Long Time Behavior of a Modified Becker-Döring System

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Abstract A modification, based on asymptotic behavior, of the Becker-Döring system is introduced in which the concentration of monomers is slaved to the concentrations of the other clusters. This modified system has the same continuum limit as the usual Becker-Döring system. For one member of the modified systems it is proved, for compact initial data, that all solutions will converge to the same self-similar form as time tends to infinity.

1 Introduction

Ostwald ripening is a coarsening process, often associated with a phase transition, in which droplets or clusters condense from a vapor phase. The Becker-Döring equations have been commonly used in an effort to understand ripening from a theoretical perspective. They provide a description of the time evolution of the concentration of cluster sizes phrased in terms of an infinite set of rate equations. The Becker-Döring equations have been fairly well studied over the years and many aspects of their behavior are well known. Nevertheless an important question remains unanswered, namely, whether or not these equations will converge to the same self similar profile for a wide class of initial data. There is some evidence from numerical simulations that the solutions of the Becker-Döring equations will indeed converge to a self similar form [2, 4, 8]. However these calculations are difficult because the rate of convergence appears to be very slow. Nevertheless, it seems possible that the Becker-Döring system has the same self similar form for a wide class of initial data.

In this paper, a modification of the Becker-Döring equations will be presented. For one member of the modified equations we will prove that, for all compactly supported initial data, the long time behavior can be described by the same self-similar form.

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Let us begin by putting this work in context by first recalling the Becker-Döring equations, which are

$$\dot{c}_j = F_{j-1} - F_j \quad \text{for } j = 2, 3, 4, \dots \tag{1}$$

where $c_j = c_j(t)$ is the concentration of clusters of size j; the monomer concentration satisfies

$$\dot{c}_1 = -2F_1 - \sum_{j=2}^{\infty} F_j. \tag{2}$$

F_j is the rate at which clusters of size j get converted to clusters of size $j + 1$. The density, ρ, is

$$\rho = \sum_{j=1}^{\infty} j c_j.$$

It is an easy check, for the Becker-Döring system that, formally, $\dot{\rho} = 0$. The fluxes take the form

$$F_j = a_j c_1 c_j - b_{j+1} c_{j+1} \quad \text{for } j = 1, 2, 3, \dots. \tag{3}$$

The existence and uniqueness of solutions was established by Ball, Carr and Penrose [1]. In addition, they prove that if the density ρ, is less than some critical density, ρ_c, the long time behavior will result in solutions converging strongly to a unique steady solution. Physically, this corresponds to a vapor. On the other hand, if $\rho > \rho_c$, the long time behavior of solutions will only result in weak convergence to the unique steady solution. The excess density will be contained in progressively larger clusters as time increases. This corresponds to coarsening. It should pointed out this scenario is only true if a_j and b_j satisfy certain growth rates [1].

A natural question is whether or not the long time behavior of the excess density can be described by a self-similar form. One approach to describing the long time behavior of the excess density is to formulate a continuum approximation of the Becker-Döring equations. Let us briefly discuss this below.

1.1 LSW Approximation

Here we briefly outline how one can obtain the LSW (Lifshitz, Slyozov, & Wagner) approximation from the Becker-Döring equations. This derivation was inspired from the work of Penrose [13]. The discussion below, however, emphasizes certain points that are needed later in this paper.

In case when $\rho > \rho_c$ the steady solution of the Becker-Döring equations is denoted γ_j where $j = 1, 2, 3, \dots$. The critical density is then

$$\rho_c = \sum_{j=1}^{\infty} j \gamma_j$$

It follows from [1] (also see [13]) that

$$\lim_{t \to \infty} c_j(t) = \gamma_j \quad \text{and} \quad \lim_{t \to \infty} F_j = 0. \tag{4}$$

