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The Becker–Döring Equations and the Lifshitz–Slyozov Theory of Coarsening

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In this paper the relation between the kinetic set of Becker–Döring (BD) equations and the classical Lifshitz–Slyozov (LS) theory of coarsening is studied. A model that resembles the LS theory but keeps some of the nucleation effects is derived. For this model a solution is described that shows how the kinetic effects explain the particular solution selected in the LS theory. By means of a renormalization procedure, a discrete group of transformations is shown to play an important role in describing the structure of the solution near the critical size of the LS theory.

KEY WORDS: Becker–Döring equations; Lifshitz–Slyozov theory; nucleation; coarsening; Fokker–Planck equations; renormalization group; asymptotics beyond all orders.

1. INTRODUCTION

The Lifshitz–Slyozov (LS) theory is used to model the formation of aggregates like liquid drops, growing crystals, spin seas and other physical problems. In all cases it is expected to describe the late-stage coarsening of the system under consideration.

In the LS theory of coarsening the growth of particles is driven by a steady diffusion field. The concentration of the magnitude that diffuses (that depends of the particular physical situation considered) is given at the surface of the agregates by the Gibbs–Thomson law. The amount of "undersaturation" that produces the growth of the aggregates is a controlling parameter that is determined by means of the conservation of mass of the aggregating material. Namely, the amount of the substance away from the

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aggregates that is avalaible to enter in the coarsening process added to the amount of substance in the aggregates should remain constant. An assumption is also made that asserts that the distance between aggregates is very large, so that the diffusion field can be obtained for each cluster assuming that it is isolated.

The LS theory relies in a self-similar solution that predicts a growth rate for the radius of the clusters of the type:

$$R(t) \sim At^{1/3} \tag{1.1}$$

Moreover, this theory also provides a detailed description of the distribution of sizes for the aggregates. As a matter of fact, in the LS theory, a family of solutions satisfying (1.1) for different values of the constant A is obtained, all of them with a similar concentration of particles. The particular distribution selected by the LS theory is picked among that family by means of a stability criteria.

Although the LS theory is very succesful in predicting the rate of growth (1.1), it is very natural to raise some mathematical questions about the model. Actually, according to that theory, there are unstable solutions arbitrarily close to the "right" solutions of the model, and it then seems natural to ask the reason that makes this particular solution of the model stable.

In this paper a Fokker–Planck approximation of the kinetic Becker–Döring (BD) model for aggregation of particles is studied. When the coefficients of this last model are selected adequately, the BD system resembles the LS model for large sizes of the clusters. However, part of the kinetic effects included in the BD equations will be kept in our approximation, since although they are small, they play an important role for sizes of the clusters larger than the critical ones in the LS theory, and are also important in determining the distribution of clusters for subcritical sizes of the aggregates. The picture that emerges from the analysis performed here is that large clusters, that are nucleated in very small quantities due to kinetic effects in the BD model, begin to grow to the rate (1.1) as soon as their size coincides with the power $At^{1/3}$. The analysis performed here predicts also that in the long term, these clusters cease to grow, and they keep their size constant for long times. The precise way in which these aggregates stop growing is precisely the factor that determines the concentration of clusters for subcritical values of the radius in the LS theory. A precise mathematical description of the way in which this happens is given later (see Section 5). Among the most relevant facts we should mention that near the critical size there exists a discrete rescaling group, and that the solution obtained here is approximately self-similar for this discrete group near that region. In particular, this implies that the "undersaturation" that drives the coarsening of the particles (denoted as $\delta(t)$), behaves as

$$\delta(t)=\frac{B}{t^{1/3}}\left[\frac{1}{4}+\frac{1}{4t}+\frac{1}{4t\ln(t)}+\frac{1}{4t\ln(t)\ln(\ln(t))}+\cdots\right],\qquad t\to\infty \tag{1.2}$$

for some suitable constant $B>0$. The first terms of the series (1.2) are obtained in the original paper by Lifshitz–Slyozov.[9] A precise meaning of the series (1.2) will be given in the Section 5 below.

A detailed description of the BD and LS models can be found in ref. 8. The LS theory is also discussed in the reviews.[15, 16] Numerical solutions of the BD model and a comparison with the LS theory are discussed in refs. 13 and 14. The analysis of the mathematical well-posedness of the BD model and its asymptotic behaviour for long times has been considered in ref. 2. A recent discussion of the connection between the LS theory and the set of Becker–Döring equations can be found in ref. 11. The existence of metastable solutions for these equations has been studied in refs. 6 and 12. The analysis of other models of coagulation equations makes the content of refs. 5 and 7.

In Section 2 of this paper the Fokker–Planck approximation that will be used here is derived. The instability of the "wrong" solutions of the LS theory will become clearer for the model considered here, and will be shown in Section 3. The construction of the solution of the Fokker–Planck equation that approaches to the self similar solution of the LS model will be derived in Sections 4 and 5 by using formal expansions. In Section 6 some concluding remarks will be given. In Appendixes A and B at the end of the paper some technical results that have been used in previous sections of the paper are proved.

We finally remark that the notation $f(x)\gg g(x)$ as $x\to\infty$ will be used repeatedly in the paper with the meaning $\lim_{x\to\infty}(g(x)/f(x))=0$.

2. DERIVATION OF THE FOKKER–PLANCK MODEL

The Becker–Döring system is an infinite set of equations that describes the variation in time of the concentration of clusters or aggregates made of l particles. The Becker–Döring model assumes that the only characteristic of the clusters that enters in its dynamics is the number of particles that compose the cluster, and not particular features as their geometry.

Denoting as $c_l(t)$ the concentration of clusters of size l at a given time t, the BD equations have the form (see ref. 3):

$$\frac{dc_l}{dt}=J_{l-1}-J_l,\qquad l\geqslant 2 \tag{2.1}$$

where the flux of clusters from size l to clusters of size $(l+1)$ is given by:

$$J_l = a_l c_l c_1 - b_{l+1} c_{l+1}, \qquad l \geq 1 \tag{2.2}$$

for some suitable coefficients a_l, b_l. The evolution equation of the concentration of monomers c_1 is not included in (2.1), but is determined by requiring the conservation of the total number of particles:

$$\sum_{l=1}^{\infty} l c_l = \rho > 0 \tag{2.3}$$

The choice of the coefficients that is considered here is made in order to obtain the LS model for large values of l, as suggested in ref. 13. More precisely, we will take:

$$a_l = l^{1/3} \tag{2.4}$$

$$b_l = a_l + q \tag{2.5}$$

where q is a suitable positive constant.

