s} \) and \( g_{r+s} \).

The last equation of part (iii) is an immediate consequence of the uniform convergence of every \( c_{r+s}^{n_k}(\cdot) \). To derive the first equation we start with:

\[
c_{1,0}^{n_k}(t) - \hat{c}_{1,0} + \int_{0}^{t} \left[ J_{1,0}(c_{n_k}(\tau)) + J_{1,0}'(c_{n_k}(\tau)) + \sum_{r+s=1}^{N-1} J_{r,s}(c_{n_k}(\tau)) \right] d\tau = \int_{0}^{t} \left[ \sum_{r+s=n_k} n_k J_{r,s}(c_{n_k}(\tau)) \right] d\tau. \tag{2.1.24}\n\]

Using the properties of \( a_{r,s} \) and \( g_{r+s} \) and equation (2.1.15) we can conclude that for all \( N, k \geq N_c \):

\[
\int_{0}^{t} \left[ \sum_{r+s=N}^{n_k} (a_{r,s} c_{n_k}(\tau) c_{1,0}^{n_k}(\tau) + b_{r+1,s} c_{r+1,s}^{n_k}(\tau)) \right] d\tau < K' \varepsilon, \tag{2.1.25}\n\]

for all \( t \in [0, T] \), where \( K' \) is independent of \( k \) and \( N \). We can pass to the limit on the left, by splitting the sum up into \( \sum_{r+s=N}^{n_k} \left( \sum_{r+s=N}^{r+s=t} \right), \) then letting \( k \to \infty \) and then \( \ell \to \infty \). This process results in

\[
\int_{0}^{t} \left[ \sum_{r+s=N}^{\infty} (a_{r,s} c(\tau) c_{1,0}(\tau) + b_{r+1,s} c_{r+1,s}(\tau)) \right] d\tau < K' \varepsilon, \tag{2.1.26}\n\]

for all \( t \in [0, T] \) and for every \( N > N_c \). This together with (2.1.24) imply

\[
|c_{1,0}(t) - \hat{c}_{1,0} + \int_{0}^{t} \left[ J_{1,0}(c(\tau)) + J_{1,0}'(c(\tau)) + \sum_{r+s=1}^{\infty} J_{r,s}(c(\tau)) \right] d\tau | < 2K' \varepsilon \tag{2.1.27}\n\]

for all \( t \in [0, T] \), \( \varepsilon \) and \( T \) are arbitrary, so \( c \) satisfies the fourth equation in (2.1.2). The same argument shows that \( c \) also satisfies the second equation.

\[\diamond\]

### 2.1.4 Conservation of densities

In the last section we showed that at least one solution of (2.1.1) existed. We do not, however, know if this solution is unique. Here we will show that the limits of identities (2.1.3) and (2.1.5) hold for all solutions of (2.1.1), for certain sequences \( g_{r,s} \). We can then use this to show that all solutions of (2.1.1) conserve the density of both type of particle, which is the conclusion of Corollary 2.1.7. Unfortunately we cannot, at present, show that the limits of (2.1.3) and (2.1.5) exist and have the form we believe them to have, for the full range of \( g_{r,s} \), so we will state the expected result as a conjecture and then prove it to be true for a restricted range of sequences. This conjecture is the equivalent of Theorem 2.5 in [2].

**Conjecture 2.1.4**

Let \( g_{r,s} \) be a given sequence and \( c \) be a solution of (2.1.1) on some interval \([0, T]\), where \( 0 < T \leq \infty \).

Suppose that for some \( t_1, t_2 \in [0, T] \), with \( t_1 < t_2 \):

\[
\int_{t_1}^{t_2} \sum_{r+s=1}^{\infty} |g_{r+1,s} - g_{r,s}| a'_{r,s} c_{r,s}(\tau) d\tau < \infty \text{ and either } \]

(a) \( g_{r,s} = O(r+s) \); \[
\int_{t_1}^{t_2} \sum_{r+s=1}^{\infty} |g_{r+1,s} - g_{r,s}| b_{r,s+1} c_{r,s+1}(\tau) d\tau < \infty \] and

\[
\int_{t_1}^{t_2} \sum_{r+s=1}^{\infty} |g_{r,s+1} - g_{r,s}| b'_{r,s+1} c_{r,s+1}(\tau) d\tau < \infty \text{ or } \]

(b) \( g_{r,s} = O(r+s^2) \); \[
\int_{t_1}^{t_2} \sum_{r+s=1}^{\infty} |g_{r+1,s} - g_{r,s}| a_{r,s} c_{r,s}(\tau) d\tau < \infty \text{ and either } \]

\[
\int_{t_1}^{t_2} \sum_{r+s=1}^{\infty} |g_{r+1,s} - g_{r,s}| b_{r,s+1} c_{r,s+1}(\tau) d\tau < \infty \] and

\[
\int_{t_1}^{t_2} \sum_{r+s=1}^{\infty} |g_{r,s+1} - g_{r,s}| b'_{r,s+1} c_{r,s+1}(\tau) d\tau < \infty \text{ or } \]
(b) for \( i = 1, 2 \), \( \sum_{r+s=1}^{\infty} g_{r,s} c_{r,s}(t_1) < \infty \); \( g_{r+1,s} \geq g_{r,s} \geq 0 \) and \( g_{r,s+1} \geq g_{r,s} \geq 0 \) for sufficiently large \( r \) and \( s \).

Then, for \( m \geq 2 \)

\[
\sum_{r+s=m}^{\infty} g_{r,s}(c_{r,s}(t_2) - c_{r,s}(t_1))
\]

\[+
\int_{t_1}^{t_2} \sum_{r+s=m}^{\infty} \left[(g_{r+1,s} - g_{r,s}) b_{r+1,s} c_{r+1,s}(\tau) + (g_{r,s+1} - g_{r,s}) b'_{r,s+1} c_{r,s+1}(\tau)\right] d\tau
\]

\[=
\int_{t_1}^{t_2} \sum_{r+s=m}^{\infty} \left[(g_{r+1,s} - g_{r,s}) a_{r,s} c_{1,0}(\tau) + (g_{r,s+1} - g_{r,s}) a'_{r,s} c_{0,1}(\tau)\right] c_{r,s}(\tau) d\tau
\]

\[+
\int_{t_1}^{t_2} \sum_{r+s=m-1}^{m-1} [g_{r+s} J_{r,s}(c(\tau)) + g_{r,s+1} J'_{r,s}(c(\tau)))] d\tau
\]  

(2.1.28)

In the limit the only difference we expect there to be between identity (2.1.3) and (2.1.5), is in the region over which the sum is taken. To simplify the notation, we will use \( \mathcal{R}(n) \) to denote the set \( \mathbb{N}^2 \cap (\mathbb{R}^2 - [0, n - 1]^2) \). By considering the schematic diagrams in Figures 2.1.1 and 2.1.2 it is easily seen that identity (2.1.3) tends to equation (2.1.28) if identity (2.1.5) tends to

\[
\sum_{m} g_{r,s}(c_{r,s}(t_2) - c_{r,s}(t_1))
\]

\[+
\int_{t_1}^{t_2} \sum_{m} \left[(g_{r+1,s} - g_{r,s}) b_{r+1,s} c_{r+1,s}(\tau) + (g_{r,s+1} - g_{r,s}) b'_{r,s+1} c_{r,s+1}(\tau)\right] d\tau
\]

\[=
\int_{t_1}^{t_2} \sum_{m} \left[(g_{r+1,s} - g_{r,s}) a_{r,s} c_{1,0}(\tau) + (g_{r,s+1} - g_{r,s}) a'_{r,s} c_{0,1}(\tau)\right] c_{r,s}(\tau) d\tau
\]

\[+
\int_{t_1}^{t_2} \sum_{s=0}^{m-1} [g_{r+s} J_{r,s}(c(\tau)) + g_{r,s+1} J'_{r,s}(c(\tau)))] d\tau
\]

(2.1.29)

as \( N \to \infty \) and \( M \to \infty \). The sequences for which Conjecture 2.1.4 can be proved to be true, are those which behave ‘like’ sequences in one variable, where that variable may be \( r \), \( s \) or \( r + s \), for large values of \( r \) and \( s \). The next definition makes this more precise.

Definition 2.1.5. Given sequences \( h_k \) and \( H_k \), where \( k \) is either \( r \), \( s \) or \( r + s \), we will say that \( g_{r,s} = V(h_k, H_k) \) if

(i) \( h_k < g_{r,s} < H_k \);

(ii) \( h_{k+1} - h_k < g_{r+1,s} - g_{r,s} < H_{k+1} - H_k \) and

(iii) \( h_{k+1} - h_k < g_{r,s+1} - g_{r,s} < H_{k+1} - H_k \),

for all \( r \) and \( s \) for which \( r + s \) is sufficiently large.

We will abbreviate \( V(-H_k, H_k) \) to \( V(H_k) \).

Theorem 2.1.6

Let \( c \) be a solution of (2.1.1) on \([0, T] \). Fixing \( k \) as either \( r \), \( s \) or \( r + s \), let \( h_k \) and \( H_k \) be sequences that satisfy the conditions on \( g_{r,s} \) made in Conjecture 2.1.4. If \( g_{r,s} = V(h_k, H_k) \) and also satisfies the conditions in Conjecture 2.1.4 then equations (2.1.28) and (2.1.29) hold.

We will prove the cases \( k = r + s \) and \( k = r \) separately (\( k = s \) is identical to \( k = r \)). In both proofs we start by showing the special case \( g_{r,s} = h_k \) first, and then use this to derive the result when \( g_{r,s} = V(h_k, H_k) \).
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Proof for $k = r + s$.
By comparing equations (2.1.3) and (2.1.28) and using the definition of a solution and the conditions of Conjecture 2.1.4 we can see that the result follows once we have shown that

$$\lim_{n \to \infty} \int_{t_1}^{t_2} \sum_{r+s=n}^n g_{r,s} [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\tau = 0$$

(2.1.30)

As explained above we first prove (2.1.30) for $g_{r,s} = h_{r+s}$.

If we replace $g_{r,s}$ in (2.1.3) with 1 and integrate we get:

$$\sum_{r+s=m}^n [c_{r,s}(t_2) - c_{r,s}(t_1)] = \int_{t_1}^{t_2} \sum_{r+s=m-1}^{m-1} [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\tau$$

$$+ \int_{t_1}^{t_2} \sum_{r+s=n}^n [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\tau$$

Parts (i) and (ii) of the definition of a solution imply that

$$\lim_{n \to \infty} \int_{t_1}^{t_2} \sum_{r+s=n}^n [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\tau = 0$$

and so

$$\sum_{r+s=m}^\infty [c_{r,s}(t_2) - c_{r,s}(t_1)] = \int_{t_1}^{t_2} \sum_{r+s=m-1}^{m-1} [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\tau.$$ 

Notice that if $h_{r+s}$ satisfies the conditions in part (a) of Conjecture 2.1.4

$$\lim_{n \to \infty} |h_{n+1}| \sum_{r+s=n+1}^\infty c_{r,s}(t_i) \leq \lim_{n \to \infty} \sum_{r+s=n+1}^\infty (r+s)c_{r,s}(t_i) = 0$$

for $i = 1, 2$, by part (i) of Definition 2.1.1. While if $h_{r+s}$ satisfies (b):

$$\lim_{n \to \infty} |h_{n+1}| \sum_{r+s=n+1}^\infty c_{r,s}(t_i) \leq \lim_{n \to \infty} \sum_{r+s=n+1}^\infty h_{r+s}c_{r,s}(t_i) = 0.$$ 

So in either case we have

$$\lim_{n \to \infty} \int_{t_1}^{t_2} \sum_{r+s=n}^n h_{n+1} [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\tau = 0$$

The result then follows for all sequences $h_{r+s}$ that satisfy the conditions of the conjecture. To establish the full result we notice that equation (2.1.3) can be rewritten as:

$$X_n(g_{r,s}) + D_{n,m}(g_{r,s}) = E_{n,m}(g_{r,s})$$

(2.1.31)

where:

$$X_n(g_{r,s}) := \int_{t_1}^{t_2} \sum_{r+s=n}^n g_{r,s} [J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau))] \, d\tau.$$ 

$$D_{n,m}(g_{r,s}) := \sum_{r+s=m}^n g_{r,s}c_{r,s}(t_2) + \int_{t_1}^{t_2} \sum_{r+s=m}^n (g_{r+1,s} - g_{r,s})b_{r+1,s}c_{r+1,s}(\tau) \, d\tau$$

$$+ \int_{t_1}^{t_2} \sum_{r+s=m}^n (g_{r,s+1} - g_{r,s})b'_{r,s+1}c_{r,s+1}(\tau) \, d\tau.$$
\[
E_{n,m}(g, r_s) := \sum_{r+s=m}^{n} g_{r,s}c_{r,s}(t_1) + \int_{t_1}^{t_2} \sum_{r+s=m-1}^{m} \left[ g_{r+1,s}a_{r+1,s}c_{r+1,s}(\tau) + g_{r,s+1}a_{r,s+1}c_{r,s+1}(\tau) \right] d\tau
\]

Since \( g_{r,s} = \mathcal{V}(h_{r+s}, H_{r+s}) \) we know that for all sufficiently large \( m \), \( D_{n,m}(g_{r,s}) > D_{n,m}(h_{r+s}) \) and \( E_{n,m}(g_{r,s}) < E_{n,m}(H_{r+s}) \) but equation (2.1.31) applies to \( h_{r+s} \) and \( H_{r+s} \) as well so

\[
E_{n,m}(h_{r+s}) - X_n(h_{r+s}) < X_n(g_{r,s}) + D_{n,m}(g_{r,s}) < E_{n,m}(H_{r+s}) \quad \text{for all large } m
\]

The assumptions on \( h \) and \( H \) and the result we have just proved, show us that \( \lim_{n \to \infty} E_{n,m}(h_{r+s}) \) and \( \lim_{n \to \infty} E_{n,m}(H_{r+s}) \) exist for all \( m \) and that \( \lim_{n \to \infty} X_n(h_{r+s}) = 0 \), hence \( \lim_{n \to \infty} D_{n,m}(g_{r,s}) \) exists and we have that for all large \( m \)

\[
E_{\infty,m}(h_{r+s}) < \lim_{n \to \infty} X_n(g_{r,s}) + D_{\infty,m}(g_{r,s}) < E_{\infty,m}(H_{r+s})
\]

so \( \lim_{n \to \infty} X_n(g_{r,s}) = 0 \)

Proof for \( k = r \)

The extension of the result from \( g_{r,s} = h_r \) to \( g_{r,s} = \mathcal{V}(h_r, H_r) \) is the same in this case as above, so we will only give the proof when \( g_{r,s} = h_r \). This time we start with equation (2.1.5) and take limits to derive equation (2.1.29).

Integrating equation (2.1.5) implies that

\[
\sum_{r=m}^{M} \sum_{s=0}^{N} h_r(c_{r,s}(t_2) - c_{r,s}(t_1)) + \int_{t_1}^{t_2} \sum_{r=m}^{M} \sum_{s=0}^{N-1} (h_{r+1} - h_r)b_{r+1,s}c_{r+1,s}(\tau) d\tau
\]

\[
= \int_{t_1}^{t_2} \sum_{s=0}^{N} h_m J_{m-1,s}(c(\tau)) d\tau
\]

\[
+ \int_{t_1}^{t_2} \sum_{r=m}^{M} \sum_{s=0}^{N-1} (h_{r+1} - h_r)a_{r,s}c_{1,0}c_{r+1,s}(\tau) d\tau
\]

\[
- \int_{t_1}^{t_2} \sum_{s=0}^{N} h_M J_{M,s}(c(\tau)) d\tau - \int_{t_1}^{t_2} \sum_{r=m}^{M} h_r J_{r,N}(c(\tau)) d\tau.
\]

Since

\[
\left| \int_{t_1}^{t_2} \sum_{r=m}^{M} h_r J_{r,N}(c(\tau)) d\tau \right| < \max_{M \geq r \geq m} |h_r| \int_{t_1}^{t_2} \sum_{r=m}^{M} |J_{r,N}(c(\tau))| d\tau
\]

and, by the definition of a solution

\[
\lim_{N \to \infty} \int_{t_1}^{t_2} \sum_{r=m}^{M} \left| J_{r,N}(c(\tau)) \right| d\tau = 0
\]

we can take the limit as \( N \to \infty \) in the above to get

\[
\begin{align*}
\sum_{r=m}^{M} \sum_{s=0}^{N} h_r(c_{r,s}(t_2) - c_{r,s}(t_1)) &+ \int_{t_1}^{t_2} \sum_{r=m}^{M} \sum_{s=0}^{\infty} (h_{r+1} - h_r)b_{r+1,s}c_{r+1,s}(\tau) d\tau \\
&= h_m \int_{t_1}^{t_2} \sum_{s=0}^{\infty} J_{m-1,s}(c(\tau)) d\tau \\
&+ \int_{t_1}^{t_2} \sum_{r=m}^{M} \sum_{s=0}^{\infty} (h_{r+1} - h_r)a_{r,s}c_{1,0}c_{r+1,s}(\tau) d\tau
\end{align*}
\]
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\[-h_M \int_{t_1}^{t_2} \sum_{s=0}^{\infty} J_{M,s}(c(\tau)) \, d\tau.\]

Replacing \(h_r\) with 1 in the above and letting \(M \to \infty\) we obtain:

\[\sum_{r=m}^{\infty} \sum_{s=0}^{\infty} (c_{r,s}(t_2) - c_{r,s}(t_1)) = \int_{t_1}^{t_2} \sum_{s=0}^{\infty} J_{m-1,s}(c(\tau)) \, d\tau.\]

So that we can use the same argument as in the last theorem to conclude that

\[\lim_{M \to \infty} h_M \int_{t_1}^{t_2} \sum_{s=0}^{\infty} J_{M,s}(c(\tau)) \, d\tau = 0.\]

Hence

\[\sum_{r=m}^{\infty} \sum_{s=0}^{\infty} h_r (c_{r,s}(t_2) - c_{r,s}(t_1)) + \int_{t_1}^{t_2} \sum_{r=m}^{\infty} \sum_{s=0}^{\infty} [(h_{r+1} - h_r) h_{r+1,s} c_{r+1,s}(\tau)] \, d\tau\]

\[= h_m \int_{t_1}^{t_2} \sum_{s=0}^{\infty} J_{m-1,s}(c(\tau)) \, d\tau + \int_{t_1}^{t_2} \sum_{r=m}^{\infty} \sum_{s=0}^{\infty} [(h_{r+1} - h_r) a_{r,s} c_{1,0} c_{r+1,s}(\tau)] \, d\tau. \quad (2.1.32)\]

Now let \(\sum'\) represent the sum \(\sum_{r=0}^{m-1} \sum_{s=m}^{N} + \sum_{r=m}^{\infty} \sum_{s=0}^{\infty}\), so \(\sum' \to \sum\), as \(N \to \infty\). Combining equations (2.1.32) with (2.1.5) will give:

\[\sum' h_r (c_{r,s}(t_2) - c_{r,s}(t_1)) + \int_{t_1}^{t_2} \sum' [(h_{r+1} - h_r) h_{r+1,s} c_{r+1,s}(\tau)] \, d\tau\]

\[= \int_{t_1}^{t_2} \sum_{r=0}^{m-1} h_r J_{r,m-1}(c(\tau)) \, d\tau + h_m \int_{t_1}^{t_2} \sum_{s=0}^{\infty} J_{m-1,s}(c(\tau)) \, d\tau\]

\[+ \int_{t_1}^{t_2} \sum_{r=m}^{\infty} \sum_{s=0}^{\infty} [(h_{r+1} - h_r) a_{r,s} c_{1,0} c_{r+1,s}(\tau)] \, d\tau\]

\[+ h_m \int_{t_1}^{t_2} \sum_{s=N+1}^{\infty} J_{m-1,s}(c(\tau)) \, d\tau - \int_{t_1}^{t_2} \sum_{r=0}^{m-1} h_r J_{r,N}(c(\tau)) \, d\tau.\]

The definition of a solution tells us that the last line of the above expression tends to zero as \(N \to \infty\) and we are left with the desired equation.

\[\diamond\]

By making the appropriate choice for \(g_{r,s}\) in above theorems we can immediately derive:

**Corollary 2.1.7**

Let \(c\) be a solution of (2.1.1) on some interval \([0,T]\), \(0 < T \leq \infty\). Then for all \(t \in [0,T]\)

\[\sum_{r+s=1}^{\infty} (r+s)c_{r,s}(t) = \sum_{r+s=1}^{\infty} (r+s)c_{r,s}(0); \quad (2.1.33)\]

\[\sum_{r+s=1}^{\infty} rc_{r,s}(t) = \sum_{r+s=1}^{\infty} rc_{r,s}(0); \quad (2.1.34)\]

\[\sum_{r+s=1}^{\infty} sc_{r,s}(t) = \sum_{r+s=1}^{\infty} sc_{r,s}(0). \quad (2.1.35)\]

Further
We first observe that Corollary 2.1.7 tells us that

\[
\sum_{r+s=m}^{\infty} (c_{r,s}(t) - c_{r,s}(0)) = \int_0^t \left\{ \sum_{r+s=m-1}^{m-1} J_{r,s}(c(\tau)) + J'_{r,s}(c(\tau)) \right\} d\tau; \tag{2.1.36}
\]

\[
\sum_{r+s=m}^{\infty} (c_{r,s}(t) - c_{r,s}(0)) = \int_0^t \left\{ \sum_{s=0}^{m-1} J_{m-1,s}(c(\tau)) + \sum_{r=0}^{m-1} J'_{r,m-1}(c(\tau)) \right\} d\tau. \tag{2.1.37}
\]

2.2 When Two Components are Equivalent to One

There are two distinct cases when the two component case of the Becker-Döring equations behave like the solutions of the one component equations. One is when the initial data contains only one type of particle. The other is when there is no important physical difference between the two types of particle. Each of these cases is considered in detail below.

2.2.1 One component system

We start by restating the one component equations, some changes have been made to the notation in order to avoid possible confusion between the systems.

\[
\begin{align*}
\dot{c}_r &= J_{r-1}(c) - J_r(c) \quad \text{if } r = 2, 3, \ldots \\
\dot{c}_1 &= -J_1(c) - \sum_{r=1}^{\infty} J_r(c)
\end{align*}
\tag{2.2.1}
\]

where \(J_r(c) = A_r c_{r-1} - B_{r+1} c_{r+1}\). Solutions to (2.2.1) are defined on the sequence space

\[
\chi^+ = \left\{ y = (y_m) : y_m \geq 0 \text{ and } \|x\|_\chi = \sum_{m=1}^{\infty} m y_m < \infty \right\}
\]

**Definition 2.2.1.** Let \(0 < T \leq \infty\). A solution \(c = (c_r)\) of (2.2.1) on \([0, T)\) is a function \(c : [0, T) \to \chi^+\)

(i) each \(c_r : [0, T) \to \mathbb{R}\) is continuous and \(\sup_{t \in [0, T)} \|c(t)\|_\chi < \infty\);

(ii) \(\int_0^t \sum_{r=1}^{\infty} A_r c_r(\tau) \, d\tau < \infty\), \(\int_0^t \sum_{r=2}^{\infty} B_r c_r(\tau) \, d\tau < \infty\) for all \(t \in [0, T)\) and

(iii) \(c_1(t) = c_1(0) - \int_0^t \left[ J_1(c(s)) + \sum_{r=1}^{\infty} J_r(c(s)) \right] ds\)

\(c_r(t) = c_r(0) + \int_0^t [J_{r-1}(c(s)) - J_r(c(s))] ds, \quad \text{For } r \geq 2\) \tag{2.2.2}

2.2.2 Starting with only one component

**Theorem 2.2.2**

(i) If \(c\) is a solution of (2.1.1) on \([0, T)\) with \(c_{r,s}(0) = 0\) if \(s \geq 1\) and \(r \geq 0\) then \((c_{r,0})\) is a solution of (2.2.1) on \([0, T)\), with \(A_k = a_{k,0}\) and \(B_{k+1} = b_{k+1,0}\), for \(k \geq 1\).

(ii)If \(c\) is a solution of (2.1.1) on \([0, T)\) with \(c_{r,s}(0) = 0\) if \(s \geq 0\) and \(r \geq 1\) then \((c_{0,s})\) is a solution of (2.2.1) on \([0, T)\), with \(A_k = a'_{0,k}\) and \(B_{k+1} = b'_{0,k+1}\), for \(k \geq 1\).

**Proof.**

(i) We first observe that Corollary 2.1.7 tells us that

\[
\sum_{r=0}^{\infty} \sum_{s=1}^{\infty} s c_{r,s}(t) = \sum_{r=0}^{\infty} \sum_{s=1}^{\infty} s c_{r,s}(0) \quad \text{for all } t \in [0, T),
\]
but $c_{r,s}(0) = 0$ if $s \geq 1$ and $r \geq 0$ and $c_{r,s}(t) \geq 0$ for all $t \in [0, T)$ so $c_{r,s}(t) = 0$ for all $s \geq 1$ and $r \geq 0$ and all $t \in [0, T)$. By substituting $c_{r,s}(t) = 0$ into Definition 2.1.1 we obtain Definition 2.2.1 with $(r, 0)$ in place of $r$. (ii) is proved in the same way.

\[\diamond\]

### 2.2.3 When both components behave the same

This situation is best imagined as having particles of two different colours, red and blue, say, but in every other respect the two types of particle are identical. So that a cluster with $r$ ‘red’ particles and $s$ ‘blue’ particles will behave the same as all the other clusters containing $r + s$ particles. To consider the implications of this we observe that: The rate at which ‘red’ particles meet and coalesce with $(r, s)$-clusters is $a_{r,s}c_{1,0}$, where $c_{1,0}c_{r,s}$ can be thought of as the rate of meeting and $a_{r,s}$ is the probability that once they’ve met they will coalesce. In the same way $a'_{r,s}$ represents the probability that a ‘blue’ particle and an $(r, s)$-cluster will coalesce on collision and so should be equal to $a_{r,s}$. Since there is no difference between an $(r, s)$-cluster and any other cluster with $r + s$ particles, $a_{r,s}$ and $a'_{r,s}$ must equal some quantity dependent only on $r + s$, $A_{r+s}$ say. On the other hand, the rate at which ‘red’ particles are lost from an $(r, s)$-cluster is $b_{r,s}c_{r,s}$ and the rate which ‘blue’ particles are lost is $b'_{r,s}c_{r,s}$. This means that the rate at which particles of any type are lost is $(b_{r,s} + b'_{r,s})c_{r,s}$. And again, since there is no difference between $(r, s)$-clusters and other clusters with $r + s$ particles, $b_{r,s} + b'_{r,s} = B_{r+s}$, for some sequence $B_m$. In view of all of this, it is reasonable to expect that whenever $a_{r,s}$, $a'_{r,s}$, $b_{r,s}$ and $b'_{r,s}$ are as described, then sums of all clusters of the same total size should be solutions of (2.2.1).

#### Theorem 2.2.3

If $a_{r,s} = a'_{r,s} = A_{r+s}$, $b_{r,s} + b'_{r,s} = B_{r+s}$ for all $r \geq 0$, $s \geq 0$ and $c$ is a solution of (2.1.1) on $[0, T)$ then $(x_m) = \left(\sum_{r=0}^{m} c_{r,m-r}\right)$ is a solution of (2.2.1) on $[0, T)$.

**Proof.**

First we notice that if $c \in X^+$ then

$$\|c\| = \sum_{m=1}^{\infty} \sum_{r=0}^{m} m |c_{r,m-r}| = \sum_{m=1}^{\infty} m |x_m| = \|x\|_X.$$ 

So $x$ maps $[0, T)$ to $\chi^+$ and $\sup_{t \in [0, T)} \|x(t)\|_X = \sup_{t \in [0, T)} \|c(t)\| < \infty$. Since each $c_{r,s}$ is continuous then any finite sum of them will be, and so $x_m : [0, T) \rightarrow \mathbb{R}$ is continuous. Which means that $(x_m)$ satisfies (i) of Definition 2.2.1.

To verify (ii) we note that (ii) of Definition 2.1.1 tells us that $\int_0^t \sum_{r+s=1}^{\infty} a_{r,s}c_{r,s}(\tau) \, d\tau < \infty$, so

$$\int_0^t \sum_{m=1}^{\infty} A_m x_m(\tau) \, d\tau < \infty.$$ 

We also know that $\int_0^t \sum_{r+s=1}^{\infty} b_{r,s}c_{r,s}(\tau) \, d\tau$ and $\int_0^t \sum_{r+s=1}^{\infty} b'_{r,s}c_{r,s}(\tau) \, d\tau$ are finite, adding these gives $\int_0^t \sum_{m=2}^{\infty} B_m x_m(\tau) \, d\tau < \infty$. Hence (ii) of Definition 2.2.1 is proved.

Finally, the next two calculations tell us that (iii) is also satisfied.

For any $m \geq 2$

$$x_m(t) = \sum_{r=0}^{m} c_{r,m-r}(t) = \int_0^t \sum_{r=0}^{m} \left[ J_{r-1,m-r}(e(\tau)) - J_{r,m-r}(e(\tau)) + J'_{r,m-r-1}(e(\tau)) - J'_{r,m-r}(e(\tau)) \right] \, d\tau$$
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Proof.

If \( m = 1 \)

\[
x_1(t) = c_{1,0}(t) + c_0(1)t = -\int_0^t \left[ J_{1,0}(\tau) + J'_{1,0}(\tau) + J_{0,1}(\tau) + J'_{0,1}(\tau) + \sum_{m=1}^\infty \sum_{r=0}^m (J_{r,m-r}(\tau) + J'_{r,m-r}(\tau)) \right] d\tau
\]

\[
= -\int_0^t \left[ A_1(c_{1,0}^2 + 2c_{1,0}c_0,1 + c_0,1) - B_2(c_2,0 + c_{1,1} + c_0,2) + \sum_{m=1}^\infty A_m(c_{1,0} + c_0,1)x_m - B_{m+1}x_{m+1} \right] d\tau
\]

We can take the our reasoning about the coefficients \( b_{r,s} \) and \( b'_{r,s} \) a stage further: Since there are \( r \) \textit{red} particles in an \((r, s)\)-cluster, out of a total of \( r + s \) particles, then given that a particle will leave the cluster there is a probability of \( \frac{r}{r + s} \) that this will be a \textit{red} particle. So \( b_{r,s} = \frac{r}{r + s}B_{r+s} \) and \( b'_{r,s} = \frac{s}{r + s}B_{r+s} \). With this additional information it is possible to start with a solution of (2.2.1) and construct a solution of (2.1.1). This is shown below.

**Theorem 2.2.4**

Suppose that \( a_{r,s} = a'_{r,s} = A_{r+s}, b_{r,s} = \frac{r}{r + s}B_{r+s} \) and \( b'_{r,s} = \frac{s}{r + s}B_{r+s} \). If \( x \) is a solution of (2.2.1) on \([0, T]\) then there exists a sequence \( \{\lambda_{r,s}\} \) such that \( \lambda_{r,s}x_{r+s} \) is a solution of (2.1.1) on \([0, T]\). Further, the only sequences for which this is true are given by \( \lambda_{r,s} = \left( \frac{r + s}{r} \right)^{\alpha} \beta^s \), where \( \alpha = \frac{\rho}{\|c(0)\|} \) and \( \beta = \frac{\sigma}{\|c(0)\|} \), where \( \rho = \sum_{r+s=1}^\infty rc_{r,s}(0) \) and \( \sigma = \sum_{r+s=1}^\infty sc_{r,s}(0) \).

**Proof.**

First note that, it follows immediately that conditions (i) and (ii) of Definition 2.1.1 apply to \( (\lambda_{r,s}x_{r+s}) \) from conditions (i) and (ii) of Definition 2.2.1. This leaves (iii), which means showing that the next three equations hold:

\[
\lambda_{1,0}x_1(t) = \lambda_{1,0}x_1(0) - \int_0^t (\lambda_{2,0}^2a_{1,0} + \lambda_{1,0}a_{0,1}a_{1,0})x_1^2(\tau) - (\lambda_{2,0}a_{2,0} + \lambda_{1,1}a'_{1,1})x_2(\tau) d\tau
\]

\[
- \int_0^t \sum_{r+s=1}^\infty [a_{r,s}x_1(\tau)x_{r+s}(\tau) - a_{r+1,s}b_{r+1,s}x_{r+s+1}(\tau)] d\tau
\]

\[
\lambda_{0,1}x_1(t) = \lambda_{0,1}x_1(0) - \int_0^t (\lambda_{1,0}a_{1,0} + \lambda_{0,1}a'_{0,1})x_1^2(\tau) - (\lambda_{1,1}a_{1,1} + \lambda_{0,2}b_{0,2})x_2(\tau) d\tau
\]
The equations we know apply are:

\[ \lambda_{r,s} x_{r+s}(t) = \lambda_{r,s} x_{r+s}(0) + \int_0^t (a_{r-1,s} \lambda_{r-1,s} + a'_{r,s-1} \lambda_{r,s-1}) x_1(t) x_{r+s-1}(\tau) \, d\tau \]

\[ - \int_0^t \lambda_{r,s} [(a_{r,s} \lambda_{r,0} + a'_{r,s} \lambda_{r,s}) x_1(t) + b_{r,s} + b'_{r,s}] x_{r+s}(\tau) \, d\tau \]

\[ + \int_0^t (\lambda_{r+1,s} b_{r+1,s} + \lambda_{r,s+1} b'_{r,s+1}) x_{r+s+1}(\tau) \, d\tau \quad \text{for } r + s \geq 2 \] (2.2.5)

The equations we know apply are:

\[ x_{r+s}(t) = x_{r+s}(0) + \int_0^t A_{r+s-1} x_1(t) x_{r+s-1}(\tau) \, d\tau \]

\[ - \int_0^t [A_{r+s} x_1(\tau) + B_{r+s}] x_{r+s}(\tau) \, d\tau \]

\[ + \int_0^t B_{r+s+1} x_{r+s+1}(\tau) \, d\tau \] (2.2.6)

\[ x_1(t) = x_1(0) - \int_0^t A_1 x_1^2(\tau) - B_2 x_2(\tau) \, d\tau \]

\[ - \int_0^t \sum_{r+s=1}^{\infty} [A_{r+s} x_1(\tau) x_{r+s}(\tau) - B_{r+s+1} x_{r+s+1}(\tau)] \, d\tau \quad \text{for } r + s \geq 2 \] (2.2.7)

Equation (2.2.6) implies equation (2.2.5) when and only when the next three difference equations are satisfied:

\[ \lambda_{r,s} = \lambda_{r-1,s} \lambda_{r,0} + \lambda_{r,s-1} \lambda_{0,1} \] (2.2.8)

\[ 1 = \lambda_{1,0} + \lambda_{0,1} \] (2.2.9)

\[ \lambda_{r,s} = \frac{r + 1}{r + s + 1} \lambda_{r+1,s} + \frac{s + 1}{r + s + 1} \lambda_{r,s+1}, \] (2.2.10)

where \( r + s \geq 2 \) and, by our conventions of notation, \( \lambda_{r,s} = 0 \) if either \( r < 0, s < 0 \) or \( r = s = 0 \). It is easily shown that the solution of (2.2.8) is

\[ \lambda_{r,s} = \left( \frac{r + s}{r} \right)^{\lambda_{1,0} \lambda_{0,1}^s} \] (2.2.11)

With this solution, equation (2.2.9) implies that equation (2.2.10) is satisfied for all \( r + s \geq 2 \). So we will only consider sequences \( \{ \lambda_{r,s} \} \) that satisfy equation (2.2.11) and (2.2.9). Since we need to have \( c_{r,s}(0) = \lambda_{r,s} x_{r+s}(0) \), if \( \lambda_{r,s} x_{r+s} \) is to be a solution of (2.1.1), we require that

\[ \rho = \sum_{m=1}^{\infty} \sum_{k=0}^{m} r c_{r,s}(0) = \sum_{m=1}^{\infty} x_{m}(0) \sum_{k=0}^{m} k \binom{m}{k} \lambda_{1,0}^k \lambda_{0,1}^{m-k} \]

\[ = \sum_{m=1}^{\infty} x_{m}(0) \left[ m \lambda_{1,0} (\lambda_{1,0} + \lambda_{0,1})^{m-1} \right] \]

\[ = \lambda_{1,0} \sum_{m=1}^{\infty} m x_{m}(0) = \lambda_{1,0} ||c(0)||. \]

So we must have that \( \lambda_{1,0} = \alpha = \frac{\rho}{||c(0)||} \), and by a similar argument that \( \lambda_{0,1} = \beta \). Note that \( \alpha + \beta = 1 \) so equation (2.2.9) is an implication of this.