Next, we introduce a variable ℓ that is chosen to be large enough so that $\gamma_\ell \ll 1$. The expression for the density is rewritten as

$$\rho = \sum_{j=1}^{\ell-1} jc_j + \sum_{j=\ell}^{\infty} jc_j.$$

In view of (4) and our choice of ℓ, the following is a good approximation for large t

$$\rho - \rho_c \approx \sum_{j=\ell}^{\infty} jc_j.$$

Since $\rho - \rho_c$, the excess density, is constant then differentiating the above equation with respect to time and using summation by parts yields

$$\sum_{j=\ell}^{\infty} F_j \approx 0, \tag{5}$$

where the approximation $F_{\ell-1} \approx 0$ for $t \gg 1$ has been used (this follows from 4). If the expression for F_j given by (3) is used in (5) we arrive at the approximation

$$c_1 \approx \frac{\sum_{j=\ell}^{\infty} b_{j+1} c_{j+1}}{\sum_{j=\ell}^{\infty} a_j c_j}. \tag{6}$$

Therefore, to study the long time behavior of the excess density it is a good approximation to solve (1) for $j \geq \ell$ while using (6) for the monomer concentration. In view of (4) and our choice of ℓ it is reasonable to take $F_{\ell-1} = 0$ as a boundary condition. Finally, we mention that the discrete system given by (1) for $j \geq \ell$ along with (6) is nothing more than a discretization of the LSW equation discussed in the next section.

1.1.1 Continuum Limit

Next we will briefly discuss how to approximate (1) combined with (6) as a partial differential equation. Let $c(x,t)$ be defined such that $c_j(t) = c(j,t)$. $a(x)$, $b(x)$, and $F(x,t)$ are defined in an analogous way. In addition we will let monomer concentration, c_1, be denoted as $u(t)$. If we assume that all of these functions are smooth in x then one has the approximation

$$F_j - F_{j-1} \approx \partial_x F$$

This indicates that (1) maybe approximated by

$$\partial_t c + \partial_x F \approx 0$$

It is convenient to rewrite the fluxes as

$$F_j = (a_j u - b_j)c_j + b_j c_j - b_{j+1} c_{j+1}$$

which are approximated as

$$F \approx (au - b)c + \partial_x(bc).$$

The above approximations are combined to give the following partial differential equation,

$$\partial_t c + \partial_x[(au - b)c] \approx \partial_{xx}^2(bc). \tag{7}$$

The continuum approximation of (6) is

$$u(t) \approx \frac{\int_\ell^\infty b(x)c(x,t)dx}{\int_\ell^\infty a(x)c(x,t)dx}$$

If we ignore the right hand side of (7) and take $\ell = 0$ we have the following approximation to the Becker-Döring system

$$\partial_t c + \partial_x[(au - b)c] = 0 \quad \text{where } u = \frac{\int_0^\infty bcdx}{\int_0^\infty acdx}. \tag{8}$$

We will henceforth refer to this as an LSW equation.

If we make the following choice

$$a = x^{1/3} \quad \text{and} \quad b = 1$$

then we obtain the well known equation

$$\partial_t c + \partial_x[(x^{1/3}u - 1)c] = 0 \quad \text{with } u = \frac{\int_0^\infty cdx}{\int_0^\infty x^{1/3}cdx}. \tag{9}$$

This is often referred to as the LSW equation for diffusion controlled coarsening. On the other hand if we choose

$$a = x \quad \text{and} \quad b = 1,$$

then we obtain the simplified LSW equation, proposed by Carr & Penrose [3],

$$\partial_t c + \partial_x[(xu - 1)c] = 0 \quad \text{with } u = \frac{\int_0^\infty cdx}{\int_0^\infty xcdx}. \tag{10}$$

The above derivation uses uncontrolled approximations. However, for a class of Becker-Döring systems Penrose [13] and Niethammer [10] systematically established that their long time behavior is governed by an LSW equation. It should also be pointed out that the LSW equation can be derived in other ways. For example, it arises naturally as a mean field model of clusters or drops connected through a diffusion field. A good review can be found in [16], but also see [9] and [11]. As a consequence, the long behavior time of the LSW equation has attracted considerable attention.

The paper of Lifshitz and Slyozov [5] establishes that the LSW equation (9) has a one parameter family of self similar solutions all with compact support. Exactly one of them is infinitely differentiable; henceforth denoted the LS self similar solution. Lifshitz and Slyozov argue that this self similar solution will be the one that is selected either when solving the LSW equation or when examining experimental results. There is some evidence for the later claim, especially for dilute systems (e.g. Marder [6]). However, the former claim has generated controversy over the years (see [12] for nice description of the history) and was only recently put to rest by Niethammer and Pego [12] who prove that it is in fact false. They prove that long time behavior of the LSW equations depends in a sensitive way on

the initial conditions, in particular on the size distribution of the largest clusters. Only for special initial conditions will the LS self similar solution be realized. A similar result was obtained by Carr and Penrose [3] for the simplified LSW equation given by (10).