Many mathematical properties of the model (2.1)–(2.5), have been studied in refs. 2 and 11 for more general choices of the coefficients. In particular, it was obtained in ref. 2 that for $\rho \leqslant \rho_0$, where ρ_0 is a critical concentration, there exists a steady state solution of (2.1)–(2.5). Using the existence of an entropy associated to the system that can be used as a Lyapunov function, it is proved there that the solutions of the evolution problem converge asymptotically to the steady state as $t \to \infty$. For $\rho > \rho_0$ it was obtained in ref. 2 that the solutions of (2.1)–(2.5) converge to the maximal steady state, uniformly on bounded sets of l. However, in this case an amount of mass $\rho - \rho_0$ escapes towards the region $l \gg 1$ as $t \to \infty$. It is then assumed that the amount of mass that is "lost" gives place to aggregates of particles of a different phase.

In this paper the dynamics of large clusters is considered. To this end, it is convenient to introduce the following notation. Let us define the discrete derivation operator given by:

$$D(x_l) = x_l - x_{l-1}, \qquad l \leqslant 2$$

The system of equations (2.1)–(2.5) can then be written as:

$$\frac{dc_l}{dt} = D(D(b_{l+1} c_{l+1})) + D((q - \eta(t)\, a_l)\, c_l), \qquad l \leqslant 2 \tag{2.6}$$

where

$$\eta(t) = c_1(t) - 1$$

For large values of l, it is natural to approximate the operator D by standard derivation operators if the variation of c_{l+1} is not too fast on the l variable. We then obtain, to the lowest order, the following Fokker–Planck equation:

$$\frac{\partial c(l,t)}{\partial t} = \frac{\partial^2}{\partial l^2}(l^{1/3}c(l,t)) + \frac{\partial}{\partial l}((q - \eta(t)\, l^{1/3})\, c(l,t)) \tag{2.7}$$

The results in ref. 2 previously described imply that there is a mass ρ_0 in the region where $l \approx 1$. Taking into account that the equation (2.7) describes the evolution of $c(l,t)$ for large values of l, it is natural to replace the condition (2.3) by:

$$\int_0^\infty lc(l,t)\, dl = \rho - \rho_0 \equiv \theta > 0 \tag{2.8}$$

that complements the equation (2.7). This last describes the behaviour of $c(l,t)$ for large values of l. To study (2.7), (2.8) we introduce a set of self-similar variables, that correspond to the natural scales of the problem obtained on dropping the second derivatives in (2.7):

$$c(l,t) = \frac{1}{(t+1)^2}\,\Phi\left(\frac{l}{t+1}, \ln(t+1)\right)$$

$$\xi = \frac{l}{t+1}, \qquad \tau = \ln(t+1) \tag{2.9}$$

$$\eta(t) = \frac{\lambda(\tau)}{(t+1)^{1/3}}$$

In this set of variables equations (2.7), (2.8) become:

$$\Phi_\tau = e^{-2\tau/3}(\xi^{1/3}\Phi)_{\xi\xi} + (q - \lambda(\tau)\,\xi^{1/3} + \xi)\,\Phi_\xi + \left(2 - \frac{\lambda(\tau)}{3}\,\xi^{-2/3}\right)\Phi \tag{2.10}$$

$$\int_0^\infty \Phi(\xi,\tau)\,\xi\, d\xi = \theta > 0 \tag{2.11}$$

The function $\lambda(\tau)$ gives a measure of the deviation of $c_1 = 1$ with respect to the equilibrium value, that in this particular case is $c_1 = 1$.

Dropping the term $e^{-2\tau/3}(\xi^{1/3}\Phi)_{\xi\xi}$ in (2.10), we obtain the classical Lifshitz–Slyozov model, written in self-similar variables. If we keep the term $e^{-2\tau/3}(\xi^{1/3}\Phi)_{\xi\xi}$, we include thereby the kinetic effects that are not taken into account in the LS theory. In order to have a well defined mathematical problem, a boundary condition at $\xi=0$ is required. The behaviour of $c(l, t)$ in the region $l \approx 1$ is given by the maximal steady state, as it was shown in ref. 2. In the situation considered here, this maximal steady state is

$$c_l^{(s)} = Q_l (z_s)^l$$
$$Q_l = \frac{\prod_{k=1}^{k=l-1} a_k}{\prod_{k=2}^{k=l} b_k} \tag{2.12}$$

where z_s is the radius of convergence of the series $\sum_{l=1}^{\infty} l Q_l z^l$. Taking into account the exponential decay of the solution (2.12) as $l \gg 1$, we deduce that, in order to match the solutions of (2.10) with these steady states, it is natural to impose the following boundary condition

$$\Phi(0, \tau) = 0 \tag{2.13}$$

and we need to complement these equations with the initial data

$$\Phi(\xi, 0) = \Phi_0(\xi) \geqslant 0 \tag{2.14}$$

Problem (2.10), (2.11), (2.13), (2.14) is well posed from a mathematical point of view (locally in time) for a large class of initial data, as will be proved in Appendix A at the end of the paper.

At this stage, it is convenient to recall some of the basic facts of the LS theory. The distribution of sizes of the aggregates is described, according to this theory, by a steady state of (2.10) without the term $e^{-2\tau/3}(\xi^{1/3}\Phi)_{\xi\xi}$, namely

$$(q - \lambda_\infty \xi^{1/3})\, \Phi_\xi + \left(2 - \frac{\lambda_\infty}{3}\, \xi^{-2/3}\right) \Phi = 0 \tag{2.15}$$

with the additional condition (2.11). There exist solutions of (2.15), (2.11) only if the real number λ_∞ satisfies

$$\lambda_\infty \geqslant \left(\frac{3\sqrt{3}\, q}{2}\right)^{2/3}$$

A stability analysis performed in ref. 9 indicates that only the choice

$$\lambda_\infty = \left(\frac{3\sqrt{3}\, q}{2}\right)^{2/3} \tag{2.16}$$

could give a stable solution. The steady distribution of clusters is then given by

$$\Phi(\xi) = C \int_{\xi}^{\lambda_\infty} \exp\left[-\frac{(2-(\lambda_\infty/3)\,u^{-2/3})}{(q-\lambda_\infty u^{1/3}+u)} \right] du \tag{2.17}$$

where $C > 0$ is selected in such a way that (2.11) holds.

3. UNSTABLE SOLUTIONS OF THE FOKKER–PLANCK MODEL

We now prove the following result

Theorem 1. There is no nonnegative solution of the problem (2.10), (2.11) such that

$$\lim_{\tau \to \infty} \lambda(\tau) > \lambda_{crit} \equiv \left(\frac{3\sqrt{3}\,q}{2} \right)^{2/3} \tag{3.1}$$

Notice that no assumption is required about the boundary condition at $\xi = 0$.