So far we found that if \( \lambda_{r,s} x_{r+s} \) is to be a solution of (2.1.1) then \( \lambda_{r,s} = \left( \frac{r + s}{r} \right)^{\alpha^* \beta^*} \). To prove that it is indeed a solution we must see that equations (2.2.3) and (2.2.4) are satisfied but this is easily shown by substitution. \( \diamond \)
2.3 Differentiability and Generalised Flows

In this section we consider the continuity and differentiability of the solutions of (2.1.1). We also introduce the weak* topology of X which is essential for a discussion on the asymptotics of the solution. It will simplify the statement of future results if we use $A_{r,s}$ represent all the four coefficients. So if we state that $A_{r,s} = O(r+s)$ we mean that $a_{r,s} = O(r+s)$, $a'_{r,s} = O(r+s)$, $b_{r,s} = O(r+s)$ and $b'_{r,s} = O(r+s)$.

2.3.1 Continuity and differentiability of solutions

The next result is stated without proof because its proof is exactly equivalent to that of Proposition 3.1 in [2]. As in [2], we will use $(\Delta h)_k$ to denote the difference between the $k$th and $(k+1)$th term of the sequence $h$, i.e. $(\Delta h)_k = h_{k+1} - h_k$.

Proposition 2.3.1

Let $c$ be a solution of (2.1.1) on $[0, T)$ for $0 < T \leq \infty$. Then $c : [0, T) \rightarrow X$ is continuous, and the series $\sum_{r+s=1}^{\infty} (r+s)c_{r,s}$ is uniformly convergent on compact intervals of $[0, T)$.

It is possible to make and prove a general statement about the differentiability of any solution $c$, which is equivalent to Theorem 3.2 in [2]. Here, however, we will only give conditions under which $c \in C^1[0, T)$ and under which $c \in C^2[0, T)$. This is because we only need these two results for our later special cases better illustrate how the proof in [2] works and what modifications need to be made for it to apply to the two component case.

(a) If $A_{r,s} = O(r+s)$ then $c_{r,s} \in C^1[0, T)$ for each $r \geq 0$ and $s \geq 0$.

(b) Suppose $A_{r,s} = V(h_{r+s})$ where $h$ is a positive sequence for which $h_m = O(m)$ and $(\Delta h)_m = O(1)$. Then $c_{r,s} \in C^2[0, T)$ for each $r \geq 0$ and $s \geq 0$.

Proof of (a).

For $r + s \geq 2$ we have, from part (iii) of the definition of a solution that:

$$c_{r,s}(t) = \int_{0}^{t} J_{r-1,s}(c(\tau)) + J'_{r-1,s}(c(\tau)) - J_{r,s}(c(\tau)) - J'_{r,s}(c(\tau)) \, d\tau$$

for $0 \leq t < T$ \hspace{1cm} (2.3.1)

The continuity of every $c_{r,s}$ implies that each $J_{r,s}(c)$ and $J'_{r,s}(c)$ are continuous so equation (2.3.1) implies that each $c_{r,s}$ with $r + s \geq 2$ is differentiable on $[0, T)$. Thus for $r + s \geq 2$:

$$\dot{c}_{r,s}(t) = J_{r-1,s}(c(t)) + J'_{r-1,s}(c(t)) - J_{r,s}(c(t)) - J'_{r,s}(c(t)) \quad \text{for} \quad 0 \leq t < T,$$

which implies that $c_{r,s} \in C^1[0, T)$. From the definition of $c_{1,0}$ it is easily seen that the same is true for it if $\sum_{r+s=2}^{\infty} a_{r,s}c_{r,s}(t)$ and $\sum_{r+s=2}^{\infty} b_{r+1,s}c_{r+1,s}(t)$ are continuous. This follows form Proposition 2.3.1 and the fact that $a_{r,s} = O(r+s)$ and $b_{r,s} = O(r+s)$. Similarly $c_{0,1} \in C^1[0, T)$.

Proof of (b).

We may conclude that $\dot{c}_{r,s} \in C^1[0, T)$ when $r + s \geq 2$ from the following:

$$\frac{dJ_{r,s}}{dt} = a_{r,s}c_{1,0}(t)c_{r,s}(t) + a_{r,s}c_{1,0}\dot{c}_{r,s}(t) - b_{r+1,s}\dot{c}_{r+1,s}(t)$$

$$\frac{dJ'_{r,s}}{dt} = a'_{r,s}c_{1,0}(t)c_{r,s}(t) + a'_{r,s}c_{1,0}\dot{c}_{r,s}(t) - b'_{r+1,s}\dot{c}_{r+1,s}(t).$$

Since $A_{r,s} = V(h_{r+s})$, $h_n = O(n) \implies A_{r,s} = O(r+s)$, Proposition 2.3.1 gives that $\sum_{r+s=2}^{\infty} A_{r,s}c_{r,s}(t)$ is uniformly convergent on compact sub-intervals of $[0, T)$. So, using the result of Theorem 2.1.6, we
Let Lemma 2.3.5 for every \( r \) (see Definition 2.3.3, below). Justification for using the term 'weak' is continuous, for all \( m \). This, however, is an immediate consequence of \( \mathcal{A}_{r,s} = \mathcal{V}(h_{r+s}), h_n = \mathcal{O}(n) \) and \( (\Delta h)_m = \mathcal{O}(1) \). Hence for every \( r \geq 0 \) and \( s \geq 0 \), \( c_{r,s} \in \mathcal{C}^2[0,T] \).

This actually proves that every \( \hat{c}_{r,s}(t) \) is differentiable, but the continuity of \( \hat{c}_{r,s}(t) \) cannot be determined without information about \( (\Delta^2 h)_m \).

2.3.2 Weak* topology

The set \( \mathbb{B}_{\rho, \sigma} = \{ x \in X : \sum_{r+s=1}^{\infty} r|x_{r,s}| \leq \rho \text{ and } \sum_{r+s=1}^{\infty} s|x_{r,s}| \leq \sigma \} \) is a compact metric space with the metric \( d(x,y) = \sum_{r+s=1}^{\infty} |x_{r,s} - y_{r,s}| \). We will define weak* convergence as convergence in this metric (see Definition 2.3.3, below). Justification for using the term 'weak*' can be found in [2]. We will use the adjective 'strong' to refer to the normed topology of \( X \). We can define weak* convergence on the whole of \( X \) as follows:

**Definition 2.3.3.** The sequence \( \{x^{(n)}\} \subset X \) converges weak* to \( x \in X \) (we will write \( x^{(n)} \rightharpoonup x \)) as \( n \to \infty \) if

(i) there exist a \( \rho \geq 0 \) and a \( \sigma \geq 0 \) such that \( x^{(n)} \in \mathbb{B}_{\rho, \sigma} \) for all \( n \geq 1 \), and

(ii) \( d(x^{(n)}, x) \to 0 \) as \( n \to \infty \).

We list some useful results about the weak* topology. Each is an immediate consequence of elementary metric space theory, and they are stated without proof. The first just states that weak* convergence of a sequence is equivalent to term-wise convergence – which was the definition chosen in [2].

**Lemma 2.3.4**

Let \( \{x^{(n)}\} \subset X \) and \( x \in X \). Then \( x_n \rightharpoonup x \) as \( n \to \infty \) iff \( \sup_n \|x^{(n)}\| < \infty \) and \( x^{(n)}_{r,s} \to x_{r,s} \) as \( n \to \infty \) for every \( r \) and \( s \) with \( r + s \geq 1 \).

The next result helps us deal with sums of the type \( \sum_{r+s=1}^{\infty} g_{r,s}c_{r,s} \).

**Lemma 2.3.5**

Let \( g_{r,s} \) be a real sequence and suppose that \( g_{r,s} = \mathcal{O}(h_k) \), where \( k \) is either \( r \), \( s \) or \( r + s \). Define the function \( S \) from \( \mathbb{B}_{\rho, \sigma} \) to \( \mathbb{R} \) by:

\[
S(x) = \sum_{r+s=1}^{\infty} g_{r,s}x_{r,s}.
\]

(i) If \( h_m = \mathcal{O}(m) \) then the function \( S \) is strongly continuous.

(ii) If \( h_m = o(m) \) then the function \( S \) is weak* continuous.

Applying this to solutions of (2.1.1) we get some additional information about the uniform convergence of the sums.
Lemma 2.3.6
Let \( c \) be a solution of (2.1.1) on \([0, T)\) and let \( \alpha_m \) be a positive sequence such that \( \alpha_m \to 0 \) as \( m \to \infty \). If \( g_{r,s} = O(\alpha_k) \) where \( k \) is either \( r, s \) or \( r + s \) then \( \sum_{r+s=1}^{\infty} k g_{r,s} c_{r,s} \) is uniformly convergent on the whole of \([0, T)\).

Finally, a result that gives us a useful combination of facts that imply strong convergence.

Lemma 2.3.7
If \( x^{(m)} \xrightarrow{\ast} x \) in \( X \) and both \( \sum_{r+s=1}^{\infty} r x^{(m)}_{r,s} \to \sum_{r+s=1}^{\infty} r x_{r,s} \) and \( \sum_{r+s=1}^{\infty} s x^{(m)}_{r,s} \to \sum_{r+s=1}^{\infty} s x_{r,s} \), then \( x^{(m)} \to x \) in \( X \).

2.3.3 Generalised flows

The definition below is taken from [2].

Definition 2.3.8. A generalised flow \( G \) on a metric space \( Y \) is a family of continuous mappings \( \varphi : [0, \infty) \to Y \) with the properties

(i) if \( \varphi \in G \) and \( \tau \geq 0 \) then \( \varphi_\tau \in G \) where \( \varphi_\tau \) is given by \( \varphi_\tau(t) = \varphi(\tau + t), \ t \in [0, \infty) \),

(ii) if \( y \in Y \), there exists at least one \( \varphi \in G \) with \( \varphi(0) = y \), and

(iii) if \( \varphi_j \in G \) with \( \varphi_j(0) \) convergent in \( Y \) as \( j \to \infty \), then there exists a subsequence \( \varphi_{j_k} \) of \( \varphi_j \) and an element \( \varphi \in G \) such that \( \varphi_{j_k}(t) \to \varphi(t) \) uniformly on compact subintervals of \([0, \infty)\).

When discussing generalised flows formed out of solutions of (2.1.1) we must distinguish between the weak and strong topologies. The next two theorems give sufficient conditions for the solutions to form a generalised flow, for each of these.

Theorem 2.3.9
Assume that \( a_{r,s} = O(r+s) \) and \( a'_{r,s} = O(r+s) \). Let \( G \) denote all solutions \( c \) of (2.1.1) on \([0, \infty)\). Then \( G \) is a generalised flow on \( X^+ \).

Proof.
Parts (i) and (ii) are immediate consequences of the Definition 2.1.1 and Theorem 2.1.3, respectively. (iii) Suppose \( c^{(j)} \) are solutions of (2.1.1) and that \( c^{(j)}(0) \to \hat{c}_0 \) as \( j \to \infty \), for some \( \hat{c}_0 \in X^+ \). We saw in the proof of Theorem 2.1.3 that when \( r+s \geq 2 \), \( |c^{(j)}_{r,s}(t)| < M_{r,s} \), for some \( M_{r,s} \), independent of \( j \) and \( t \). So there is a subsequence of \( c^{(j)} \), which we will denote as \( c^{(k)} \), and a function \( c : \mathbb{R}^+ \to X^+ \) such that: \( c(0) = \hat{c}_0 \) and, for \( r+s \geq 2 \), \( c_{r,s}(t) \to c_{r,s}(t) \) as \( k \to \infty \), uniformly on compact subintervals of \([0, T)\). To show that this is also true of \( c^{(k)}_{r,s} \) and \( c^{(k)'}_{r,s} \) (or at least for a subsequence of these) we continue in the same vein as Theorem 2.1.3 and show that both \( c^{(k)}_{r,s} \) and \( c^{(k)'}_{r,s} \) are Cauchy sequences. To help in this we observe that Corollary 2.1.7 gives:

\[
\begin{align*}
&c^{(k)}_{1,0}(t) + c^{(k)}_{0,1}(t) = \sum_{r+s=1}^{M-1} (r+s)c^{(k)}_{r,s}(0) - \sum_{r+s=2}^{M-1} (r+s)c^{(k)}_{r,s}(t)
&\quad - \sum_{r+s=M}^{\infty} (r+s)\left[c^{(k)}_{r,s}(t) - c^{(k)}_{r,s}(0)\right]
\end{align*}
\] (2.3.3)

We know that \( \left\{ \sum_{r+s=1}^{M-1} (r+s)c^{(k)}_{r,s}(0) \right\} \) and \( \left\{ \sum_{r+s=2}^{M-1} (r+s)c^{(k)}_{r,s}(t) \right\} \) are Cauchy. To see that

\( \left\{ \sum_{r+s=M}^{\infty} (r+s)\left[c^{(k)}_{r,s}(t) - c^{(k)}_{r,s}(0)\right] \right\} \) is also, observe that equation (2.1.28) with \( g_{r,s} = r+s \) gives

\[
\sum_{r+s=M}^{\infty} (r+s)\left[c^{(k)}_{r,s}(t) - c^{(k)}_{r,s}(0)\right] + \int_{t}^{t} \sum_{r+s=M}^{\infty} b_{r+1,s}c^{(k)}_{r+1,s}(\tau) + b'_{r,s+1}c^{(k)}_{r,s+1}(\tau) d\tau
\]
\begin{equation}
\begin{aligned}
&= \int_0^t c^{(k)}_1(\tau) \sum_{r+s=M} a_{r,s} c^{(k)}_{r,s}(\tau) \, d\tau + \int_0^t c^{(k)}_{0,1}(\tau) \sum_{r+s=M} a'_{r,s} c^{(k)}_{r,s}(\tau) \, d\tau \\
&\quad + \int_0^t M \sum_{r+s=M-1} J_{r,s}(c^{(k)}(\tau)) + J'_{r,s}(c^{(k)}(\tau)) \, d\tau
\end{aligned}
\end{equation}

This is sufficiently similar to equation (2.1.16), for us to be able to copy over the proof of Theorem 2.1.3, from equation (2.1.16) onwards, with \( g_{r,s} \) replaced with \( r+s \). Hence we can conclude that, not only are \( c^{(k)}_1 \) and \( c^{(k)}_{0,1} \) Cauchy and converge to \( c_{1,0} \) and \( c_{0,1} \) uniformly on compact sub-intervals of \([0, \infty)\) but that \( c \) is a solution of (2.1.1).

\textbf{Theorem 2.3.10}

Assume that \( A_{r,s} = o(r+s) \). For \( \rho > 0, \sigma > 0 \), let \( G_{\rho,\sigma} \) denote all solutions \( c \) of (2.1.1) on \([0, \infty)\), with \( c(0) \in \mathbb{B}^+_{\rho,\sigma} \). Then \( G_{\rho,\sigma} \) is a generalised flow on \( \mathbb{B}^+_{\rho,\sigma} \).

\textbf{Proof.}

Again, it is only necessary to show that part (iii) of Definition 2.3.8 is true. Let \( c^{(j)} \) be a sequence of solutions with \( c^{(j)}(0) \xrightarrow{\star} c_0 \) as \( j \to \infty \). We have already seen from Proposition 2.3.2 (a) that \( c^{(j)} \in C^1[0,\infty) \), so \( \dot{c}^{(j)}_r \) exists for all \( j, r \) and \( s \). Since \( A_{r,s} < O(r+s) \), equation (2.1.33) gives that \( \dot{c}^{(j)}_{r,s}(t) \) is absolutely bounded, independently of \( j \) and \( t \). Hence the Arzela-Ascoli Theorem give us a subsequence \( c^{(k)} \) of \( c^{(j)} \) and a function \( c : [0, \infty) \to X^+ \) such that \( c^{(k)}(t) \xrightarrow{\star} c_{r,s}(t) \) as \( k \to \infty \), uniformly on compact subintervals of \([0, \infty)\). It is then straight forward to check that \( c \) satisfies (i), (ii) and the equations of (iii) for which \( r+s \geq 2 \) of Definition 2.1.1. To see that \( c_{1,0} \) and \( c_{0,1} \) also satisfy the relevant equations in (iii), we note that Lemma 2.3.5 (ii) and \( A_{r,s} = o(r+s) \) combine to tell us that
\[
x \mapsto \sum_{r+s=2} A_{r,s} x_{r,s} \text{ is a weak* continuous function.}
\]

\[
2.4 \text{ Equilibria}
\]

\textbf{2.4.1 Set of all equilibria}

From this point on we assume that \( A_{r,s} > 0 \) for all \( r \) and \( s \) for which \( r+s \geq 1 \) and the coefficients satisfy the detailed balancing condition:

\[
\frac{a_{r,s}}{b_{r+1,s}} = \frac{a'_{r+1,s}}{b'_{r+1,s+1}} = \frac{a'_{r,s}}{b'_{r,s+1}} = \frac{a_{r,s+1}}{b_{r+1,s+1}}.
\]

This can be thought of as saying, that given that a \( (r,s) \)-cluster has changed into a \( (r+1,s+1) \)-cluster, then it is equally likely that a type-I monomer joined the cluster first followed by a type II, as that a type-II joined followed by a type-I.

Solutions of (2.1.1) that satisfy \( J_{r,s}(c) = J'_{r,s}(c) = 0 \), for all \( r \) and \( s \) with \( r+s \geq 1 \), are equilibrium solutions. Now \( J_{r,s}(c) = J'_{r,s}(c) = 0 \) is equivalent to

\[
\frac{c_{r+1,s}}{c_{r,s}} = \frac{a_{r,s}}{b_{r+1,s}} c_{1,0} \quad \text{and} \quad \frac{c_{r,s+1}}{c_{r,s}} = \frac{a'_{r,s}}{b'_{r,s+1}} c_{0,1};
\]

both of which cannot be satisfied unless equation (2.4.1) holds. These equations imply that

\[
c_{r,s} = Q_{r,s} c_{1,0} c_{0,1}^s
\]

where \( Q_{r,s} = \prod_{j=0}^{r-1} \frac{a_{j,s}}{b_{j+1,s}} \prod_{j=0}^{s-1} \frac{a'_{0,j}}{b'_{0,j+1}} \). At present, it cannot be proved, in general, that all equilibria have zero fluxes. However a formal calculation* gives that

\[
* \text{See equation (2.1.3).}
\]
\[
\sum_{r+s=2}^{\infty} \dot{c}_{r,s} \ln \left( \frac{c_{r,s}}{Q_r s_{r+1,0} s_0} \right) = - \sum_{r+s=1}^{\infty} J_{r,s}(c) \ln \left( \frac{a_{r,s} c_0 c_{r,s}}{b_{r+1,s} s_{r+1,1}} \right) \sum_{r+s=1}^{\infty} J'_{r,s}(c) \ln \left( \frac{a'_{r,s} c_0 c_{r,s}}{b'_{r+1,s} s_{r+1,1}} \right)
\] (2.4.3)

Each summand on the right of this equation has the form \((x - y)(\ln x - \ln y)\), which is non-negative for all positive values of \(x\) and \(y\). Hence, if \(c\) is an equilibrium solution of (2.1.1) then every \(J_{r,s}(c)\) and \(J'_{r,s}(c)\) must be zero. A corollary of Theorem 2.5.5 (page 50) is that equation (2.4.3) holds when sufficiently strong assumptions are made about the coefficients. We therefore conjecture that all equilibrium solutions satisfy (2.4.2) and from now on will only consider those equilibria that do.

For a distribution of the form \(Q_{r,s} w^r z^s\) to be a solution of (2.1.1) \(w\) and \(z\) must be such that \(Q_{r,s} w^r z^s \in X^+\), i.e.

\[
F(w, z) := \sum_{r+s=1}^{\infty} rQ_{r,s} w^r z^s < \infty \quad (2.4.4)
\]

\[
G(w, z) := \sum_{r+s=1}^{\infty} sQ_{r,s} w^r z^s < \infty. \quad (2.4.5)
\]

The sets \(\Theta = \{(w, z) \in \mathbb{R}^2 : w \geq 0, z \geq 0 \text{ and } F(w, z) < \infty\}\) and \(\Xi = \{(w, z) \in \mathbb{R}^2 : w \geq 0, z \geq 0 \text{ and } G(w, z) < \infty\}\) are therefore of interest to us. If \(S\) is a set then we will use \(\bar{S}\) to denote the closure of that set; \(S^0\) to denote the interior of the set and \(\partial S\) to denote the boundary of the set.

In this section we will first discuss \(\Theta^0\) and this will automatically give us the form of \(\partial \Theta\). It will then be possible to write down the \(\Xi^i\) and \(\partial \Xi\). Following this we will give four examples to show the range of possible sets that \(\Theta\) and \(\Xi\) may be. We conclude by describing \(\Theta \cap \Xi\). Throughout it will be assumed that \(w \geq 0\) and \(z \geq 0\).

By noting that

\[
F(w, z) = \sum_{r=1}^{\infty} rQ_{r,1} w^r + \sum_{r=1}^{\infty} rQ_{r,2} w^r + \cdots = w \sum_{s=1}^{\infty} Q_{1,s} z^s + 2w^2 \sum_{s=1}^{\infty} Q_{2,s} z^s + \cdots,
\]

it is possible to see that \(F(w, z)\) will not be finite if either of the following four conditions are satisfied.

\[
w > \inf_{s \geq 0} \left[ \limsup_{r \to \infty} Q_{r,s}^{1/r} \right]^{-1} =: \bar{w}_c, \quad z > \inf_{s \geq 0} \left[ \limsup_{r \to \infty} \left( \sum_{r=1}^{\infty} Q_{r,s} w^r \right)^{1/s} \right]^{-1} =: z_c(w);
\]

\[
z > \inf_{s \geq 1} \left[ \limsup_{r \to \infty} Q_{r,s}^{1/r} \right]^{-1} =: \bar{z}_c \quad \text{or} \quad w > \inf_{s \geq 0} \left[ \limsup_{r \to \infty} \left( \sum_{r=1}^{\infty} Q_{r,s} z^s \right)^{1/r} \right]^{-1} =: w_c(z).
\]

Alternatively, we can see that \(F(w, z) < \infty\) if \(w < \bar{w}_c\) and \(z < z_c(w)\), or if \(z > \bar{z}_c\) and \(w < w_c(z)\).

We will not consider the case where \(\Theta^0 = \emptyset\), so we assume that

\[
\sup_{s \geq 0} \limsup_{r \to \infty} Q_{r,s}^{1/r} < \infty \quad \text{which is equivalent to} \quad \sup_{r \geq 0} \limsup_{s \to \infty} Q_{r,s}^{1/s} < \infty; \quad (2.4.6)
\]

which means that \(\bar{w}_c > 0\) and \(\bar{z}_c > 0\). Hence \(z_c(\cdot)\) and \(w_c(\cdot)\) are defined on some interval of the positive real line. To describe \(\Theta\) in as concise a way as possible, we need to extend the definition of the functions \(z_c\) and \(w_c\) to the whole of the non-negative real line. First observe that while \(w < \bar{w}_c\), \(w \mapsto \sum_{r=1}^{\infty} rQ_{r,s} w^r\) is a continuous non-decreasing function and that \(\sum_{r=1}^{\infty} rQ_{r,s} w^r \geq Q_{n,s} w^n\) for any \(n \geq 1\). Hence as \(w \downarrow 0\), \(\limsup_{s \to \infty} \left( \sum_{r=1}^{\infty} rQ_{r,s} w^r \right)^{1/s} \) does not decrease and is bounded above by
Later on we will be interested in\[\limsup_{s \to \infty} \frac{Q_{r,s}^{1/s}}{z} \]for every \(r \geq 1\), and so
\[
0 < \lim_{w \to 0} \left[ \limsup_{s \to \infty} \left( \sum_{r=1}^{\infty} rQ_{r,s} w^r \right)^{1/s} \right]^{-1} \leq z_c. 
\]This is the value we will assign to \(z_{c_1}(0)\). The fact that \(w \mapsto \limsup_{s \to \infty} \left( \sum_{r=1}^{\infty} rQ_{r,s} w^r \right)^{1/s} \) is non-decreasing also tells us that either: \(\limsup_{s \to \infty} \left( \sum_{r=1}^{\infty} rQ_{r,s} w^r \right)^{1/s} < \infty\) for every \(w > 0\), or that there is a unique value of \(w, \alpha_1\), say, such that the limit is finite for all positive values of \(w\) below \(\alpha_1\) but diverges for all \(w > \alpha_1\). From which we can make the following definitions

\[
z_{c_1}(w) = \begin{cases} 
\lim_{w \to 0} \left[ \limsup_{s \to \infty} \left( \sum_{r=1}^{\infty} rQ_{r,s} w^r \right)^{1/s} \right]^{-1} & \text{if } w = 0 \\
\limsup_{s \to \infty} \left( \sum_{r=1}^{\infty} rQ_{r,s} w^r \right)^{1/s}^{-1} & \text{if } 0 < w < \alpha_1 \\
0 & \text{if } \alpha_1 \leq w,
\end{cases}
\]

and, if \(\beta_0\) is the value of \(z\) above which \(\limsup_{r \to \infty} \left( \sum_{s=0}^{\infty} Q_{r,s} z^s \right)^{1/r}\) diverges,

\[
w_{\beta_0}(z) = \begin{cases} 
\lim_{z \to 0} \left[ \limsup_{r \to \infty} \left( \sum_{s=0}^{\infty} Q_{r,s} z^s \right)^{1/r} \right]^{-1} & \text{if } z = 0 \\
\limsup_{r \to \infty} \left( \sum_{s=0}^{\infty} Q_{r,s} z^s \right)^{1/r}^{-1} & \text{if } 0 < z < \beta_0 \\
0 & \text{if } \beta_0 \leq z.
\end{cases}
\]

Hence

\[
\Theta^\circ = \{(w, z) : 0 < w < \tilde{w}_c, 0 < z < z_{c_1}(w)\} \cup \{(w, z) : 0 < z < z_{c_1}(w) ; 0 < w < z_{c_0}(w)\} \\
\partial \Theta = \{(w, z_{c_1}(w)) : 0 \leq w \leq \min\{\alpha_1, \tilde{w}_c\}\} \cup \{(w_{\beta_0}(z), z) : 0 \leq z \leq \min\{\beta_0, z\}\} \\
\cup \left\{(w, 0) : 0 \leq w \leq \limsup_{r \to \infty} \left( \sum_{s=0}^{\infty} Q_{r,s} w^r \right)^{1/r} \right\} \cup \{(0, z) : 0 \leq z\} \\
\cup \left\{(w, z) : 0 \leq w \leq w_{c_0}(z_{c_1})\right\} \cup \{(\tilde{w}_c, z) : 0 \leq z \leq z_{c_1}(\tilde{w}_c)\}
\]

Later on we will be interested in \(\partial \Theta \setminus L_\Theta\), where \(L_\Theta\) denotes the section of the \(w\) and \(z\) axes which border the interior of \(\Theta\); i.e.

\[
L_\Theta = \{(w, 0) : 0 \leq w \leq w_{c_0}(0)\} \cup \{(0, z) : 0 \leq z \leq z_{c_1}(0)\}
\]

The sketch in Figure 2.4.1 illustrates each of the quantities and functions described above.

By following the same reasoning for \(G(w, z)\) we find that

\[
\Xi^\circ = \{(w, z) : 0 < w < \tilde{w}_c, 0 < z < z_{c_0}(w)\} \cup \{(w, z) : 0 < z < \tilde{z}_c, 0 < w < z_{c_1}(w)\} \\
\partial \Xi = \{(w, z_{c_0}(w)) : 0 \leq w \leq \min\{\alpha_0, \tilde{w}_c\}\} \cup \{(w_{c_1}(z), z) : 0 \leq z \leq \min\{\beta_1, \tilde{z}_c\}\} \\
\cup \left\{(0, z) : 0 \leq z \leq \limsup_{s \to \infty} \left( \sum_{r=0}^{\infty} Q_{r,s} z^r \right)^{1/r} \right\} \cup \{(w, 0) : 0 \leq w\}
\]
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Figure 2.4.1: Sketch of the region of equilibria with finite type-I density.

\[ \cup \{ (w, z) : 0 \leq w \leq w_{c_1}(z_c) \} \cup \{ (w, z) : 0 \leq z \leq z_{c_0}(w_c) \} \]

\[ L_\Xi = \{ (w, 0) : 0 \leq w < w_{c_1}(0) \} \cup \{ (0, z) : 0 \leq z < z_{c_0}(0) \}, \]

where \( \alpha_0 \) is the value of \( w \) above which \( \limsup_{r \to \infty} \left( \sum_{s=0}^{\infty} Q_{r,s} w^r \right)^{1/s} \) diverges; \( \beta_1 \) is the value of \( z \) above which \( \limsup_{r \to \infty} \left( \sum_{s=0}^{\infty} s Q_{r,s} z^s \right)^{1/r} \) diverges;

\[
z_{c_0}(w) = \begin{cases} 
\lim_{w \to 0} \left[ \limsup_{s \to \infty} \left( \sum_{r=0}^{\infty} Q_{r,s} w^r \right)^{1/s} \right]^{-1} & \text{if } w = 0 \\
\limsup_{r \to \infty} \left( \sum_{s=0}^{\infty} s Q_{r,s} z^s \right)^{1/r} & \text{if } 0 < w < \alpha_0 \\
0 & \text{if } \alpha_0 \leq w
\end{cases}
\]  (2.4.11)

and

\[
w_{c_1}(z) = \begin{cases} 
\lim_{z \to 0} \left[ \limsup_{r \to \infty} \left( \sum_{s=1}^{\infty} s Q_{r,s} z^s \right)^{1/r} \right]^{-1} & \text{if } z = 0 \\
\limsup_{r \to \infty} \left( \sum_{s=1}^{\infty} s Q_{r,s} z^s \right)^{1/r} & \text{if } 0 < z < \beta_1 \\
0 & \text{if } \beta_1 \leq z
\end{cases}
\]  (2.4.12)

We are principally concerned with \( \Theta \cap \Xi \) and we will consider this set after the following four examples (see Lemma 2.4.5). The first is the most important because it is physically motivated, see equation (1.2.3) on page 4.

**Example 2.4.1.** If \( Q_{r,s} = \exp(k_1 r + k_2 s) \exp \left[ K(v_1 r + v_2 s)^{2/3} \right] \frac{r^s}{(r+s)^{r+s}} \) then \( \Theta^c = \Xi^c = \{ (w, z) : 0 < w < e^{-k_1}, 0 < z < e^{-k_2} \} \).
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Proof. First note that \( \limsup_{r \to \infty} Q_{r,s}^{1/r} = e^{k_1} \) for all values of \( s \geq 0 \) and \( \limsup_{s \to \infty} Q_{r,s}^{1/s} = e^{k_2} \) for all values of \( r \geq 0 \), so \( \bar{w}_c = w_c = e^{-k_1} \) and \( \bar{z}_c = z_c = e^{-k_2} \). Next consider

\[
F(w, z) = \sum_{m=0}^{\infty} \sum_{r=0}^{m} r \exp \left[ \frac{K(v_1r + v_2(m-r))(2/3)}{m^m} \right] \frac{r^r(m-r)^{m-r}}{m^m} [e^{k_1}w]^r [e^{k_2}z]^{m-r}.
\]

If we assume, w.l.o.g., that \( e^{k_1}w \geq e^{k_2}z \) then

\[
F(w, z) \leq \sum_{m=0}^{\infty} \left[ \frac{m(m+1)}{2} e^{K' m^{2/3}} \right] [e^{k_1}w]^m.
\]

Hence, \( F(w, z) < \infty \) if \( w < e^{-k_1} \) and \( z < e^{-k_2} \). A similar calculation can be performed on \( G \) and the result follows.

The next example is a more general form of the systems of ‘red’ and ‘blue’ particles we discussed in Section 2.2.3

Example 2.4.2. If \( Q_{r,s} = q_{r,s} \left( \frac{r+s}{r} \right) a^r b^s \), where \( a > 0, b > 0 \) and \( q_{r,s} \) is a positive sequence with \( \limsup_{n \to \infty} q_{r,s}^{1/n} < \infty \) then \( \Theta^o = \Xi^o = \{(w, z) : w, z > 0 \text{ and } aw + bz < k\} \), where \( k := \left[ \limsup_{n \to \infty} q_{r,s}^{1/n} \right]^{-1} \).

Proof. This is an immediate consequence of:

\[
F(w, z) = \sum_{m=0}^{\infty} \sum_{r=0}^{m} r q_{m,r} \left( \frac{m}{r} \right) (aw)^r (bz)^{m-r} = aw \sum_{m=0}^{\infty} m q_{m,r} \cdot (aw + bz)^{m-1}.
\]

The next two examples, while artificial, are given to show the range of possible forms \( \Theta \) and \( \Xi \) can take. Example 2.4.3 shows that \( \Theta \) is not necessarily equal to \( \Xi \) and Example 2.4.4 shows that \( \Theta \) and \( \Xi \) may be unbounded.

Example 2.4.3. If \( Q_{r,s} = (s + 1)^{-r} \) then \( \Theta^o = \{(w, z) : 0 < w < 1, 0 < z < 1\} \) and \( \Xi^o = \{(w, z) : 0 < w < 2, 0 < z < 1\} \).