If we are to believe the numerical simulations, it seems reasonable to conclude that the long time behavior of a Becker-Döring system cannot be completely described in terms of an LSW equation with arbitrary initial conditions. As pointed out by Niethammer [10] (see Sect. 1.5.4) the Becker-Döring system must somehow create the correct initial conditions for the corresponding LSW equation. One possibility is to include the diffusion term and study (7) instead of (8) with the idea that the diffusion term will serve to "prepare the initial data". In this way, the long time behavior could be described by the self similar behavior. This idea has been investigated by Meerson [7], Rubinstein and Zaltzman [14], and Veláquez [15].

In the previous section we argued that the long time behavior of the excess density can be approximated by the system

$$\dot{c}_j = F_{j-1} - F_j \quad \text{for } j = \ell, \ell+1, \ell+2, \ldots \tag{11}$$

where $F_{\ell-1} = 0$, F_j for $j \geq \ell$ is given by (3), c_1 is given by (6) and ℓ is chosen so that $\gamma_\ell \ll 1$. In many respects, (11) is no better an approximation to the Becker-Döring system than is the LSW equation. However, (11) has the advantage that it retains the discrete nature of the Becker-Döring system. In what follows we shall argue that the discreteness can have an important effect on the self similar behavior. To explore this issue we will introduce a modification of the Becker-Döring system which is somewhat simpler and should retain the essential characteristics with respect to the long time behavior but is more amenable to analysis.

2 Modified Becker-Döring Systems

Based on the preceding discussion we introduce a modification of the Becker-Döring system which is as follows. The form of the flux is the same, namely

$$F_j = a_j u c_j - b_{j+1} c_{j+1} \quad \text{for } j = 0, 1, 2, \ldots \tag{12}$$

with added restriction $a_0 = 0$. In these equations c_j represents the concentration of clusters of size $j + 1$ and u denotes the monomer concentration. The time evolution of c_j is given by

$$\dot{c}_j = F_{j-1} - F_j \quad \text{for } j = 1, 2, 3, \ldots \tag{13}$$

Motivated by (6), the monomer concentration is taken to be

$$u = \frac{\sum_{j=1}^{\infty} b_j c_j}{\sum_{j=1}^{\infty} a_j c_j}. \tag{14}$$

We shall call the set of equations given by (12), (13), and (14) modified Becker-Döring systems.

The "density" for this modified Becker-Döring is

$$\rho = \sum_{j=1}^{\infty} j c_j.$$

It easy to show that, formally, $\dot{\rho} = 0$.

We remark that one can view the modified Becker-Döring system as some sort of long time approximation to the Becker-Döring system or a first order (in space) upwind discretization of the generalized LSW system given by (8). It should be pointed out that the only stationary solution of this modified system is $c_j = 0$, $j = 1, 2, 3, \ldots$.

2.1 A Modified Becker-Döring System

Carr and Penrose [3] were motivated to arrive at their simplified LSW equation (10) because it could be solved exactly. Here a similar path will be followed and we will consider the modified Becker-Döring system with $a_j = j$ and $b_j = 1$ which as it turns out can be solved exactly. As pointed out in Ref. [3] this case is probably not physical but nevertheless the insight we gain maybe useful in other situations.

With this choice the modified Becker-Döring system we propose to study is

$$\dot{c}_j + u(jc_j - (j-1)c_{j-1}) - (c_{j+1} - c_j) = 0 \quad \text{for } j = 1, 2, 3, \ldots \tag{15}$$

where the monomer concentration is given by

$$u = \frac{\sum_{j=1}^{\infty} c_j}{\sum_{j=1}^{\infty} jc_j}. \tag{16}$$

The c_j's are normalized so that $\rho = 1$ and the equation for the monomer concentration becomes

$$u = u(t) = \sum_{j=1}^{\infty} c_j. \tag{17}$$

Equations (15) and (17) can be viewed as a discretization of (10). It convenient to rewrite (15) and (17) using