Proof of Theorem 1. We denote as $\xi_1(\tau), \xi_2(\tau)$ the roots of the equation

$$q - \lambda(\tau)\,\xi^{1/3} + \xi = 0$$

such that $0 < \xi_1(\tau) < \xi_2(\tau) < \infty$. It is readily seen that (3.1) implies that $\xi_1(\tau), \xi_2(\tau)$ exist for τ large enough. Let us write

$$\xi_{2,\infty} = \lim_{\tau \to \infty} \xi_2(\tau)$$

Some simple computations show that (2.10) may be written as

$$\begin{aligned} \Phi_\tau = {} & ((\xi_{2,\infty})^{1/3}\, e^{-2\tau/3} + a(\xi, \tau))(\Phi)_{\xi\xi} \\ & + \left(\left(1 - \frac{\lambda_\infty(\xi_{2,\infty})^{-2/3}}{3} \right)(\xi - \xi_{2,\infty}) + b(\xi, \tau) \right) \Phi_\xi \\ & + \left(2 - \frac{\lambda_\infty(\xi_{2,\infty})^{-2/3}}{3} + c(\xi, \tau) \right) \Phi \end{aligned} \tag{3.2}$$

where

$$\lim_{\tau \to \infty} \lambda(\tau) \equiv \lambda_\infty$$

and

$$|a(\xi, \tau)| \leqslant C\, |\xi - \xi_{2,\infty}|\, e^{-2\tau/3} \tag{3.3}$$

$$|b(\xi, \tau)| \leqslant \varepsilon(\tau) + C\, |\xi - \xi_{2,\infty}|^2 \tag{3.4}$$

$$|c(\xi, \tau)| \leqslant \varepsilon(\tau) + C\, |\xi - \xi_{2,\infty}|^2 \tag{3.5}$$

where $\lim_{\tau \to \infty} \varepsilon(\tau) = 0$ and $C > 0$ is a fixed constant.

We now fix $\tau_0 > 0$ large enough. Let us denote as $\Psi(\xi, \tau)$ the solution of Eq. (3.2) in the set $\xi \in (\xi_{2,\infty} - \varepsilon_0, \xi_{2,\infty} + \varepsilon_0)$, $\tau > \tau_0$ with $\varepsilon_0 > 0$ small, that satisfies the boundary conditions

$$\Psi(\xi_{2,\infty} \pm \varepsilon_0, \tau) = 0 \tag{3.6}$$

and the initial data

$$\Psi(\xi, \tau_0) = \begin{cases} 1, & |\xi - \xi_{2,\infty}| < \varepsilon_0/2 \\ 0, & |\xi - \xi_{2,\infty}| \geqslant \varepsilon_0/2 \end{cases} \tag{3.7}$$

where the dependence of Ψ on τ_0 is assumed, but it will not be explicitly written for simplicity. Using the classical maximum principle for parabolic equations, the following upper estimate is easily obtained

$$\Psi(\xi, \tau_0) \leqslant e^{\tau - \tau_0} \tag{3.8}$$

Let us consider the function

$$\tilde{\Psi}(\xi, \tau) = e^{3(\tau - \tau_0)} G(u)$$

with

$$G(u) = \int_u^\infty e^{-\alpha v^2/2}\, dv$$

and

$$u = \frac{\xi - \xi_{2,\infty} - \varepsilon_0/2}{(3/2(e^{-2\tau_0/3} - e^{-2\tau/3}))^{1/2}}$$

where $\alpha = 1/3(\xi_{2,\infty})^{1/3}$, and $0 < \mu < \min\{1/3, (1 - \lambda_\infty(\xi_{2,\infty})^{-2/3}/3)\}$. It is not difficult to check that $\tilde{\Psi}(\xi, \tau)$ defines a supersolution for (3.2) in the region $\xi \in (\xi_{2,\infty} + \varepsilon_0/2, \xi_{2,\infty} + \varepsilon_0)$, $\tau > \tau_0$ if ε_0 is selected small enough and τ_0 is sufficiently large. To this end, it has to be verified that

$$\begin{aligned}\tilde{\Psi} \geqslant{} & ((\xi_{2,\infty})^{1/3} e^{-2\tau/3} + a(\xi, \tau))(\tilde{\Psi})_{\xi\xi} \\ & + \left(\left(1 - \frac{\lambda_\infty(\xi_{2,\infty})^{-2/3}}{3}\right)(\xi - \xi_{2,\infty}) + b(\xi, \tau)\right) \tilde{\Psi}_\xi \\ & + \left(2 - \frac{\lambda_\infty(\xi_{2,\infty})^{-2/3}}{3} + c(\xi, \tau)\right) \tilde{\Psi}\end{aligned}$$

that follows after some simple computations by using (3.3)–(3.5). Taking into account that $\tilde{\Psi}$ satisfies the boundary conditions (3.6), as well as (3.7) and (3.8), the following estimate follows

$$0 \leqslant \Psi(\xi, \tau) \leqslant C \exp(-2\gamma e^{\mu\tau})\, e^{3(\tau - \tau_0)}$$

if $3\varepsilon_0/4 \leqslant \xi - \xi_0 \leqslant \varepsilon_0$, $\tau \geqslant \tau_0$, where $\gamma > 0$ is a suitable constant depending on ε_0. A similar bound can be obtained in the region $-3\varepsilon_0/4 \geqslant \xi - \xi_0 \geqslant -\varepsilon_0$ with a symmetric argument. Classical regularizing effects for parabolic equations then imply a bound of the form

$$|\Psi_\xi(\xi_{2,\infty} \pm \varepsilon_0, \tau)| \leqslant C \exp(-\gamma e^{\mu\tau}) \tag{3.9}$$

if $\tau \geqslant \tau_0$. By definition Ψ solves (2.10). Integrating this equation in the interval $(\xi_{2,\infty} - \varepsilon_0, \xi_{2,\infty} + \varepsilon_0)$, it turns out that

$$\frac{d}{d\tau}\left(\int_{\xi_{2,\infty}-\varepsilon_0}^{\xi_{2,\infty}+\varepsilon_0} \Psi(\xi, \tau)\, d\xi\right) = \int_{\xi_{2,\infty}-\varepsilon_0}^{\xi_{2,\infty}+\varepsilon_0} \Psi(\xi, \tau)\, d\xi + e^{-2\tau/3}[\xi^{1/3}\Psi_\xi]_{\xi_{2,\infty}-\varepsilon_0}^{\xi_{2,\infty}+\varepsilon_0}$$

and taking into account (3.9), it follows that $\int_{\xi_{2,\infty}-\varepsilon_0}^{\xi_{2,\infty}+\varepsilon_0} \Psi(\xi, \tau)\, d\xi$ grows exponentially fast. In order to conclude the argument, we notice that for any given function Ψ satisfying the hypothesis of Theorem 1, the strong maximum principle implies that $\Psi(\cdot, \tau_0)$ becomes strictly positive in the interval $(\xi_{2,\infty} - \varepsilon_0, \xi_{2,\infty} + \varepsilon_0)$. We can then use the function $\beta\Psi$ as a subsolution for $\beta > 0$ small enough. Thus $\int_{\xi_{2,\infty}-\varepsilon_0}^{\xi_{2,\infty}+\varepsilon_0} \Phi(\xi, \tau)\, d\xi$ grows exponentially fast, but this contradicts (2.11), whence Theorem 1 follows.