Proof. Note that \( \limsup_{r \to \infty} Q_{r,s}^{1/r} = [s + 1]^{-1} \) while \( \limsup_{s \to \infty} Q_{r,s}^{1/s} = 1 \), so \( z_c = \bar{z}_c = 1 \),

\[
w_c = \inf_{s \geq 1} \left[ \limsup_{r \to \infty} Q_{r,s}^{1/r} \right]^{-1} = 2 \text{ and } \bar{w}_c = \inf_{s \leq 0} \left[ \limsup_{r \to \infty} Q_{r,s}^{1/r} \right]^{-1} = 1.
\]

Now

\[
F(w, z) = \sum_{s=0}^{\infty} z^s \sum_{r=1}^{\infty} \left( \frac{w}{s + 1} \right)^r = \sum_{s=0}^{\infty} z^s \left( \frac{w}{1 - \frac{w}{s + 1}} \right)^r \text{ provided } w < 1,
\]

\[
\lim_{r \to 0} (r)^{m-r} = 1.
\]

\[
\lim_{s \to \infty} (s)^{m-s} = 1.
\]

\[
\lim_{r \to 0} (r)^{m-r} = 1.
\]

\[
\lim_{s \to \infty} (s)^{m-s} = 1.
\]
so $F(w, z)$ will converge if $w < 1$ and $z < 1$ but will diverge if either $w \geq 1$ or $z \geq 1$. This shows that $\Theta$ is as claimed. For $\Xi$ we perform the same calculation on $G$:

$$G(w, z) = \sum_{s=1}^{\infty} sz^s \sum_{r=0}^{\infty} \left( \frac{w}{s+1} \right)^r$$

$$= \sum_{s=1}^{\infty} sz^s \frac{w}{s+1}$$

provided $w < 2$,

and we can see that $G(w, z)$ will converge if $w < 2$ and $z < 1$ but will diverge if either $w \geq 2$ or $z \geq 1$. 

\[ \Box \]

**Example 2.4.4.** If $Q_{r,s} = \frac{(s + 1)^r}{r!}$ then $\Theta^0 = \Xi^0 = \{(w, z) : 0 < w, z \text{ and } z < e^{-w}\}$

**Proof.**

The result follows immediately from observing that

$$F(w, z) = \sum_{s=0}^{\infty} z^s \sum_{r=1}^{\infty} \frac{1}{r!} [(s + 1)w]^r = \sum_{s=0}^{\infty} (s + 1)z^s e^{(s+1)w}$$

$$G(w, z) = \sum_{s=0}^{\infty} sz^s e^{(s+1)w}$$

\[ \Box \]

**Lemma 2.4.5**

Let $E(w, z) := \sum_{r+s=1}^{\infty} Q_{r,s}w^rz^s$, $\Gamma := \{(w, z) : 0 \leq w, z \text{ and } E(w, z) < \infty\}$ and $\Lambda(Q) := \{(w, z) : 0 \leq w \leq \bar{w}_c, 0 \leq z \leq \bar{z}_c\}$. Then $\Theta^0 \cap \Xi^0 = \Gamma^0$ and $\partial \Gamma = (\partial \Theta) \cap (\partial \Xi)$. Further $\Gamma^0 = \Theta^0 \cap \Lambda(Q) = \Xi^0 \cap \Lambda(Q)$.

The statement of Lemma 2.4.5 is most easily understood in terms of the sketches given in Figure 2.4.2.

**Proof.**

It follows from the arguments used to find $\Theta$ that:

$$\Gamma^0 = \{(w, z) : 0 < w \leq \bar{w}_c, 0 < z < z_{c0}(w)\} = \{(w, z) : 0 < w < w_{c0}(z), 0 < z < \bar{z}_c\}$$

and

$$\partial \Gamma = \{(w, z_{c0}(w)) : 0 \leq w \leq \min(\alpha_0, \bar{w}_c) \cup \{w_{c0}(z), z) : 0 \leq z \leq \min(\beta_0, \bar{z}_c)\}$$

$$\cup \left\{(w, 0) : 0 \leq w \leq \limsup_{r \to \infty} Q_{r,\beta_0}^{-1} \right\} \cup \left\{(0, z) : 0 \leq z \leq \limsup_{s \to \infty} Q_{0,s}^{-1} \right\}$$

$$\cup \{(w, \bar{z}_c) : 0 \leq w \leq w_{c1}(\bar{z}_c)\} \cup \{(\bar{w}_c, z) : 0 \leq z \leq z_{c1}(\bar{w}_c)\}.$$ 

The result then follows. 

\[ \Box \]

An immediate consequence of this result is that $\Theta$ and $\Xi$ only differ when either $\bar{w}_c \neq w_c$ or $\bar{z}_c \neq z_c$. It is also clear that the functions $z_{c0}$ and $z_{c1}$ are equal, as are $w_{c0}$ and $w_{c1}$; hence $\alpha_0 = \alpha_1$ and $\beta_0 = \beta_1$.

### 2.4.2 Finding equilibria of given densities

Having described the set of all equilibria the next point of interest is, to find the equilibrium distribution which has a density of type-I particles of a given value $\rho > 0$ and a type-II density of $\sigma > 0$. In other words to solve the simultaneous equations:

$$F(w, z) = \rho$$

$$G(w, z) = \sigma$$

(2.4.13)

The main aim of this section is to prove the claim that, equations (2.4.13) do not always have a solution but when they do it is unique. First we will show that if $F$ and $G$ are truncated after finitely many terms, then the equations can always be solved uniquely.
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Lemma 2.4.6
For all \( N \geq 1 \), the simultaneous equations

\[
F^{(N)}(w, z) := \sum_{r,s=0}^{N} rQ_{r,s}w^r z^s = \rho \tag{2.4.14}
\]

\[
G^{(N)}(w, z) := \sum_{r,s=0}^{N} sQ_{r,s}w^r z^s = \sigma
\]

have a unique solution for every value of \( \rho > 0 \) and \( \sigma > 0 \).

We will give a detailed proof of this result because the calculations performed within it are useful to the solution of the main problem. We first define the notation that will be used:

- \( \alpha^{(N)}_\rho \) is the unique positive root of \( \sum_{r=1}^{N} rQ_{r,0} w^r = \rho \) and \( \beta^{(N)}_\sigma \) is the unique positive root of \( \sum_{s=1}^{N} sQ_{0,s} z^s = \sigma \).
- \( f^{(N)}_\rho : \{0, \alpha^{(N)}_\rho \} \to \mathbb{R}^+ \) is the function for which \( f^{(N)}_\rho(a) \) is the single positive root of \( \sum_{r,s=0}^{N} rQ_{r,s} a^r z^s = \rho \) and similarly, \( g^{(N)}_\sigma : \mathbb{R}^+ \to [0, \beta^{(N)}_\sigma] \) is such that \( g^{(N)}_\sigma(a) \) is the positive root of \( \sum_{r,s=0}^{N} sQ_{r,s} a^r z^s = \sigma \).

Proof.
Using the notation just given the statement is equivalent to saying that

\[
f^{(N)}_\rho(w) = g^{(N)}_\sigma(w) \tag{2.4.15}
\]

has a unique solution.

First note that \( f^{(N)}_\rho(a) \to \infty \) as \( a \to 0 \) and that \( g^{(N)}_\sigma(0) \) is the solution of \( \sum_{s=1}^{N} sQ_{0,s} z^s = \sigma \), i.e. \( g^{(N)}_\sigma(0) = \beta^{(N)}_\sigma \). Hence for all \( \varepsilon > 0 \) sufficiently small \( f^{(N)}_\rho(\varepsilon) > g^{(N)}_\sigma(\varepsilon) \). Now note that for all \( a \geq 0 \)

\( g^{(N)}_\sigma(a) > 0 \) while the definition of \( \alpha^{(N)}_\rho \) gives that \( F^{(N)}(\alpha^{(N)}_\rho, 0) = \rho \) so \( f^{(N)}_\rho(\alpha^{(N)}_\rho) = 0 \). Hence \( f^{(N)}_\rho(\alpha^{(N)}_\rho) < g^{(N)}_\sigma(\alpha^{(N)}_\rho) \). This means that there is at least one solution to equation (2.4.15) in the interval \((\varepsilon, \alpha^{(N)}_\rho)\).
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We can show that this solution is unique by considering the gradients of \(f^{(N)}(\rho)\) and \(g^{(N)}(\sigma)\) at roots of equation (2.4.15). The definitions of \(f^{(N)}(\rho)\) and \(g^{(N)}(\sigma)\) give

\[
\sum_{r,s=0}^{N} rQ_{r,s} w^{r}[f^{(N)}(\rho)]^{s} = \rho
\]

\[
\sum_{r,s=0}^{N} sQ_{r,s} w^{r}[g^{(N)}(\sigma)]^{s} = \sigma,
\]

so implicit differentiation then gives

\[
\frac{df^{(N)}(\rho)}{dw} = -\frac{f^{(N)}(\rho)}{w} \cdot \sum_{r,s=0}^{N} r^{2}Q_{r,s} w^{r}[f^{(N)}(\rho)]^{s}
\]

\[
\frac{dg^{(N)}(\sigma)}{dw} = -\frac{g^{(N)}(\sigma)}{w} \cdot \sum_{r,s=0}^{N} s^{2}Q_{r,s} w^{r}[g^{(N)}(\sigma)]^{s}
\]

Let \(\bar{w}\) denote a solution of equation (2.4.15) and let \(z = f^{(N)}(\bar{w})\). The uniqueness of \(\bar{w}\) would be proved if

\[
\frac{df^{(N)}(\rho)}{dw} \bigg|_{w=\bar{w}} < \frac{dg^{(N)}(\sigma)}{dw} \bigg|_{w=\bar{w}}
\]

(2.4.16)

were show to be true, but equation (2.4.16) is equivalent to

\[
\left( \sum_{r,s=1}^{N} rsQ_{r,s} \bar{w}^{r}z^{s} \right)^{2} < \left( \sum_{r=0,s=1}^{N} s^{2}Q_{r,s} \bar{w}^{r}z^{s} \right) \cdot \left( \sum_{r,s=1}^{N} r^{2}Q_{r,s} \bar{w}^{r}z^{s} \right)
\]

(2.4.17)

However,

\[
S_{1} := \left( \sum_{r,s=1}^{N} rsQ_{r,s} \bar{w}^{r}z^{s} \right)^{2}
\]

\[
= \sum_{i,j,r,s}^{N} 2ijrsQ_{i,j}Q_{r,s} \bar{w}^{i+r}z^{j+s} + \sum_{k=1}^{N} k^{4}Q_{k,k} \bar{w}^{k}z^{k}
\]

where as

\[
S_{2} := \left( \sum_{r,s=1}^{N} s^{2}Q_{r,s} \bar{w}^{r}z^{s} \right) \cdot \left( \sum_{i=1,j=0}^{N} i^{2}Q_{i,j} \bar{w}^{i}z^{j} \right)
\]

\[
= \left( \sum_{s=1}^{N} s^{2}Q_{0,s} \bar{w}^{s} \right) \left( \sum_{i=1,j=0}^{N} i^{2}Q_{i,j} \bar{w}^{i}z^{j} \right) + \left( \sum_{r,s=1}^{N} s^{2}Q_{r,s} \bar{w}^{r}z^{s} \right) \left( \sum_{i=1}^{N} i^{2}Q_{i,0} \bar{w}^{i} \right)
\]

(\#)

\[
+ \sum_{i,j,r,s}^{N} (i^{2}s^{2} + j^{2}r^{2})Q_{i,j}Q_{r,s} \bar{w}^{i+r}z^{j+s} + \sum_{k=1}^{N} k^{4}Q_{k,k} \bar{w}^{k}z^{k}
\]
Hence $S_2 - S_1$ is the value of line (+) more than $\sum (si - jr)^2 Q_{ij} Q_{rs} \bar{w}^{i+r} z^{j+s}$ and so is strictly positive, which proves the inequality given in (2.4.16) and so the result.

We next consider what happens to the graphs of $f^{(N)}_\rho$ and $g^{(N)}_\sigma$, $\theta^{(N)}_\rho$ and $\xi^{(N)}_\sigma$ respectively, as $N \to \infty$. Lemma 2.4.7 proves that

$$\theta^{(N)}_\rho \to \{(w, z) \in \Theta : F(w, z) = \rho\} \cup \{(w, z) \in \partial\Theta \setminus L_\Theta : F(w, z) < \rho\}$$

$$\xi^{(N)}_\sigma \to \{(w, z) \in \Sigma : G(w, z) = \sigma\} \cup \{(w, z) \in \partial\Sigma \setminus L_\Sigma : G(w, z) < \sigma\},$$

where the definition of set convergence is explicitly given in the lemma. Lemma 2.4.8 will tell us that

Lemma 2.4.7. The simultaneous solution to equations (2.4.14), either tends to the solution of (2.4.13) or approaches the section of the boundary of $\Gamma$ where both $F(w, z) \leq \rho$ and $G(w, z) \leq \sigma$.

(i) For every $w \in \left(0, \liminf_{N \to 0} \alpha^{(N)}_\rho\right)$ there exists a $z \geq 0$ such that $f^{(N)}_\rho(w) \to z$ as $N \to \infty$ and where either $F(w, z) = \rho$, or $z = z_0(w)$ and $F(w, z) < \rho$.

(ii) For every $z \geq 0$ there exists a $w \in \left(0, \liminf_{N \to 0} \alpha^{(N)}_\rho\right)$ such that $f^{(N)}_\rho(w) \to z$ as $N \to \infty$ and where either $F(w, z) = \rho$, or $w = w_0(z)$ and $F(w, z) < \rho$.

Proof for (i)a.

Fix the value of $w$. Then which of the two alternatives, the limit of $f^{(N)}_\rho(w)$ will take depends on whether $F(w, z_0(w)) \geq \rho$ or $F(w, z_0(w)) < \rho$.

Figure 2.4.3: Sketches illustrating the convergence of $\theta^{(N)}_\rho$ as $N \to \infty$. 
If \( F(w, z_{\rho_0}(w)) \geq \rho \) (which includes the case where \( F(w, z_{\rho_0}(w)) \) diverges) then \( F(w, z) = \rho \) has a unique solution. Denote this solution \( f^N_\rho(w) \). We will show that \( f^N_\rho(w) \to f_\rho(w) \) as \( N \to \infty \). First note that as \( N \) increases \( f^N_\rho(w) \) decreases, strictly, and since \( f^N_\rho(w) \geq 0 \) then \( \lim_{M \to \infty} f^M_\rho(w) \) exists. Now

\[
0 \leq \rho - \sum_{r=1, s=0}^N r Q_{r,s} w^r \left( \lim_{M \to \infty} f^M_\rho(w) \right)^s \]

\[
= \sum_{r=1, s=0}^N r Q_{r,s} w^r \left\{ [f_\rho(w)]^s - \left[ \lim_{M \to \infty} f^M_\rho(w) \right] \right\} + \sum_{r \in \mathcal{R}(N)} r Q_{r,s} w^r [f_\rho(w)]^s
\]

\[
< \sum_{r=1, s=0}^N r Q_{r,s} w^r \left\{ \left[ f^M_\rho(w) \right]^s - \left[ \lim_{M \to \infty} f^M_\rho(w) \right] \right\} + \frac{\varepsilon}{2} \quad \text{for all } M > 0 \text{ and all large } N
\]

\[
< \frac{\varepsilon}{2} \quad \text{for all large } M.
\]

Hence

\[
\lim_{N \to \infty} \sum_{r=1, s=0}^N r Q_{r,s} w^r \left[ \lim_{M \to \infty} f^M_\rho(w) \right]^s = \rho \quad \text{but the solution of }
\]

\[
\sum_{r=1, s=0}^N r Q_{r,s} w^r z^s = \rho \quad \text{is unique, so } f_\rho(w) = \lim_{M \to \infty} f^M_\rho(w).
\]

If \( F(w, z_{\rho_0}(w)) < \rho \) then note that for all \( N > 0 \)

\[
F^N(w, z_{\rho_0}(w)) < \lim_{M \to \infty} F^M(w, z_{\rho_0}(w)) = F(w, z_{\rho_0}(w)) < \rho = F^N(w, f^N_\rho(w))
\]

So, for all \( N > 0 \), \( z_{\rho_0}(w) < f^N_\rho(w) \). For any \( z > z_{\rho_0}(w) \), \( F(w, z) \) diverges, i.e. \( F^N(w, z) \not\to \infty \) as \( N \to \infty \), so for all large \( N \), \( f^N_\rho(w) < z \). Hence \( f^N_\rho(w) \to z_{\rho_0}(w) \) as \( N \to \infty \). \( \diamond \)

**Lemma 2.4.8**

If \( (\tilde{w}^N_\rho, \tilde{z}^N_\rho) \) is the solution of equations (2.4.14) then either:

(a) \((\tilde{w}^N_\rho, \tilde{z}^N_\rho) \to (\tilde{w}_{\rho, \sigma}, \tilde{z}_{\rho, \sigma}) \) as \( N \to \infty \), where \((\tilde{w}_{\rho, \sigma}, \tilde{z}_{\rho, \sigma}) \) is the unique solution of equations (2.4.13) in \( \Gamma^c \cup L^c \), or

(b) there is no solution to equations (2.4.13) in \( \Gamma^c \cup L^c \), and

\[
\text{dist} \left\{ (\tilde{w}^N_{\rho, \sigma}, \tilde{z}^N_{\rho, \sigma}), \left\{ (a, b) \in \partial \Gamma \setminus L : F(a, b) \leq \rho, G(a, b) \leq \sigma \} \right\} \to 0 \quad \text{as } N \to \infty \quad (2.4.20)
\]

**Proof.**

The subscript \( \rho, \sigma \) will be dropped to clarify the notation. Suppose that

\[
\text{dist} \left\{ \tilde{w}^N, \tilde{z}^N \right\}, \partial \Gamma \setminus L \neq 0 \quad \text{as } N \to \infty
\]

Lemma 2.4.7 tells us that \( \text{dist} \left\{ \left\{ (w_i^N, z_i^N) \right\}, \Gamma \right\} \to 0 \), so there must be a subsequence of \( \left\{ (w_i^N, z_i^N) \right\} \), which is contained in \( \Gamma^c \cup L^c \) and bounded away from \( \partial \Gamma \setminus L \). Now \( F^N \) and \( G^N \) converge to \( F \) and \( G \) uniformly on compact subsets of \( \Gamma^c \cup L \). This means that, for sufficiently large \( N \), all \( \left\{ (w_i^N, z_i^N) \right\} \) are in \( \Gamma^c \cup L^c \) bounded away from \( \partial \Gamma \setminus L \). Since \( 0 \leq \tilde{w}^N \leq \alpha^N_\rho \), \( 0 \leq \tilde{z}^N \leq \beta^N_\rho \) and \( \alpha^N_\rho \) and \( \beta^N_\rho \) are both decreasing sequences, then \( \left\{ (\tilde{w}^N, \tilde{z}^N) \right\} \) must have a convergent subsequence. This subsequence will converge to a solution of equations (2.4.13) because \( F^N \) and \( G^N \) are uniformly convergent; in fact

\[
\text{dist} \left\{ \left\{ (w_i^N, z_i^N) \right\}, \left\{ (x, y) \in \Gamma^c \cup L : F(x, y) = \rho, G(x, y) = \sigma \} \right\} \to 0 \quad \text{as } N \to \infty \quad (2.4.21)
\]

We can show that there is only one solution to equations (2.4.13) in \( \Gamma^c \cup L^c \) by the same argument as we used to show that the solution of (2.4.14) was unique in Lemma 2.4.6. So we have shown that \( \text{dist} \left\{ \left\{ (w_i^N, z_i^N) \right\}, \partial \Gamma \setminus L \right\} \neq 0 \) implies option (a). If

\[
\text{dist} \left\{ \left\{ (w_i^N, z_i^N) \right\}, \partial \Gamma \setminus L \right\} \to 0 \quad \text{as } N \to \infty,
\]
then Lemma 2.4.7 gives us that equation (2.4.20) is also true. If under these circumstances equations (2.4.13) did have a solution in $\Gamma^o \cup L_{\Gamma}$ then the uniform convergence of $F^{(N)}$ and $G^{(N)}$ would give that $(\hat{w}^N, \hat{z}^N) \to (\hat{w}, \hat{z})$ as $N \to \infty$ and so contradict equation (2.4.20).

In Lemma 2.4.9, below, we describe a situation where equations (2.4.13) do have a solution, while Figure 2.4.4 gives sketches of circumstances under which the equations will not have a solution in $\Gamma^o \cup L_{\Gamma}$.

![Figure 2.4.4: Sketches of situations where no point has both its densities equal to given values.](image)

**Lemma 2.4.9**

Assume that there exist $\alpha > 0$ and $\beta > 0$ such that

$$B = \{(w, z) : 0 < w < \alpha, 0 < z < \beta\} \subset \Gamma^o.$$

If $\rho \leq F(\alpha, 0)$ and $\sigma \leq G(0, \beta)$ then there is a unique solution to equations (2.4.13) in $\Gamma^o \cup L_{\Gamma}$.

**Proof.**

We have already seen in the proof of Lemma 2.4.8 that if there is a solution in $\Gamma^o \cup L_{\Gamma}$ then it will be unique. The circumstances given here, however, are such that there must be at least one solution – by similar arguments used to show existence in the finite case, see Lemma 2.4.6. The sketch in Figure 2.4.5 is enough to see how to make the necessary alterations.

2.5 **Lyapunov Functions**

In this section we will show that a certain class of functions are Lyapunov functions of the system in (2.1.1).

2.5.1 **Continuity and boundedness**

For $c \in X^+$ let

$$V(c) = \sum_{r+s=1}^\infty c_{r,s} \left[ \ln \left( \frac{c_{r,s}}{Q_{r,s}} \right) - 1 \right],$$

(2.5.1)

where the summand is defined to be zero when $c_{r,s} = 0.$
Lemma 2.5.1
The function
\[ U(c) = \sum_{r+s=1}^{\infty} c_{r,s} [\ln (c_{r,s}) - 1], \] (2.5.2)
is finite and weak* continuous on \( X^+ \).

Proof.
Note that for any \( \varepsilon \in (0, 1) \), there is a constant \( K > 0 \) such that
\[ x|\ln(x)| \leq K \left( x^{1-\varepsilon} + x^{1+\varepsilon} \right). \] (2.5.3)
So for any \( N \geq 1 \)
\[
\left| \sum_{r+s=1}^{N} c_{r,s} [\ln (c_{r,s}) - 1] \right| \leq K \sum_{r+s=1}^{N} \left( c_{r,s}^{1-\varepsilon} + c_{r,s}^{1+\varepsilon} \right) + \sum_{r+s=1}^{N} c_{r,s} \]
\[
\leq K \left( \sum_{r+s=1}^{N} (r+s)c_{r,s} \right)^{1-\varepsilon} \left( \sum_{m=1}^{N} m^{-(1-\varepsilon)/\varepsilon} \right)^{\varepsilon} + \|c\|,
\]
using Hölder’s inequality. So by setting \( \varepsilon < \frac{1}{2} \), we see that
\[
\sum_{r+s=1}^{N} |c_{r,s} [\ln (c_{r,s}) - 1]| \leq K'\|c\| \quad \text{for all } N \geq 1,
\]
which proves that \( U \) is absolutely convergent in \( X^+ \).
To show weak* continuity, suppose that the sequence \( c^{(j)} \in X^+ \) converges weakly to \( c \in X^+ \), then consider:
\[
\left| U(c^{(j)}) - U(c) \right| \leq \sum_{r+s=1}^{M} c_{r,s}^{(j)} \ln(c_{r,s}^{(j)}) - \sum_{r+s=1}^{M} c_{r,s} \ln(c_{r,s}) + \sum_{r+s=M+1}^{\infty} \left| c_{r,s}^{(j)} - c_{r,s} \right| \\
+ K \sum_{r+s=M+1}^{\infty} \left( c_{r,s}^{(j)} \right)^{1+\varepsilon} + K \sum_{r+s=M+1}^{\infty} (c_{r,s})^{1+\varepsilon} \\
+ K \left[ \sum_{m=M+1}^{\infty} (r+s) \left( c_{r,s}^{(j)} + c_{r,s} \right) \right]^{1-\varepsilon} \left[ \sum_{m=M+1}^{\infty} m^{-(1-\varepsilon)/\varepsilon} \right]^{\varepsilon}.
\]
2.5. LYAPUNOV FUNCTIONS

The first line can be made arbitrarily small by setting \( j \) sufficiently large, while the last two lines will become small if \( M \to \infty \).

By noticing that

\[
V(c) = U(c) - \sum_{r+s=1}^{\infty} r c_{r,s} \ln \left( \frac{Q_{r,s}^{1/r}}{w^{r} z^{s}} \right),
\]

we can see that, if

\[
\sup_{s \geq 0} \left\{ \limsup_{r \to \infty} Q_{r,s}^{1/s} \right\} < \infty, \quad \dagger
\]

then \( V \) is bounded below on \( B_{p,\sigma}^{+} \), and if

\[
\inf_{s \geq 0} \left\{ \liminf_{r \to \infty} Q_{r,s}^{1/r} \right\} > 0, \quad \ddagger
\]

then \( V \) is bounded above on \( B_{p,\sigma}^{+} \).

For any \( w > 0 \) and \( z > 0 \) we define

\[
V_{w,z}(c) = \sum_{r+s=1}^{\infty} r c_{r,s} \left[ \ln \left( \frac{c_{r,s}}{Q_{r,s}^{1/r} w^{r} z^{s}} \right) - 1 \right].
\]

(2.5.6)

\( V_{w,z} \) has the same boundedness properties as \( V \) on \( B_{p,\sigma}^{+} \), because

\[
V_{w,z}(c) = V(c) + \ln(w) \sum_{r+s=1}^{\infty} r c_{r,s} - \ln(z) \sum_{r+s=1}^{\infty} s c_{r,s}.
\]

In order to study the asymptotic behaviour of the solutions of (2.1.1), we need to know about the weak* continuity of the functions \( V_{w,z} \). The next theorem will give us the necessary information, but it requires us to make additional assumptions about \( Q_{r,s} \). These are

\[
\lim_{r \to \infty} Q_{r,s}^{1/r} = \frac{1}{w_{c}} \quad \text{for all } s \geq 0
\]

(2.5.7)

and

\[
\lim_{s \to \infty} Q_{r,s}^{1/s} = \frac{1}{z_{c}} \quad \text{for all } r \geq 0.
\]

(2.5.8)

When we assume that (2.5.7) and (2.5.8) hold it will often be convenient to rewrite \( Q_{r,s} \) as \( K_{r,s} \left( \frac{1}{w_{c}} \right)^{r} \left( \frac{1}{z_{c}} \right)^{s} \). One consequence of this is that

\[
\left( \sum_{r=1}^{\infty} Q_{r,s} w^{r} \right)^{1/s} = \frac{1}{z_{c}} \left[ \sum_{r=1}^{\infty} \left( \frac{K_{r,s}^{1/r}}{w_{c}} \right)^{r} \right]^{1/s} \to \frac{1}{z_{c}} \quad \text{as } s \to \infty
\]

(2.5.9)

because (2.5.7) is equivalent to \( \lim_{r \to \infty} K_{r,s}^{1/r} = 1 \) for all \( s \geq 0 \). Hence \( z_{c_{0}}(w) = z_{c} \) for all \( w \in [0, w_{c}] \), and in the same way we can show that \( w_{c_{0}}(z) = w_{c} \) for all \( z \in [0, z_{c}] \). Using the notation of Section 2.4.1 we can say that (2.5.7) and (2.5.8) imply that \( \Gamma = \Theta = \Xi = \Lambda(Q) \). Out of the examples considered in that section, Example 2.4.1 is the only one the satisfy all four of the above conditions; that is equations (2.5.4), (2.5.5), (2.5.7) and (2.5.8).

\[\textbf{Theorem 2.5.2}\]

Assume (2.5.7) and (2.5.8) hold. Then \( V_{w,z} \) is weak* continuous for every \( z > 0 \) and \( V_{w,z} \) is weak* continuous for every \( w > 0 \).

\[\dagger\text{Note that } \sup_{s \geq 0} \left\{ \limsup_{r \to \infty} Q_{r,s}^{1/s} \right\} < \infty \iff \sup_{r \geq 0} \left\{ \limsup_{s \to \infty} Q_{r,s}^{1/r} \right\} < \infty.\]

\[\ddagger\text{Similarly } \inf_{s \geq 0} \left\{ \liminf_{r \to \infty} Q_{r,s}^{1/r} \right\} > 0 \iff \inf_{r \geq 0} \left\{ \liminf_{s \to \infty} Q_{r,s}^{1/s} \right\} > 0.\]
Proof.
Note that
\[
V_{w,z}(c) = U(c) - \sum_{r+s=1}^{\infty} c_{r,s} \ln \left( Q_{r,s}^w z^s \right) \\
= U(c) - \sum_{r+s=1}^{\infty} c_{r,s} \ln \left[ K_{r,s} \left( \frac{z}{z_c} \right)^s \right].
\]

Lemma 2.3.5 (ii) told us that \( y \mapsto \sum g_{r,s} y_{r,s} \) was weak* continuous when \( g_{r,s} = O(h_r) \) and \( |h_s| = o(r) \). Now observe that
\[
\frac{1}{r} \ln \left[ K_{r,s} \left( \frac{z}{z_c} \right)^s \right] = \ln \left[ K_{r/s} \left( \frac{z}{z_c} \right)^{s/r} \right] \to 0 \quad \text{as } r \to \infty, \text{ for all } s \geq 0.
\]
So \( V_{w,z} \) is weak* continuous. The weak* continuity of \( V_{w,z} \) is proved in a similar way.

\[\Box\]

Let \( H_{m,n}(w,z) := \sum_{r+s=1}^{\infty} r^m s^n Q_{r,s}^w z^s \) and note that, if \( (w,z) \in \Gamma^0 \cup L^r \) then \( H_{m,n}(w,z) < \infty \) for all \( m \geq 0, n \geq 0 \). With this notation \( E = H_{0,0}, F = H_{1,0} \) and \( G = H_{0,1} \). Let \( c^w,z \) denote the equilibrium distribution \( (Q_{r,s}^w z^s) \), then we can rewrite \( V_{w,z_0}(c^w,z) \) as
\[
V_{w,z_0}(c^w,z) = \ln \left( \frac{w}{w_0} \right) H_{1,0}(w,z) + \ln \left( \frac{z}{z_0} \right) H_{0,1}(w,z) - H_{0,0}(w,z)
\]

**Proposition 2.5.3:** gives details about the first derivatives of \( V_{w,z_0}(c^w,z) \). It deals with the derivatives on \( \Gamma^0, L^r \) and \( \partial \Gamma \setminus L^r \) separately; and the case for \( \partial \Gamma \setminus L^r \) is considered only when \( \Gamma = \Lambda(Q) \).

(i) If \((w,z) \in \Gamma^0 \) then
\[
\left[ \begin{array}{c} \frac{\partial}{\partial w} (V_{w,z_0}(c^w,z)) \\ \frac{\partial}{\partial z} (V_{w,z_0}(c^w,z)) \end{array} \right] = \left[ \begin{array}{c} \frac{1}{w} H_{2,0}(w,z) + \frac{1}{z} H_{1,1}(w,z) \\ \frac{1}{z} H_{1,1}(w,z) + \frac{1}{w} H_{0,2}(w,z) \end{array} \right] \left[ \begin{array}{c} \ln \left( \frac{w}{w_0} \right) \\ \ln \left( \frac{z}{z_0} \right) \end{array} \right].
\]

(ii) (a) If \( 0 \leq w < \limsup_{r \to \infty} Q_{r,0}^{1/r} \) then
\[
\frac{d}{dw} (V_{w,z_0}(c^{w,0})) = \frac{1}{w} \ln \left( \frac{w}{w_0} \right) H_{2,0}(w,0).
\]

(b) If \( 0 \leq z < \limsup_{s \to \infty} Q_{0,s}^{1/s} \) then
\[
\frac{d}{dz} (V_{w,z_0}(c^{0,z})) = \frac{1}{z} \ln \left( \frac{z}{z_0} \right) H_{0,2}(0,z).
\]

(iii) Suppose that \( \Gamma = \{(w,z) : 0 \leq w \leq w_c, 0 \leq z \leq z_c\} \) then:

(a) if \( 0 < w \leq w_c \) then
\[
\frac{d}{dw} (V_{w,z_0}(c^{w,z})) = \frac{1}{w} \ln \left( \frac{w}{w_0} \right) H_{2,0}(w,z_c) + \frac{1}{w} \ln \left( \frac{z}{z_0} \right) H_{1,1}(w,z_c),
\]

\[5\text{Lemma 2.4.5 defined } E \text{ by } E(w,z) = \sum_{r+s=1}^{\infty} Q_{r,s}^w z^s.\]
(b) and if $0 < z \leq z_c$ then
\[
\frac{d}{dz}(V_{w_0,z_0}(e^{w_{c,z}})) = \frac{1}{z} \ln \left( \frac{w_c}{w_0} \right) H_{1,1}(w_c, z) + \frac{1}{z} \ln \left( \frac{z}{z_0} \right) H_{0,2}(w_c, z).
\]

Proof.
(i) If $(w, z) \in \Gamma^\circ$ then \(\frac{\partial H_{m,n}}{\partial w}(w, z) = \frac{1}{w} H_{m+1,n}(w, z)\) and \(\frac{\partial H_{m,n}}{\partial z}(w, z) = \frac{1}{z} H_{m,n+1}(w, z)\). So
\[
\frac{\partial}{\partial w}(V_{w_0,z_0}(e^{w_{c,z}})) = \frac{1}{w} H_{1,0}(w, z) + \frac{1}{w} \ln \left( \frac{w}{w_0} \right) H_{2,0}(w, z) + \frac{1}{w} \ln \left( \frac{z}{z_0} \right) H_{0,2}(w, z) - \frac{1}{w} H_{1,0}(w, z)
\]
\[= \left[ \frac{1}{w} H_{2,0}(w, z) \right] \ln \left( \frac{w}{w_0} \right) \left[ \ln \left( \frac{z}{z_0} \right) \right].\]

The same calculation can be performed for \(\frac{\partial}{\partial z}(V_{w_0,z_0}(e^{w_{c,z}}))\) and the result is then obtained.

(ii) Note that
\[
V_{w_0,z_0}(e^{w_{c,0}}) = \sum_{r=1}^{\infty} Q_r,0 w_r \left[ \ln \left( \frac{w_r}{w_c} \right) - 1 \right] = \ln \left( \frac{w}{w_c} \right) H_{1,0}(w, 0) - H_{0,0}(w, 0).
\]

Since \(w \in (0, \limsup_{r \to \infty} Q_r,0)\), \(\frac{d}{dw} H_{m,n}(w, 0) = \frac{1}{w} H_{m+1,n}(w, 0)\). The result then follows.

Parts (ii)b, (iii)a and (iii)b can be proved in a similar way.

\[\diamond\]

2.5.2 Energy equations

Before showing that \(t \mapsto V(c(t))\) is a non-increasing function, we need to show that, for non-zero initial data, all \(c_{r,s}(t)\) are strictly positive for all \(t > 0\).

**Theorem 2.5.4**

Suppose that \(A_{r,s} > 0\). Let \(c\) be a solution of (2.1.1) on \([0, T]\), with \(c(0) \neq 0\).

(i) If \(c_{r,s}(0) \neq 0\) for some \(r > 0, s > 0\) then \(c_{r,s}(t) > 0\) for all \(t > 0\) and all \(r \geq 0, s \geq 0\).

(ii) If \(c_{r,0}(0) \neq 0\) for some \(r \geq 1\) then \(c_{r,0}(t) > 0\) for all \(t > 0\) and all \(r \geq 1\).

(iii) If \(c_{0,s}(0) \neq 0\) for some \(s \geq 1\) then \(c_{0,s}(t) > 0\) for all \(t > 0\) and all \(s \geq 1\).