$$h_j = h_j(t) = \sum_{m=j}^{\infty} c_m \tag{18}$$

to obtain

$$\dot{h}_j + u(t)(j-1)(h_j - h_{j-1}) - (h_{j+1} - h_j) = 0 \tag{19}$$

where $j = Z^+$ and $u(t) = h_1$. It follows by the application of summation by parts on $\sum_{j=1}^{\infty} jc_j = 1$ that

$$\sum_{j=1}^{\infty} h_j = 1. \tag{20}$$

Next we observe that since $\dot{h}_1$ does not depend on h_0, we can, therefore, consider (19) for all $j \in Z$ without changing any solution of (19) for $j \in Z^+$ (Z denotes the set of all integers and Z^+ the set of all positive integers). We will therefore consider (19) for $j \in Z$ with initial conditions

$$h_j(0) = \begin{cases} g_j & \text{for } j > 0 \\ 0 & \text{otherwise.} \end{cases} \tag{21}$$

By virtue of (18) it follows that

$$g_1 \geq g_2 \geq g_3 \geq \cdots. \tag{22}$$

In addition we will assume that g_j will decay faster that any polynomial for large j. More precisely we demand

$$\lim_{j\to\infty} j^p g_j = 0 \quad \text{for all } p \in Z^+. \tag{23}$$

Finally, we point out that when solving (19) and (21) $h_j(t)$, will be nonzero for $j \leq 0$. Nevertheless, the evolution of h_j for $j \leq 0$ has no effect on h_j for $j > 0$. We shall see, however, it is more convenient to consider (19) for $j \in Z$ rather than Z^+.

2.2 Solution of the Initial Value Problem

In this section, the initial value problem for (19) and (21) will be solved. When considering discrete problems it is natural to consider the discrete Fourier transform of h_j,

$$\widehat{h}(k) = \sum_{j=-\infty}^{\infty} h_j e^{-ijk} \tag{24}$$

and its inverse

$$h_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ijk}\widehat{h}(k)dk. \tag{25}$$

For our purpose it is useful to modify this as follows; we let $e^{ik} = 1 + i\omega$ and make the definition $H(\omega) \equiv \widehat{h}(k)$ then (24) becomes

$$H(\omega) = \sum_{j=-\infty}^{\infty} h_j (1 + i\omega)^{-j}$$

and (25) becomes

$$h_j = \frac{1}{2\pi} \int_B H(\omega)(1 + i\omega)^{j-1}d\omega \tag{26}$$

where B is a circle of radius one that encloses the point $\omega = i$.

Equation (19) is multiplied by $1/(1 + i\omega)^j$ and summed over all $j \in Z$ to obtain

$$\partial_t H - u(t)\omega\partial_\omega H = (u(t) + i\omega)H$$

with initial conditions

$$H(\omega, 0) = H_0(\omega) = \sum_{j=1}^{\infty} \frac{g_j}{(1 + i\omega)^j}. \tag{27}$$

The partial differential equation for H can be solved by the method of characteristics. Let

$$U = U(t) = \int_0^t u(s)ds \quad \text{and} \quad v = v(t) = \int_0^t e^{-U(s)}ds, \tag{28}$$

then we have

$$H(\omega, t) = e^U H_0(\omega e^U) \exp(i\omega v e^U).$$

Combining the above result with (26) we arrive at

$$h_j = \frac{1}{2\pi} \int_B H_0(\omega e^U) \exp(i\omega e^U)(1+i\omega)^{j-1} d\omega.$$

Next, we let $\theta = \omega e^U$ and use (27) to obtain

$$h_j = \frac{e^{-v}}{2\pi} \sum_{m=1}^{\infty} \int_B \frac{g_m}{(1+i\theta)^m} e^{(1+i\theta)v}(1+i\theta\dot{v})^{j-1} d\theta. \tag{29}$$

It is apparent we will have an explicit expression for h_j once $v(t)$ is known. To determine $v(t)$ we note that since $u(t) = h_1$ it follows that

$$u = \frac{e^{-v}}{2\pi} \sum_{j=1}^{\infty} \int_B \frac{g_j}{(1+i\theta)^j} e^{(1+i\theta)v} d\theta.$$