Theorem 1 rules out the possibility of $\lambda(\tau)$ being asymptotically larger than λ_{crit}. It cannot be asymptotically smaller either, although a rigorous proof of this fact would not be provided here. However a heuristic argument relying on the WKB method will be given that shows that it is not possible to have that

$$\lim_{\tau \to \infty} \lambda(\tau) = \lambda_\infty < \lambda_{crit} \equiv \left(\frac{3\sqrt{3}\,q}{2}\right)^{2/3} \tag{3.10}$$

Indeed, let us assume that (3.10) takes place. Then Eq. (2.10) approaches to

$$\Phi_\tau = e^{-2\tau/3}(\xi^{1/3}\Phi)_{\xi\xi} + (q - \lambda_\infty \xi^{1/3} + \xi)\,\Phi_\xi + \left(2 - \frac{\lambda_\infty}{3}\xi^{-2/3}\right)\Phi \tag{3.11}$$

where now $\lambda_\infty < \lambda_{crit}$. Let us denote as $G(\xi, \tau, \tau_0, R)$ the solution of (3.11), (2.13) for $\tau > \tau_0$ with initial data

$$\Phi(\xi, \tau_0) = \delta(\xi - R) \tag{3.12}$$

Let us also pick τ_0 large enough in order to be able to approximate (2.10) by (3.11). When $\tau_0 \gg 1$, the coefficient in front of the term containing second order derivatives is very small, and we can use the WKB method in order to approximate $G(\xi, \tau, \tau_0, R)$. The problem can be made simpler by introducing a new space variable

$$y = \xi^{5/6} \tag{3.13}$$

that transforms (3.11), (3.12) into

$$\Phi_\tau = e^{-2\tau/3}\left[\frac{25}{36}\Phi_{yy} + \frac{5}{12y}\Phi_y - \frac{2}{9y^2}\Phi\right] + \frac{5}{6}(q - \lambda_\infty y^{1/5} + y)\,\Phi_y + \left(2 - \frac{\lambda_\infty}{3}y^{-4/5}\right)\Phi \tag{3.14}$$

$$\Phi(y, \tau_0) = \frac{5}{6R^{1/6}}\,\delta(y - R^{5/6}) \tag{3.15}$$

For $\tau \to \tau_0^+$, $y \approx R^{5/6}$, we approximate this problem by another with constant coefficients. Then to the lowest order

$$\Phi(y, \tau) \approx \frac{e^{\tau_0/3}}{2R^{1/6}\sqrt{\pi(\tau - \tau_0)}}\exp\left(-\frac{9e^{2\tau_0/3}(y - R^{5/6})^2}{25(\tau - \tau_0)}\right) \tag{3.16}$$

as $\tau \to \tau_0^+$, $|y - R^{5/6}| \to 0$. The classical WKB method suggests to expand the function Φ as

$$\Phi = \exp(e^{2\tau_0/3}(S_0 + e^{-2\tau_0/3} S_1 + \cdots)) \tag{3.17}$$

The approximation until the order S_0 defines the so called "geometric optic" approximation and the approximation until the term S_1 defines the "physical optics approximation" of Φ. It turns out that the function S_0 satisfies the usual Hamilton–Jacobi equation associated to the hamiltonian

$$H(y, p, \tau - \tau_0) = -\frac{25e^{-2(\tau - \tau_0)/3}}{36} p^2 - \frac{5}{6}(q - \lambda_\infty y^{1/5} + y)\, p \tag{3.18}$$

and the function S satisfies a transport equation. Both equations can be analyzed by means of a careful analysis of the corresponding characteristics that are given by

$$\begin{aligned} \frac{dy}{d\tau} &= \frac{\partial H}{\partial p} = -\frac{5}{6}(q - \lambda_\infty y^{1/5} + y) \\ \frac{dp}{d\tau} &= -\frac{\partial H}{\partial y} = \frac{5}{6}\left(1 - \frac{\lambda_\infty}{5} y^{-4/5}\right) p \end{aligned} \tag{3.19}$$

The evolution of the function S_0 along the solutions of (3.19) is described by

$$\frac{dS_0}{d\tau} = L \equiv p\frac{dy}{d\tau} - H = -\frac{25e^{-2(\tau - \tau_0)/3}}{36} p^2 \tag{3.20}$$

A detailed analysis of (3.19) and (3.20) taking into account that we are interested matching with (3.16) shows that the Green function $G(\xi, \tau, \tau_0, R)$ is concentrated along a curve that propagates along the corresponding characteristic that starts at the point $\xi = R$ and approaches towards the origin. The Green function spreads a little amount in space due to the diffussion to a region of size $R^{1/3}e^{-(\tau - \tau_0)}$. The WKB approximation breaks down near the origin where, however, a standard boundary layer analysis can be made. If R is large the corresponding characteristics approach towards the origin exponentially fast. In this case the Green function $G(\xi, \tau, \tau_0, R)$ can be approximated as

$$\begin{aligned} G(\xi, \tau, \tau_0, R) &\sim \frac{Ce^{(3/2)(\tau - \tau_0)}}{R^{1/6}} \exp\left(-\frac{1}{4}(R^{-1/6}e^{(\tau - \tau_0)/2}(\xi - Re^{-(\tau - \tau_0)}))^2\right) \\ &\sim e^{(\tau - \tau_0)}\, \delta(\xi - Re^{-(\tau - \tau_0)}) \end{aligned} \tag{3.21}$$

where the value of the coefficient on front of the Dirac mass has been taken exactly as $e^{(\tau-\tau_0)}$ because a simple integration of (3.14) shows that the mass of the Green function grows exponentially.

We can then write the following representation formula for the solution of (3.14)

$$\Phi(\xi,\tau)=\int_0^\infty G(\xi,\tau,\tau_0,\lambda)\,\Phi(\lambda,\tau_0)\,d\lambda$$

and taking into account (3.21) it follows the approximation for $\Phi(\xi,\tau)$

$$\Phi(\xi,\tau)=e^{2(\tau-\tau_0)}\Phi(\xi e^{(\tau-\tau_0)},\tau_0)$$

Notice that as soon as the characteristics arrive to the region $\xi=O(1)$, they cross the line $\xi=0$ in a time of order unity, and the mass of the Green function becomes negligible (a fact that is not taken into account by the approximation $\xi\sim Re^{-(\tau-\tau_0)}$). Then

$$\int_0^\infty \xi\Phi(\xi,\tau)\,d\xi\approx\int_{e^{(\tau-\tau_0)}}^\infty e^{2(\tau-\tau_0)}\xi\Phi(\xi e^{(\tau-\tau_0)},\tau_0)\,d\xi=\int_{e^{2(\tau-\tau_0)}}^\infty \xi\Phi(\xi,\tau_0)\,d\xi$$

and this last integral approaches to zero as $\tau-\tau_0\to\infty$, that contradicts (2.11), whence it is not possible to have $\lambda_\infty<\lambda_{crit}$. Notice that a crucial fact is the approximation (3.21). The key point in the argument is the lost of mass for the Green function near the origin as the time grows.