**Proof.**

We will prove (ii) first and will proceed by contradiction. Suppose \(c_{r,0}(\tau) = 0\) with \(\tau \in (0, T)\). If \(r > 1\) then
\[
\dot{c}_{r,0} = \gamma_{r,0} - \eta_{r,0} c_{r,0},
\]
where \(\gamma_{r,0} := a_{r-1,0} c_{r-1,0} + b_{r+1,0} c_{r+1,0} + b'_{r,1} c_{r,1}\) and \(\eta_{r,0} := a_{r,0} c_{1,0} + b_{r,0} + a'_{r,0} c_{0,1}\). So
\[
0 = c_{r,0}(\tau) \exp \left( \int_0^\tau \eta_{r,0}(\zeta) d\zeta \right) = c_{r,0}(0) + \int_0^\tau \exp \left( \int_0^\tau \eta_{r,0}(\zeta) d\zeta \right) \gamma_{r,0}(t) dt,
\]
which implies that $a_{r-1,0}c_{1,0}(t)c_{r-1,0}(t) = 0$ for a.e. $t \in (0, \tau)$. Since $c_{1,0}$ and $c_r$ are continuous and $\alpha_{r,s} > 0$, then either $c_{1,0}(\tau) = 0$ or $c_{r-1,0}(\tau) = 0$. If the latter then induction leads us to the former, so $c_{1,0}(\tau) = 0$. Let $\eta_{1,0}(t) := a_1 c_{1,0}(t) + \sum_{r+s=1} a_{r,s} c_{r,s}(t)$ and $\gamma_{1,0}(t) := b_2 c_{2,0}(t) + b_{1,1} c_{1,1}(t) + \sum_{r+s=1} b_{r+1,s} c_{r+1,s}(t)$, then

$$
\dot{c}_{1,0}(t) = -c_{1,0}(t) \eta_{1,0}(t) + \gamma_{1,0}(t)
$$

$$
\implies c_{1,0}(\tau) \exp \left( \int_0^\tau \eta_{1,0}(\zeta) d\zeta \right) = c_{1,0}(0) + \int_0^\tau \gamma_{1,0}(t) \exp \left( \int_0^t \eta_{1,0}(\zeta) d\zeta \right) dt = 0.
$$

Hence $\gamma_{1,0}(t) = 0$ for a.e. $t \in (0, \tau)$ and $c_{1,0}(0) = 0$, which implies that $c_r(s)$ is also 0 for a.e. $t \in (0, \tau)$ and all $r \geq 2$ and $s \geq 0$, but $c_{r,s}$ are all continuous so $c_r(s) = 0$ for all $t \in [0, \tau]$. In particular all $c_r(0) = 0$ for all $r \geq 1$, which contradicts the original assumption.

To prove (iij) we again, assume for the purpose of contradiction, that $c_{r,s}(\tau) = 0$ for some $\tau \in (0, T)$ and some $r \geq 1$, $s \geq 1$. So

$$
0 = c_{r,s}(\tau) \exp \left( \int_0^\tau \eta_{r,s}(\zeta) d\zeta \right)
$$

$$
= c_{r,s}(0) + \int_0^\tau \exp \left( \int_0^t \eta_{r,s}(\zeta) d\zeta \right) \gamma_{r,s}(t) dt,
$$

where $\eta_{r,s}$ and $\gamma_{r,s}$ have the expected definitions. This implies that $a_{r,s-1} c_{1,0}(t) c_{r,s-1}(t) = 0$ for a.e. $t \in [0, \tau]$, the continuity of the $c_{r,s}$’s then implies that either $c_{0,1}(\tau) = 0$ or $c_{r,s-1}(\tau) = 0$. If the latter then induction leads to $c_{1,0}(\tau) = 0$ and this in turn leads to $c_{1,0}(\tau) = 0$. We saw above that this implies that $\gamma_{1,0}(t) = 0$ for a.e. $t \in [0, \tau]$. This together with continuity of each $c_{r,s}$ would imply that $c_{r,s}(0) = 0$ for every $r \geq 1$ and $s \geq 0$ which is a contradiction. So the former alternative must apply, i.e. $c_{0,1}(\tau) = 0$, but this will give that $\gamma_{0,1}(t) = 0$ for a.e. $t \in [0, \tau]$, which implies that $c_{r,s}(0) = 0$ for every $r \geq 0$ and $s \geq 1$ another contradiction.

\begin{theorem}
Suppose that (2.5.4), (2.5.5) hold and that $A_{r,s} > 0$, $A_{r,s} = O((r+s)^\alpha)$ for some $\alpha \in (0, 1)$. Let $c$ be a solution of (2.1.1) on some interval $[0, T)$, $0 < T \leq \infty$, with $c_{r,s}(0) > 0$ for some $r \geq 1$, $s \geq 1$. Then

$$
V(c(t)) + \int_0^t D(c(\tau)) d\tau = V(c(0)) \quad \text{for all } t \in [0, T),
$$

where

$$
D(c) := \sum_{r+s=1}^{\infty} \left( a_{r,s} c_{1,0} c_{r,s} - b_{r+1,s} c_{r+1,s} \right) \ln \left( \frac{a_{r,s} c_{1,0} c_{r,s}}{b_{r+1,s} c_{r+1,s}} \right)
$$

$$
+ \sum_{r+s=1}^{\infty} \left( a^\prime_{r,s} c_{0,1} c_{r,s} - b^\prime_{r,s+1} c_{r,s+1} \right) \ln \left( \frac{a^\prime_{r,s} c_{0,1} c_{r,s}}{b^\prime_{r,s+1} c_{r,s+1}} \right)
$$

(2.5.11)

\end{theorem}

\begin{proof}
For $n \geq 1$ define

$$
V^{(n)}(c) = \sum_{r+s=1}^{n} \ln \left( \frac{c_{r,s}}{Q_{r,s}} \right) - 1
$$

$$
D^{(n)}(c) = \sum_{r+s=1}^{n} \left( a_{r,s} c_{1,0} c_{r,s} - b_{r+1,s} c_{r+1,s} \right) \ln \left( \frac{a_{r,s} c_{1,0} c_{r,s}}{b_{r+1,s} c_{r+1,s}} \right)
$$

(2.5.12)

\end{proof}
2.5. LYAPUNOV FUNCTIONS

By Theorem 2.5.4 and the identity (2.1.3) we can see that

\[ V^{(n)}(c) = \sum_{r+s=1}^{n-1} J_{r,s} \ln \left( \frac{a_{r,s} c_{0,1}}{b_{r,s+1}} \right) + J_{r,s} \ln \left( \frac{a_{r,s} c_{0,1} c_{r,s}}{b_{r,s+1} c_{r,s+1}} \right) \]

or

\[ V^{(n)}(c) = - D^{(n)}(c) - \sum_{r+s=1}^{n-1} J_{r,s} \ln \left( \frac{c_{r+1,s}}{Q_{r+1,s}} \right) + J_{r,s} \ln \left( \frac{c_{r,s}}{Q_{r,s}} \right) \]

Since Theorem 2.5.4 gives us that \( c_{1,0}(t) > 0, c_{0,1}(t) > 0 \) for all \( t \in [\tau, T] \), where \( \tau > 0 \), we can say

\[ \inf_{\eta \in [\tau, t]} \{ \ln(c_{1,0}(\eta)) \} \int_{\tau}^{t} \left| \sum_{r+s=1}^{\infty} J_{r,s} \ln(c(\eta)) \right| d\eta \leq \left| \int_{\tau}^{t} \ln(c_{1,0}(\eta)) \sum_{r+s=1}^{\infty} J_{r,s} \ln(c(\eta)) d\eta \right| \leq \sup_{\eta \in [\tau, t]} \{ \ln(c_{1,0}(\eta)) \} \int_{\tau}^{t} \left| \sum_{r+s=1}^{\infty} J_{r,s} \ln(c(\eta)) \right| d\eta. \]

This means that

\[ \lim_{n \to \infty} \int_{\tau}^{t} \ln(c_{1,0}(\eta)) \sum_{r+s=1}^{\infty} J_{r,s} \ln(c(\eta)) d\eta = 0, \]

and in the same way

\[ \lim_{n \to \infty} \int_{\tau}^{t} \ln(c_{0,1}(\eta)) \sum_{r+s=1}^{\infty} J'_{r,s} \ln(c(\eta)) d\eta = 0. \]

Since we have assumed that (2.5.4) and (2.5.5) hold then a similar calculation, using equation (2.1.30), will give:

\[ \lim_{n \to \infty} \int_{\tau}^{t} \sum_{r+s=1}^{n} J_{r,s} \ln(Q_{r,s}) d\eta = \lim_{n \to \infty} \int_{\tau}^{t} \sum_{r+s=1}^{n} J_{r,s} \ln(Q_{r+1,s}) d\eta = 0, \]

\[ \lim_{n \to \infty} \int_{\tau}^{t} \sum_{r+s=1}^{n} J'_{r,s} \ln(Q_{r,s}) d\eta = \lim_{n \to \infty} \int_{\tau}^{t} \sum_{r+s=1}^{n} J'_{r,s} \ln(Q_{r,s+1}) d\eta = 0. \]

We will next find bounds for the terms of the form \( \int_{\tau}^{t} \sum_{r+s=1}^{n} J_{r,s} \ln(c_{r,s}(\eta)) d\eta \). Note that for sufficiently large values of \( m, -J_{r,m-r} \ln(c_{r,m-r}) \leq a_{r,m-r} c_{1,0} c_{r,m-r} \ln(c_{r,m-r}) \). Since \( A_{r,s} = \)
O((r + s)^n) we can write

\[- \sum_{r = 0}^{m} J_{r,m-r} \ln(c_{r,m-r}) \leq Km^{\alpha} \sum_{r = 0}^{m} c_{r,m-r} |\ln(c_{r,m-r})|.
\]

Now for any \( \gamma \in (0, 1) \) there is an \( \varepsilon_\gamma > 0 \) such that \( x \in (0, \varepsilon_\gamma) \implies x |\ln(x)| < x^\gamma \) and Proposition 2.3.1 tells us that \( m \sum_{r=0}^{m} c_{r,m-r}(\eta) \to 0 \) as \( m \to \infty \), uniformly on compact sub-intervals of \([0, T)\). So, given \( \varepsilon_\gamma > 0 \) we can find an \( M_\gamma \) such that \( m > M_\gamma \implies \sum_{r=0}^{m} c_{r,m-r}(\eta) < \varepsilon_\gamma \) for all \( \eta \in [0, t] \). Hence

\[- \sum_{r = 0}^{m} J_{r,m-r} \ln(c_{r,m-r}) \leq Km^{\alpha} \sum_{r = 0}^{m} (c_{r,m-r})^\gamma < Km^{\alpha} \left( \sum_{r = 0}^{m} c_{r,m-r} \right)^\gamma \cdot m^{1-\gamma} = Km^{1+\alpha-2\gamma} \left( m \sum_{r=0}^{m} c_{r,m-r}(\eta) \right)^\gamma.
\]

This means that \(- \int_{\tau}^{t} \sum_{r = 0}^{m} J_{r,m-r}(c(\eta)) \ln(c_{r,m-r}(\eta)) \, d\eta \leq o(1) \) and similarly

\[- \int_{\tau}^{t} \sum_{r = 0}^{m} J_{r,m-r}(c(\eta)) \ln(c_{r,m-r}(\eta)) \, d\eta \leq o(1).
\]

We can see that

\[- \int_{\tau}^{t} \sum_{r = 0}^{m} J_{r,m-r}(c(\eta)) \ln(c_{r+1,m-r}(\eta)) \, d\eta \geq o(1)
\]

by observing that for sufficiently large \( m \),

\[- J_{r,m-r}(c) \ln(c_{r+1,m-r}) \geq -b_{r+1,m-r} c_{r+1,m-r} |\ln(c_{r+1,m-r})|\]

and then using the same calculation as the last case. This all means that

\[\int_{\tau}^{t} D^{(n)}(c(\eta)) \, d\eta + o(1) \leq V^{(n)}(c(\tau)) - V^{(n)}(c(t)) \leq \int_{\tau}^{t} D^{(n-1)}(c(\eta)) \, d\eta + o(1).
\]

So by the monotone convergence theorem

\[\int_{\tau}^{t} D(c(\eta)) \, d\eta = V(c(\tau)) - V(c(t)),
\]

but \( c \) and \( V \) are continuous, so we can derive (2.5.10) by letting \( \tau \to 0 \).

If the solutions of (2.1.1) were known to be unique, it would be possible to prove that (2.5.10) held as an inequality under far more general conditions. This is given in the next theorem, it is the equivalent to Theorem 4.8 in [2].

**Theorem 2.5.6**

Let the hypotheses of Theorem 2.1.3, (2.5.4) and (2.5.5) hold, and suppose that \( c_0 \neq 0 \) and \( V(c_0) < \infty \). Then there exists a solution \( c \) of (2.1.1) on \([0, \infty)\) with \( c(0) = c_0 \) satisfying

\[V(c(t)) + \int_{0}^{t} D(c(\tau)) \, d\tau \leq V(c(0)) \quad \text{for all } t \in [0, T).
\]

In [2] this was proved by showing that the solution constructed in the proof of Theorem 2.1.3 satisfied (2.5.12). We can write down precisely the same arguments in this case.
2.6 Asymptotic Behaviour of Solutions

It has not been possible to work out the full asymptotic behaviour of solutions of (2.1.1). It can be proved, however, with certain assumptions, that solutions tend weakly to one of the equilibrium solutions described in Section 2.4. And we can find equilibrium distributions that minimise the Lyapunov function, and this is sufficiently strong evidence to conjecture a statement about the convergence of c.

2.6.1 Weak’ convergence

The following theorem relies heavily on the “invariance principle”, described in [2], which we will repeat here: Let G be a generalised flow, then \( V : Y \to \mathbb{R} \) is called a Lyapunov function if \( t \to V(\varphi(t)) \) is non-increasing on \([0, \infty)\) for each \( \varphi \in G \). If \( V \) is continuous and the positive orbit of \( \varphi, \mathcal{P}^+(\varphi) := \{ \varphi(t) : t \geq 0 \} \), is relatively compact then the \( \omega \)-limit set of \( \varphi, \omega(\varphi) = \{ y \in Y : \varphi(t_j) \to y \text{ for some sequence } t_j \to \infty \} \), consists of complete orbits along which \( V \) has the constant value \( \lim_{t \to \infty} V(\varphi(t)) \). A standard topological result also gives that if \( \mathcal{P}^+(\varphi) \) is relatively compact then \( \text{dist}(\varphi(t), \omega(\varphi)) \to 0 \) as \( t \to \infty \).

Theorem 2.6.1

Assume that \( A_{r,s} > 0, A_{r,s} = \mathcal{O}((r + s)\alpha) \) for some \( \alpha \in (0, 1) \) and that (2.5.4), (2.5.5), (2.5.7) and (2.5.8) hold, and further suppose that \( 0 < w_c < \infty, 0 < z_c < \infty \). Let \( c \) be a solution of (2.1.1) on \([0, \infty)\) and let \( \rho_0 = \sum_{r+s=1}^\infty r c_{r,s}(0), \sigma_0 = \sum_{r+s=1}^\infty s c_{r,s}(0) \). Then \( c(t) \xrightarrow{t} e^{w_z} \) as \( t \to \infty \), for \( (w, z) \in \Gamma \) such that \( F(w, z) \leq \rho_0 \) and \( G(w, z) \leq \sigma_0 \).

Proof.

If \( \rho_0 = 0 \) and \( \sigma_0 = 0 \) then \( c(t) = 0 \) for all \( t \geq 0 \) which implies that \( c(t) \to 0 \) as \( t \to \infty \). If \( \rho_0 > 0 \) and \( \sigma_0 = 0 \) then Theorem 2.2.2 showed that \( (c_{r,0}) \) is a solution of (2.2.1) on \([0, \infty)\), and Theorem 5.5 of [2] gives the result. Similarly when \( \rho_0 = 0 \) and \( \sigma_0 > 0 \). So suppose that \( \rho_0 > 0 \) and \( \sigma_0 > 0 \), then: from Theorem 2.3.10 we know that \( \mathcal{G}_{\rho_0, \sigma_0} \) is a generalised flow of \( \mathbb{B}^+_{\rho_0, \sigma_0} \); Theorem 2.5.2 tells us that \( V_{w, z} \) and \( V_{w, z_c} \) are continuous on \( \mathbb{B}^+_{\rho_0, \sigma_0} \), for every \( z > 0, w > 0 \) and Theorem 2.5.5 plus Corollary 2.1.7 gives

\[
V_{w, z}(c(t)) + \int_0^t D(c(\tau)) d\tau = V_{w, z}(c(0)) \quad \text{for all } t \in [0, \infty),
\]

and

\[
V_{w, z_c}(c(t)) + \int_0^t D(c(\tau)) d\tau = V_{w, z_c}(c(0)) \quad \text{for all } t \in [0, \infty).
\]

Since \( \sum_{r+s=1}^\infty (r+s)c_{r,s}(t) \) is bounded then \( \mathcal{P}^+(c) \) is relatively compact in \( \mathbb{B}^+_{\rho_0, \sigma_0} \). We can now apply the invariance principle to conclude that \( \omega(c) \) is non-empty and consists of solutions of (2.1.1), \( d(\cdot) \), along which \( V_{w, z} \) takes the constant value \( V_{w, z}^\infty = \lim_{t \to \infty} V_{w, z}(c(t)) \) and \( V_{w, z_c} \) takes the value \( V_{w, z_c}^\infty = \lim_{t \to \infty} V_{w, z_c}(c(t)) \). This means that \( \int_0^t D(d(\tau)) d\tau \to 0 \) for all \( t \geq 0 \), and so \( d_{r,s}(t) = Q_{r,s} d_{1,0}(t)^* d_{0,1}(t)^* \) for all \( t \geq 0 \). Corollary 2.1.7 says that both densities \( \sum_{r+s=1}^\infty r d_{r,s}(t) \) and \( \sum_{r+s=1}^\infty s d_{r,s}(t) \) are conserved and Lemma 2.4.8 says that there is at most one solution to

\[
\begin{align*}
F(w, z) &= \sum_{r+s=1}^\infty r d_{r,s}(0) \\
G(w, z) &= \sum_{r+s=1}^\infty s d_{r,s}(0)
\end{align*}
\]

Hence \( d_{r,s}(t) = Q_{r,s} w^r z^s \) for all \( t \geq 0 \) for some \( (w, z) \in \Gamma \); i.e., \( \omega(c) \) consists of equilibrium points \( e^{w_z} \), for which \( V_{w, z}(e^{w_z}) = V_{w, z_0}^\infty \) for every \( z_0 > 0 \) and \( V_{w, z_c}(e^{w_z}) = V_{w, z_c}^\infty \) for every \( w_0 > 0 \). The results of Proposition 2.5.3 plusLemma 2.4.8 tell us that \( \omega(c) = \{ e^{w_z} \} \) for a unique point \( (w, z) \in \Gamma \) such that \( F(w, z) \leq \rho_0 \) and \( G(w, z) \leq \sigma_0 \). \( \diamond \)

2.6.2 Minimising the Lyapunov functions

We have just seen that a solution of (2.1.1) tends weakly to some unique equilibrium point. The best guess of which equilibrium point it tends to is the point that minimises \( V \) over \( X_{\rho, \sigma} \), while ‘losing’ as
little of their original density as possible. The following Theorem finds these points; it is the equivalent of Theorem 4.4 in [2].

For \(0 \leq \rho < \infty\), \(0 \leq \sigma < \infty\) define \(X_{\rho,\sigma}^+ = \left\{ x \in X^+: \sum_{r+s=1}^{\infty} r x_{r,s} = \rho, \sum_{r+s=1}^{\infty} s x_{r,s} = \sigma \right\} \).

**Theorem 2.6.2**

Assume (2.5.4) and (2.5.5) hold

(i) If there is a \((w, z) \in \Gamma\) such that \(F(w, z) = \rho\) and \(G(w, z) = \sigma\) then \(e^{w, z}\) is the unique minimiser of \(V\) on \(X_{\rho,\sigma}^+\) and of \(V_{w, z}\) on \(X^+\). Any minimising sequence of \(V\) on \(X_{\rho,\sigma}^+\) will converge strongly to \(e^{w, z}\).

Assume further that \(\frac{1}{w_{c}} = \lim_{r \to \infty} Q_{r,0}^{1/r} \ast \) and \(\frac{1}{z_{c}} = \lim_{s \to \infty} Q_{0,s}^{1/s} \ast \).

(ii) Suppose that there is a \(\rho, \sigma \in (0, w_{c})\) such that \(F(\alpha_{\rho}, \zeta_{\sigma}) = \rho\) and \(G(\alpha_{\rho}, \zeta_{\sigma}) < \sigma\) then:

\[
\inf_{c \in X_{\rho,\sigma}^+} V_{\alpha_{\rho}, \zeta_{\sigma}}(c) = V_{\alpha_{\rho}, \zeta_{\sigma}}(e^{\alpha_{\rho}, \zeta_{\sigma}})
\]

\[
\inf_{c \in X_{\rho,\sigma}^+} V(c) = V(e^{\alpha_{\rho}, \zeta_{\sigma}}) + \ln(\zeta_{\sigma})[\sigma - G(\alpha_{\rho}, \zeta_{\sigma})].
\]

If \(c^{j}\) is a minimising sequence of \(V\) or \(V_{\alpha_{\rho}, \zeta_{\sigma}}\) in \(X_{\rho,\sigma}^+\) then \(c^{j} \xrightarrow{\ast} e^{\alpha_{\rho}, \zeta_{\sigma}}\) as \(j \to \infty\), but the convergence is not strong.

(iii) Suppose that there is a \(\beta_{\sigma} \in (0, \zeta_{\sigma})\) such that \(F(\bar{w}_{c}, \beta_{\sigma}) < \rho\) and \(G(\bar{w}_{c}, \beta_{\sigma}) = \sigma\) then:

\[
\inf_{c \in X_{\rho,\sigma}^+} V_{\bar{w}_{c}, \beta_{\sigma}}(c) = V_{\bar{w}_{c}, \beta_{\sigma}}(e^{\bar{w}_{c}, \beta_{\sigma}})
\]

\[
\inf_{c \in X_{\rho,\sigma}^+} V(c) = V(e^{\bar{w}_{c}, \beta_{\sigma}}) + \ln(\bar{w}_{c})[\rho - F(\bar{w}_{c}, \beta_{\sigma})].
\]

If \(c^{j}\) is a minimising sequence of \(V\) or \(V_{\bar{w}_{c}, \beta_{\sigma}}\) in \(X_{\rho,\sigma}^+\) then \(c^{j} \xrightarrow{\ast} e^{\bar{w}_{c}, \beta_{\sigma}}\) as \(j \to \infty\), but the convergence is not strong.

(iv) Suppose that \(F(\bar{w}_{c}, \bar{z}_{c}) < \rho\) and \(G(\bar{w}_{c}, \bar{z}_{c}) < \sigma\) then:

\[
\inf_{c \in X_{\rho,\sigma}^+} V_{\bar{w}_{c}, \bar{z}_{c}}(c) = V_{\bar{w}_{c}, \bar{z}_{c}}(e^{\bar{w}_{c}, \bar{z}_{c}})
\]

\[
\inf_{c \in X_{\rho,\sigma}^+} V(c) = V(e^{\bar{w}_{c}, \bar{z}_{c}}) + \ln(\bar{w}_{c})[\rho - F(\bar{w}_{c}, \bar{z}_{c})] + \ln(\bar{z}_{c})[\sigma - G(\bar{w}_{c}, \bar{z}_{c})].
\]

If \(c^{j}\) is a minimising sequence of \(V\) or \(V_{\bar{w}_{c}, \bar{z}_{c}}\) in \(X_{\rho,\sigma}^+\) then \(c^{j} \xrightarrow{\ast} e^{\bar{w}_{c}, \bar{z}_{c}}\) as \(j \to \infty\), but the convergence is not strong.

Note that the situation where \(\Lambda(Q) \setminus \Gamma \neq \emptyset\) and \(F(w, z) < \rho, G(w, z) < \sigma\) for all \((w, z) \in \partial \Gamma\) is not covered by this theorem. At present we do not know enough to even conjecture a result. Figure 2.6.1 shows sketches of typical examples for each of the four cases that are covered above. The graphs of \(f_{\rho}^{(N)}\) and \(g_{\sigma}^{(N)}\), for a large value of \(N\), are shown rather than \(f_{\rho}\) and \(g_{\sigma}\) because this gives a an indication of why the result is true, and why the missing case is so difficult to predict. The black dot indicates the point that \((\bar{w}_{\rho, \sigma}^{(N)}, \bar{z}_{\rho, \sigma}^{(N)})\) is believed to converge to and the point which generates the minimising equilibrium distribution described in the theorem.

**Proof of (i).**

The function \(c_{r,s} \mapsto c_{r,s} \ln \left( \frac{c_{r,s}}{Q_{r,s}w^{r}z^{s}} \right) - 1\) attains a unique minimum at \(c_{r,s}^{w, z} = Q_{r,s}w^{r}z^{s}\). Hence \(e^{w, z}\) is the unique minimum of \(V_{w, z}\) on \(X^+\) and of \(V\) on \(X_{\rho,\sigma}^+\). Further, if \(c^{j}\) is a minimising sequence

\*Recall that \(\bar{w}_{c} := \inf_{z} \left[ \limsup_{r \to \infty} Q_{r,s}^{1/r} \right]^{-1}\), and similarly for \(\bar{z}_{c}\).
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Figure 2.6.1: Sketches of points that minimise the Lyapunov function, for an example where \( z_c > \bar{z}_c \) and \( w_c = \bar{w}_c \).

of \( V \) on \( X^+_{\rho,\sigma} \), then each \( c_{r,s} \rightarrow Q_{r,s}w^rz^s \) as \( j \rightarrow \infty \), i.e. \( c \rightharpoonup c^w/z \) as \( j \rightarrow \infty \). However \( F(w, z) = \rho = \sum_{r+s=1}^{\infty} rc^j_{r,s} \) and \( G(w, z) = \sigma = \sum_{r+s=1}^{\infty} sc^j_{r,s} \) for all \( j \geq 1 \), so Lemma 2.3.7 implies that \( c^j \rightharpoonup c^w/z \). \( \square \)

Proof of (ii).

By (i) we know that \( V_{\alpha, z_c}(c) \geq V_{\alpha, z_c}(c^{\alpha, z_c}) \) for every \( c \in X^+ \). We will prove the result by giving a sequence \( c^j \in X^+_{\rho,\sigma} \) which converges weakly to \( c^{\alpha, z_c} \). Define \( c^j \) by:

\[
c^j_{r,s} = Q_{r,s}c^j_{r,s} + \delta_{j,s}\delta_{0,r} \left( \frac{\sigma - G(\alpha, \bar{z}_c)}{j} \right),
\]

where \( \delta_{j,s}\delta_{0,r} = \begin{cases} 1 & \text{if } s = j \text{ and } r = 0 \\ 0 & \text{otherwise} \end{cases} \) and note that \( \sum_{r+s=1}^{\infty} rc^j_{r,s} = F(\alpha, \bar{z}_c) = \rho \) and \( \sum_{r+s=1}^{\infty} sc^j_{r,s} = G(\alpha, \bar{z}_c) + (\sigma - G(\alpha, \bar{z}_c)) = \sigma \), so \( c^j \in X^+_{\rho,\sigma} \) and \( c^j \rightharpoonup c^{\alpha, z_c} \). Now

\[
V_{\alpha, z_c}(c^j) = V_{\alpha, z_c}(c^{\alpha, z_c}) + \varepsilon_j
\]

where

\[
\varepsilon_j = \left[ Q_{0,s}\bar{z}_c^s + \left( \frac{\sigma - G(\alpha, \bar{z}_c)}{s} \right) \right] \left[ \ln \left( \frac{Q_{0,s}\bar{z}_c^s - \sigma - G(\alpha, \bar{z}_c)}{Q_{0,s}\bar{z}_c^s} \right) - 1 \right] + Q_{0,s}\bar{z}_c^s.
\]

Since \( \lim_{s \to \infty} Q_{0,s}^{1/s} = (\bar{z}_c)^{-1} \) we can see that \( \varepsilon_j \to 0 \) as \( s \to \infty \), and so

\[
\inf_{c \in X^+_{\rho,\sigma}} V_{\alpha, z_c}(c) = V_{\alpha, z_c}(c^{\alpha, z_c}).
\]

Equation (2.6.4) then follows from this and the definition of \( V_{w,z} \).

If \( c^j \) is a general minimising sequence of \( V \) on \( X^+_{\rho,\sigma} \), then \( V_{\alpha, z_c}(c^j) \to V_{\alpha, z_c}(c^{\alpha, z_c}) \) as \( j \to \infty \), and so is a minimising sequence of \( V_{\alpha, z_c} \) on \( X^+_{\rho,\sigma} \). This and part (i) imply that \( c^j_{r,s} \rightharpoonup \alpha_{r,s} \) for each \( r \geq 0, s \geq 0 \), i.e. \( c^j \rightharpoonup c^{\alpha, z_c} \). Convergence cannot be strong because \( \|c^j\| = \sum_{r+s=1}^{\infty} (r+s)c^j_{r,s} = \rho + \sigma \), whereas \( \|c^{\alpha, z_c}\| = F(\alpha, \bar{z}_c) + G(\alpha, \bar{z}_c) < \rho + \sigma \). \( \square \)

(iii) and (iv) can be proved in a similar way using

\[
c^j_{r,s} = Q_{r,s}w^r\beta^s_\sigma + \delta_{0,s}\delta_{j,r} \left( \frac{\rho - F(\bar{w}_c, \beta_\sigma)}{j} \right)
\]
and \( C_{r,s}^t = Q_{r,s} \bar{w}^t_{c} \bar{z}^t_{c} + \delta_{0,s} \delta_{j,r} \left( \frac{\rho - F(\bar{w}_{c}, \bar{z}_{c})}{j} \right) \)
\[ + \delta_{0,r} \delta_{j,s} \left( \frac{\sigma - G(\bar{w}_{c}, \bar{z}_{c})}{j} \right), \]
respectively.

\[ \text{Conjecture 2.6.3} \]
Assume that \( A_{r,s} > 0, A_{r,s} = O((r + s)\alpha) \) for some \( \alpha \in (0,1) \) and that equations (2.5.4), (2.5.5), (2.5.7) and (2.5.8) hold. Let \( c \) be a solution of (2.1.1) on \([0, \infty)\) and let \( \rho_0 = \sum_{r+s=1}^{\infty} rc_{r,s}(0), \)
\[ \sigma_0 = \sum_{r+s=1}^{\infty} sc_{r,s}(0). \]

(i) If there is a \((w, z) \in \Gamma\) such that \( F(w, z) = \rho_0 \) and \( G(w, z) = \sigma_0 \) then \( c(t) \to c^{w,z}, \) as \( t \to \infty. \)

(ii) Suppose that there is an \( \alpha_\rho \in (0, w_c) \) such that \( F(\alpha_\rho, z_c) = \rho_0 \) and \( G(\alpha_\rho, z_c) < \sigma_0 \) then \( c(t) \to c^{w_\rho, z_c}, \) as \( t \to \infty. \)

(iii) Suppose that there is a \( \beta_\sigma \in (0, z_c) \) such that \( F(w_c, \beta_\sigma) < \rho_0 \) and \( G(w_c, \beta_\sigma) = \sigma_0 \) then \( c(t) \to c^{w_c, \beta_\sigma}, \) as \( t \to \infty. \)

(iv) Suppose that \( F(w_c, z_c) = \rho_0 \) and \( G(w_c, z_c) = \sigma_0 \) then \( c(t) \to c^{w_c, z_c}, \) as \( t \to \infty. \)

The hypotheses of the conjecture are those of both Theorem 2.6.1 and Theorem 2.6.2. In all the proofs of the equivalent theorem for the one-component system (Theorem 5.6 in [2], Theorem 5 in [26] and Theorem 5.11 in [27]) it was necessary to make further assumptions on the coefficients and to assume that the solutions of the equations where unique to the initial data.
Chapter 3

Metastable Solutions of the Finite Becker-Döring Equations

In this Chapter we construct a class of metastable solutions to the finite systems of Becker-Döring equations. This gives theoretical backing to the claim made in [22] and [13] that numerical solutions of a truncated Becker-Döring system are metastable. The work follows along roughly the same lines as those used by Penrose in [12], where he showed that the full Becker-Döring system had metastable solutions. Proving results for the infinite system is simpler than for the finite case because it is possible to construct monotonic bounds on the solutions. Here we have found non-monotonic bounds that play the same rôle as Penrose’s bounds but their construction is technically complex. The first section is intended to give the reader an overview of chapter’s contents.

3.1 Preliminaries

In this section we state the properties of the truncated Becker-Döring equations, describe the notation used and summarise the results that are proved in the later sections.

3.1.1 The finite Becker-Döring equations

The Becker-Döring equations are:

\begin{equation}
\begin{align*}
\dot{c}_1 &= -J_1 - \sum_{r=1}^{N-1} J_r \\
\dot{c}_r &= J_{r-1} - J_r & \text{for } r = 2, 3, \ldots, N-1 \\
\dot{c}_N &= J_{N-1}.
\end{align*}
\end{equation}

The following statements about the finite system (3.1.1) are easily established. Given \( c(0) \):

1. The system has a unique solution.

2. Density \( \sum_{r=1}^{N} rc_r(t) \) is conserved over time. That is \( \rho := \sum_{r=1}^{N} rc_r(0) = \sum_{r=1}^{N} rc_r(t) \) for all \( t \geq 0 \).

3. \( V(c) = \sum_{r=1}^{N} c_r \left[ \ln \left( \frac{c_r}{Q_r z^r} \right) - 1 \right] \), where \( Q_r = \frac{a_{r-1} a_{r-2} \cdots a_1}{b_r b_{r-1} \cdots b_2} \) and \( z \) is the unique solution of \( \sum_{r=1}^{N} r Q_r z^r = \rho \), is a Lyapunov function.
4. \( \{c_r(t)\} \to \{Q_r \bar{z}^r\} \) as \( t \to \infty \).

An important property of \( \{a_r Q_r \bar{z}^r\} \) is that, under certain assumptions on \( \{a_r\} \) and \( \{b_r\} \) (e.g. H3–I in Section 3.1.4), if \( \bar{z} > z_* \) then it has a unique local minimum and if \( \bar{z} \leq z_* \) then it is non-increasing. When \( \{Q_r \bar{z}^r\}^{\infty}_{r=1} \) has a local minimum we denote the value of \( r \) at which it attains it by \( \bar{\ell}(\bar{z}) \). (In [12] and [24] \( \ell^* \) was used).

### 3.1.2 Metastability

The introduction gave motivation for defining a metastable chemical solution\(^\dagger\) as one:

(a) where the total concentration of super-critical clusters is at most exponentially small but will eventually become algebraically small;

(b) where it will take at least an exponentially long time for this to happen, and

(c) where it is highly unlikely that the concentration of super-critical clusters will ever decrease by an algebraically small amount.

Here we need a definition of a metastable solution of (3.1.1), so in this section we will show how to adapt the above to what is needed.

We first note that because we are using asymptotic scales (replacing ‘very small’ with ‘at most exponentially small’), it is only possible to talk about solutions being metastable, once their behaviour has been compared to that of a sequence of solutions whose densities tend to \( \rho_* \). In other words a solution \( c \) can only be said to be metastable if it belongs to a class of metastable solutions \( \{c(\rho) : \rho \in (\rho_* , \mathcal{P})\} \), for some \( \mathcal{P} > \rho_* \). In [12], Penrose showed that a class of solutions with specific initial data were metastable. M. Kreer in [24] showed that another set of initial data was also metastable and then showed that if this data were perturbed by a exponentially small amount then the solution would remain metastable. We will incorporate this perturbation result into our definition of metastability by first giving the definition of a metastable class of solutions, \( \{\mathcal{R}_\rho\} \), where each \( \mathcal{R}_\rho \) is a subset of the space of all possible configurations. A metastable class of solutions is then defined to be one for which \( c(\rho)(0) \in \mathcal{R}_\rho \) for each \( \rho \in (\rho_* , \mathcal{P}) \).