In the above expression, the integrals are easily evaluated using the calculus of residues to reveal

$$u = e^{-v} \sum_{j=1}^{\infty} \frac{g_j v^{j-1}}{(j-1)!}. \tag{30}$$

It follows from (28) that $\dot{v} = \exp(-U)$ and $\ddot{v} = -\dot{v}u$. Therefore one has

$$\frac{\ddot{v}}{\dot{v}} = e^{-v} \sum_{j=1}^{\infty} \frac{g_j v^{j-1}}{(j-1)!}.$$

This maybe integrated once in v to obtain

$$\dot{v} = e^{-v} \left(1 + \sum_{p=1}^{\infty} \frac{\alpha_p v^p}{p!} \right) \quad \text{where } \alpha_p = \sum_{m=p+1}^{\infty} g_m, \tag{31}$$

where we have used (20). Let us now return to (29) and deduce an expression for h_j in terms of $v = v(t)$. To begin we rewrite (29) as

$$h_j = e^{-v} \sum_{m=1}^{\infty} g_m I_m \tag{32}$$

with

$$I_m = \frac{1}{2\pi i} \int_{B_0} \frac{e^{zv}(z\dot{v} + 1 - \dot{v})^{j-1}}{z^m} dz \tag{33}$$

where B_0 is a closed path in the complex plane the encloses the origin. The expression for I_m can be evaluated using the calculus of residues. We find for $j \in Z^+$ that

$$I_1 = (1 - \dot{v})^{j-1},$$

$$I_2 = (1 - \dot{v})^{j-1} v + (j-1)(1 - \dot{v})^{j-2}\dot{v},$$

and in general

$$I_m = \sum_{k=1}^{m} \frac{1}{(m-k)!} \binom{j-1}{k-1} (1-\dot{v})^{j-k} \dot{v}^{k-1} v^{m-k}.$$

Upon substituting the above expression into (32) one finds

$$h_j = e^{-v} \sum_{k=1}^{\infty} \binom{j-1}{k-1} (1-\dot{v})^{j-k} \dot{v}^{k-1} S_k$$

where

$$S_k = \sum_{m=k}^{\infty} \frac{g_m v^{m-k}}{(m-k)!}.$$

Finally we use the expression for u, (30), to obtain

$$h_j = u(1-\dot{v})^{j-1} + e^{-v} \sum_{k=2}^{\infty} \binom{j-1}{k-1} (1-\dot{v})^{j-k} \dot{v}^{k-1} S_k. \tag{34}$$

3 Asymptotic Behavior of Solutions

3.1 A Simple Case

We observe that if

$$g_j = \begin{cases} 1 & \text{for } j = 1 \\ 0 & \text{otherwise} \end{cases} \tag{35}$$

then the equation for v becomes

$$\dot{v} = e^{-v}.$$

Recalling that $v(0) = 0$ it easy to see that the solution for v is

$$v = \log(1+t).$$

If we substitute the above formula for v into (30) we obtain

$$u = \frac{1}{1+t}.$$

Finally we use the expressions for u and v combined with (35) in (34) to obtain the following solution to our modified Becker-Döring equation

$$h_j = \frac{1}{1+t} \left(\frac{t}{1+t} \right)^{j-1}.$$

Next, the asymptotic behavior will be examined. Notice that since $(1-t^{-1})^t = e + O(t^{-1})$ as $t \to \infty$ then we can write

$$h_j = t^{-1} H_1(j/t, t)$$

where

$$H_1(J,t) = e^{-J}(1 + O(t^{-1})) \quad \text{as } t \to \infty \text{ provided } J = O(1).$$

It is clear that h_j converges to a self similar solution at a linear rate.

3.2 A More General Result

The differential equation (31) does not have an explicit solution, however, we are able to obtain an asymptotic solution with enough accuracy for our needs. We will consider initial data of the form given by (27) with the added restrictions

$$g_j = 0 \quad \text{for } j > N + 1 \tag{36}$$

and

$$g_1 > g_2 > \cdots > g_{N+1}. \tag{37}$$

We remark that in terms of the densities (36) and (37) can be expressed as:

$$c_j = 0 \quad \text{for } j > N + 1$$

and

$$c_j > 0 \quad \text{for } j = 1, 2, \ldots, N + 1.$$

In material that follows it will proved that, for the initial conditions described above, the solution of (19) converges to the self-similar solution $h_j = t^{-1}\exp(-j/t)$. In addition, the rate of convergence will be shown to be logarithmic in time.