4. THE CASE $\lambda(\tau)\approx\lambda_{crit}$

In this section the approximations that are used to obtain a solution that converges asymptotically as $\tau\to\infty$ to the self-similar LS solution are described. The two main ingredients of the approach developed here are the following

(1) The nucleation effects produce for τ large an exponential tail with the form

$$\Phi(\xi,\tau)\approx\exp(-\tfrac{9}{25}e^{2\tau/3}\xi^{5/3}(1+o(1)))\qquad\text{as}\quad\xi\to\infty\tag{4.1}$$

(2) For $\tau\to\infty$ the effect of the term $e^{-2\tau/3}(\xi^{1/3}\Phi)_{\xi\xi}$ in (2.10) can be neglected, and (2.10) can be approximated by

$$\Phi_\tau=(q-\lambda(\tau)\,\xi^{1/3}+\xi)\,\Phi_\xi+\left(2-\frac{\lambda(\tau)}{3}\,\xi^{-2/3}\right)\Phi\tag{4.2}$$

Assumption (1) is very natural from a physical point of view. In fact, in the original set of variables it just means that for large clusters $l \gg 1$ the concentration has the distribution

$$c_l(t) \approx \exp\left(-\frac{9}{25}\frac{l^{5/3}}{t}(1+o(1))\right)$$

that is a typical kinetic distribution of clusters that can be expected from Eq. (2.7). Mathematically, it is not hard to justify (4.1), at least for fast decaying initial data. Actually, on introducing the new space variable

$$\eta = e^{\tau/3}\xi^{5/6}$$

Eq. (2.10) becomes

$$\Phi_\tau = \frac{25}{36}\Phi_{\eta\eta} + \frac{5}{12\eta}\Phi_\eta - \frac{2}{9\eta^2}\Phi + \left(\frac{5qe^{6\tau/15}}{\eta^{1/5}} - \frac{5\lambda(\tau)\, e^{4\tau/15}\eta^{1/5}}{6} + \frac{\eta}{2}\right)\Phi_\eta + \left(2 - \frac{\lambda(\tau)\, e^{4\tau/15}}{\eta^{4/5}}\right)\Phi \tag{4.3}$$

The dominant terms of this equation as $\eta \to \infty$ are

$$\Phi_\tau \approx \frac{25}{36}\Phi_{\eta\eta} + \frac{\eta}{2}\Phi_\eta + 2\Phi$$

This equation can be transformed in a classical diffusion equation by means of the change of variables

$$y = \frac{\eta}{\sqrt{1-e^{-\tau}}}$$

$$s = 1 - e^{-\tau}$$

whence for compactly supported initial data there holds

$$\Phi(\xi, \tau) \approx \exp\left(-\frac{9}{25}\frac{e^{2\tau/3}\xi^{5/3}}{1-e^{-\tau}}(1+o(1))\right)$$

as $\eta \to \infty$. If we take $\tau \gg 1$, (4.1) follows.

The term $o(1)$ that appears in the exponent of (4.1) depends very strongly on the initial data. However, from the point of view of the accuracy of the expansions that will be obtained in this paper (4.1) will be enough.

Assumption (2) is very natural when we take into account the smallness of the coefficient $e^{-2\tau/3}$ in the term $e^{-2\tau/3}(\xi^{1/3}\Phi)_{\xi\xi}$. Some care is needed, however in the regions where $\Phi_{\xi\xi}$ is large, a fact to be reckoned with for the solutions described here when $\xi \approx q/2$. Actually, it will be checked "a posteriori" that the assumption (2) holds for the solutions obtained below. In some simple parabolic equations like $u_t = e^{-\gamma\tau}u_{xx} + Au_x$, $\gamma > 0$, it can be easily seen that the fundamental solution can be approximated by the corresponding fundamental solution for the hyperbolic equation in which the diffusive term is dropped. Similar results can be expected for more general equations like (4.3), but a general proof of such result will not be provided here.

The simplified Eq. (4.2) can be studied by using characteristics. Let us denote as $g(\tau; \tau; \xi_0)$ the solution of the problem

$$\begin{aligned} \frac{dg}{d\tau} &= -(q - \lambda(\tau)\, g^{1/3} + g) \\ g(\tau_0; \tau_0; \xi_0) &= \xi_0 \end{aligned} \tag{4.4}$$

The dependence on $\lambda(\tau)$, although essential in the forthcoming argument, will not be made explicit by notational simplicity. Notice that the solutions of (4.4) decay exponentially fast for g large. On the other hand, in the LS self-similar solution $\lambda(\tau) = \lambda_{crit}$. We then assume $\lambda(\tau) \approx \lambda_{crit}$ in (4.4). In this case the behaviour of $g(\tau; \tau_0; \xi_0)$ is very sensitive to small changes of $\lambda(\tau)$, since the equation

$$q - \lambda_{crit}\, g^{1/3} + g = 0$$

has a double zero at $g = q/2$. In particular, if $\lambda(\tau)$ is slightly above the value λ_{crit}, the equation $q - \lambda(\tau)\, g^{1/3} + g = 0$ has two roots, the largest one being stable. For $\lambda(\tau)$ slightly below λ_{crit} the equation $q - \lambda(\tau)\, g^{1/3} + g = 0$ has not roots, and all the solutions of (4.4) would cross to the region $g < q/2$ as $\tau \to \infty$. In particular, the time that the function $g(\tau; \tau_0; \xi_0)$ remains close to the critical line $g = q/2$ is very sensitive on $\lambda(\tau)$. This fact will play an essential role in our argument here, and will be made more precise later.

Notice that in terms of the function g defined by (4.4), the solution of (4.2) satisfying (4.1) is given by

$$\Phi(\xi, \tau) \approx \exp\left(\int_{\tau_0}^{\tau} \left(2 - \frac{\lambda(s)}{3}\, g(s; \tau_0; \xi_0)\right) ds\right) \exp\left(-\frac{9}{25}\, e^{2\tau_0/3}(\xi_0)^{5/3}\right) \tag{4.5}$$

as $\tau \to \infty$ where

$$\xi = g(\tau; \tau_0; \xi_0)$$

and τ_0 is selected large enough to assert the validity of (4.1) and $\tau \gg \tau_0$. Note also that we use the fact that, as $\tau \to \infty$, the values of ξ_0 that we need to take in order to have $\xi > 0$ are those with $\xi_0 \gg 1$. Indeed, notice that the function $g(\tau; \tau_0; \xi_0)$ reaches the value $g = 0$ for finite τ, since otherwise we would have that $g \to q/2$ as $\lambda(\tau) \to \lambda_{crit}$. Then, by (4.5), Φ would grow exponentially in the region $\xi \approx q/2$, and the same would happen with $\int_0^\infty \xi \Phi(\xi, \tau)\, d\xi$, that contradicts (2.8).