The equivalence of (a) above and M I below is can be seen, by noting that the size of a critical cluster is the size where the concentration of super-critical clusters will eventually become algebraically small.

It is not possible to discuss the likelihood of return to the metastable region fully, without treating \( c \) as a random variable and this is beyond the scope of the existing theory. However both systems (infinite and finite) of Becker-Döring equations have Lyapunov/free-energy functions, see 3 above. So we know that if \( V(c(t)) < \min(V(\mathcal{R}_\rho)) \) (where \( \mathcal{R}_\rho \) is the metastable region) then the solution is not in \( \mathcal{R}_\rho \) and cannot be at any later time. This fact motivates the weakening of (c) above to M III below.

**Definition 3.1.1.** A class of regions \( \{\mathcal{R}_\rho : \rho \in (\rho_* , \mathcal{P})\}, \ (x_r) \in \mathcal{R}_\rho \implies \sum_{r=1}^{N} r x_r = \rho \), for some \( \mathcal{P} > \rho_* \) is said to be metastable if

\[
\begin{align*}
M I \quad (x_r) &\in \mathcal{R}_\rho \implies \sum_{r=\ell(\bar{z})+1}^{N} r x_r \text{ is at most exponentially small but } \sum_{r=\ell(\bar{z})+1}^{N} r Q_r \bar{z}^r \text{ is at least algebraically small.} \\
M II \quad \text{If } c(0) \in \mathcal{R}_\rho \text{ then } t_\rho := \inf\{t : c(t) \notin \mathcal{R}_\rho\} \text{ is at least exponentially large.} \\
M III \quad \text{There exists a continuous function } V : \mathbb{R}^N \to \mathbb{R}^+ \text{ and an } S_\rho \text{ such that, if } c(0) \in \mathcal{R}_\rho \text{ then} \\
&\quad (a) \ V(c(s)) \in V(\mathcal{R}_\rho) \quad \forall s < S_\rho , \text{ and}
\end{align*}
\]

\(^\dagger\)Where \( z_* \) is the radius of convergence of \( \sum_{r=1}^{\infty} r Q_r \bar{z}^r \).

\( ^\dagger \)To avoid ambiguity when the word ‘solution’ is used to mean a solute dissolved in a solvent we will say ‘chemical solution’ and the word ‘solution’ by itself will mean a solution of an equation(s).
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(b) \( c(s) \notin \mathcal{R}_\rho \ \forall s > S_\rho \).

A class of solutions \( \{ c_\rho : \rho \in (\rho_s, \mathcal{P}) \} \) is metastable if \( c_\rho(0) \in \mathcal{R}_\rho \) for every \( \rho \in (\rho_s, \mathcal{P}) \) and \( \mathcal{R}_\rho \) is a metastable class of regions. A subset of configuration space is metastable if it is an element in a metastable class of regions, and a solution metastable if it belongs to a class of metastable solutions.

The definition of the asymptotic expressions, such as ‘at least exponentially large’, are given below.

**Definition 3.1.2.** Let \( f \) be a real valued function defined on an interval \( (\rho_s, \rho) \). Then:

- \( f(\rho) \) is at least exponentially large if there is a \( \varepsilon > 0 \) and a \( \eta > 0 \) such that \( f(\rho) > e^{(\rho - \rho_s) - \eta} \ \forall \rho \in (\rho_s, \rho_s + \varepsilon) \)
- \( f(\rho) \) is at least algebraically large if there is a \( \varepsilon > 0 \) and a \( \eta > 0 \) such that \( f(\rho) > (\rho - \rho_s)^{-\eta} \ \forall \rho \in (\rho_s, \rho_s + \varepsilon) \)
- \( f(\rho) \) is at least algebraically small if there is a \( \varepsilon > 0 \) and a \( \eta > 0 \) such that \( f(\rho) > (x - a)^n \ \forall \rho \in (\rho_s, \rho_s + \varepsilon) \)
- \( f(\rho) \) is at least exponentially small if there is a \( \varepsilon > 0 \) and a \( \eta > 0 \) such that \( f(\rho) > e^{-(\rho - \rho_s) - \eta} \ \forall \rho \in (\rho_s, \rho_s + \varepsilon) \)

Equivalent definitions are given to expressions such as ‘at most exponentially large’. We will only say that \( f \) is exponentially large if there is an \( \varepsilon, \eta' \) and \( \eta \) such that \( e^{(\rho - \rho_s) - \eta'} < f(\rho) < e^{(\rho - \rho_s) - \eta} \ \forall \rho \in (\rho_s, \rho_s + \varepsilon) \). Similarly for the other terms.

### 3.1.3 The Penrose strategy

In the introduction we outlined how Penrose proved that certain solutions of (1.1.1) were metastable. In this section we describe how that strategy is applied to the finite case. The key element in defining \( \mathcal{R}_\rho \) and in proving that it is metastable, is to establish upper and lower bounds on the solution of (3.1.1). These bounds only hold for a finite time \( T \), though. A sketch is given in Figure 3.1.1.

![Figure 3.1.1: Sketch of the temporary lower and upper bounds on c. The solid lines represent the bounds and the dotted line the equilibrium distribution](image)

\( \mathcal{R}_\rho \) is then defined as consisting of distributions \( \{ x_r \} \) of density \( \rho \) and where for \( r \leq \ell(\bar{z}) \), \( x_r \) is exponentially close and below \( U_r \) and for \( r > \ell(\bar{z}) \), \( x_r \) is exponentially close and above \( L_r \).
Proving that M I and M III hold is then a matter of calculation. To prove M II we first note that the growth of super-critical clusters is controlled by the size of $J_{t}(z)$. While the bounds hold, $J_{t}(z) \leq J^{*}(z) := a_{t}U_{t} - b_{t+1}L_{t+1}$, we will show that $J^{*}$ is at most exponentially small and so for every $r > \ell(z)$, $c_{r}(t)$ remains very close to $L_{r}$. Since density is conserved the ‘growth’ of super-critical clusters is balanced by the ‘depletion’ of sub-critical clusters and so for every $r > \ell(z)$, $c_{r}(t)$ remains close to $U_{r}$. In other words $c(t)$ remains in $\mathcal{R}_{p}$ until either an exponentially long time has passed or the bounds break down. We can use the ‘smallness’ of $J^{*}$ to show that breakdown of the bounds will also take an exponentially long time. Hence M II holds.

### 3.1.4 Hypothesises for $a_{r}$ and $b_{r}$

It will be necessary to make assumptions about the behaviour of $a_{r}$ and $b_{r}$. These are listed below, for $r = 2, 3, \ldots$:

- **H3-1** $\frac{b_{r}}{a_{r}} > \frac{b_{r+1}}{a_{r+1}}$.
- **H3-2** $\frac{a_{r}}{r} > \frac{a_{r+1}}{r+1}$.
- **H3-3** $A' \leq a_{r} \leq A r^{\alpha}$ for some $A' > 0$, $A > 0$ and $\alpha \in [0, 1)$.
- **H3-4** $z_{s} \exp \left( \frac{G_{1}'}{r^{\beta_{1}}(r-1)^{k_{1}}} \right) \leq \frac{b_{r}}{a_{r}} \leq z_{s} \exp \left( \frac{G_{1}}{r^{\beta_{1}}(r-2)^{k_{1}}} \right)$ for some $z_{s} > 0$, $G_{1}', G_{1} > 0$ and $\beta_{1}, \beta_{1} \in (0, 1)$.
- **H3-5** $\frac{b_{r+1}/a_{r+1}}{b_{r}/a_{r}} \leq \exp \left( -\frac{G_{2}}{r^{1+\beta_{2}}} \right)$ for some $G_{2} > 0$ and $\beta_{2} \in (0, 1)$. (Note that this implies H3-1.)

In order to illustrate clearly the different aspects of the metastable behaviour of the numerical solutions in Chapter 4, it is necessary to use two different, though similar, sets of coefficients. These are described in the example below. The coefficients used in [13] are case B below. Physical justifications for considering either of these cases is given in [12].

**Example 3.1.3.** If either:

- **Case A** $b_{r} := \exp \left( \frac{1}{r^{\beta_{1}}} \right)$ and $a_{r} := 1$ for all $r$, or

- **Case B** $b_{r} := \exp \left( (r-1)^{k_{1}} (r-2)^{k_{2}} \right)$ and $a_{r} := 1$ for all $r$,

then each of the above hypotheses are satisfied.

**Proof for Case A.**

Clearly H3-1 and H3-2 hold and the the other hypotheses hold with the constants taking the values: in H3-3, $A' = A = 1$ and $\alpha = 0$; in H3-4 $z_{s} = 1$, $G_{1}' = G_{1} = 1$ and $\beta_{1}' = \beta_{1} = \frac{1}{2}$ and in H3-5 $G_{2} = \frac{1}{2}$ and $\beta_{2} = \frac{3}{2}$.

**Proof for Case B.**

Clearly H3-1 and H3-2 hold and the the other hypotheses can be seen to hold once the constants have been set at the following values: in H3-3, $A' = A = 1$ and $\alpha = 0$; in H3-4 $z_{s} = 1$, $G_{1}' = \frac{2}{3}$, $G_{1} = 2 \frac{2}{3}$ and $\beta_{1}' = \beta_{1} = \frac{1}{3}$ and in H3-5 $G_{2} = \frac{2}{3}$ and $\beta_{2} = \frac{1}{3}$.

We will illustrate some of the results below by referring back these cases.
3.1.5 Constant flux

In the introduction we saw that the distributions with constant flux ($J_r = \text{const.}$, for all $r \geq 1$) were very important to the study of metastability. The value of this constant flux corresponds to the nucleation rate of the original Becker-Döring theory of metastability. Here we will perform some of the basic calculations on the constant flux distributions that are useful when constructing the upper-bound. The following algebraic identity is the starting point of most of these calculations.

**Proposition 3.1.4**

$$J_r = a_r c_1 c_r - b_{r+1} c_{r+1}$$

for $r = 1, \cdots, N - 1$

$$\iff c_r = Q_r c_1' \left(1 - \sum_{k=1}^{r-1} \frac{J_k}{a_k Q_k c_1' k + 1}\right)$$

for $r = 1, \cdots, N$

**Proof.**

$$\sum_{k=1}^{r-1} \frac{J_k}{a_k Q_k c_1' k + 1} = \frac{c_r}{Q_r c_1'} - \frac{c_{r+1}}{Q_r c_1'} - \frac{c_r}{Q_r c_1'}$$

for $r = 1, \cdots, N - 1$

$$\iff c_r = Q_r c_1' \left(1 - \sum_{k=1}^{r-1} \frac{J_k}{a_k Q_k c_1' k + 1}\right)$$

for $r = 1, \cdots, N$

**Corollary 3.1.5**

If \(\{c_r\}_1^N\) has a constant nucleation rate \(J\) then

$$c_r = Q_r c_1' \left(1 - J \sum_{k=1}^{r-1} \frac{1}{a_k Q_k c_1' k + 1}\right)$$

for $r = 1, \cdots, N - 1$

From now on we will use the following notation:

$$A_k(z) := \frac{1}{a_k Q_k z^{k+1}}$$

and

$$M_r(z, J) := Q_r z^r \left(1 - J \sum_{k=1}^{r-1} A_k(z)\right).$$

The upper bound on the solutions is made up of three sections, the first of which is of the form $M_r(z, J)$. The upper bound used in [12] and described in the Introduction is $f_r(z) = M_r \left(\frac{z - \frac{b_r}{a_r}}{z \sum_{k=1}^{r-2} A_k(z) - \frac{b}{a_r} \sum_{k=1}^{r-2} A_k(z)}\right)$.

The Lemma 3.1.8 shows that, when H3–1 holds, the sequence \(\{a_r, M_r(z, J)\}\) behaves in a similar way to \(\{a_r Q_r z^r\}\). The behaviour of \(\{a_r Q_r z^r\}\) is summarised in the next lemma.

**Lemma 3.1.6**

Assuming H3–1:

(i) If $z > \frac{b_r}{a_r}$ then $\ell(z)$ is not defined and \(\{a_r, Q_r z^r\}\) is increasing;

(ii) If $\ell(z)$ is defined then \(\{a_r, Q_r z^r\}\) in decreasing for $r \leq \ell(z)$ and increasing for $r \geq \ell(z)$;

(iii) If $z_s \geq z$ then $\ell(z)$ is not defined and \(\{a_r, Q_r z^r\}\) is decreasing.

The results follow immediately from the observation that:

$$a_r Q_r z^r = a_{r-1} Q_{r-1} z^{r-1} \times \frac{a_r}{b_r} z$$

Before we prove the equivalent results concerning \(\{a_r, M_r(z, J)\}\) we define

$$q_r(z) := \frac{z - \frac{b_r}{a_r}}{z \sum_{k=1}^{r-1} A_k(z) - \frac{b}{a_r} \sum_{k=1}^{r-2} A_k(z)}.$$
and show that \( \{q_r(z)\}_{r=1}^\infty \) is increasing.

**Lemma 3.1.7**

Assuming H3–1:

(i) \( \{q_r(z)\} \) is increasing in \( r \), with \( q_\ell(z) \leq 0 \) and \( q_{\ell+1}(z) > 0 \).

(ii) For any fixed \( r > 1 \), \( \frac{d}{dz}(q_r(z)) > 0 \).

**Proof.**

We will first show that \( -D_r(z) := \sum_{k=1}^{r-1} A_k(z) - \frac{b_r}{a_r} \sum_{k=1}^{r-2} A_k(z) > 0 \)

\[
z \sum_{k=1}^{r-1} A_k(z) - \frac{b_r}{a_r} \sum_{k=1}^{r-2} A_k(z) = \sum_{k=1}^{r-1} \frac{1}{a_k Q_k z^k} - \frac{b_r}{a_r} \sum_{k=1}^{r-2} \frac{1}{a_k Q_k z^{k+1}}
\]

\[
= \frac{1}{a_1 z^r} + \sum_{k=2}^{r-1} \frac{1}{z^k} \left( \frac{1}{a_k Q_k} - \frac{b_r}{a_r} \frac{1}{a_{k-1} Q_{k-1}} \right)
\]

\[
= \frac{1}{a_1 z} + \sum_{k=2}^{r-1} \frac{1}{a_{k-1} Q_{k-1} z^k} \left( \frac{b_k}{a_k} - \frac{b_r}{a_r} \right)
\]

(3.1.2)

By H3–1, all terms in (3.1.2) are positive. Hence the sign of \( q_r(z) \) is the same as the sign of \( z - \frac{b_r}{a_r} \).

i.e. \( q_r(z) \leq 0 \) for all \( r < \ell \) and \( q_r(z) > 0 \) for all \( r > \ell \).

We will complete the proof of part (i) by showing that \( q_{r+1}(z) - q_r(z) > 0 \).

\[
q_{r+1}(z) - q_r(z) = \left[ \left( \frac{z}{a_r} \right) \left( \frac{z}{a_r} \right) \right] \left( \sum_{k=1}^{r-1} A_k - \frac{b_r}{a_r} \sum_{k=1}^{r-2} A_k \right) - \left( \sum_{k=1}^{r-1} A_k - \frac{b_r}{a_r} \sum_{k=1}^{r-2} A_k \right)
\]

\[
= \left( \frac{z}{a_r} \right) \left( \frac{z}{a_r} \right) \left( \sum_{k=1}^{r-1} A_k - \frac{b_r}{a_r} \sum_{k=1}^{r-2} A_k \right)
\]

\[
= -A_r z^2 + \frac{b_r}{a_r} \left( A_r + A_{r-1} - \frac{b_r}{a_r} A_{r-1} \right) \div D_{r+1}D_r
\]

We began by showing that \( D_r > 0 \) and H3–1 tells us that \( \left[ \frac{b_r}{a_r} - \frac{b_{r+1}}{a_{r+1}} \right] \geq 0. \) Hence \( q_{r+1}(z) - q_r(z) > 0 \).

Part (ii) is proved by observing that since \( D_r = \frac{-1}{a_1} + \sum_{k=2}^{r-1} \frac{z^{-k}}{a_{k-1} Q_{k-1}} \left( \frac{b_k}{a_k} - \frac{b_r}{a_r} \right) \) then the coefficients of \( z^{-k} \) are positive and so \( \frac{d}{dz}(D_r(z)) < 0 \). Finally, by noting that \( \frac{d}{dz} \left( z - \frac{b_r}{a_r} \right) = 1 \), we clearly see that \( \frac{d}{dz}q_r > 0 \).
Lemma 3.1.8
Assuming \( H3{-1} \):

(i) If \( \{q_r(z)\} \) is bounded above and \( J > \sup \{q_r(z)\} \) then \( \{a_rM_r(z,J)\} \) is decreasing;

(ii) If there is a \( k \) such that \( q_k(z) < J < q_{k+1}(z) \) then \( \left\{a_rM_r(z,J)\right\}_{r=1}^{k} \) is decreasing and \( \left\{a_rM_r(z,J)\right\}_{r=k}^{\infty} \) is increasing;

(iii) If \( J = q_k(z) \) then \( \left\{a_rM_r(z,J)\right\}_{r=1}^{k-1} \) is decreasing, \( a_{k-1}M_{k-1} = a_kM_k \) and \( \left\{a_rM_r(z,J)\right\}_{r=k}^{\infty} \) is increasing;

(iv) If \( J < q_2 \) then \( \{a_rM_r(z,J)\} \) is increasing.

Proof.
All of the above follow from:

\[
a_rM_r - a_{r-1}M_{r-1} = a_rQ_rz^{r-1} \left[ z \left( 1 - J \sum_{k=1}^{r-1} A_k(z) \right) - \frac{b_r}{a_r} \left( 1 - J \sum_{k=1}^{r-2} A_k(z) \right) \right] \]

\[
= a_rQ_rz^{r-1} \left[ \left( z - \frac{b_r}{a_r} \right) - J \left( z \sum_{k=1}^{r-1} A_k(z) - \frac{b_r}{a_r} \sum_{k=1}^{r-2} A_k(z) \right) \right] \]

\[
= a_rQ_rz^{r-1} [q_r - J] D_r \quad \checkmark
\]

3.1.6 Construction of the bounds

When constructing the upper bound we need to control the position of the turning point of \( \{a_rM_r(z,J)\} \).
Lemma 3.1.8 shows us that given \( z \) and \( k \), the sequence will attain its minimum at \( r = k \) if
\( q_k(z) \leq J \leq q_{k+1}(z) \). The value of \( z \) must also be carefully selected; it must satisfy:

\[
\sum_{r=1}^{m(z)} rQ_rz^r > \rho
\]

where \( m(z) := \max \left\{ r : \frac{b_r}{a_r} - \frac{b_r}{a_r} \leq z > \frac{b_{r+1}}{a_{r+1}} - \frac{b_{r+1}}{a_{r+1}} \right\} \), and where \( \gamma > \frac{1+b'_{r} y}{1-y} \). We will use \( \omega_r \) to denote \( \frac{b_r}{a_r} - \frac{b_r}{a_r} \).

Theorem 3.3.1 on page 72 states that if: \( H3{-2} \) to \( H3{-5} \) hold, \( z \) satisfies the condition above; \( N \geq m(z) \); \( z_e < z \); \( \ell^* \) is some integer between \( \ell(z) \) and \( \ell(z_e) =: \ell_e \) and \( J \in (q_{\ell-e-1}, q_{\ell^*}] \), then

\[
U_r(z, z_e, J, \ell^*) = \begin{cases} M_r(z, J) & \text{for } 1 \leq r \leq \ell^* \\ b_rM_r(z, J) & \text{for } \ell^* \leq r \leq \ell_e + 1 \\ b_rM_r(z, J) & \text{for } \ell_e + 1 \leq r \leq N \end{cases}
\]

will be an upper bound to any solution \( c(t) \) for which \( c(0) \leq U(z, z_e, J, \ell^*) \), and \( t \) satisfying \( t < \min \{ \inf \{ s : c_1(s) < z_e \}, \inf \{ s : c_N(s) > U_N \} \} \). Figure 3.3.1 on page 72 shows a sketch of \( U_r \).

Theorem 3.3.3 on page 75 states that if \( I \geq \max \{q_N(y), 0\} \) and \( c(0) \geq M(y, I) \) then \( c(t) \geq M(y, I) \) while \( t < \inf \{ s : c_1(s) < y \} \). Figure 3.1.1 on page 59 shows a sketch of both an upper and a lower bound.

\[\footnote{When } \gamma > \frac{1+b_{r} y}{1-y} \text{, then } \frac{b_r}{a_r} > \omega_r > \frac{b_{r+1}}{a_{r+1}} \text{ for all sufficiently large } r \text{ and so there will be no loss of meaning if } \omega_r \text{ is read as } \frac{b_r}{a_r} \text{ and } m(z) \text{ is read as } \ell(z). \text{ See Corollary 3.2.5 for exact statement.} \]
3.1.7 Definition of \( \{ R_\rho : \rho \in (\rho_\delta, P) \} \)

When defining a class of regions \( \{ R_\rho : \rho \in (\rho_\delta, P) \} \), it is necessary to state explicitly how \( z_c, z_0 \) and \( N \) depend on \( \rho \). Once these have been given we define \( R_\rho \) as the set of all distributions \( \{ x_r \}_{r=1}^N \) which satisfy:

\[
\sum_{r=1}^N r x_r = \rho;
\]

b. for some \( J \geq 0 \) and \( \ell^* \) satisfying the conditions for an upper bound (see above or Theorem 3.3.1) we have that:

\[
x_r \leq U_r(z, z_c, J, \ell^*) \quad \text{for} \quad 1 \leq r \leq N
\]

and \( U_r(z, z_c, J, \ell^*) - x_r \) is at most exponentially small \( \quad \text{for} \quad 1 \leq r \leq \ell(z_c) \);

c. for some \( y \leq z_c \) and \( I \) which satisfy the conditions for a lower bound (see above or Theorem 3.3.3) we have that:

\[
x_r \geq L_r(y, I) \quad \text{for} \quad 1 \leq r \leq N
\]

and \( x_r - L_r(y, I) \) is at most exponentially small \( \quad \text{for} \quad \ell(z_c) < r \leq N \).

In the following results we only consider those classes where \( z \) is such that \( \sum_{r=1}^{m(z)} r Q_r z^r \geq \rho \) but \( \sum_{r=1}^{m(z)} r Q_r z^r - \rho \) is at most exponentially small; \( N \) is algebraically large and \( N \geq m(z)^{\gamma} \) and \( z_c \) is the unique solution of \( \sum_{r=1}^{N} r Q_r w^r = \rho \). In Chapter 4 we will look at the classes where \( z = \min \{ w : \sum_{r=1}^{m(w)} r Q_r w^r = \rho \} \) and \( N = m^\gamma(z) \left( \frac{2 - \rho}{\rho - \rho_\delta} \right)^{1/4} \); we vary \( \gamma \) to compare the behaviour of different classes.

3.2 Technical Results

3.2.1 Estimates

In order to perform the calculations necessary to show that \( \{ R_\rho \} \) satisfies M I to M III, we need bounds on various quantities, such as \( Q_r \omega_r^* \). These are established here. They are also useful in proving that the \( z \)'s of the upper bound exist.

Lemma 3.2.1

Assuming H3–3, H3–4, H3–5–:

(i) For all \( r \geq 2 \) \( \quad \Gamma \exp \left( \frac{G_1}{1 - \beta_1} r^{1 - \beta_1} \right) \leq a_r Q_r z_r^* \leq \Gamma' \exp \left( - \frac{G'_1}{1 - \beta'_1} r^{1 - \beta'_1} \right) \)

where \( \Gamma = a_1 z_a \exp \left( \frac{G_1}{\beta_1} \right) \) and \( \Gamma' = a_1 z_a \exp \left( \frac{G'_1}{1 - \beta'_1} 2^{1 - \beta'_1} \right) \).

(ii) For all \( r \geq 2 \) \( a_r Q_r \omega_r^* \leq a_r Q_r \left( \frac{b_r}{\alpha_r} \right) r \leq \Gamma_2 \exp \left( - \frac{G_2}{1 - \beta_2} r^{1 - \beta_2} \right) \)

where \( \Gamma_2 = \frac{a_1}{a_2} b_2 \exp \left( \frac{G_2}{\beta_2} 2^{1 - \beta_2} \right) \).

(iii) Both \( \lim_{r \to \infty} \sum_{k=1}^{r} k^2 Q_k \left( \frac{b_r}{\alpha_r} \right)^k \) and \( \lim_{r \to \infty} \sum_{k=1}^{r} k^2 Q_k \omega_r^k \) are finite.

(iv) Provided that \( \gamma > \frac{1 + \beta'_1}{1 - \alpha} \), then there exist an \( R_1 \in \mathbb{N} \) and a \( H > 0 \) such that for all \( r \geq R_1 \)

\( \omega_r > z_a \exp \left( \frac{H}{r^{\gamma'_1}} \right) \).
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(v) There exist an \( R_2 \in \mathbb{N} \) and a \( \zeta > 0 \) such that for all \( r \geq R_2 \)
\[
\sum_{k=r+1}^{\infty} k Q_k z_k^k < e^{-r^\zeta}
\]

Proof.

(i) This is calculated directly:
\[
Q_r = \frac{a_r}{a_r} \prod_{k=2}^{r} \frac{a_k}{a_k} \leq \frac{a_1 z_s}{a_r z_s} \prod_{k=2}^{r} e^{-G_1/k^\alpha} = \frac{a_1 z_s}{a_r z_s} \exp \left( -G_1 \sum_{k=2}^{r} \frac{1}{k^\alpha} \right)
\]
Similarly
\[
Q_r \geq \frac{a_1 z_s}{a_r z_s} \exp \left( -G_1 \sum_{k=2}^{r} \frac{1}{k^\alpha} \right)
\]
Now \( 1/x^\beta \) is a decreasing function for all positive \( x \) and all positive \( \beta \). Hence
\[
\left( \frac{1-\beta}{1-\beta} - \frac{2^{1-\beta}}{1-\beta} \right) = \int_2^r \frac{1}{x^\beta} dx < \int_2^{r+1} \frac{1}{x^\beta} dx
\]
\[
< \sum_{k=2}^{r} \frac{1}{k^\beta} \leq \int_1^r \frac{1}{x^\beta} dx = \left( \frac{r^{1-\beta}}{1-\beta} - \frac{1}{1-\beta} \right)
\]
(3.2.1)
Substituting this into the above gives the result.

(ii) Recall \( \omega_r = \frac{b_r}{a_r} - \frac{b_r/r^r}{a_r/r} < \frac{b_r}{a_r} \). Hence
\[
Q_r \omega_r ^r \leq Q_r \left( \frac{b_r}{a_r} \right)^r = \frac{a_1}{a_r} \prod_{k=2}^{r} \frac{b_k}{a_k} \frac{b_r}{a_r}
\]
\[
= \frac{a_1}{a_r} \prod_{k=2}^{r-1} \left[ \frac{b_k+1/a_k}{b_k/a_k} \right]^k \frac{b_2}{a_2}
\]
\[
\leq \frac{a_1}{a_r} \prod_{k=2}^{r-1} \exp \left( -G_2 k \right) \frac{b_2}{a_2}
\]
\[
= \frac{a_1}{a_r} \exp \left( -G_2 \sum_{k=2}^{r-1} \frac{1}{k^\beta} \right) \frac{b_2}{a_2}
\]
but equation (3.2.1) implies that
\[
\frac{a_1}{a_r} \exp \left( -G_2 \sum_{k=2}^{r-1} \frac{1}{k^\beta} \right) \frac{b_2}{a_2} \leq \frac{a_1}{a_r} \frac{a_2}{a_2} \left[ \exp \left( G_2 \frac{2^{1-\beta}}{1-\beta} \right) \times \exp \left( -G_2 \frac{2^{1-\beta}}{1-\beta} \right) \right].
\]
so
\[
a_r Q_r \omega_r ^r < a_r Q_r \left( \frac{b_r}{a_r} \right)^r \leq \Gamma_2 \exp \left( -G_2 \frac{2^{1-\beta}}{1-\beta} \right)
\]

(iii) From part (ii): \( \sum_{k=1}^{r} k^g Q_k \omega_k ^k \leq \sum_{k=1}^{r} k^2 Q_k \left( \frac{b_r}{a_r} \right)^k \) but \( \left( \frac{b_r}{a_r} \right) \leq \left( \frac{b_k}{a_k} \right) \) for every \( k \leq r \) and \( a_k \leq A k^\alpha \) for every \( k \geq 1 \). So
\[
\sum_{k=1}^{r} k^2 Q_k \omega_k ^k \leq \sum_{k=1}^{r} k^2 Q_k \left( \frac{b_k}{a_k} \right)^k \leq \Gamma_2 \sum_{k=1}^{r} k^2 Q_k \left( \frac{b_r}{a_r} \right)^k \left( \frac{b_k}{a_k} \right) \times \exp \left( -G_2 \frac{2^{1-\beta}}{1-\beta} \right).
\]
The function \( f(x) = x^{2+\alpha} \exp \left( -G_2 \frac{2^{1-\beta}}{1-\beta} \right) \) has a local maximum at \( x = \left( \frac{2+\alpha}{G_2} \right)^{\frac{1}{1-\beta}} \) and is decreasing for all \( x > \left( \frac{2+\alpha}{G_2} \right)^{\frac{1}{1-\beta}} \). So, defining \( r_1 \) as the least integer greater than \( \left( \frac{2+\alpha}{G_2} \right)^{\frac{1}{1-\beta}} \),
we can say that
\[
\sum_{k=1}^{r} k^2 Q_k \omega_k^2 < \Lambda_2 \sum_{k=1}^{r_1} k^{2+\alpha} \exp \left( -\frac{G_2}{1 - \beta_2} k^{1-\beta_2} \right) + \Lambda_2 \sum_{k=r_1+1}^{r} k^{2+\alpha} \exp \left( -\frac{G_2}{1 - \beta_2} k^{1-\beta_2} \right)
\]
\[
< \text{con.} + \Lambda_2 \int_{r_1}^{r} x^{2+\alpha} \exp \left( -\frac{G_2}{1 - \beta_2} x^{1-\beta_2} \right) \, dx
\]
\[
= \text{con.} + \frac{\Lambda_2}{1 - \beta_2} \int_{r_1-\beta_2}^{r-\beta_2} y^{2+\beta_2+\alpha} \exp \left( -\frac{G_2}{1 - \beta_2} y \right) \, dy
\]
Clearly \( \lim_{r \to \infty} \int_{r_1-\beta_2}^{r-\beta_2} y^{2+\beta_2+\alpha} \exp \left( -\frac{G_2}{1 - \beta_2} y \right) \, dy \) is finite, so the result follows. \( \diamond \)

(iv) Recall \( \gamma = \frac{b_r}{a_r} \frac{b_r-\gamma/r}{a_r/r} - \frac{b_r-\gamma/r}{a_r/r} \) and \( \frac{b_r-\gamma/r}{a_r/r} \leq \frac{b_r}{a_r} \) since \( \gamma > \frac{1 + \beta_1'}{1 - \alpha} > 1 \)

Hence
\[
\omega_r \geq \frac{b_r}{a_r} \left( 1 - \frac{A}{A' \gamma^{(1-\alpha)-1}} \right)
\]
\[
\geq z_s \exp \left( \frac{G_1'}{2 \gamma} \right) \left[ 1 - \frac{A}{A' \gamma^{(1-\alpha)-1}} \right]
\]
\[
\geq z_s \exp \left( \frac{G_1'}{2 \gamma} \right) \left[ 1 + \frac{G_1'}{2 \gamma} \right] \left[ 1 - \frac{A}{A' \gamma^{(1-\alpha)-1}} \right]
\]
Now \( \gamma > \frac{1 + \beta_1'}{1 - \alpha} \), hence there exists a \( R_1 \) such that
\[
r > R_1 \implies \frac{G_1'}{2 \gamma} > \frac{A}{A' \gamma^{(1-\alpha)-1}} + \frac{AG_1'}{2 A' \gamma^{(1-\alpha)+\beta_1'-1}}.
\]
so
\[
\omega_r > z_s \exp \left( \frac{G_1'}{2 \gamma} \right) \quad \text{for all } r > R_1
\]
\( \diamond \)

(v) From part (i) \( \sum_{k=r+1}^{N} kQ_k z_k^k < \Gamma' \sum_{k=r+1}^{N} k^{1+\alpha} \exp \left( -\frac{G_1'}{1 - \beta_1} k^{1-\beta_1} \right) \) Now for all
\[
x > \left( \frac{1 + \alpha}{G_1'} \right)^{1-\beta_1'}, \text{ the function } f(x) = x^{1+\alpha} \exp \left( -\frac{G_1'}{1 - \beta_1} x^{1-\beta_1} \right) \text{ is decreasing. Let } r_2 \text{ be the least}
\]
integer greater than \( \left( \frac{1 + \alpha}{G_1'} \right)^{1-\beta_1'}, \text{ then } r > r_2 \text{ will imply that}
\[
\sum_{k=r+1}^{N} kQ_k z_k^k < \Gamma' \int_{r}^{N} x^{1+\alpha} \exp \left( -\frac{G_1'}{1 - \beta_1} x^{1-\beta_1} \right) \, dx.
\]
So \( \lim_{N \to \infty} \sum_{k=r+1}^{N} kQ_k z_k^k \) exists and
\[
\sum_{k=r+1}^{\infty} kQ_k z_k^k < \frac{\Gamma'}{G_1'} \left( \frac{1-\beta_1'}{G_1'} \right)^{1-\beta_1'} \int_{r}^{\infty} y^{1-\beta_1} \exp \left( -\frac{G_1'}{1 - \beta_1} y \right) \, dy
\]
\[
< P(r'^{-\beta_1'}) \exp \left( -\frac{G_1'}{1 - \beta_1} r'^{-\beta_1'} \right),
\]
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for some polynomial $P$. So there is a $R_2(\zeta)$ such that

$$r > R_2 \iff \sum_{k=r+1}^{\infty} kQ_k z_s^k < e^{-r^c}$$

for any $\zeta < 1 - \beta_1'$

\[ \diamond \]

**Corollary 3.2.2**

If $H3-3, H3-4, H3-5$ hold and $\gamma > \frac{1 + \beta_1'}{1 - \alpha}$ then

$$\lim_{r \to \infty} \omega_r = z_s$$

and

$$\lim_{r \to \infty} \sum_{k=1}^{r} kQ_k \omega_r^k = \rho_s$$

**Proof.**

By (iv) above $\omega_r > z_s \exp\left(\frac{H}{p\beta_1}\right)$ for all $r > R_1$ and since $\omega_r < \frac{b_r}{a_r}$ for all $r$, it follows that

$$\lim_{r \to \infty} \omega_r = z_s.$$

To establish the other limit, first note that:

$$\sum_{k=1}^{r} kQ_k \omega_r^k = \sum_{k=1}^{r} kQ_k (\omega_r^{k-1} + \omega_r^{k-2} z_s + \cdots + \omega_r z_s^{k-2} + z_s^{k-1})(\omega_r - z_s) = \sum_{k=r+1}^{\infty} kQ_k z_s^k.$$

Then, since $\omega_r > z_s$, we can use part (iii) to derive:

$$(\omega_r - z_s) < \omega_r^{k-2} z_s + \cdots + \omega_r z_s^{k-2} + z_s^{k-1})(\omega_r - z_s)$$

$$< (\omega_r - z_s) \max_{r \in \mathbb{N}} \left\{ \sum_{k=1}^{r} k^2 Q_k \left( \frac{b_r}{a_r} \right)^k \right\} =: K(\omega_r - z_s).$$

We now use (iv) to say that for $r > R_1$, $\frac{z_s}{2} (\omega_r - z_s) > \frac{z_s}{2} \left( \frac{H}{p\beta_1} \right)$ and there exists an $R_3 \in \mathbb{N}$ such that $\frac{z_s}{2} \left( \frac{H}{p\beta_1} \right) > e^{-r^c}$, for all $r > R_3$. Combining all of these gives, for $r > \max\{R_1, R_2, R_3\}$:

$$\frac{1}{2} (\omega_r - z_s) < \sum_{k=1}^{r} kQ_k \omega_r^k - \rho_s < K(\omega_r - z_s)$$

and from this we conclude that

$$\lim_{r \to \infty} \sum_{k=1}^{r} kQ_k \omega_r^k = \rho_s.$$

\[ \diamond \]

**Corollary 3.2.3**

If $H3-3, H3-4, H3-5$ hold then

$$\lim_{r \to \infty} \sum_{k=1}^{r} kQ_k \left( \frac{b_r}{a_r} \right)^k = \rho_s.$$

**Proof.**

By the same arguments to those we used above we see that:

$$\left( \frac{b_r}{a_r} - z_s \right) - \sum_{k=r+1}^{\infty} kQ_k z_s^k < \sum_{k=1}^{r} kQ_k \left( \frac{b_r}{a_r} \right)^k - \rho_s < K \left( \frac{b_r}{a_r} - z_s \right)$$

and so for all $r > \max\{R_1, R_2, R_3\}$ we have that:

$$\frac{1}{2} \left( \frac{b_r}{a_r} - z_s \right) < \sum_{k=1}^{r} kQ_k \left( \frac{b_r}{a_r} \right)^k - \rho_s < K \left( \frac{b_r}{a_r} - z_s \right).$$

From which the result follows. 

\[ \diamond \]
Lemma 3.2.4
If $H3-2$, $H3-3$, $H3-4$, $H3-5$ hold and $\gamma > \frac{1+\beta_1}{1-\alpha}$ then there exists a monotonically increasing sequence $\{r_j\} \subset \mathbb{N}$ such that both $\{\omega_{r_j}\}_{r_j=R}^\infty$ and $\left\{\sum_{k=1}^r kQk^r_c\right\}_{r_j=R}^\infty$ are monotonically decreasing, for some sufficiently large $R \in \mathbb{N}$.