3.2.1 Behavior of v

For the class of initial data described above (31) becomes

$$\dot{v} = e^{-v}p(v) \quad \text{where } p(v) = 1 + \sum_{j=1}^{N} \frac{\alpha_j v^j}{j!}. \tag{38}$$

At this time is also convenient to rewrite the expression for the monomer concentration (30) as

$$u = e^{-v}q(v) \quad \text{where } q(v) = \sum_{j=1}^{N+1} \frac{g_j v^{j-1}}{(j-1)!}. \tag{39}$$

We observe that both p and q are Nth order polynomials and they satisfy the following relationship

$$q(v) = p(v) - p'(v). \tag{40}$$

Next we let $\psi = \psi(t)$ satisfy the following equation

$$e^{-\psi}q(\psi) = \frac{1}{t + \tau}. \tag{41}$$

In what follows we shall prove that

$$v(t) = \psi(t) + o\left(\frac{1}{\log t}\right) \quad \text{as } t \to \infty \tag{42}$$

provided τ is chosen sufficiently large. Before the above result is verified let us establish some properties of ψ. By rewriting (41) as

$$\psi = \log(t + \tau) + \log(q(\psi))$$

one can show

$$\psi = \log(t + \tau) + \log(q(\log(q(\log(t + \tau) \cdots.$$

It follows from the definition of q that

$$g_1 \leq q(\psi) \leq g_1 e^{\psi g_2/g_1},$$

If the above inequality is multiplied by $e^{-\psi}$ and (41) is used, the following estimate can be obtained

$$\log[(t + \tau)g_1] \leq \psi \leq \log[(t + \tau)g_1]/(1 - g_2/g_1).$$

This implies

$$\psi = O(\log t) \quad \text{as } t \to \infty. \tag{43}$$

The proof of (42) begins by introducing the following new variable as follows

$$v(t) = \psi(t) - r(t). \tag{44}$$

If we substitute (44) into (31) we obtain the following ordinary differential equation for r

$$\dot{r} = e^{-\psi} p(\psi) - e^{-\psi+r} p(\psi - r) + \frac{G(\psi)}{t + \tau} \equiv F(t, r, \tau) \tag{45}$$

where

$$G(\psi) = \frac{(p'(\psi))^2 - p(\psi)p''(\psi)}{q(\psi)(q(\psi) - q'(\psi))}.$$

Since $v(0) = 0$ it follows that the initial condition for (45) is

$$r(0) = r_0 \quad \text{where } e^{-r_0} q(r_0) = \frac{1}{\tau}. \tag{46}$$

For $\tau > 1$ there exists a unique positive value of r_0. We note that the numerator of G is a polynomial in ψ of order $2N - 2$ whereas the denominator is a polynomial of order $2N$. This combined with (43) implies

$$G(\psi(t)) = O\left(\frac{1}{\log^2 t}\right) \quad \text{as } t \to \infty. \tag{47}$$

It follows from (39) and (36–37) that q and $q - q'$ are both positive. We also observe $(p')^2 - pp'' = -p^2(p'/p)'$. Since $p = p(\psi)$ is polynomial of finite order it follows that p'/p must be a deceasing function for sufficiently large values of ψ therefore we have

$G(\psi) > 0$ provided that ψ is sufficiently large. Since $\psi(t) > r_0$ for all $t > 0$ we can pick τ sufficiently large so that $G(\psi) > 0$ for all $t > 0$ (recall r_0 is an increasing function of τ). For this choice of τ we have $F(t, 0, \tau) > 0$. Since $r(0) = r_0 > 0$ then $r \geq 0$.