We then need to select $\lambda(\tau)$ such that (2.8) holds, whence by (4.5) we require

$$\int_0^\infty \xi \exp\left(\int_{\tau_0}^\tau \left(2 - \frac{\lambda(s)}{3}\, g(s; \tau_0; \xi_0)\right) ds\right) \exp\left(-\frac{9}{25}\, e^{2\tau_0/3}(\xi_0)^{5/3}\right) = 0 \qquad (4.6)$$

This provides an integral equation for $\lambda(\tau)$ that describes the asymptotics of this function as $\tau \to \infty$. Actually, we can simplify (4.6) further. To this end, we argue as follows. If $\tau \to \infty$, the values of ξ_0 that enter in (4.6) satisfy $\xi_0 \gg 1$. The factor $\exp(-(9/25)\, e^{2\tau_0/3}(\xi_0)^{5/3})$ is then very small. In order to have (4.6), function $g(\tau; \tau_0; \xi_0)$ needs to remain stacked in the region $\xi \approx q/2$ for a long time, in which the factor $\exp(\int_{\tau_0}^\tau (2 - (\lambda_s/3)\, g(s; \tau_0; \xi_0))\, ds)$ has time to increase Φ until values of order one. Notice that near the critical line, $(2 - (\lambda(s)/3)\, g(s; \tau_0; \xi_0)) \approx 1$. On the other hand, for large values of ξ_0 the function g is close to $\xi_0 e^{-(\tau - \tau_0)}$ until g becomes of order one. Denoting as τ_1 the time in which the function g is close to the critical value $\xi \approx q/2$, we would have

$$\xi_0 \approx e^{(\tau_1 - \tau_0)}$$

Using (4.5), and taking into account that the change in the function Φ is not very relevant during the time that the function g needs to reduce its value from ξ_0 until $\xi = O(1)$ it follows that near the critical line one has that, to the leading order

$$\Phi(\xi, \tau) \approx e^{(\tau - \tau_1)} \exp(-\tfrac{9}{25}\, e^{2\tau_0/3} e^5/3(\tau_1 - \tau_0)), \qquad \text{for} \quad \tau \gg \tau_1 \gg \tau_0 \qquad (4.7)$$

In order to make this function of order one we would need

$$(\tau - \tau_1) \approx e^{(5/3)\,\tau_1}$$

where we just keep the leading term.

Summarizing, we have obtained that for large values of τ the problem (4.6) can be approximated to the leading order by the following one:

Find $\lambda(\tau)$ such that the function $g(\tau; \tau_0; \xi_0)$ that reaches the region $g \approx q/2$ for times of order τ_1 remains stacked at the line $\xi \approx q/2$ during a time of order $T(\tau_1) \approx e^{(5/3)\,\tau_1}$.

Once the function $T(\tau_1)$ has been found, the function g takes values in the region $g \approx q/2$. It is then natural to approximate Eq. (4.4) by the dominant terms near the critical line. We then replace (4.4) by the ordinary differential equation

$$\frac{dg}{d\tau} = -\frac{1}{3q}\left(g - \frac{q}{2}\right)^2 - \varepsilon(\tau)\left(\frac{q}{2}\right)^{1/3} \tag{4.8}$$

where

$$\varepsilon(\tau) = \lambda(\tau) - \lambda_{crit}$$

The solutions of Eq. (4.8) can become $\pm\infty$ for finite values of τ. The time that the corresponding solutions g spend to take on all values until $g = O(1)$ is of order unity, and it is then negligible compared with $T(\tau_1)$. Then, with the same precision that in the case of the previous approximations, we can reformulate the approximate problem in the following way:

Find $\varepsilon(\tau)$ such that the solution of (4.8) satisfying

$$g(\tau_1) = +\infty \tag{4.9}$$

verifies

$$g(\tau_1 + T(\tau_1)) = -\infty \tag{4.10}$$

where

$$T(\tau_1) = e^{(5/3)\tau_1} \tag{4.11}$$

We notice that, once this problem has been solved, the corresponding function Φ given by (4.5) yields the behaviour of the selfsimilar LS solution for $\xi < q/2$. Indeed, let us denote by τ_2 a characteristic time where

$$\varepsilon(\tau_2) \ll \left(g - \frac{q}{2}\right)^2 \ll 1 \tag{4.12}$$

It is readily seen that $\tau_2 \approx \tau_1 + T(\tau_1) \approx T(\tau_1)$. Since the choice of $T(\tau_1)$ implies that Φ becomes of order one for $\tau \approx \tau_1 + T(\tau_1)$, using (4.7) we obtain that along the characteristic line $\xi = g$ there holds

$$\Phi \approx k \exp(\tau - \tau_2)$$

and on the other hand, using (4.8) we deduce from (4.12)

$$g \approx \frac{q}{2} + \frac{3q}{(\tau - \tau_2)}$$

for $\tau < \tau_2$. Using the fact that $\xi = g$, we readily obtain that for each fixed value of τ

$$\Phi \sim k \exp\left(\frac{1}{3q(\xi - q/2)}\right)$$

as $\xi \to (q/2)^-$. It is readily seen that this behaviour coincides with the asymptotic behaviour of the LS self-similar solution near the critical line. Moreover, if we now integrate by characteristics equation (4.2) beginning with this asymptotic behaviour near the critical line, we recover the self-similar solution of the LS theory. The boundary condition (2.13) does not play an important role, since the direction of the convective term allows to connect the value obtained for the LS theory at $\xi = 0$ with the boundary condition $\Phi(0, \tau) = 0$ as can be seen by means of standard boundary layer theory.

We then need to solve the problem (4.8), (4.9), (4.10), (4.11), that contains all the main features of the model (2.10), (2.11), (2.13) near the critical line. As was previously indicated, that problem has an extreme sensitivity to small variations of $\varepsilon(\tau)$ in (4.8). A solution for (4.8), (4.9), (4.10), (4.11) will be obtained in the next pages using the invariance of the problem under a suitable discrete group of transformations.

5. A RENORMALIZATION PROCEDURE

In this section the problem given by (4.8), (4.9), (4.10), (4.11) is solved by taking advantage of a particular invariance of this system under a suitable rescaling group. We can eliminate the numerical constants in the problem by means of the change of variables

$$y = \frac{1}{2} + \frac{1}{3q}\left(g - \frac{q}{2}\right)$$

$$s = \tau - \tau_1$$

$$\delta(s) = \frac{\varepsilon(\tau)}{3 \cdot 2^{1/3} \cdot q^{2/3}}$$

$$R = \tau_1$$

that transforms (4.8), (4.9), (4.10), (4.11) into the following problem. Find $\delta(s)$ such that

$$\frac{dy}{ds} = -\left(y - \frac{1}{2}\right)^2 - \delta(s+R) \tag{5.1}$$

$$y(0) = +\infty \tag{5.2}$$

$$y(T(R)) = -\infty \tag{5.3}$$

where

$$T(R) = e^{\beta R}, \qquad \beta = \tfrac{5}{3} \tag{5.4}$$

Notice that $\delta(s+R)$ is basically $\lambda(\tau)$.