While this result is an immediate corollary to 3.2.2, we will give a constructive proof because the information this gives about $\{r_j\}$ is useful in Section 3.4.1.

Proof.
We define $\{r_j\}$ inductively: $r_1 = \text{ceil} \left( \frac{4G_1}{C_1} \right)$ and $r_{j+1} = \text{ceil} \left( \frac{4G_1}{C_1} r_j^\beta_1 \right)$. Where ceil$(x)$ is the least integer greater than or equal to $x$.

So $r_j^{\beta_1} \geq \left[ \frac{4G_1}{C_1} \right]^{\beta_1} r_j^\beta_1 \implies z_a \exp \left( \frac{1}{2} G_1 r_j \right) \geq z_a \exp \left( \frac{G_1}{r_j^{\beta_1}} \right)$. Hence for $r_j > R_1$

$$\omega_r \leq \omega_{r_j} \exp \left( - \frac{G_1}{2r_j^\beta_1} \right) < \omega_{r_j} \quad (3.2.2)$$

This means that $\left\{ \omega_{r_j} \right\}_{r_j=R_1}^{\infty}$ is decreasing.

To show that $\left\{ \sum_{k=1}^r kQ_k^r c \right\}_{r_j=R}^{\infty}$ is decreasing we calculate that for sufficiently large $r_j$:

$$\sum_{k=1}^{r_j} kQ_k^r c - \sum_{k=1}^{r_{j+1}} kQ_k^r c > (\omega_{r_j} - \omega_{r_{j+1}}) - \sum_{k=r_{j+1}+1}^{r_j} a_k Q_k \left( \frac{b_{r_{j+1}}}{a_{r_{j+1}}} \right)^k$$

$$> \omega_{r_j} \left[ 1 - \exp \left( - \frac{G_1}{2r_j^\beta_1} \right) \right] - \frac{r_{j+1}}{a_{r_{j+1}}} \omega_{r_j} \left[ \frac{b_{r_{j+1}}}{a_{r_{j+1}}} \right]$$

$$> \omega_{r_j} \left[ G_1 \right]^{\beta_1} - \frac{4G_1}{C_1} \left( \frac{2\beta_1/\beta_1}{r_j^\beta_1} - \frac{1}{A_r a_{r_j}} \right) \omega_{r_j} \left( \frac{b_{r_{j+1}}}{a_{r_{j+1}}} \right)$$

$$> \text{con.} r_j^{\beta_1} \exp \left( - \frac{G_2}{1-\beta_2} r_j^{1-\beta_2} \right) > 0 \quad \diamond$$

Under certain circumstances Lemma 3.2.4 is true for $\{r_j\} = \mathbb{N}$. Two such cases are given below.

Lemma 3.2.5
If $H3-3$, $H3-4$, $H3-5$ hold and $\gamma > \frac{2+\beta_1}{1-\alpha}$ then there exists an $R \in \mathbb{N}$ such that $r > R$ implies that

$$\frac{b_{r+1}}{a_{r+1}} < \omega_r < \frac{b_r}{a_r}$$

and $\left\{ \sum_{k=1}^r kQ_k^r c \right\}_{r_j=R}^{\infty}$ is monotonically decreasing.

Proof.
For all $r \geq 2$ we have that $\omega_r < \frac{b_r}{a_r}$. To establish that $\omega_r > \frac{b_{r+1}}{a_{r+1}}$ we make the following calculation, for sufficiently large $r$:

$$\omega_r = \frac{b_{r+1}}{a_{r+1}} + \frac{b_r}{a_r} - \frac{b_{r+1}}{a_{r+1}} \left( \frac{b_r}{a_r} \right) \left( \frac{b_r}{a_r} \right)$$

$$> \frac{b_{r+1}}{a_{r+1}} + \frac{b_r}{a_r} \left( 1 - \exp \left( - \frac{G_2}{r^{1-\beta_2}} \right) \right) - \frac{A}{A^\gamma(1-\gamma)} \omega_{r_j} \exp \left( \frac{G_1}{r^{1-\beta_2}} \right)$$
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\[ \frac{b_{r+1}}{a_{r+1}} + \left[ \frac{\text{con.}}{r^{1+\beta_2}} - \frac{\text{con.}}{r^{\gamma(1-\alpha)-1}} \right] \]

So if \( \gamma > \frac{2+\delta}{1-\alpha} \) then \( \omega_r > \frac{b_r}{a_{r+1}} \) for all sufficiently large \( r \).

The monotonicity of \( \left\{ \sum_{k=1}^{r} k Q_k \omega_r^k \right\} \) is proved in a similar way to that used in the last Lemma.

That is, by observing that

\[ \sum_{k=1}^{r} k Q_k \omega_r^k - \sum_{k=1}^{r+1} k Q_k \omega_r^k > (\omega_r - \omega_{r+1}) - (r+1)Q_{r+1} \omega_r^{r+1} > \]

\[ \frac{\text{con.}}{r^{1+\beta_2}} - \frac{\text{con.}}{r^{\gamma(1-\alpha)-1}} \frac{(r+1) \exp \left( -\frac{G_2}{1-\beta_2} r^{1-\beta_2} \right)}{r^{1+\beta_2}} > 0, \]

for a sufficiently large \( r \).

**Lemma 3.2.6**

If \( H3\beta-3, H3\beta-4, H3\beta-5 \) hold; \( a_r = A r^\alpha \) for all \( r \geq 1 \) and there exist a \( G'_2 > 0 \) and a \( \beta_2' \in (0, \beta_2) \) such that \( \frac{b_{r+1}/a_{r+1}}{b_r/a_r} \geq \exp \left( -\frac{G'_2}{r^{1+\beta_2'}} \right) \) then if \( \gamma > 1 + \frac{\beta_2'}{1-\alpha} \) then there exists a \( R \) such that \( \{\omega_r\}_{r=R}^{\infty} \) and \( \{\sum_{k=1}^{r} k Q_k \omega_r^k\}_{r=R}^{\infty} \) are decreasing.

Note that both sets of coefficients in Example 3.1.3 satisfy the conditions of this Lemma, with \( A = 1, \alpha = 0, G'_2 = 4 - 2\frac{\delta}{r} \) and \( \beta_2' = \frac{2}{5} \).

**Proof.**

Writing \( \delta \) in place of \( (\gamma-1)(1-\alpha)\) -

\[ \omega_{r+1} - \omega_r < \frac{b_r}{a_r} \left[ \exp \left( -\frac{G_2}{r^{1+\beta_2}} \right) - 1 \right] + \frac{b_r}{a_r} \left[ \left( r \right) - \left( r + 1 \right) \right] \left[ \left( \frac{r}{r+1} \right)^\delta \exp \left( -\frac{G_2}{1+\gamma} \sum_{k=r+1}^{\infty} \frac{1}{k^{1+\beta_2}} \right) \right] \]

then for sufficiently large \( r \):

\[ \omega_{r+1} - \omega_r < z_r \left[ \left( \frac{G_2}{2r^{1+\beta_2}} \right) + \frac{b_r/a_r}{r^\delta} \left[ 1 - \left( 1 - \frac{\delta}{r} \right) \exp \left( -\frac{G_2}{r} \int_{r-1}^{(r+1)^\gamma} \frac{1}{x^{1+\beta_2}} dx \right) \right] \right] \]

\[ < \frac{z_r G_2}{2r^{1+\beta_2}} + \frac{b_r/a_r}{r^\delta} \left[ 1 - \left( 1 - \frac{\delta}{r} \right) \left[ 1 - \frac{G_2}{\beta_2' r^{1+\beta_2'}} \left( 1 \right) \right] \right] \]

\[ < \frac{z_r G_2}{2r^{1+\beta_2}} + \frac{b_r/a_r}{r^\delta} \left[ 1 - \left( 1 - \frac{\delta}{r} \right) \left[ 1 - \frac{G_2'}{\beta_2' r^{1+\beta_2'}} \left( 1 + \frac{2\gamma \beta_2'}{r} - 1 + \gamma \frac{\beta_2'}{r} \right) \right] \right] \]

\[ < \frac{z_r G_2}{2r^{1+\beta_2}} + \frac{b_r/a_r}{r^\delta} \left[ \frac{\delta}{r} + 3G_2' \right] \]

\[ < \frac{\text{con.}}{r^{1+\beta_2}} + \frac{\text{con.}}{r^{\delta+1}} \]

so if \( \delta > \beta_2' \), i.e. if \( \gamma > 1 + \frac{\beta_2'}{1-\alpha} \), then for sufficiently large \( r \): \( \omega_{r+1} - \omega_r < 0 \).

We can use the same argument as in Lemma 3.2.5 to also conclude that the sequence \( \left\{ \sum_{k=1}^{r} k Q_k \omega_r^k \right\} \) is eventually decreasing.

The only time we will need to use the exact form of \( \{\omega_r\} \) is when showing that \( m(z) \) is algebraically large. Elsewhere \( \{\omega_r\} \) could be replaced with any sequence \( \{\nu_r\} \) for which:
PI  \( \nu_r \leq \frac{b_r}{a_r} \) for every \( r \geq 2 \);

PI II \( \{\nu_r\} \) is eventually monotonically decreasing and converges to \( z_s \), and

PI III \( \left\{ \sum_{k=1}^{\infty} kQ_k\omega_k^b \right\} \) is eventually monotonically decreasing and converges to \( \rho_s \).

So once we have defined \( m : [z_s, \omega_R] \to \mathbb{N} \) as the value of \( r_j \geq R \) (where \( r_j \) is as defined in Lemma 3.2.4) for which \( \omega_{r_{j+1}} < w \leq \omega_{r_j} \), it is possible to clarify the notation by writing \( \omega_r \) in place of \( \omega_{r_j} \).

3.2.2 The existence of \( z \)

The next Lemma shows that it is possible to construct an upper bound for every value of \( \rho \in (\rho_s, \mathcal{P}) \), where \( \mathcal{P} := \sum_{k=1}^{R} kQ_k\omega_k^b \). \( R \) is as in Lemma 3.2.4.

**Lemma 3.2.7**

Assume that hypotheses H3–3 H3–4 and H3–5 hold and that \( \gamma > \frac{1+\beta_1}{1-\alpha} \). Then, for every \( \rho \in [\rho_s, \mathcal{P}] \) there is at least one \( z_\rho \) which satisfies \( \sum_{r=1}^{m(\rho)} rQ_r\omega_r^b = \rho \). Further

\[
\min\left\{ w : \sum_{k=1}^{m(w)} kQ_k\omega_k^b = \rho \right\} \to z_s \text{ as } \rho \searrow \rho_s
\]

**Proof.**

Lemma 3.2.4 gives that \( \sum_{k=1}^{r} kQ_k\omega_k^b \searrow \rho_s \) as \( r \to \infty \).

Hence, for every \( \rho \in [\rho_s, \mathcal{P}] \) there exists \( r_\rho \geq R \) such that

\[
\sum_{k=1}^{r_\rho} kQ_k\omega_k^b < \rho \leq \sum_{k=1}^{r_\rho+1} kQ_k\omega_k^b
\]

Note that \( r_\rho \) is uniquely defined and that \( r_\rho \not\to \infty \) as \( \rho \searrow \rho_s \).

Now the function \( z \mapsto \sum_{k=1}^{r_\rho} kQ_k\omega_k^b \) is continuous and increasing, so-

\[
(\omega_{r_{\rho+1}}, \omega_{r_\rho}) \ni (\omega_\rho) \mapsto (\text{bijection}) \mapsto \left( \sum_{k=1}^{r_\rho} kQ_k\omega_k^b \right) \ni \left( \sum_{k=1}^{r_\rho+1} kQ_k\omega_k^b \right) \ni \rho
\]

So there is a unique value of \( z \in (\omega_{r_{\rho+1}}, \omega_{r_\rho}] \), \( \omega_\rho \), say, such that \( \sum_{k=1}^{r_\rho} kQ_k\omega_k^b = \rho \) and because \( \omega_\rho \in (\omega_{r_{\rho+1}}, \omega_{r_\rho}] \) and \( \left\{ \omega_r \right\}_{r=R}^{\infty} \) is decreasing, the definition of \( m(z) \) gives \( r_\rho = m(\omega_\rho) \). Since \( r_\rho \) is uniquely defined then so is \( \omega_\rho \) and because \( \omega_{r_{\rho+1}} < z_\rho \leq \omega_{r_\rho} \) we know that \( z_\rho \searrow z_s \) as \( \rho \searrow \rho_s \).

The proof is completed by showing that \( z_\rho \) is the minimum of the set \( \left\{ w : \sum_{k=1}^{m(w)} kQ_k\omega_k^b = \rho \right\} \). To help visualise this, Figure 3.2.1 shows a sketch of the graph of \( z \mapsto \sum_{k=1}^{r_\rho} kQ_k\omega_k^b \).

---

5Figure 4.1.1 on page 91 shows graphs of \( \{\omega_r\} \) against \( \left\{ \sum_{k=1}^{r} kQ_k\omega_k^b \right\} \) for both sets of coefficients given in Example 3.1.3.
3.3. **BOUNDS**

Throughout this section we assume that all the Hypotheses H3–2 to H3–5 hold and that \( \gamma > \frac{1 + \beta'}{1 - \alpha}. \)
3.3.1 Upper bounds on $c(t)$

Theorem 3.3.1

Suppose that: $z$ has the property $\sum_{r=1}^{m(z)} r Q_r z^r \geq \rho = \sum_{r=1}^{N} r c_r(0); \; N \geq \max\{m(z), \ell(z) + 1\}; \; z_e < z; \; \ell^* \in \mathbb{N} and \; \ell(z) \leq \ell^* \leq \ell(z_e) =: \ell_e; \; and \; J \in (q_{\ell-1}(z), q_{\ell_e}(z)]$. Then define

$$U_r(z, z_e, J, \ell^*) := \begin{cases} M_r(z, J) & \text{for } 1 \leq r \leq \ell^* \\ b_r M_r(z, J) \frac{1}{b_j} & \text{for } \ell^* < r \leq \ell_e + 1 \\ b_{\ell_e+1} M_r(z, J) \frac{1}{b_{\ell_e+1} Q_{\ell_e+1} z_{\ell_e}^r} & \text{for } \ell_e + 1 \leq r \leq N \end{cases}$$

$$T := \min\{\inf\{t : c_1(t) < z_e\}, \inf\{t : c_N(t) > U_N\}\}.$$ 

If $c_r(0) \leq U_r$ for $1 \leq r \leq N$ then $c_r(t) \leq U_r$ for $1 \leq r \leq N$ and all $t \in [0, T)$.

It is helpful to keep the following sketch of $U$ in mind while reading the proof of this result.

\[ \begin{array}{c}
\text{represents the upper bound } U_r \\
\text{represents an equilibrium distribution } Q_r z_e^r
\end{array} \]

**Figure 3.3.1:** A sketch of the upper bound, $U_r(z, z_e, J, \ell^*)$ against $r$.

**Proof.**

We will first prove the result for the following system of equations

\[
\begin{align*}
\dot{x}_1 &= -J_1(x) - \sum_{k=1}^{N-1} J_k(x) - \varepsilon x_1 \\
\dot{x}_r &= J_{r-1}(x) - J_r(x) - \varepsilon x_r \\
\dot{x}_N &= J_{N-1}(x) - \varepsilon x_N
\end{align*}
\]

(3.3.1)

where $J_r(x) = a_r x_1 x_r - b_{r+1} x_{r+1}$. Note the following:-

1. By arguments in [2], $x_r(0) \geq 0 \implies x_r(t) \geq 0 \; \forall t > 0$ and for $1 \leq r \leq N$. 
(2) \[ \sum_{k=1}^{N} k \dot{x}_k = -\varepsilon \sum_{k=1}^{N} k x_k \implies \sum_{k=1}^{N} k x_k(t) = e^{-\varepsilon t} \sum_{k=1}^{N} k x_k(0) \text{ i.e. } \rho(t) = e^{-\varepsilon t} \rho(0). \]

We proceed by contradiction, so suppose that, \( S := \min \{ \inf_{s \in \mathcal{X}} \{ s : x_r(s) > U_r \} \} < T, \) and that this minimum is attained at \( r = j. \) Then, since all \( x_r \) are continuous, \( x_j(S) = U_r, \) for some \( S' < S, \) \( x_j(t) < U_r \) \( \forall t \in [S', S) \) and for some \( S'' > S, \) \( x_j(t) > U_r \) \( \forall t \in (S, S'') \); which implies that \( \dot{x}_j(S) \geq 0. \)

Now suppose \( j = 1, \) so \( x_1(S) = U_1 = z \) and for all \( r \neq 1 \) \( x_r \leq U_r := \)

\[
\dot{x}_1(S) = -2a_1z^2 + b_2x_2 + \sum_{k=2}^{N-1} a_k \frac{b_k}{a_k} z x_k + b_N x_N - \varepsilon z
\]

\[
= -2a_1z^2 + b_2x_2 + \sum_{k=2}^{m(z)} a_k \left( \frac{b_k}{a_k} - z \right) Q_k z^k
\]

\[- \sum_{k=2}^{m(z)} a_k \frac{b_k}{a_k} z k Q_k z^k - k x_k + b_N x_N - \varepsilon z
\]

By noting the following

(1) H3–1 and H3–2 gives that \( \left\{ a_r \frac{b_k}{a_k} - z \right\} \frac{\ell(z)}{r} \) is decreasing;

(2)

(i) \( a_k \frac{b_k}{a_k} - z \geq 0 \forall k \leq \ell(z); \)

(ii) \( a_k \frac{b_k}{a_k} - z < 0 \forall k \geq \ell(z) + 1, \) and

(3) for \( k \leq \ell^*(> m): x_k \leq M_k < Q_k z^k, \) so \( (Q_k z^k - x_k) > 0 \forall k \leq m \)

we can conclude that

\[
\dot{x}_1(S) \leq -2a_1z^2 + b_2M_2 + \sum_{k=2}^{m(z)} (a_{k-1}Q_k z^{k-1} - a_k Q_k z^{k+1})
\]

\[- a_m \frac{b_m}{a_m} - z \sum_{k=2}^{m(z)} k Q_k z^k - k x_k + b_N x_N - \varepsilon z
\]

By assumption on \( z \) we know that

\[
\sum_{k=1}^{m(z)} k Q_k z^k \geq \rho \geq \rho e^{-\varepsilon S} = \sum_{k=1}^{N} k x_k(S)
\]

and so \(- \sum_{k=2}^{m} k(Q_k z^k - x_k) \leq -z - \sum_{m+1}^{N} k x_k. \) Hence

\[
\dot{x}_1(S) \leq -2a_1z^2 + b_2Q_2z^2 + a_1Q_1z^2 - a_m Q_m z^{m+1} - a_m z \frac{b_m}{a_m} - z \frac{m}{m}
\]

\[- a_m \frac{b_m}{a_m} - z \sum_{k=m+1}^{N} k x_k + \sum_{k=m+1}^{N-1} a_k \frac{b_k}{a_k} z k x_k + b_N x_N - \varepsilon z
\]
\[
\leq -a_m Q_m z^{m+1} - a_m z \left( \frac{b_m}{a_m} - z \right) + \frac{N-1}{m} \sum_{k=m+1}^N \left[ \frac{b_k}{a_k} - \frac{b_m}{a_m} \right] k x_k
\]

\[
+ \left[ \frac{b_N}{N} - a_m \left( \frac{b_m}{a_m} - z \right) \right] N x_N - \varepsilon z.
\]

From the previous remark we know that \[\left[ a_k \left( \frac{b_k}{a_k} - \frac{b_m}{a_m} \right) \right] \leq 0, \forall k \geq m + 1.\] So,

\[
\dot{x}_1(S) \leq \left[ \frac{b_N}{N} - a_m \left( \frac{b_m}{a_m} - z \right) \right] N x_N - \varepsilon z = \left[ \frac{b_N}{N} - \frac{b_m}{m} + \frac{a_m z}{m} \right] N x_N - \varepsilon z
\]

\[
\leq -\varepsilon z < 0.
\]

This contradicts \(x_1(s) \geq 0\). So \(j \neq 1\).

If \(1 < j < \ell^*\) then

\[
\dot{x}_j(S) = a_j x_j - (a_j x_1 + b_j M_j + b_{j+1} x_{j+1}) - \varepsilon M_j
\]

but by the assumption \(J \in (q_{e-1}(z), q_e(z))\) and Lemma 3.1.8, we know that \((a_j x_1 + b_j M_j) > 0\) for all \(j \leq \ell^* - 1\). Hence

\[
\dot{x}_j(S) \leq (a_j x_1 + b_j M_j) - b_j M_j + b_{j+1} M_{j+1} - \varepsilon M_j,
\]

which contradicts \(x_j(s) \geq 0\).

If \(j = \ell^*\) then

\[
\dot{x}_{\ell^*}(S) \leq (a_{\ell^*-1} M_{\ell^*-1} - a_{\ell^*} M_{\ell^*}) x_1 - b_{\ell^*} M_{\ell^*} + b_{\ell^*+1} x_{\ell^*+1} \left( \frac{1}{b_{\ell^*+1}} - \varepsilon M_j \right)
\]

but \(J \leq q_{\ell^*}(z) \implies (a_{\ell^*-1} M_{\ell^*-1} - a_{\ell^*} M_{\ell^*}) < 0\) so

\[
\dot{x}_{\ell^*}(S) \leq -b_{\ell^*} M_{\ell^*} + b_{\ell^*} M_{\ell^*} - \varepsilon M_{\ell^*} < 0.
\]

If \(\ell^* + 1 \leq j \leq \ell_e\) then

\[
\dot{x}_j(S) \leq \left( \frac{a_j}{b_j - 1} - a_j \right) x_1 - b_j x_{\ell^*}(z, J) \frac{1}{b_j} x_1 - b_j x_{\ell^*}(z, J) \frac{1}{b_j} x_1 - \varepsilon x_j(S)
\]

\[
\leq b_{\ell^*} M_{\ell^*} (z, J) \left( \frac{a_j}{b_j - 1} - a_j \right) x_1 - \varepsilon x_j(S) < -\varepsilon x_j(S) < 0.
\]

If \(j = \ell_e + 1\) then

\[
\dot{x}_{\ell_e+1}(S) \leq b_{\ell^*} M_{\ell^*} (z, J) \left( \frac{a_{\ell_e}}{b_{\ell_e}} - \frac{a_{\ell_e+1}}{b_{\ell_e+1}} \right) Q_{\ell_e+1} Q_{\ell_e+1} x_{\ell_e+1}
\]
3.3. BOUNDS

Our result gives that 

\[ \frac{b_{r+1}}{b_{r+1} + Q_{r+1}z_{r+1}z_{r+2}} - \frac{b_{r+2}}{b_{r+1} + Q_{r+1}z_{r+1}z_{r+2} + 1} \int_{x_{r+1}} \leq b_r, M_r(z, J) \left[ \left( \frac{a_{r+1}}{a_r} \right) z_e - 1 + \frac{a_{r+1}Q_{r+1}z_{r+1}z_{r+2}}{b_{r+1}Q_{r+1}z_{r+1}z_{r+2} + 1} \right] - \varepsilon x_{r+1}(S) \]

We use a similar method to the one used in the last theorem. So the result is first proved for the

Corollary 3.3.2

Let \( z \) and \( J \) be as above, suppose that \( N \geq m^\gamma(z) \), \( \ell^* \geq \ell(z) \) and define:

\[
U_r(z, J, \ell^*) := \begin{cases} 
M_r(z, J) & \text{for } 1 \leq r \leq \ell^* \\
\frac{b_r, M_r(z, J)}{b_r} & \text{for } \ell^* < r \leq N 
\end{cases}
\]

\[
T := \inf \{ t : c_N(t) > U_N \}.
\]

Then \( c_r(0) \leq U_r \) for \( 1 \leq r \leq N \) \( \Rightarrow c_r(t) \leq U_r \) for \( 1 \leq r \leq N \) and for all \( t \in [0, T] \)

This follows from the arguments given above. We state the result to show that the only effect \( N \) being less than \( \ell(z) \) + 1 has on the bounds is to change their algebraic form in the expected way. The asymptotic results, however, only apply when \( N > \ell(z) \) – see section 3.4.1 – and so only Theorem 3.3.1 is relevant there. This is in marked contrast to the infinite system, where classes of solutions can be shown to be metastable using either \( U_r(z, 0, \ell(z) + 1) \) or \( M_r(z, J) \) – see [24] and [12] respectively.

3.3.2 Lower bounds on \( c(t) \)

Theorem 3.3.3

Define \( L_r = M_r(y, I) \) for \( 1 \leq r \leq N \) where \( I \geq q_N(y) \geq 0 \) and \( T' = \inf \{ s : c_1(s) < y \} \). Then \( c_r(0) \geq L_r \) for \( 1 \leq r \leq N \) \( \Rightarrow c_r(t) \geq L_r \) for \( 1 \leq r \leq N \) and for \( t \leq T' \)

Proof.

We use a similar method to the one used in the last theorem. So the result is first proved for the system

\[
\begin{align*}
\dot{y}_1 &= -J_1(y) - \sum_{k=1}^{N-1} J_k(y) + \varepsilon y_1 \\
\dot{y}_r &= J_{r-1}(y) - J_r(y) + \varepsilon y_r \\
\dot{y}_N &= J_{N-1}(y) + \varepsilon y_N
\end{align*}
\]

(3.3.3)

where \( J_r(y) = a_r y_1 y_r - b_{r+1} y_{r+1} \). The result is then proved by letting \( \varepsilon \to 0 \).

For the purposes of contradiction suppose \( S < T' \) where \( S = \min \{ \inf \{ s : y_r(s) < L_r \} \} \) and that the minimum is attained at \( r = j \). The definition of \( T' \) gives that \( j \neq 1 \), otherwise \( S = T' \).
If \(1 < j < N\) then
\[
\hat{y}_j(S) = a_{j-1}y_1y_{j-1} - (a_jy_1 + b_j)M_j(y, I) + b_{j+1}y_{j+1} + \varepsilon M_j(y, I)
\]
\[\geq (a_{j-1}M_j - a_jM_j)y_1 - b_jM_j + b_{j+1}M_{j+1} + \varepsilon M_j,
\]
but \(I \geq q_N(y)\) so \((a_{j-1}M_j - a_jM_j) > 0\) for \(j \leq N\). Hence
\[
\hat{y}_j(S) \geq (a_{j-1}M_j - a_jM_j)y - b_jM_j + b_{j+1}M_{j+1} + \varepsilon M_j = I - I + \varepsilon M_j = \varepsilon M_j > 0.
\]
Now \(S = \inf\{s : y_j(s) < L_j\}\) so \(y_j(S) = M_j(y, I)\) and there exist \(S'\) and \(S''\) such that \(y_j(t) > M_j(y, I)\), \(\forall t \in (S'', S)\) and \(y_j(t) < M_j(y, I)\), \(\forall t \in (S, S')\), which means that \(\hat{y}_j(S) < 0\). This is a contradiction.

If \(j = N\)
\[
\hat{y}_N(S) = a_N^{-1}y_1y_{N-1} - b_N M_N(y, I) + \varepsilon M_N(y, I)
\]
\[\geq a_N^{-1}M_N^{-1}y - b_N M_N + \varepsilon M_N = I + \varepsilon M_N > 0,
\]
which contradicts \(S = \inf\{s : y_N(s) < L_N\}\) \(\implies \hat{y}_N(S) < 0\).

Corollary 3.3.4
If \(c_r(0) \geq Q_r\left(\frac{b_N}{a_N}\right)^r\) for \(1 \leq r \leq N\) then \(c_r(t) \geq Q_r\left(\frac{b_N}{a_N}\right)^r\) for \(1 \leq r \leq N\) and for all \(t \geq 0\).

Proof.
First note that \(Q_r\left(\frac{b_N}{a_N}\right)^r = M_r\left(\frac{b_N}{a_N}\right)\) and \(q_N\left(\frac{b_N}{a_N}\right) = 0\). So the proof of Theorem 3.3.3 gives
us that if \((y_r)\) is the solution of the system (3.3.3) and if \(y_r(0) \geq Q_r\left(\frac{b_N}{a_N}\right)^r\) for \(1 \leq r \leq N\) then
\[y_r(t) \geq Q_r\left(\frac{b_N}{a_N}\right)^r\]
for \(1 \leq r \leq N\) and for all \(0 \leq t \leq T'\) where \(T' = \inf\left\{t : y_1(t) < \left(\frac{b_N}{a_N}\right)\right\}\).

Suppose that \(T' < \infty\) then \(\hat{y}_1(T') < 0\) but, if \(y = \frac{b_N}{a_N}\) then
\[
\hat{y}_1(T') = -2a_1y^2 + b_2y^2 + \sum_{k=2}^{N-1} a_k \left(\frac{b_k}{a_k} - y\right) y_k + b_N y N + \varepsilon y.
\]
However \(y = \frac{b_N}{a_N} \leq \frac{b_r}{a_r}\) for \(2 \leq r \leq N\), so
\[
\hat{y}_1(T') \geq -2a_1y^2 + b_2Q_2y^2 + \sum_{k=2}^{N-1} a_k \left(\frac{b_k}{a_k} - y\right) Q_ky^k + b_N Q_N y^N + \varepsilon y
\]
\[= \varepsilon y > 0,
\]
which is a contradiction. So \(T' = \infty\) for every \(\varepsilon > 0\). Hence by letting \(\varepsilon \to 0\) we have proved the result.

3.3.3 Upper bounds on the growth of super-critical clusters

Theorem 3.3.5
If \(c_r(0) \leq U_r(z, z_c, J, \ell^*)\), where \(z, z_c, J, \ell^*\) and \(N\) satisfy the conditions of Theorem 3.3.1 then for all \(t \in [0, T)\)
\[(i) \quad S_0(t) - S_0(0) \leq J^*_N t.
\]
\[ S_1(t) - S_1(0) \leq \begin{cases} J_1^* \left[ (1 + \lambda t)^{(2-\alpha)} - 1 \right] \frac{1}{\alpha} \left( \frac{A}{\lambda^2} \right)^{\frac{1}{\alpha}} & \text{if } \alpha \in (0, 1) \\ J_1^* t^2 + [ (\ell_e + 1) J_1^* + A z S_0(0) ] t & \text{if } \alpha = 0 \end{cases} \]

where \( J_1^* := a_{\ell_e} z U_{\ell_e} \), and \( \lambda := \frac{A z (S_0(0)/J_1^*) + \ell_e + 1}{\ell_e} \).

(iii) If it is also true that \( c_r(0) \geq L_r(y, I) \) where \( y \) and \( I \) satisfy the conditions of Theorem 3.3.3 then

\[ S_1(t) - S_1(0) \leq N J^* t + \sum_{k=\ell_e+1}^{N} (N - k) [ c_r(0) - L_r(y, I) ], \]

where \( J^* := a_{\ell_e} z U_{\ell_e} - b_{\ell_e+1} L_{\ell_e+1} \).

**Proof.**

Note that, since \( c_r(0) \leq U_r \) Theorem 3.3.1 tells us that \( t < T \implies c_r(t) \leq U_r \).