Next we shall establish that $\lim_{t \to \infty} r(t) \log t = 0$. By examining the properties of p and q one can verify that $(e^{-\psi} p(\psi))'' > 0$. Therefore the following inequality is true

$$e^{-\psi} p(\psi) - e^{-\psi+r} p(\psi - r) < -\frac{r}{t+\tau}. \tag{48}$$

Upon combining (45) and (48), the following differential inequality is obtained

$$\dot{r} \leq -\frac{r}{t+\tau} + \frac{G(\psi)}{t+\tau} \quad \text{for } t > 0. \tag{49}$$

The above inequality is integrated in time to deduce the following estimate

$$0 \leq r \leq \frac{\tau r_0}{t+\tau} + \frac{1}{t+\tau} \int_0^t G(\psi(s)) ds. \tag{50}$$

The lower bound follows from the discussion below (47). One can establish, using L'Hospital's rule together with (47) and (50), that

$$r(t) = o\left(\frac{1}{\log t}\right) \quad \text{as } t \to \infty. \tag{51}$$

This completes the proof of (42).

3.2.2 Behavior of $\dot{v}$ and u

With the behavior of v now known we can use (38) and (39) to find the asymptotic behavior of $\dot{v}$ and u. To begin, we substitute (44) into (38) to obtain

$$\dot{v} = e^{-\psi+r} p(\psi - r). \tag{52}$$

It follows from (41) and (40) that

$$e^{-\psi} p(\psi) = \frac{1}{t+\tau}\left(1 + \frac{p'(\psi)}{q(\psi)}\right). \tag{53}$$

Therefore we can write (52) as

$$\dot{v} = \frac{1}{t+\tau}\left(1 + \frac{p'(\psi)}{q(\psi)}\right) + e^{-\psi+r} p(\psi - r) - e^{-\psi} p(\psi). \tag{54}$$

We recall that $\psi = O(\log t)$; since both p and q are polynomials of the same order we have $p'(\psi)/q(\psi) = O(1/\log t)$. This combined with (48) and (51) in (54) yields

$$\dot{v} = \frac{1}{t+\tau}\left(1 + O\left(\frac{1}{\log t}\right)\right). \tag{55}$$

A similar argument shows

$$u = \frac{1}{t+\tau}\left(1 + o\left(\frac{1}{\log t}\right)\right). \tag{56}$$

3.2.3 Behavior of h_j

With the above results we can now determine the long time behavior of h_j. For the case at hand we have

$$h_j = u(1 - \dot{v})^{j-1} + e^{-v} \sum_{k=2}^{N+1} \binom{j-1}{k-1} S_k (1 - \dot{v})^{j-k} \dot{v}^{k-1}. \tag{57}$$

We define the rescaled size

$$J = j/t$$

and note

$$\binom{j-1}{k-1} \frac{1}{t^{k-1}} = \frac{J^{k-1}}{(k-1)!} + O(t^{-1}). \tag{58}$$

Next we use a Taylor expansion to obtain

$$e^{-v} S_k(v) = e^{-\psi + r} S_k(\psi - r) = e^{-\psi} S_k(\psi)[1 + O(r)].$$

The above equation is rewritten, using (41), as

$$e^{-v} S_k(v) = \frac{1}{t + \tau} \frac{S_k(\psi)}{q(\psi)} [1 + O(r)].$$

We observe that $S_k(\psi)$ is a polynomial of order $N + 1 - k$ and recall $q(\psi)$ a polynomial of order N. This combined with (43) and (51) yields for $k \geq 2$

$$e^{-v} S_k(v) = \frac{1}{t + \tau} O\left(\frac{1}{(\log t)^{k-1}}\right) \quad \text{as } t \to \infty. \tag{59}$$

One can use (55) to show

$$(1 - \dot{v})^{j-k} \dot{v}^{k-1} = \frac{e^{-J}}{t^{k-1}} \left[1 + O\left(\frac{1}{\log t}\right)\right] \quad \text{as } t \to \infty. \tag{60}$$

We now substitute (56), (58), (59), and (60) into (57) to obtain

$$h_j = t^{-1} H(j/t, t)$$

where

$$H(J, t) = e^{-J}[1 + E(J, t)] \quad \text{as } t \to \infty \text{ provided } J = O(1)$$

with

$$E(J, t) = O\left(\frac{1}{\log t}\right) + \sum_{k=2}^{N+1} \frac{J^{k-1}}{(k-1)!} O\left(\frac{1}{(\log t)^{k-1}}\right).$$

We note that $\lim_{t \to \infty} E(J, t) = 0$. This implies that for the initial conditions (36–37) the solution of (19) converges to the self-similar form $h_j = t^{-1} \exp(-j/t)$. In addition the rate of convergence is logarithmic in time. This indicates the rate of convergence is rather slow. This is consistent with the observations of Meerson *et al.* [8].