A. A Discrete Group of Transformations

The key property of the problem (5.1), (5.2), (5.3), (5.4) that will be used here is its invariance under the following transformation

$$y(s) = \frac{1}{2} + \frac{e^{-\tilde{s}}\tilde{y}(\tilde{s})}{(R+1)} \tag{5.5}$$

$$s = (R+1)(e^{\tilde{s}} - 1) \tag{5.6}$$

$$\delta(s) = \frac{1}{(s+1)^2}\left[\frac{1}{4} + \tilde{\delta}(\ln(s+1))\right] \tag{5.7}$$

$$R = e^{\tilde{R}} - 1 \tag{5.8}$$

$$T(R) = (R+1)(e^{\tilde{T}(\tilde{R})} - 1) \tag{5.9}$$

that defines a new set of variables $\tilde{s}$, $\tilde{y}$, $\tilde{\delta}$, $\tilde{R}$, $\tilde{T}$. Notice that (5.6), (5.7) and (5.8) imply

$$\delta(s+R) = \frac{e^{-2\tilde{s}}}{(R+1)^2}\left[\frac{1}{4} + \tilde{\delta}(\tilde{s} + \tilde{R})\right]$$

Using this expression and (5.5), (5.6) in (5.1) we obtain

$$\frac{e^{-\tilde{s}}}{(R+1)}\frac{d}{d\tilde{s}}\left[\frac{e^{-\tilde{s}}}{(R+1)}\tilde{y}\right] = -\frac{e^{-2\tilde{s}}}{(R+1)^2}(\tilde{y}(\tilde{s}))^2 - \frac{e^{-2\tilde{s}}}{(R+1)^2}\left[\frac{1}{4} + \tilde{\delta}(\tilde{s} + \tilde{R})\right]$$

that after some simple computations yields

$$\frac{d\tilde{y}}{d\tilde{s}} = -\left(\tilde{y} - \frac{1}{2}\right)^2 - \tilde{\delta}(\tilde{s} + \tilde{R}) \tag{5.10}$$

On the other hand, (5.6) implies that $s = 0$ becomes $\tilde{s} = 0$. Using thus (5.5), we obtain

$$\tilde{y}(0) = +\infty \tag{5.11}$$

and finally (5.5), (5.6), (5.9) imply

$$\tilde{y}(\tilde{T}(\tilde{R})) = -\infty \tag{5.12}$$

Notice that (5.10), (5.11), (5.12) give the invariance of (5.1)–(5.4) under (5.5)–(5.9).

B. Analysis of a Bidimensional Iteration Map

We need to understand the properties of the iteration map defined by means of (5.8), (5.9) on the quadrant $\mathbb{R}^+ \times \mathbb{R}^+$. To this end, we write the corresponding transformation as

$$S\colon (R, T) \to \left(\ln(R+1), \ln\left(1 + \frac{T}{R+1}\right)\right) \tag{5.13}$$

Some simple properties of the iteration S defined by means of (5.13) are the following

(1) The only fixed point of S in $\mathbb{R}^+ \times \mathbb{R}^+$ is $(R, T) = (0, 0)$.

(2) The variables R, T decrease in each iteration.

(3) For any (R, T) there holds

$$\lim_{N \to \infty} S^N(R, T) = (0, 0)$$

(4) The transformation S is invertible. The inverse of S is given by

$$S^{-1}\colon (R, T) \to (e^R - 1, (R+1)(e^T - 1))$$

and one has that

$$\lim_{N \to \infty} S^{-N}(R, T) = \lim_{N \to \infty} (S^{-1})^N (R, T) = (+\infty, +\infty)$$

It is important to understand the structure of the curves in the quadrant $\mathbb{R}^+ \times \mathbb{R}^+$ that are invariant under the transformation S. we are interested in graph-like curves in $\mathbb{R}^+ \times \mathbb{R}^+$ with the form

$$T = f(R) \tag{5.14}$$

The curve defined by (5.14) is invariant under S if and only if the function f satisfies the functional equation

$$f(R) = (R+1)[e^{f(\ln(R+1))} - 1] \tag{5.15}$$

It is easily seen that we can obtain solutions of this equation if we prescribe the values of f in any interval of the form $[R_0, e^{R_0} - 1)$ with $R_0 > 0$, just by iteration of (5.15). In particular the solutions of (5.15) could be extremely oscillatory and also very irregular.

It is natural to expect the existence of a particular class of solutions of (5.15) that are not oscillatory as $R \to 0^+$. To wit, let us assume that f is smooth enough near the origin. Using Taylor expansion, it should be possible to make the following approximation

$$f(\ln(R+1)) \approx f\left(R - \frac{R^2}{2}\right) \approx f(R) - \frac{R^2}{2} f'(R)$$

We then write (5.15) as

$$\begin{aligned} f(R) &\approx (R+1)[e^{f(R)} e^{-(R^2/2) f'(R)} - 1] \\ &\approx f(R) + Rf(R) - \frac{R^2}{2} f'(R) + O(f(R))^2) \end{aligned}$$

We then approximate (5.15) by the differential equation

$$\frac{R}{2} f'(R) = f(R) + O\left(\frac{f(R)^2}{R}\right)$$

whose solutions behave in the form

$$f(R) \approx CR^2$$

as $R \to 0$, where $C \geqslant 0$ is an arbitrary constant. This argument is made precise in the following theorem.

Theorem 2. For each constant $C \geqslant 0$ there exists an unique solution of (5.15), that we will denote as f_C, such that

$$\lim_{R \to 0^+} \frac{f_C(R)}{R^2} = C \tag{5.16}$$

The solution f_C is infinitely differentiable in $\mathbb{R}^+$ and is monotonically increasing in the R variable. Moreover, if $C_1 < C_2$, there holds

$$f_{C_1}(R) < f_{C_2}(R)$$

The functions f_C depend continuously on the C variable.

The proof of Theorem 2 will be given in Appendix B.

There are other properties of the functional equation (5.15) that it is worth noticing. If $C = 0$ in (5.16) then $f \equiv 0$. Furthermore, when $C \to 0^+$ the solutions of (5.15) approach to zero in compact sets of R. We then formally obtain in the equation (5.15) the linear approximation

$$f(R) = (R+1)\, f(\ln(R+1)) \tag{5.17}$$

This equation can be easily solved by iteration. Its solution is the following function

$$f(R) = CQ(R) \tag{5.18}$$

where $Q(R)$, that plays an important role in the iteration S defined in (5.13), is given by

$$Q(E) = 4e^{2\gamma} \prod_{k=0}^{\infty} \left[g_k(R)\, e^{-2/k+1} \right] \tag{5.19}$$

where γ is Euler's constant, and the family of functions $g_k(R)$ is defined inductively as follows

$$\begin{aligned} g_0(R) &= R + 1 \\ g_{k+1}(R) &= p(g_k(R)), \qquad k = 0, 1, 2,... \\ p(\zeta) &= 1 + \ln(\zeta) \end{aligned} \tag{5.20}$$

Some properties of the functions Q, g_k that will be used later are collected in the following result that will be proved in Appendix B.