(i) We can derive the inequality

\[ S_0(t) \leq S_0(0) + J_1^* t \tag{3.3.4} \]

from the following calculation:

\[ \sum_{k=\ell_e+1}^{N} \dot{c}_k(t) = \sum_{k=\ell_e+1}^{N-1} (J_{k-1} - J_k) + J_N = J_{\ell_e} (c(t)) \]

\[ \leq a_{\ell_e} c_1(t) c_{\ell_e}(t) \leq a_{\ell_e} z U_{\ell_e} = J_1^* . \]

(ii) When \( \alpha \in (0, 1) \) the inequality

\[ S_1(t) \leq S_1(0) + J_1^* \left[ (1 + \lambda t)^{(2-\alpha)} - 1 \right] \frac{1}{\alpha} \left( \frac{A}{\lambda^2} \right)^{\frac{1}{\alpha}} \tag{3.3.5} \]

can be derived in the following way.

\[ \sum_{k=\ell_e+1}^{N} k \dot{c}_k(t) = \sum_{k=\ell_e+1}^{N-1} k (J_{k-1} - J_k) + NJ_{N-1} = (\ell_e + 1) J_{\ell_e} + \sum_{k=\ell_e+1}^{N-1} J_k \]

\[ \leq (\ell_e + 1) J_1^* + \sum_{k=\ell_e+1}^{N} a_{\ell_e} c_1(t) c_k(t) \]

\[ \leq (\ell_e + 1) J_1^* + A z \sum_{k=\ell_e+1}^{N} k^\alpha c_k(t) \]

\[ \leq (\ell_e + 1) J_1^* + A z \left( \sum_{k=\ell_e+1}^{N} c_k(t) \right)^{\alpha} \left( \sum_{k=\ell_e+1}^{N} k c_k(t) \right)^{(1-\alpha)} \tag{3.3.6} \]

That is

\[ \hat{S}_1(t) \leq \left[ (\ell_e + 1) J_1^* + A z S_0(t) \right]^{(1-\alpha)} \left[ (\ell_e + 1) J_1^* + A z S_1(t) \right]^{\alpha} . \tag{3.3.7} \]

Substituting (3.3.4) into (3.3.7) and integrating, will give

\[ \frac{[(\ell_e + 1) J_1^* + A z S_1(t)]^{(1-\alpha)}}{A z (1-\alpha)} - \frac{[(\ell_e + 1) J_1^* + A z S_0(t)]^{(1-\alpha)}}{A z (1-\alpha)} \leq \]
\[ \frac{(l_e + 1)J^*_1 + AzS_0(0) + AzJ^*_1 e}{AzJ^*_1(2 - \alpha)} - \frac{(l_e + 1)J^*_1 + AzS_0(0)}{AzJ^*_1(2 - \alpha)}, \]

which may be rearranged to give
\[ \left( \frac{l_e + 1)J^*_1 + AzS_1(t)}{AzJ^*_1(1 - \alpha)} \right) = \left[ \left( l_e + 1)J^*_1 + AzS_1(0) \right) \right]^{(1 - \alpha)} + J^*_1 \left( \frac{1 - \alpha}{2 - \alpha} \right) \left( AzS_0(0) + AzJ^*_1 e \right)^{(2 - \alpha)} - 1. \]

Hence
\[ \left( l_e + 1)J^*_1 + AzS_1(t) \right) \leq \left( l_e + 1)J^*_1 + AzS_1(0) \right) + J^*_1 \left( \frac{1 - \alpha}{2 - \alpha} \right) \left( AzS_0(0) + AzJ^*_1 e \right)^{(2 - \alpha)} - 1. \]

which is equivalent to (3.3.5).

When \( \alpha = 0 \) the calculation above may be repeated up to the inequality (3.3.6) which becomes
\[ \sum_{k=k_{e+1}}^{N} kC_k(t) \leq (l_e + 1)J^*_1 + Az \sum_{k=k_{e+1}}^{N} c_k(t). \]

Hence
\[ S_1(t) - S_1(0) \leq \int_{0}^{t} (l_e + 1)J^*_1 + AzS_0(s)ds \]
\[ \leq \left( l_e + 1)J^*_1 + AzS_0(t) \right) t + J^*_1 t^2. \]  


(iii) First note that \( S_1(t) - S_1(0) = \sum_{r=r_{e+1}}^{N} r(c_r(t) - L_r(y,I)) + \sum_{r=r_{e+1}}^{N} r(c_r(0) - L_r(y,I)) \) and since \( t < T < T' \) Theorem 3.3.3 gives that \( c_r(t) \geq L_r(y,I) \). Hence
\[ S_1(t) - S_1(0) \leq N \sum_{r=r_{e+1}}^{N} (c_r(t) - L_r) - \sum_{r=r_{e+1}}^{N} r(c_r(0) - L_r(y,I)) \]
\[ = N(S_0(t) - S_0(0)) + \sum_{r=r_{e+1}}^{N} (N - r) (c_r(0) - L_r(y,I)) \]
\[ \leq N(a_{e+1} z U_{e+1} - b_{e+1} L_{e+1})t + \sum_{r=r_{e+1}}^{N} (N - r) (c_r(0) - L_r(y,I)). \]

\[ \Box \]

3.4 Asymptotic Behaviour as \( \rho \searrow \rho_s \)

As was mentioned in Section 3.1 each class \( \{ R_{\rho} : \rho \in (\rho_s, P) \} \) has explicit definitions of \( z, N, \) and \( z_e \) as functions of \( \rho \) associated with it and we gave conditions on these functions which ensure that the main results apply. However many of the preliminary results hold under weaker conditions and so there is a progressive strengthening of the assumptions of the statements in this section. We start by finding the smallest system size for which there are super-critical clusters. An immediate corollary to these calculations is that an asymptotic statement with respect to \( \rho \searrow \rho_s \) is equivalent to one
with respect to $z \setminus z_s$. This then enables us to translate the estimates given in Lemma 3.2.1 into asymptotic results. We then have all the prerequisite results needed to prove that $M\ II$ holds, in the way described in Section 3.1.3. One further lemma is needed to give estimates for the Lyapunov function and then we can conclude that $\{R_\rho : \rho \in (\rho_s, \tilde{P})\}$ is metastable.

Throughout the Section we assume that hypotheses $H3\ - 2$ to $H3\ - 5$ hold and that $\gamma > \frac{1 + \beta_1}{1 - \alpha}$.

Whatever the definition is given to $N(\rho)$, $z_\epsilon(\rho)$ will always taken to be the unique solution of $\sum_{k=1}^N kQkw^k = \rho$; i.e. $z_\epsilon(\rho) = \hat{z}$, the equilibrium value of $c_1(t)$.

### 3.4.1 Minimum system size

Recall that super-critical clusters were defined as all those clusters with more than $\ell(\hat{z})$ particles – see Figure 3.1.1 on page 59. Which means that only systems where $N > \ell(\hat{z})$ have super-critical clusters. Since $\ell(\hat{z})$ depends on $N$, we need to prove that the inequality holds, at least for a class of systems with densities arbitrarily close to $\rho_s$. We will in fact show that the inequality holds whenever $N > m^*(\hat{z}_P)$ and this comes from establishing a connection between $m(w)$ and $\ell(w)$, but before this can be done we need to check that many of the results that apply to $\omega_r$ also apply to $\frac{b_w}{a_r}$.

#### Lemma 3.4.1

Assume that $H3\ - 3$, $H3\ - 4$, $H3\ - 5$ hold, then there is some $R'$ for which $\left\{ \sum_{k=1}^r kQ_k \left( \frac{b_k}{a_r} \right)^k \right\}_{r=R'}^\infty$ is decreasing.

**Proof.**

The result follows from the calculation below.

\[
\sum_{k=1}^r kQ_k \left( \frac{b_k}{a_r} \right)^k - \sum_{k=1}^{r-1} kQ_k \left( \frac{b_{r-1}}{a_{r-1}} \right) < rQ_r\omega_r - \left( \frac{b_{r-1}}{a_{r-1}} - \frac{b_r}{a_r} \right) < \frac{\Gamma r^r}{A'} \exp \left( - \frac{G_2}{1 - \beta_2} r^{1 - \beta_2} \right) - \frac{b_{r-1}}{a_{r-1}} - \frac{b_r}{a_r} < 0 \quad \text{for } r \text{ sufficiently large} \quad \diamond
\]

#### Lemma 3.4.2

Assume that hypotheses $H3\ - 3$ $H3\ - 4$ and $H3\ - 5$ hold. Then, for every $\rho \in \left[ \rho_s, \sum_{k=1}^{R'} kQ_k \left( \frac{b_k}{a_r} \right)^k \right]$ there is at least one $y_\rho$ which satisfies $\sum_{r=1}^{\ell(z_P)} rQ_r y_r^r = \rho$. Further

\[
\min \left\{ w : \sum_{k=1}^{\ell(w)} kQ_k w^k = \rho \right\} \to z_s \quad \text{as } \rho \searrow \rho_s.
\]

**Proof.**

The function $\ell$ is defined in the same way as $w$ only in relation to the sequence $\left\{ \frac{b_w}{a_r} \right\}$ rather than $\{\omega_r\}$. Hypotheses $H3\ - 4$ and $H3\ - 5$ give that $\left\{ \frac{b_w}{a_r} \right\}$ is eventually decreasing and tends to $z_s$ as $r \to \infty$.

Corollary 3.2.3 and Lemma 3.4.1 combined tell us that $\left\{ \sum_{k=1}^r kQ_k \left( \frac{b_k}{a_r} \right)^k \right\}$ is eventually decreasing and tends to $\rho_s$. This means that $\left\{ \frac{b_w}{a_r} \right\}$ has properties P II and P III from page 70. Which all means that the proof of Lemma 3.2.7 can be re-used here. \quad \diamond

To obtain a more precise connection between $\ell$ and $m$ we use the exact form of the subsequence $r_j$; which was defined in the proof of Lemma 3.2.4 inductively by: $r_1 = \text{ceil} \left( \frac{\frac{G_1}{G_2}}{2^{\frac{1}{2}}} \right)$ and
\[r_{j+1} = \text{ceil} \left( \frac{\ln \left( \frac{r_j}{2} \right)}{G_1} \right)^{1/\beta_1} \] We then saw that there existed an \( R \in \mathbb{N} \) such that both \( \left\{ \omega_{r_j} \right\}_{r_j=R}^\infty \) and
\[\sum_{k=1}^{r_j} k Q_k \omega_R^k_{r_j=R} \] are monotonically decreasing. The following Lemmas apply to those functions of \( z(\rho) \) where \( z(\rho) < \omega_R \) and \( 0 < \sum_{k=1}^{m(\rho)} k Q_k z(\rho)^k - \rho \leq \min\{\kappa(\rho - \rho_0), \rho - \rho\} \), for some \( \kappa \geq 0 \). We will use \( \rho' \) to denote \( \sum_{k=1}^{m(\rho)} k Q_k z(\rho)^k \).

**Lemma 3.4.3**
There exist constants \( D', D, E', E > 0 \) and \( \eta', \eta > 0 \) such that for any \( w \) sufficiently close to \( z_s \):

(i) \( D'(w - z_s)^{-\eta'} < m(w) < D(w - z_s)^{-\eta} \) and

(ii) \( E'(w - z_s)^{-1/\beta_1'} < \ell(w) < D(w - z_s)^{-1/\beta_1} \).

**Proof of (i).**
The definition of \( m(w) \) is that \( m(w) = r_j \) if
\[\omega_{r_{j+1}} < w \leq \omega_{r_j} \]
Now \( \omega_{r_j} < \frac{b_{r_j}}{\omega_{r_j}} \leq z_s \exp \left( \frac{G_1}{r_{j+1}} \right) \Rightarrow r_j < \left[ \frac{G_1}{\ln \left( \frac{1}{\omega_{r_j}} \right)} \right]^{1/\beta_1} \) and if \( w \) is sufficiently close to \( z_s \) then
\[\ln \left( \frac{w}{z_s} \right) > \frac{w - z_s}{z_s} \text{. So } m(w) < \left[ \frac{2z_s G_1}{w - z_s} \right] ^{1/\beta_1} \text{. Lemma 3.2.1 (iv) tells us that} \]
\[\omega_{r_{j+1}} > z_s \exp \left( \frac{G_1'}{r_{j+1}} \right) > z_s \exp \left[ \frac{\frac{G_1'}{r_{j+1}}}{\left( \frac{4G_1'}{G_1} (1/\beta_1) \right) \left( r_j(\beta_1'/\beta_1) + 1 \right) \beta_1} \right] \],
which may be re-arranging to give:
\[m(z) > \left( \frac{\frac{G_1'}{4}}{\ln \left( \frac{w}{z_s} \right)} \right)^{1/\beta_1} - 1 \left( \frac{G_1'}{4G_1} \right)^{1/\beta_1} \left( w - z_s \right)^{-\beta_1'/\beta_1^2} \text{.} \]
So for \( w \) sufficiently close to \( z_s \) we have that
\[m(z) > \left( \frac{G_1'}{4} \right)^{1/\beta_1} - \left( \frac{G_1'}{4G_1} \right)^{1/\beta_1} \left( w - z_s \right)^{-\beta_1'/\beta_1^2} \text{.} \]

**Note** that the above proof can easily be modified to apply when \( r_j = \mathbb{N} \).

**Proof of (ii).**
The definition of \( \ell(w) \) together with hypothesis H3–4 imply that
\[z_s \exp \left( \frac{G_1'}{(\ell + 1)/\beta_1} \right) < w \leq z_s \exp \left( \frac{G_1}{\ell/\beta_1} \right) \text{.} \]
This can be rearranged to become
\[\left[ \frac{G_1'}{\ln \left( \frac{w}{z_s} \right)} \right]^{1/\beta_1} - 1 < \ell(w) \leq \left[ \frac{G_1}{\ln \left( \frac{z_s}{w} \right)} \right]^{1/\beta_1} \text{.} \]
So if $w$ is sufficiently close to $z_s$ then
\[ \frac{1}{2}(z_s G_1') \frac{1}{\beta_i}(w - z_s)^{-1/\beta_i} < \ell(w) \leq (2z_s G_1') \frac{1}{\beta_i}(w - z_s)^{-1/\beta_i} \]

Lemma 3.4.4
For $\rho \in [\rho_s, \mathcal{P}]$ sufficiently close to $\rho_s$:

(i) \[ \frac{1}{2(\kappa + 1)}(z(\rho) - z_s) < \rho - \rho_s < K(z(\rho) - z_s) \]

(ii) \[ \frac{1}{2}(y_\rho - z_s) < \rho - \rho_s < K(y_\rho - z_s) \]

where $y_\rho = \min \{ w : \sum kQ_k w^k = \rho \}$ and $K = \max_{r \in \mathbb{N}} \left\{ \sum_{k=1}^{r} k^2 Q_k \left( \frac{b_{k+1}}{a_k} \right)^k \right\}$.

Proof of (i).
\[ \rho' - \rho_s = \sum_{k=1}^{m(z)} kQ_k (z^k - z_s^k) - \sum_{k=m+1}^{\infty} kQ_k z_s^k \]
so we have that:
\[ \frac{1}{\kappa + 1} [(z - z_s) - \exp(-m(z)]) < \frac{1}{\kappa + 1} (\rho' - \rho_s) < \rho - \rho_s < (\rho' - \rho_s) < K(z - z_s). \]

Now $\sum_{k=1}^{m(z)} kQ_k z^k = \rho' \rightarrow \rho_s$ as $\rho \rightarrow \rho_s$ and this implies that $z \rightarrow z_s$. So by setting $\rho$ sufficiently close to $\rho_s$ we can ensure that:
\[ [(z - z_s) - \exp(-m(z))] < (z - z_s) - \exp(-D'(z - z_s)) < \frac{1}{2}(z - z_s). \]

Hence we have the desired result that:
\[ \frac{1}{2(\kappa + 1)}(z - z_s) < \rho - \rho_s < K(z - z_s) \]

Proof of (ii).
This follows in the same way, using $\rho - \rho_s = \sum_{k=1}^{\ell(y_\rho)} kQ_k (y_\rho^k - z_s^k) - \sum_{k=\ell+1}^{\infty} kQ_k z_s^k$ and the result of Lemma 3.4.2 that $y_\rho \rightarrow z_s$.

Corollary 3.4.5
If $\gamma > \max \left\{ \left( \frac{\beta_i}{\beta_i} \right)^2, \frac{1 + \beta_i}{1 - \alpha} \right\}$ then for all $\rho \in [\rho_s, \mathcal{P}]$ sufficiently close to $\rho_s$, $\ell(y_\rho) < m(z)^\gamma$. Hence $N \geq m(z)^\gamma \implies \ell(z_c) < N$.

Proof.
Using Lemmas 3.4.3 and 3.4.4 we can say that for $\rho$ sufficiently close to $\rho_s$:
\[ \ell(y_\rho) < \frac{E}{(y_\rho - z_s)^{1/\beta_i}} < \frac{K^{1/\beta_i}E}{(\rho - \rho_s)^{1/\beta_i}} \]
\[ < \frac{(2(\kappa + 1)K)^{1/\beta_i} E}{(z - z_s)^{1/\beta_i}} < (2(\kappa + 1)K)^{1/\beta_i} E \left( \frac{m(z)}{D'} \right)^{1/(\beta_1 \gamma')} \]
\[ < \text{con.} m(z) \left( \frac{a_{k+1}}{a_k} \right)^2 < m(z)^\gamma \]

If $N \geq m(z)^\gamma$ then the above tells us that $N \geq \ell(y_\rho) + 1$, so by Lemma 3.4.1
\[ \sum_{k=1}^{N} kQ_k \left( \frac{b_N}{a_N} \right)^k \leq \sum_{k=1}^{\ell+1} kQ_k \left( \frac{b_{\ell+1}}{a_{\ell+1}} \right)^k < \rho = \sum_{k=1}^{N} kQ_k z_s^k, \]
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which implies that \( \frac{b_N}{a_N} < z_c \), but this means that \( N \geq \ell(z_c) + 1 \).

We can now define \( \mathcal{P} \) as the greatest value less than \( \mathcal{P} \) for which, all the Lemmas in this section apply for every \( \rho \in (\rho_s, \mathcal{P}) \). From now on, whatever the definition of \( z(\rho) \), the function \( N(\rho) \) is assumed to be greater than \( m(z(\rho))^\gamma \), where \( \gamma > \max \left\{ \left( \frac{\beta_1}{\beta_1} \right)^2 \frac{1 + \beta_1}{1 - \alpha} \right\} \). This means that \( \rho \in (\rho_s, \mathcal{P}) \implies N > \ell(z) \) and so all the systems considered will have super-critical clusters in their equilibrium state.

3.4.2 Asymptotic estimates

Lemma 3.4.6

(i) \( z - z_e \) is at least algebraically small.

(ii) \( \sum_{k=1}^{N} \frac{N}{z_e} \) is at least algebraically small.

The notation in the following proof is a little clearer if we note that, since \( N > m(z(\rho))^\gamma \), then \( \gamma > \max 0 \).

Proof of (i).

By definition \( \sum_{k=1}^{N} kQ_k z^k = \rho . \) So \( NQ_N z^N < \rho \) implies, by Lemma 3.2.1 (i), that

\[
\Gamma \exp \left( -\frac{G_1}{1 - \beta_1} N^{1-\beta_1} + N \ln \left( \frac{z_e}{z_s} \right) \right) < \frac{\rho A}{N^{1-\alpha}}. \]

Now \( N \to \infty \) as \( \rho \to \rho_s \), so for \( \rho \) sufficiently close to \( \rho_s \) we have that

\[
N \ln \left( \frac{z_e}{z_s} \right) < \frac{G_1}{1 - \beta_1} N^{1-\beta_1} \implies \ln \left( \frac{z_e}{z_s} \right) < \frac{G_1}{(1 - \beta_1)N^{\beta_1}} \leq \frac{G_1}{(1 - \beta_1)E_2} (\rho - \rho_s)^{\mu \beta_1}.
\]

Note that \( \mu \beta_1 = \gamma \left( \frac{\beta_1}{\beta_1} \right)^2 = 1 + \delta \) for some \( \delta > 0 \), and since \( N \to \infty \) as \( \rho \to \rho_s \) we know that \( z_e \to z_s \). Hence there is an \( \varepsilon > 0 \) such that

\[
\rho - \rho_s < \varepsilon \implies z_e - z_s < (\rho - \rho_s)^{1+\delta} \quad \text{for some } \delta > 0.
\]

So there exists \( \varepsilon' > 0 \) such that, \( \rho - \rho_s < \varepsilon' \) implies that

\[
z - z_e = (z - z_s) - (z_e - z_s) > (\rho - \rho_s) \left( \frac{1}{K} - (\rho - \rho_s)^\delta \right) > \frac{1}{2K}(\rho - \rho_s)
\]

Proof of (ii).

This follows from the calculation given below.

\[
\rho - \rho_s < \sum_{k=1}^{N} kQ_k (z_e^k - z_s^k) + \sum_{k=\ell_e+1}^{N} kQ_k z^k_e < (z_e - z_s)K + \sum_{k=\ell_e+1}^{N} kQ_k z^k_e < K(\rho - \rho_s)^{1+\delta} + \sum_{k=\ell_e+1}^{N} kQ_k z^k_e
\]

Lemma 3.4.7

If \( N \) is at most algebraically large then
3.4. ASYMPTOTIC BEHAVIOUR AS $\rho \searrow \rho_S$

(i) $Q_N z_c^N$ is at least algebraically small.

(ii) $\sum_{\ell' = 1}^N Q_{\ell'} z_c^{\ell'}$ is at least algebraically small.

(iii) Both $a_m Q_m z^m$ and $J^* = a_{\ell_c} z U_{\ell_c}(z, z, J, \ell')$ (for $J \geq 0$) are at most exponentially small.

(iv) $\sum_{r = m+1}^N |\ln(Q_r z^r)|$ is algebraically large.

Proof of (i).

From the definition of $\ell_c \{ rQ_r z_c^r \}_{r = \ell_c}^\infty$ is increasing so $\sum_{k = \ell_c+1}^N kQ_k z_c^k < N^2 Q_N z_c^N$. From the last result $\sum_{k = \ell_c+1}^N kQ_k z_c^k$ is at least algebraically small and $N$ is assumed to be algebraically large.

Proof of (ii).

$\sum_{k = \ell_c+1}^N Q_k z_c^k > Q_N z_c^N$.

Proof of (iii).

By definition of $m$, $z \leq \omega_m < \left( \frac{b_m}{a_m} \right)$ and Lemma 3.2.1 (ii) gives that

$$a_m Q_m \left( \frac{b_m}{a_m} \right) ^m \leq \Gamma_2 \exp \left( - \frac{G_2}{1 - \beta_2} m^{1-\beta_2} \right)$$

and this quantity is exponentially small since $m(z)$ is algebraically large (Lemma 3.4.3 plus Lemma 3.4.4). Therefore $a_m Q_m z^m$ is at most exponentially small. The result for $J^*$ follows from the next calculation:

$$a_{\ell_c} z U_{\ell_c} = \frac{a_{\ell_c}}{b_{\ell_c}} z b_{\ell_c} M_{\ell_c}(J, \ell') \leq \frac{a_{\ell_c}}{b_{\ell_c}} z a_{\ell_c}^{-1} M_{\ell_c-1}(J, \ell')$$

$$\leq \frac{z}{z_s} \exp \left( - \frac{G_1}{1 - \beta_1} \right) \times a_m Q_m z^m < a_m Q_m z^m \quad \Box$$

Proof of (iv).

$$\max \left\{ \ln(Q_r z^r) \right\} = \max \left\{ m \left| \ln(Q_m^m z^m) \right|, \ell \left| \ln(Q_\ell^\ell z^\ell) \right|, N \left| \ln(Q_N^N z^N) \right| \right\}.$$  Lemma 3.2.1 (i) gives that

$$\frac{\Gamma a_r}{z_s} \exp \left( - \frac{G_1}{1 - \beta_1} r^{\beta_1} \right) \leq Q_r^r \leq \frac{\Gamma' a_r}{z_s} \exp \left( - \frac{G_1'}{(1 - \beta') r^{\beta'_1}} \right),$$

for sufficiently large $r$. Hence

$$\frac{z}{2z_s} \exp \left( - \frac{G_1}{1 - \beta_1} r^{\beta_1} \right) \leq Q_r^r z \leq 2z \exp \left( - \frac{G_1'}{(1 - \beta') r^{\beta'_1}} \right)$$

$$\ln \left( \frac{z}{2z_s} \right) \leq \frac{G_1}{1 - \beta_1} r^{\beta_1} \leq \ln \left( Q_r^r z \right) \leq \ln \left( 2z \right) - \frac{G_1'}{(1 - \beta') r^{\beta'_1}}.$$

The result then follows from noting that $m, \ell$ and $N$ are algebraically large.

$\Box$
3.4.3 Metastability of \( \{ \mathcal{R}_\rho : \rho \in (\rho_s, \mathcal{P}) \} \)

From now on we assume that \( z = \min \left\{ w : \sum_{r=1}^{m(w)} rQ_r w^r = \rho' \right\} \) where \( \rho' \geq \rho \) but \( \rho' - \rho \) is at most exponentially small; \( N \) is algebraically large and \( N \geq m(z)\).

\( \mathcal{R}_\rho \) is made up of those distributions \( \{ x_r \} \) for which:

- a. \( \sum_{r=1}^{N} r x_r = \rho; \)
- b. for some \( J \geq 0 \) and \( \ell^* \) satisfying the conditions for Theorem 3.3.1, we have that:
  \[
  x_r \leq U_r(z, z_e, J, \ell^*) \quad \text{for } 1 \leq r \leq N \\
  \text{and } U_r(z, z_e, J, \ell^*) - x_r \text{ is at most exponentially small for } 1 \leq r \leq \ell(z_e); 
  \]
- c. for some \( y \leq z_e \) and \( I \) which satisfying the conditions for Theorem 3.3.3, we have that:
  \[
  x_r \geq L_r(y, I) \\
  \text{and } x_r - L_r(y, I) \text{ is at most exponentially small for } \ell(z_e) < r \leq N. 
  \]

**Lemma 3.4.8**

\( \mathcal{R}_\rho \) is not empty for any \( \rho \in (\rho_s, \mathcal{P}) \).

**Proof.**

We define \( \bar{w} = \min \left\{ w : \sum_{r=1}^{m(w)} rQ_r w^r = \rho \right\} \) then show that \( x_r = \begin{cases} Q_r \bar{w}^r & 1 \leq r \leq m(\bar{w}) \\
0 & m(\bar{w}) + 1 \leq r \leq N \end{cases} \) is an element of \( \mathcal{R}_\rho \). Part a. is then automatically satisfied and part c. follows immediately from noting that \( y = 0 \) and \( I = 0 \) satisfy the necessary conditions. We will show part b. applies for \( J = 0 \) and \( \ell^* = \ell(z) + 1 \).

Since \( \rho' \geq \rho \) we know that \( z \geq \bar{w} \) which in turn implies that \( Q_r \bar{w}^r \leq U_r(z, z_e, 0, \ell + 1) \) for \( 1 \leq r \leq \ell(z) + 1 \). Now, \( m(\bar{w}) \leq \ell(z) \) so we have that \( x_r \leq U_r(z, z_e, 0, \ell + 1) \) for \( 1 \leq r \leq N \).

Lemma 3.4.7 (iii) gives that \( U_r(z, z_e, 0, \ell + 1) \) is at most exponentially small for \( m(z) \leq r \leq \ell_e \).

Hence \( U_r - x_r \) is at most exponentially small for \( m(z) < r \leq \ell_e \).

We know that \( U_r - x_r \) is at most exponentially small for \( 1 \leq r \leq m(z) \) from the following:

\[
\sum_{r=1}^{m(z)} r(U_r - x_r) = \rho' - \sum_{r=1}^{m(z)} r x_r = (\rho' - \rho) + \sum_{r=m(z)+1}^{N} r x_r \leq (\rho' - \rho) + NmQ_m z^m 
\]

**Corollary 3.4.9**

If \( X_r := \begin{cases} Q_r z^r & \text{for } 1 \leq r \leq m(z) \\
0 & \text{for } m(z) + 1 \leq r \leq N \end{cases} \) and \( X \in \mathcal{R}_\rho \) then \( |x_r - X_r| \) is at most exponentially small for \( 1 \leq r \leq N \).

**Proof.**

Since \( x \in \mathcal{R}_\rho \) we know that \( x \) is at most exponentially far from some

\[
B_r := \begin{cases} U_r(z, z_e, J, \ell^*) & \text{for } 1 \leq r \leq \ell_e \\
L_r(y, I) & \text{for } \ell^* + 1 \leq r \leq N 
\end{cases}
\]

For \( m(z) + 1 \leq r \leq N \), the conditions on \( y \), and \( I \) together with Lemma 3.4.7 (iii) give that \( B_r \leq Q_m z^m \) and so \( |B_r - X_r| \) is at most exponentially small.

For \( 1 \leq r \leq m(z) \) the same calculation as was used in Lemma 3.4.8 gives

\[
\sum_{r=1}^{m(z)} r(X_r - B_r) \leq (\rho' - \rho) + N^2 Q_m z^m. 
\]

So \( |B_r - X_r| \) is at most exponentially small.
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**Theorem 3.4.10**

Let $\{x_r\}_{r=1}^N \in \mathcal{R}_\rho$. If $\{c_r\}_{r=1}^N$ is the solution of equation (3.1.1) with $c_r(0) = x_r$ for $1 \leq r \leq N$ then for each $r$ $|c_r(t) - c_r(0)|$ will remain exponentially small until $t$ becomes exponentially large but at some time $|c_r(t) - c_r(0)|$ will become at least algebraically small.

**Proof.**

Use $f(\rho)$ to denote $\sum_{r=1}^{\ell_\epsilon} r(U_r - x_r)$ and $g(\rho)$ to denote $\sum_{r=\ell_\epsilon+1}^N (x_r - L_r)$. Since $N$ is at most algebraically large both $f$ and $g$ are at most exponentially small.

We will now show that if $t < T'$ then $|c_r(t) - c_r(0)|$ is exponentially large. Hence $t \to T'$ will remain exponentially small until $t$ becomes exponentially large. We know that all the bounds hold while $t < T$, where $T = \min \{\inf \{t : c_1(t) < z_e\}, \inf \{t : c_N(t) > U_N\}\}$. First we suppose that $T = \inf \{t : c_N(t) > U_N\}$ and denote this value by $T''$. So, if $t < T''$ then

$$c_N(t) - L_N < \sum_{r=\ell_\epsilon+1}^N [c_r(t) - L_r(y,I)] = S_0(t) - S_0(0) + \sum_{r=\ell_\epsilon+1}^N c_r(0) - L_r(y,I),$$

and $S_0(t) - S_0(0) < J^*t$ and $\sum_{r=\ell_\epsilon+1}^N c_r(0) - L_r(y,I) = g(\rho)$, so

$$c_N(T'') - L_N - g(\rho) < J^*T'' .$$

We obtain

$$T'' > \frac{Q_N z_e^N - L_N(y,I) - g(\rho)}{J^*}$$

by substituting $c_N(T'') > Q_N z_e^N$ into (3.4.1) and re-arranging the inequality. Theorem 3.4.6 tells us that $\frac{Q_N z_e^N - L_N(y,I) - g(\rho)}{J^*}$ is exponentially large.

Now suppose that $T = T' = \inf \{t : c_1(t) < z_e\}$. Since density is conserved we know that

$$\sum_{r=1}^t r(c_r(0) - c_r(t)) = S_1(t) - S_1(0).$$

So

$$\sum_{r=1}^{\ell_\epsilon} r(U_r - c_r(t)) = S_1(t) - S_1(0) + \sum_{r=\ell_\epsilon+1}^\ell r(U_r - c_r(t)),$$

but if $t < T'$ then $z - c_1(t) < \sum_{r=1}^\ell r(U_r - c_r(t))$. Hence $z - c_1(T') \leq NJ^*T' + (N - \ell_\epsilon)g + f$, which implies that

$$T' > \frac{(z - z_e) - (f + (N - \ell_\epsilon)g)}{NJ^*}$$

By Theorem 3.4.6 and the assumptions on $x_r, T'$ is at least exponentially large. Hence $T$ is at least exponentially large.

We will now show that if $r < \ell_\epsilon$ and $t < T$ then $|c_r(0) - c_r(t)|$ is exponentially small. We first observe that, for $r < \ell_\epsilon$ and $t < T$

$$U_r - c_r(t) < \sum_{r=1}^{\ell_\epsilon} r(U_r - c_r(t)) = S_1(t) - S_1(0) + \sum_{r=\ell_\epsilon+1}^\ell r(U_r - c_r(0)),$$

so $U_r - c_r(t) < NJ^*t + (N - \ell_\epsilon)g + f$. This means that

$$-f(\rho) < c_r(0) - U_r \leq c_r(0) - c_r(t) \leq U_r - c_r(t) < NJ^*t + (N - \ell_\epsilon)g + f,$$
which implies that
\[ |c_r(t) - c_r(0)| \leq NJ^* t + (N - \ell_r) g + f. \]

Hence if \( r < \ell \) then \( |c_r(t) - c_r(0)| \) will remain exponentially small for an exponentially long time.

Further, if \( r < (\ln \ell) \frac{1}{\ell} \), then:
\[
Q_r z_r' > Q_r z_r > \frac{\Gamma}{\alpha_r} \exp \left( - \frac{G_1}{1 - \beta_1 r^1} \right) > \frac{\Gamma}{A(\ln \ell) r^{\beta_1}} \times \frac{1}{r^{\beta_1}} \tag{3.4.2}
\]

So if \( r < (\ln \ell) \frac{1}{\ell} \), then \( Q_r z_r' = \lim_{t \to \infty} c_r(t) \) is at least algebraically small.

Inequalities (3.4.3) and (3.4.2) combine with the fact that \( \lim_{\rho \to \rho_\infty} (\ln \ell) \frac{1}{\ell} \to \infty \) to say that, for every

Lemma 3.4.11 reveals exponentially close to \( c_r(0) \) for an exponentially long time but eventually moves an algebraically small distance away.

(a) If \( \sum_{r=1}^N r c_r(0) = \rho \) then \( V(c) = \sum_{r=1}^N \left( \frac{c_r}{Q_r z_r'} - 1 \right) + \sum_{r=1}^N Q_r z_r' \) is a Lyapunov function of the system.

(b) If \( x, y \in \mathcal{R}_\rho \) then \( |V(x) - V(y)| \) is at most exponentially small.

(c) If \( x \in \mathcal{R}_\rho \) then \( V(x) \) is at least algebraically small.

**Proof of (a).**
\[
\frac{dV}{dt} = \sum_{r=1}^N \dot{c}_r \ln \left( \frac{c_r}{Q_r z_r'} \right) \text{ but } \dot{c}_1 = -\sum_{r=2}^N \dot{c}_r
\]

So
\[
\frac{dV}{dt} = \sum_{r=2}^N \dot{c}_r \ln \left( \frac{c_r}{Q_r c_r'} \right) = -\sum_{r=1}^{N-1} J_r \ln (a_r c_r c_r) - \ln (b_{r+1} c_{r+1})) < 0.
\]

The proof is completed by noting that \( V \) has a single global minimum at \( Q_r z_r' \).