This self similar form was also found by Carr and Penrose for (10) as should be expected. However, they also prove that the asymptotic behavior of (10) for compact initial conditions depends on the order of the zero at the leading edge of the support. In particular, $t^{-1}\exp(-x/t)$ is only realized when the initial condition goes to zero exponentially fast as one approaches the leading edge of the support. Our result establishes for the discrete form of (10) that asymptotic behavior is the same for *all* compactly supported initial conditions. Therefore, the discrete nature of (15) provides a mechanism to select the same self similar profile for all compactly supported initial conditions.

4 Conclusions

In this paper a modified version of the Becker-Döring equations has been introduced. This approximation can viewed in two ways. The first is that it can be thought of as a first order upwind discretization of the corresponding LSW equations. It can also be thought of a system of equations that approximates the long time behavior of the Becker-Döring equations in which the monomer concentration is slaved to the concentrations of the other clusters. We are able to prove, for one member of these modified Becker-Döring equations, that the long time behavior is described by the same self similar form for compact initial conditions. The results show that the convergence rate is logarithmically slow. This work suggests that it might be easier to understand the long time behavior of Becker-Döring systems by examining the associated modified system rather than the corresponding LSW equation.

References

1. Ball, J., Carr, J., Penrose, O.: The Becker-Döring cluster equations: basic properties and asymptotic behavior of solutions. Commun. Math. Phys. **104**, 109–116 (1988)
2. Bonilla, L.L., Carpio, A., Farjoun, Y., Neu, J.C.: Asymptotic and numerical studies of the Becker-Döring model for transient homogeneous nucleation. Markov Process. Relat. Fields **12**, 341–365 (2006)
3. Carr, J., Penrose, O.: Asymptotic behavior of solutions to a simplified Lifshitz-Slyozov equation. Physica D **124**, 166–176 (1998)
4. Carr, J., Duncan, D.B., Walshaw, C.H.: Numerical approximation of a meta-stable system. IMA J. Numer. Anal. **15**, 505–521 (1995)
5. Lifshitz, I.M., Slyozov, V.V.: The kinetics of precipitation from supersaturated solid solutions. J. Phys. Chem. Solids **19**, 35–50 (1961)
6. Marder, M.: Correlations and Ostwald ripening. Phys. Rev. A **36**, 858–872 (1987)
7. Meerson, B.: Fluctuations provide strong selection in Ostwald ripening. Phys. Rev. E **60**, 3072–3075 (1999)
8. Meerson, B., Sander, L., Smereka, P.: The role of discrete particle noise in the Ostwald ripening. Eur. J. Phys. **72**, 604–610 (2005)
9. Niethammer, B.: Derivation of the LSW theory for Ostwald ripening by homogenization methods. Arch. Ration. Mech. Anal. **147**, 119–178 (1999)
10. Niethammer, B.: On the evolution of large clusters in the Becker-Döring model. J. Nonlinear Sci. **13**, 115–155 (2003)
11. Niethammer, B., Otto, F.: Ostwald Ripening: The screening length revisited. Calc. Var. PDE **13**, 867–902 (1999)
12. Niethammer, B., Pego, R.L.: Non-self-similar behavior in the LSW theory of Ostwald ripening. J. Stat. Phys. **95**, 867–902 (1999)

13. Penrose, O.: The Becker-Döring equations at large times and their connection with the LSW theory of coarsening. J. Stat. Phys. **89**, 305–320 (1997)
14. Rubinstein, I., Zaltzman, B.: Diffusional mechanism of strong selection in Ostwald ripening. Phys. Rev. E **61**, 709–717 (2000)
15. Veláquez, J.J.L.: The Becker-Döring equations and the Lifshitz-Slyozov theory of coarsening. J. Stat. Phys. **92**, 195–236 (1998)
16. Voorhees, P.W.: The theory of Ostwald ripening. J. Stat. Phys. **38**, 231–252 (1985)