**Proof of (b).**
Corollary 3.4.9 tells us that \( x \) is at most an exponentially small distance away from \( X_r \) such that
\[
X_r = \begin{cases} Q_r z_r' & \text{for } 1 \leq r \leq m(z) \\ 0 & \text{for } m(z) + 1 \leq r \leq N. \end{cases}
\]

This together with the conditions on \( J \) give us that there is a sequence \( \{\varepsilon_r\} \) of non-negative at most exponentially small terms such that \( x_r = \begin{cases} Q_r z_r' - \varepsilon_r & \text{for } 1 \leq r \leq m(z) \\ \varepsilon_r & \text{for } m(z) + 1 \leq r \leq N, \end{cases} \) and so
\[
|V(x) - V(X)| = \begin{align*}
&= \sum_{r=1}^N x_r \left[ \ln \left( \frac{x_r}{Q_r z_r'} \right) - 1 \right] - \sum_{r=1}^{m(z)} r Q_r z_r' \ln \left( \frac{z}{z_{c_r}} \right) - Q_r z_r' \\
&= \sum_{r=1}^N x_r \left[ \ln \left( \frac{x_r}{Q_r z_r'} \right) - 1 \right] - (\rho - \rho_0) \ln \left( \frac{z}{z_{c_r}} \right) + \sum_{r=1}^{m(z)} Q_r z_r' \\
&\leq \sum_{r=1}^m (Q_r z_r' - \varepsilon_r) \ln \left( 1 - \frac{\varepsilon_r}{Q_r z_r'} \right) \\
&\quad + \sum_{r=m+1}^N \varepsilon_r \ln \left( \frac{\varepsilon_r}{Q_r z_r'} \right) + \sum_{r=1}^N (\rho - \rho_0) \ln \left( \frac{z}{z_{c_r}} \right)
\end{align*}
\]
Theorem 3.4.12

Lemma 3.4.7 (ii) gives that

$$\sum_{r=1}^{m} Q_r z^r \left(1 - \frac{\varepsilon_r}{Q_r z^r}\right) \ln \left(1 - \frac{\varepsilon_r}{Q_r z^r}\right) + \sum_{r=m+1}^{N} \varepsilon_r \ln (\varepsilon_r)$$

$$+ \max\{\varepsilon_r\} \sum_{r=m+1}^{N} |\ln (Q_r z^r)| + \sum_{r=1}^{N} \varepsilon_r + (\rho' - \rho) \left|\ln \frac{z}{z_c}\right|$$

If $0 \leq x \leq 1$ then $|x \ln(x)| \leq 2x^\frac{1}{2}$ and $|(1 - x) \ln(1 - x)| \leq x$ so

$$|V(x) - V(X)| \leq \sum_{r=1}^{m} \varepsilon_r + \sum_{r=m+1}^{N} 2e^{-\frac{x}{2}} + \max\{\varepsilon_r\} \sum_{r=m+1}^{N} |\ln (Q_r z^r)| + \sum_{r=1}^{N} \varepsilon_r + (\rho' - \rho) \left|\ln \frac{z}{z_c}\right|$$

So $|V(x) - V(X)|$ is at most exponentially small for all $x \in \mathcal{R}_\rho$. Since

$$|V(x) - V(y)| \leq |V(x) - V(X)| + |V(y) - V(X)|,$$

we can see that $|V(x) - V(y)|$ is at most exponentially small, for all $x, y \in \mathcal{R}_\rho$. \hfill \Box

Proof of (c).

First note that $V(x) \geq ||V(X)| - |V(x) - V(X)||$ where $X$ is as above, so the result is proved if we know that $V(X)$ is at least algebraically small.

$$V(X) = \rho' \ln \left(\frac{z}{z_c}\right) - \sum_{r=1}^{m} Q_r (z^r - z_c^r) + \sum_{r=m+1}^{N} Q_r z_c^r,$$

for $\rho$ sufficiently close to $\rho_*$. Hence,

$$V(X) \geq$$

$$\rho' \left[\frac{z - z_c}{z_c} - \frac{(z - z_c)^2}{2z_c^2}\right] - \sum_{r=1}^{m} (z - z_c) Q_r (z^{r-1} + z_c z^{r-2} + \cdots + z_c^{r-2} z + z_c^{r-1}) + \sum_{r=m+1}^{N} Q_r z_c^r$$

$$\geq \rho'(z - z_c) \left[\frac{1}{z_c} - \frac{z - z_c}{2z_c^2}\right] - (z - z_c) \frac{\rho'}{z_c} + \sum_{r=m+1}^{N} Q_r z_c^r$$

$$= \rho' \left[\frac{z - z_c}{2z_c^2}(z_c - (z - z_c))\right] + \sum_{r=m+1}^{N} Q_r z_c^r$$

$$\geq \rho' \left[\frac{(z - z_c)^2}{2z_c^2}(z_c - (z - z_c))\right] + \sum_{r=m+1}^{N} Q_r z_c^r,$$

for $\rho$ sufficiently close to $\rho$. Therefore

$$V(X) \geq \sum_{r=m+1}^{N} Q_r z_c^r$$

and so by Lemma 3.4.7 (ii), $V(X)$ is at least algebraically small. \hfill \Box

Theorem 3.4.12

$\{\mathcal{R}_\rho : \rho \in (\rho, \mathcal{P})\}$ is a metastable class of regions.

Proof.

We need to show that M I to M III on page 58 hold.

M I holds because the definition of $\mathcal{R}_\rho$ gives that $\sum_{r=1}^{N} r x_r$ is at most exponentially small and Lemma 3.4.7 (ii) gives that $\sum_{r=1}^{N} r Q_r z^r$ is at least algebraically small.
Theorem 3.4.10 tells us that M II holds.

For M III: Lemma 3.4.11 tells us that while any two points in $V(R_{\rho})$ are at most an exponentially small distance apart, all points in $V(R_{\rho})$ are at least an algebraically small distance away from $0 = \lim_{t \to \infty} V(c(t))$ so there exists an $S$ such that $V(c(S)) < \min\{V(R_{\rho})\}$ and so $c(t) \not\in R_{\rho}$ for all $t \geq S$. Now $R_{\rho}$ is connected and $V$ is continuous so $V(R_{\rho})$ is connected. Which means that if $\min\{V(R_{\rho})\} < V(c(t)) < \max\{V(R_{\rho})\}$ then $V(c(t)) \in V(R_{\rho})$. Hence there is an $S_{\rho}$ such that:

\[
\begin{array}{ll}
\text{If } c(0) & \in R_{\rho} \quad \text{then } V(c(t)) \in V(R_{\rho}) \quad \text{for } t < S_{\rho} \\
\text{but } c(t) & \not\in R_{\rho} \quad \text{for } t > S_{\rho}
\end{array}
\]
Chapter 4

Numerics

In this Chapter we see how the analytic results just proved compare with numerical approximations. We will use both sets of coefficients given in Example 3.1.3 and give a sample of numerical solutions of the Becker-Döring equations taken from classes of solutions that we have proved to be metastable. We will then use numerical approximations to test if all the hypotheses of Theorem 3.3.1 are needed. We will also see that while the analytic results give poor estimates to the numerical solutions, they do give an indication of when metastable behaviour can be expected.

4.1 Definition of the classes

A full description of a class of the metastable regions \( \{ R_{\rho} : (\rho, \mathcal{P}) \} \) needs explicit formula for: the coefficients \((a_r)\) and \((b_r)\); the functions \(z(\rho)\), \(N(\rho)\) and \(z_s(\rho)\), and \(\mathcal{P}\). We give these below, together with descriptions of how their values may be calculated.

The coefficients used are those from Example 3.1.3, namely:

- **Case A** \( b_r := \exp \left( \frac{1}{r^{\frac{1}{3}}} \right) \) and \( a_r := 1 \) for all \( r \);
- **Case B** \( b_r := \exp \left[ (r - 1)^{\frac{1}{3}} - (r - 2)^{\frac{1}{3}} \right] \) and \( a_r := 1 \) for all \( r \),

We will not be considering systems with more than 5,000 equations. So whenever we need to calculate the value of an infinite sum, we will approximate it by adding up the first 10,000 terms. In this way this we can find an approximate value for \( s \). In case A, \( \rho_s \approx 4.167 \) and in case B, \( \rho_s \approx 4.8981 \); in both these cases \( z_s = 1 \).

In Lemma 3.2.6 we saw that there exists an \( R_{\gamma} \) such that both \( \{ \omega_r \}_{r=R_{\gamma}}^{\infty} \) and \( \left\{ \sum_{k=1}^{r} k Q_k \omega_r^k \right\}_{r=R_{\gamma}}^{\infty} \) are decreasing, provided \( \gamma > 1 + \frac{br}{\rho_s} = \frac{4}{3} \). This means that \( m(w) \) is well defined, as the value of \( r \) for which \( \omega_{r+1} < w \leq \omega_r \), provided \( w \in (z_s, \omega_{R_{\gamma}}) \). Hence we can define \( z(\rho) = \min \left\{ w : \sum_{r=1}^{m(w)} r Q_r w^r = \rho \right\} \).

For reasons given in Section 4.3 we give slightly different definitions to \( N(\rho) \) in the two cases:

- **Case A** \( N(\rho) = \text{ceil} \left( m^\gamma(z(\rho)) \left[ \frac{\rho - \rho_s}{\rho - \rho_s} \right]^{0.25} \right) \),
- **Case B** \( N(\rho) = \text{ceil} (m^\gamma(z(\rho))) \),
where \( \text{cei}(x) \) is the least integer greater than \( x \). In both cases \( z_e(\rho) \) is defined as the solution of
\[
\sum_{r=1}^{N(\rho)} r Q_r w^r = \rho.
\]

In Section 3.4, \( \mathcal{P} \) was defined as the largest value of \( \rho \) for which the all the results of the lemmas and corollaries in Section 3.4.1 were true. Only Lemmas 3.4.1 and 3.4.2 and Corollary 3.4.5 are relevant here, and \( \rho \in \left[ \rho_s, \sum_{k=1}^{R_s} k Q_k \left( \frac{b_r}{a_r} \right)^k \right] \) implies that the first two of these apply. So we define \( \mathcal{P} \) as the largest value less than \( \bar{\mathcal{P}} := \sum_{k=1}^{R_s} k Q_k \left( \frac{b_r}{a_r} \right)^k \), for which:
\[
\rho \in (\rho_s, \mathcal{P}) \implies N(\rho) > \ell(y_0),
\]
where \( \ell(y_0) \) is the value of \( r \) for which \( \sum_{k=1}^{r+1} k Q_k \left( \frac{b_r}{a_r} \right)^k < \rho < \sum_{k=1}^{r} k Q_k \left( \frac{b_r}{a_r} \right)^k \).

To calculate an approximate value of \( \mathcal{P} \) we found the numerical solution of:
\[
N(\rho) = \min_{r \geq R_s} \left\{ \sum_{k=1}^{r} k Q_k \left( \frac{b_r}{a_r} \right)^k \geq \rho \right\}.
\]
The results of this calculation, for various values of \( \gamma \) are given in the table below. The values of \( \bar{\mathcal{P}} \) are also given for reference.

### Case A

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>1.35</th>
<th>1.40</th>
<th>1.45</th>
<th>1.50</th>
<th>1.55</th>
<th>1.60</th>
<th>1.65</th>
<th>1.70</th>
<th>1.75</th>
<th>1.80</th>
</tr>
</thead>
</table>

### Case B

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>1.35</th>
<th>1.40</th>
<th>1.45</th>
<th>1.50</th>
<th>1.55</th>
<th>1.60</th>
<th>1.65</th>
<th>1.70</th>
<th>1.75</th>
<th>1.80</th>
</tr>
</thead>
</table>

* Values are not available because \( R_\gamma > 10,000 \).

Finding the value of \( z \) from \( \rho \) means performing calculations that mimic the proof of Lemma 3.2.7. We find the \( r_\rho \geq R \) such that \( \sum_{k=1}^{r_\rho} k Q_k w^k_r \geq \rho \geq \sum_{k=1}^{r_\rho+1} k Q_k w^k_{r+1} \), then solve \( \sum_{k=1}^{r_\rho} k Q_k w^k = \rho \). Figure 4.1.1 shows the plots of \( \{\omega_r\}^10^4_{r=R^\prime-1} \) against \( \left\{ \sum_{k=1}^{r} k Q_k w^k \right\}_{r=R^\prime-1}^{10^4} \) for a variety of values of \( \gamma \), where \( R^\prime \) is the least value of \( r \) for which \( \{\omega_k\}_{k=r}^{\infty} \) is decreasing.

This calculation automatically gives \( m(z) = r_\rho \), from which \( N(\rho) \), thence \( z_e(\rho) \), can be evaluated.

### 4.2 The initial data

In [12] Penrose proved that those solutions of the Becker-Döring equations, \( c \), for which
\[
c_r(0) = \begin{cases} M_r \left( z, \sum_{k=1}^{\infty} A_k(z)^{-1} \right) & 1 \leq \ell(z) \\ Q_r z^r_s & r \geq \ell(z) + 1 \end{cases}
\]
4.2. THE INITIAL DATA

Figure 4.1.1: $\omega_r$ against $\sum_{k=1}^r k Q_k \omega^k$, for $\gamma = 1.35, 1.4, \ldots, 1.8$.

were metastable. In view of this we use:

$$c_1(0) = M_r \left( z_0, \left[ \sum_{k=1}^{N-1} A_k(z_0) \right]^{-1} \right) = M_r(z_0, J_0(z_0))$$

where $z_0$ is the unique solution of $\sum_{r=1}^N r M_r(z_0, J_0(z_0)) = \rho$. In all cases considered here $z_0 \leq z(\rho)$.

We can prove that $\{M_r(z_0, J_0)\} \in \mathcal{R}_\rho$ by noting that:

$$L_r(z_c, J_0(z_c)) \leq M_r(z_0, J_0(z_0)) \leq U_r(z, z_c, q_{\ell+1}(z), \ell_c + 1)$$

and:

$$J_0(w) = \frac{1}{\sum_{k=1}^{N-1} A_k(w)} > q_N(w) = \frac{1}{\sum_{k=1}^{N-1} A_k(w) + A_N \left( w - \frac{q_N}{m_N} \right)^{-1}}$$

so $\{M_r(w, J_0(w))\}_{r=1}^N$ is non-increasing. An argument similar to the one in Lemma 3.4.8 can then be used.

In [13] Carr et al point out a very strong similarity between the approximate value of $c_1(t)$ in the metastable phase and the solution, $w$, of:

$$\sum_{k=1}^{\ell(w)} kQ_kw^k = \rho,$$
which is $y_p$ from Lemma 3.4.2. We note here that:

$$0 = \sum_{k=1}^{m(z)} kQ_k z^k - \sum_{k=1}^{\ell(y_p)} kQ_k y_p^k > (z - y_p) - (\ell(y_p) - m(z))m(z)Q_m(z)y_p^m(z)$$

$$\implies z - y_p < (N - m)mQ_m z^m,$$

so $z - y_p$, as well as $z - z_0$, is at most exponentially small. Which means that there are sets of initial data $x \in \mathcal{R}_\rho$ with $x_1 = y_p$.

### 4.3 Running the program

Numerical solutions of (3.1.1) were found for the above coefficients and initial data using a program written by Duncan and Walshaw, which is described and used in [22] and [13]. The results of which will be given in the next section. Here we discuss the restrictions on the choice of values of $\rho$ caused by, either the limitations of the program or our wish to compare its results with the bounds proved in Section 3.3.

The main limitation on running simulations is that the program has an impractically long running time for certain values of $N$ and $\rho$. This effect’s dependence on these parameters is not fully understood but it can be largely avoided by only considering systems where $N \leq 5,000$. Table 4.1 contains the numerical solutions of $N(\rho) = 5000$.

We could only expect meaningful results when $z_0 - z_c > \text{numerical error}$. As an approximation to this, we consider only those systems for which:

$$z - z_c > 10^{-4} \gg \text{truncation error}.$$

The program is written to in such a way that truncation error $\lesssim 10^{-4}$. The range of values for which $z(\rho) - z_c(\rho) > 10^{-4}$ has both upper and lower limits, numerical approximations of these are given in Table 4.2. The larger the value of $N$ the greater the width of these ranges. This is why the factor $\left[\frac{p}{p - p_c}\right]^{0.25}$ was placed in the definition of $N(\rho)$ in case A. If the same definition for $N$ was used in case B the reduced choice in Table 4.1 cancels out any improvements made here.

We will show plots of the numerical approximations of $c_1(t)$ and compare these with the bound on $c_1(t)$ which Theorem 3.4.10 prove to be:

$$c_1(t) > (c_1(0) - f - (N - \ell_c)g) - NJ^*t$$

for $t \geq \min \left\{ \frac{(z - z_c) - (f + (N - \ell_c)g)}{NJ^*}, \frac{Q_N z_c^N - L_N(y, l) - g(\rho)}{J^*} \right\} =: \tau_\rho$

where $f = \sum_{r=1}^{\ell_c} r(U_r - c_r(0))$ and $g = \sum_{r=\ell_c+1}^{N} (c_r(0) - L_r)$. We saw in Section 4.2 that $f$ and $g$ were at most exponentially small, so we only wish consider those values of $\rho$ for which $f$ and $g$ have become ‘numerically small’. To be specific we restrict ourselves to those values of $\rho$ for which:

$$\max\{f, (N - \ell_c)g\} < \frac{z - z_c}{10}$$

Table 4.3 gives the numerical solutions of $\max\{f, (N - \ell_c)g\} = \frac{z - z_c}{10}$.

Table 4.4 shows the values of $\rho$ that are in the intersection of the above ranges. Unfortunately these ranges are cut even further because values at the lower end have very long running times. In fact for $\gamma \geq 1.60$ there is effectively no range left and in case B, $\gamma = 1.55$, $\rho \geq 7.14$. This is the reason for considering case A, rather than only using the coefficients used in [13].
4.3. RUNNING THE PROGRAM

<table>
<thead>
<tr>
<th>Case</th>
<th>$\gamma$</th>
<th>$1.35$</th>
<th>$1.40$</th>
<th>$1.45$</th>
<th>$1.50$</th>
<th>$1.55$</th>
<th>$1.60$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\rho &gt;$</td>
<td>4.3727</td>
<td>4.9668</td>
<td>5.5973</td>
<td>6.2265</td>
<td>6.8845</td>
<td>7.5764</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.65</td>
<td>1.70</td>
<td>1.75</td>
<td>1.80</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>8.3176</td>
<td>9.1430</td>
<td>10.0564</td>
<td>11.1139</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* Value is not available because $N(\rho) \leq 5,000 \implies \rho < \sum_{k=1}^{10^4} kQ_k \omega_k^{\rho_k}$.

Table 4.1: Values of $\rho \in (\rho_s, P)$ for which $N(\rho) \leq 5,000$.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\gamma$</th>
<th>$1.40$</th>
<th>$1.45$</th>
<th>$1.50$</th>
<th>$1.55$</th>
<th>$1.60$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\rho = $</td>
<td>N.A.*</td>
<td>5.6022</td>
<td>6.3150</td>
<td>7.0665</td>
<td>7.8745</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.65</td>
<td>1.70</td>
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<tr>
<td></td>
<td></td>
<td>8.7746</td>
<td>9.8110</td>
<td>11.0372</td>
<td>12.4986</td>
<td></td>
</tr>
</tbody>
</table>

Values are not available because $z(\rho) - z_e(\rho) < 10^{-4}$.

Table 4.2: Values of $\rho \in (\rho_s, P)$ for which $z(\rho) - z_e(\rho) \geq 10^{-4}$.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\gamma$</th>
<th>$1.50$</th>
<th>$1.55$</th>
<th>$1.60$</th>
<th>$1.65$</th>
<th>$1.70$</th>
<th>$1.75$</th>
<th>$1.80$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\rho &lt; $</td>
<td>6.8089</td>
<td>8.1782</td>
<td>8.6918</td>
<td>8.5806</td>
<td>N.A.*</td>
<td>N.A.**</td>
<td>N.A.**</td>
</tr>
</tbody>
</table>

* Values are not available because $\max \{ f, (N - \ell_e)g \} < \frac{e_0}{10}$.
** Values are not available because it was not possible to calculate $e_0$.

Table 4.3: Values of $\rho \in (\rho_s, P)$ for which $\max \{ f, (N - \ell_e)g \} < \frac{e_0}{10}$.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\gamma$</th>
<th>$1.55$</th>
<th>$1.60$</th>
<th>$1.65$</th>
<th>$1.70$</th>
<th>$1.75$</th>
<th>$1.80$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\rho &lt; $</td>
<td>7.2454</td>
<td>8.3361</td>
<td>8.7076</td>
<td>N.A.*</td>
<td>N.A.*</td>
<td>N.A.*</td>
</tr>
</tbody>
</table>

* From Table 4.1 $\rho > 8.7746$ while from Table 4.3, $\rho < 8.7076$.

Table 4.4: Values of $\rho$ for which all the above restrictions apply.
4.4 Results

Figures 4.4.1, 4.4.2 and 4.4.3 show plots of the numerical approximations of \( c_1(t) \) against \( \log_{10}(t) \). For each plot of \( c_1(t) \) we also show the lower bound given in Equation (4.3.1) and mark the point \((\log_{10}(t_\rho), c_1(t_\rho))\), after which the bound may not hold, with a ‘+’. We have also found the first time the numerical value of \( c_1(t) \) drops below 1.0001\( z_e \); this is the numerical equivalent of \( t_\rho \) and is denoted \( T_\rho \).

\[
\begin{array}{|c|c|c|c|c|c|}
\hline
\rho & r_\rho = m(z) & z(\rho) & N(\rho) & z_e(\rho) & t_\rho & T_\rho \\
\hline
6.76 & 132 & 1.1220 & 1686 & 1.1219 & 2.0574 \times 10^8 & 2.2518 \times 10^{12} \\
6.72 & 138 & 1.1207 & 1809 & 1.1203 & 1.7192 \times 10^9 & 4.3306 \times 10^{13} \\
6.68 & 145 & 1.1194 & 1956 & 1.1181 & 1.2014 \times 10^{10} & 4.8449 \times 10^{14} \\
6.64 & 152 & 1.1180 & 2108 & 1.1157 & 5.4814 \times 10^{10} & 2.4849 \times 10^{15} \\
6.60 & 160 & 1.1167 & 2286 & 1.1131 & 2.3087 \times 10^{11} & 1.4568 \times 10^{16} \\
\hline
\end{array}
\]

\[
\begin{align*}
\text{log}_{10}(t) & \quad c_1(t) \\
0 & \quad 1.113 \\
2 & \quad 1.115 \\
4 & \quad 1.117 \\
6 & \quad 1.118 \\
8 & \quad 1.119 \\
10 & \quad 1.121 \\
12 & \quad 1.122 \\
14 & \quad 1.123 \\
16 & \quad 1.124 \\
18 & \quad 1.125 \\
\end{align*}
\]

\[
\begin{align*}
\rho = 6.76 & \quad \text{is the solution } c_1(t), \text{ for } t < t_\rho \\
+ & \quad \text{is the point } (\log(t_\rho), c_1(t_\rho)) \\
\cdots & \quad \text{is the solution } c_1(t), \text{ for } t > t_\rho \\
\cdots & \quad \text{is the lower bound to } c_1(t): (c_1(0) - f - (N - \ell_e)g) - NJ^*t \text{ for } t < t_\rho \\
\cdots & \quad \text{is a line drawn at the height of } z_e(\rho).
\end{align*}
\]

Figure 4.4.1: Case A, \( \gamma = 1.50 \)

4.5 Conjectured bounds

Looking at the work in Section 3.3 and Section 3.4 we can see that, the only time that the conditions \( \rho \leq \sum_{k=1}^{m(z)} kQkz^k \) and \( N > m(z)^\gamma \) were used explicitly, was in Theorem 3.3.1 and there only to show that \( c_1(t) < U_1 \) for all \( t < T \). The numerical evidence (here and in [13] and [22]) suggests that not only is \( c_1(t) < z \) but that \( c_1(t) < 0 \) for all \( t < T \). So it is reasonable to make the following conjecture:
4.5. CONJECTURED BOUNDS

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>$r_\rho = m(z)$</th>
<th>$z(\rho)$</th>
<th>$N(\rho)$</th>
<th>$z_\epsilon(\rho)$</th>
<th>$t_\rho$</th>
<th>$T_\rho$</th>
</tr>
</thead>
<tbody>
<tr>
<td>8.0</td>
<td>89</td>
<td>1.1573</td>
<td>1162</td>
<td>1.1407</td>
<td>7.9695 $\times 10^4$</td>
<td>6.5267 $\times 10^{10}$</td>
</tr>
<tr>
<td>7.8</td>
<td>102</td>
<td>1.1522</td>
<td>1455</td>
<td>1.1315</td>
<td>4.6713 $\times 10^5$</td>
<td>7.4556 $\times 10^{11}$</td>
</tr>
<tr>
<td>7.6</td>
<td>118</td>
<td>1.1470</td>
<td>1849</td>
<td>1.1221</td>
<td>3.0970 $\times 10^6$</td>
<td>7.9543 $\times 10^{13}$</td>
</tr>
<tr>
<td>7.4</td>
<td>138</td>
<td>1.1415</td>
<td>2393</td>
<td>1.1125</td>
<td>2.5177 $\times 10^7$</td>
<td>3.0807 $\times 10^{16}$</td>
</tr>
<tr>
<td>7.2</td>
<td>162</td>
<td>1.1357</td>
<td>3118</td>
<td>1.1033</td>
<td>2.6749 $\times 10^8$</td>
<td>N.A.</td>
</tr>
</tbody>
</table>

Figure 4.4.2: Case A, $\gamma = 1.55$
\[ r_\rho = m(z) \]

<table>
<thead>
<tr>
<th>( \rho )</th>
<th>( r_\rho = m(z) )</th>
<th>( z(\rho) )</th>
<th>( N(\rho) )</th>
<th>( z_e(\rho) )</th>
<th>( t_\rho )</th>
<th>( T_\rho )</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.22</td>
<td>182</td>
<td>1.0654</td>
<td>3185</td>
<td>1.0650</td>
<td>( 1.3934 \times 10^9 )</td>
<td>( 1.0482 \times 10^{14} )</td>
</tr>
<tr>
<td>7.20</td>
<td>189</td>
<td>1.0650</td>
<td>3376</td>
<td>1.0641</td>
<td>( 4.9429 \times 10^9 )</td>
<td>( 4.0877 \times 10^{14} )</td>
</tr>
<tr>
<td>7.18</td>
<td>197</td>
<td>1.0646</td>
<td>3600</td>
<td>1.0630</td>
<td>( 1.4999 \times 10^{10} )</td>
<td>( 1.8598 \times 10^{15} )</td>
</tr>
<tr>
<td>7.16</td>
<td>204</td>
<td>1.0642</td>
<td>3801</td>
<td>1.0621</td>
<td>( 3.4727 \times 10^{10} )</td>
<td>( 5.5076 \times 10^{15} )</td>
</tr>
<tr>
<td>7.14</td>
<td>212</td>
<td>1.0638</td>
<td>4034</td>
<td>1.0610</td>
<td>( 7.9791 \times 10^{10} )</td>
<td>( 2.8497 \times 10^{16} )</td>
</tr>
</tbody>
</table>

The table above lists the values of \( \rho \), \( r_\rho = m(z) \), \( z(\rho) \), \( N(\rho) \), \( z_e(\rho) \), \( t_\rho \), and \( T_\rho \). The figure below shows the graph of \( c_1(t) \) against \( \log_{10}(t) \) for different values of \( \rho \). The solid line indicates \( c_1(t) \) for \( t < t_\rho \), the dashed line is the point \((\log(t_\rho), c_1(t_\rho))\), the dotted line is \( c_1(t) \) for \( t > t_\rho \), the dashed-dotted line is the lower bound to \( c_1(t) \): \( (c_1(0) - f - (N - \ell_e)g) - NJ^*t \) for \( t < t_\rho \), and the dash-dot-dotted line is a line drawn at the height of \( z_e(\rho) \).

Figure 4.4.3: Case B, \( \gamma = 1.55 \)
Conjecture 4.5.1

Suppose that: \( N \geq \ell(z_e) + 1; \ z_e < \ell; \ \ell^* \in \mathbb{N} \) and \( \ell(z) \leq \ell^* \leq \ell_e; \) and \( J \in (q_{\ell^* - 1}(z), q_{\ell^*}(z)]. \) Then define

\[
U_r(z, z_e, J, \ell^*) := \begin{cases} 
M_r(z, J) & \text{for } 1 \leq r \leq \ell^* \\
\frac{b_r M_r(z, J)}{b_r} & \text{for } \ell^* < r \leq \ell_e + 1 \\
\frac{b_r M_r(z, J)}{b_{\ell_e + 1}} Q_r z_e^r & \text{for } \ell_e + 1 \leq r \leq N \\
\end{cases}
\]

\[ T := \min\{\inf\{t : c_1(t) < z_e\}, \inf\{t : c_N(t) > U_N\}\}. \]

If \( c_r(0) \leq U_r \) for \( 1 \leq r \leq N \) then \( c_r(t) \leq U_r \) for \( 1 \leq r \leq N \) and all \( t \in [0, T). \)

If the conjecture were true we would be able to prove the main results of Section 3.4, provided:

1. \( N(\rho) > \ell(y_\rho) =: \ell_\rho, \) and \( N(\rho) \) is algebraically large;
2. \( z_e(\rho) = \bar{z}; \)
3. \( [z(\rho) - z_e(\rho)] \setminus 0 \) as \( \rho \to \rho_s \) but is at least algebraically small.

Any remaining references to \( m(z) \) and \( \omega_r \) can be replaced with \( \ell(z) \) and \( \frac{b_r}{\alpha_r}, \) respectively.

Example 4.5.2. If \( c_1(t) < z \) for all \( t < T \) then the class \( \{R_\rho : \rho \in (\rho_s, \overline{\rho})\}, \) defined by \( N(\rho) = 10\ell_\rho \) and \( z(\rho) = z_\rho + 0.2(z_e - z_\rho), \) is metastable for both case A and case B; where \( \overline{\rho} = \max_{\rho \in \mathbb{N}} \left\{ \sum_{k=1}^r kQ_k \frac{b_k}{\alpha_k} \right\}. \)

This follows immediately from the comments above.

Example 4.5.3. If \( c_1(t) < z \) for all \( t < T \) then the class \( \{R_\rho : \rho \in (\rho_s, \overline{\rho})\}, \) defined by \( N(\rho) = 10\ell_\rho \) and \( z(\rho) = \overline{z_0}, \) is metastable for both case A and case B; where \( \overline{z_0} \) is the same as before, i.e. the solution of \( \sum_{r=1}^N rM_r \left( \overline{z_0}, \left[ \sum_{k=1}^{N-1} A_k(z_0) \right]^{-1} \right) = \rho. \)

Proof.

We saw above that \( \{M_r(z_0, J_0)\} \) is decreasing so we can see that \( z_0 - z_e \) is at least algebraically large by arguments similar to those used in Lemma 3.4.8.

### 4.6 An a priori test for metastability

By comparing \( t_\rho \) and \( T_\rho \) in the tables attached to Figures 4.4.1, 4.4.2 and 4.4.3 we can see that while \( t_\rho \) is a poor estimate of \( T_\rho, \) the two quantities do have the same qualitative behaviour. The results of Section 3.4 already tell us that a ‘large’ value of \( t_\rho \) implies the presence of metastability, so we may conjecture that, a ‘small’ value of \( t_\rho \) implies a loss of the metastable plateau. Unfortunately the definition of \( t_\rho^* \) contains \( f \) and \( g \) and they cause \( t_\rho \) to be negative for the range of values of \( \rho \) that interest us. So we consider the quantity \( s_\rho := \min \left\{ \frac{z - z_e}{N_\rho}, \frac{Q_N z^N - L_N(y, f)}{y^2} \right\} \) instead. This is not as arbitrary as it might first appear since one can always pick initial data for which, \( f = g = 0 \) and \( |s_\rho - t_\rho| \) is at most exponentially small, as \( \rho \to \rho_s. \)

We will test this using the Examples 4.5.2 and 4.5.3, with Case B coefficients and the following initial data:

For Example 4.5.2: \( c_{0\rho} = M_r(z, J_0) \) where \( J_0 \) is the solution of \( \sum_{r=1}^N rM_r(z, J) = \rho, \)

i.e. \( J_0 = \frac{\sum_{r=1}^N rQ_r z^r - \rho}{\sum_{r=1}^N rQ_r z^r \sum_{k=1}^{N-1} A_k(z)}. \)

\[ t_\rho^* := \min \left\{ \frac{(z - z_e) - f + \alpha(z_e - y)}{N_\rho}, \frac{Q_N z^N - L_N(y, f) - g}{y^2} \right\}. \]
For Example 4.5.3: \( c_r(0) = M_r \left( z_0, \left[ \sum_{k=1}^{N-1} A_k(z_0) \right]^{-1} \right) \).

The tables below show the values of \( s_\rho \) for Examples 4.5.2 and 4.5.3, using Case B coefficients.

<table>
<thead>
<tr>
<th>( \rho )</th>
<th>10</th>
<th>15</th>
<th>20</th>
<th>25</th>
<th>30</th>
<th>35</th>
</tr>
</thead>
<tbody>
<tr>
<td>( s_\rho ) for Ex. 4.5.2</td>
<td>6.1392 \times 10^5</td>
<td>24.911</td>
<td>20.634</td>
<td>4.2708</td>
<td>1.3083</td>
<td>0.4140</td>
</tr>
<tr>
<td>( s_\rho ) for Ex. 4.5.3</td>
<td>3.2380 \times 10^2</td>
<td>7.3631</td>
<td>2.079</td>
<td>1.0039</td>
<td>0.5325</td>
<td>0.2763</td>
</tr>
</tbody>
</table>

From which we see that if the conjecture is true, with ‘small’= \( O(1) \), we will see metastable type behaviour at values of \( \rho \) far above those seen in earlier figures or in [22] and [13]. This is indeed what we see in Figures 4.6.1 and 4.6.2, where we show the numerical approximations of \( c_1(t) \). We have found the first time, \( S_\rho \), the numerical solution of \( c_1 \) drops below 0.1\% of its initial value and marked the point \((\log_{10}(S_\rho), c_1(S_\rho))\) with a ‘+’. This may be regarded as a measure of the length of the metastable plateau.

<table>
<thead>
<tr>
<th>( \rho )</th>
<th>( z(\rho) )</th>
<th>( N(\rho) )</th>
<th>( z_\rho(\rho) )</th>
<th>( s_\rho )</th>
<th>( S_\rho )</th>
</tr>
</thead>
<tbody>
<tr>
<td>38</td>
<td>1.1546</td>
<td>380</td>
<td>1.1289</td>
<td>0.17</td>
<td>1.0667 \times 10^4</td>
</tr>
<tr>
<td>35</td>
<td>1.1429</td>
<td>500</td>
<td>1.1191</td>
<td>0.41</td>
<td>1.0667 \times 10^2</td>
</tr>
<tr>
<td>30</td>
<td>1.1314</td>
<td>660</td>
<td>1.1095</td>
<td>1.31</td>
<td>9.6244 \times 10^2</td>
</tr>
<tr>
<td>25</td>
<td>1.1224</td>
<td>330</td>
<td>1.1020</td>
<td>4.27</td>
<td>3.3798 \times 10^3</td>
</tr>
<tr>
<td>20</td>
<td>1.1130</td>
<td>1070</td>
<td>1.0941</td>
<td>20.63</td>
<td>2.4807 \times 10^4</td>
</tr>
</tbody>
</table>

Figure 4.6.1: Solutions for Example 4.5.2
4.6. An a priori test for metastability

<table>
<thead>
<tr>
<th>$\rho$</th>
<th>$z(\rho)$</th>
<th>$N(\rho)$</th>
<th>$z_e(\rho)$</th>
<th>$s_\rho$</th>
<th>$S_\rho$</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>1.1448</td>
<td>660</td>
<td>1.1095</td>
<td>0.53</td>
<td>$3.6401 \times 10^4$</td>
</tr>
<tr>
<td>25</td>
<td>1.1387</td>
<td>830</td>
<td>1.1020</td>
<td>1.00</td>
<td>$6.7399 \times 10^4$</td>
</tr>
<tr>
<td>20</td>
<td>1.1318</td>
<td>1070</td>
<td>1.0941</td>
<td>2.21</td>
<td>$3.6708 \times 10^2$</td>
</tr>
<tr>
<td>15</td>
<td>1.1230</td>
<td>1480</td>
<td>1.0849</td>
<td>7.36</td>
<td>$9.2203 \times 10^2$</td>
</tr>
<tr>
<td>10</td>
<td>1.1036</td>
<td>3010</td>
<td>1.0678</td>
<td>323.80</td>
<td>$3.5505 \times 10^4$</td>
</tr>
</tbody>
</table>

Figure 4.6.2: Solutions for Example 4.5.3
Bibliography