Theorem 3. The infinite product that defines the function Q in (5.19) converges. Moreover, there holds

$$\lim_{R \to 0} \frac{Q(R)}{R^2} = 1 \tag{5.21}$$

For each value of n and for any $\sigma > 0$ arbitrarily small, funcion $Q(R)$ satisfies

$$\begin{gathered} R \ln(R) \ln(\ln(R)) \ldots . \ln(\ln(..n.times..(\ln R))) \ll Q(R) \\ Q(R) \ll R \ln(R) \ln(\ln(R)) \ldots . [\ln(\ln(..n.times..(\ln R)))]^{1+\sigma} \end{gathered} \tag{5.22}$$

as $R \to \infty$.

For each fixed value of R, the asymptotic behaviour of the functions $g_k(R)$ as $k \to \infty$ is given by

$$g_k(R) = 1 + \frac{2}{k} + \frac{4 \ln(k)}{3k^2} + \frac{\mu(R)}{k^2} + O\left(\frac{1}{k^3}\right) \tag{5.23}$$

where $\mu(R)$ is a function increasing on R.

Formula (5.22) states that the function $Q(R)$ formally satisfies

$$Q(R) \sim R \ln(R) \ln(\ln(R)) \ldots . \ln(\ln(\ldots . (\ln R))) \ldots .$$

as $R \to \infty$. It is important to notice that the approximation of the solutions of (5.15) by means of (5.18) for $C \to 0^+$ only valid for not very large values of R. In fact, the approximation (5.18) breaks down if $CQ(R) \approx 1$. In any case this discussion will not be pursued here, since we will not need to study in detail the functions $f_C(R)$ as $C \to 0^+$.

We need however to study the asymptotic properties of the equation (5.15) as $R \to \infty$. To this end, it is convenient to introduce a suitable auxiliary function whose main properties are described in the following

Theorem 4. There exists an unique function $H \in C^\infty(\mathbb{R})$ such that

$$H(\zeta) = \ln(1 + H(\zeta + 1)) \tag{5.24}$$

$$H(\zeta) \sim -\frac{2}{\zeta}, \qquad \zeta \to -\infty \tag{5.25}$$

$$H(0) = 1 \tag{5.26}$$

Such a function H is (strictly) monotonically increasing, and it satisfies

$$H(\zeta+\sigma) \gg H(\zeta) \tag{5.27}$$

as $\zeta \to +\infty$ for any $\sigma > 0$.

The proof of this Theorem will also be given in Appendix B.

Condition (5.26) is just a normalization property. It is convenient to think of the function H when $\zeta \to +\infty$ as given by:

$$\exp(\exp(\ldots\zeta \text{ times}\ldots\exp(0)))$$

Condition (5.27) indicates that the function H grows extremely fast for large values of ζ if the argument of the function is slightly increased.

Besides providing a useful technical tool in the study of Eq. (5.15), function H will be important here because it gives a simple method of describing the asymptotic behaviour of the functions $f_C(R)$ defined in Theorem 2. The following result is the key point that explains the usefulness of the functions $f_C(R)$ in the analysis of the problem (5.1), (5.2), (5.3), (5.4).

Theorem 5. The asymptotic behaviour of the function $f_C(R)$ as $R \to \infty$ is given by:

$$H^{-1}(f_C(R)) \sim (H^{-1}(R) + 2C) \tag{5.28}$$

The proof of Theorem 5 will be given in Appendix B.

It is relevant for the study of the problem under consideration to remark that (5.24) readily implies

$$g(x) \equiv H(H^{-1}(x)+1) = e^x - 1 \tag{5.29}$$

C. Solution of (5.1)–(5.4)

We now use the previous results to solve (5.1), (5.2), (5.3), (5.4). As a preliminary step, we show how to solve the problem (5.1), (5.2), (5.3) where the function $T(R)$ satisfies

$$T(R) = f_C(R) \tag{5.30}$$

instead of (5.4), where f_C is as in Theorem 2. With this particular choice of $T(R)$, problem (5.1), (5.2), (5.3) is invariant under the transformation (5.5)–(5.9). It is then natural to look for a solution of the problem in this particular case which is invariant under that discrete set of transformations. We now have that

$$\delta(s)=\frac{1}{(s+1)^2}\left[\frac{1}{4}+\delta(\ln(1+s))\right]$$

Iterating this formula we deduce

$$\delta(s)=\lim_{N\to\infty}\left\{\frac{1}{4}\sum_{k=0}^{N}\frac{1}{(g_0(s)\,g_1(s)\cdots g_k(s))^2}+\frac{\delta(\log(g_N(s)))}{(\prod_{k=0}^{N}g_k(s))^2}\right\} \tag{5.31}$$

where the functions $g_k(s)$ are defined as in (5.20). Using (5.23), we readily see that the series in (5.31) converges. Then

$$\delta(s)=\frac{1}{4}\sum_{k=0}^{\infty}\frac{1}{(g_0(s)\,g_1(s)\cdots g_k(s))^2}+\lim_{N\to\infty}\left[\frac{\delta(\ln(g_N(s)))}{(\prod_{k=0}^{N}g_k(s))^2}\right] \tag{5.32}$$

In order to compute the last limit, we write

$$\prod_{k=0}^{N}g_k(s)=\prod_{k=0}^{N}\left[g_k(s)\,e^{-2/k+1}\right]\prod_{k=0}^{N}e^{2/k+1}\sim\tfrac{1}{4}Q(s)\,N^2 \tag{5.33}$$

as $N\to\infty$, where Q is defined in (5.19).

On the other hand (5.23) implies $\ln(g_N(s))\to 0$ as $N\to\infty$. We then need to compute the asymptotics of $\delta(s)$ as $s\to 0$. Using (5.30) and (5.16) we obtain $T(R)\sim CR^2$ as $R\to 0^+$. Notice that in (5.1) we need to solve the equation for $0<s<T(R)\ll R$. It then follows that, if $\delta(s)$ is smooth enough near the origin, then $\delta(s+R)\approx\delta(R)$ in Eq. (5.1) if $R\to 0^+$. The problem (5.1)–(5.3) can be solved with this approximation to obtain

$$y(s,R)=\frac{1}{2}-\frac{\pi}{CR^2}\tan\left(\pi\left(\frac{s}{CR^2}-\frac{1}{2}\right)\right) \tag{5.34}$$

$$\delta(R)=\frac{\pi^2}{C^2R^4} \tag{5.35}$$

Using (5.35) and (5.33), it then follows

$$\lim_{N\to\infty}\left(\frac{\delta(\ln(g_N(s)))}{(\prod_{k=0}^{N}g_k(s))^2}\right)=\frac{\pi^2}{16C^2(Q(s))^2}$$

whence

$$\delta(s) = \frac{1}{4} \sum_{k=0}^{\infty} \frac{1}{(g_0(s)\, g_1(s) \cdots g_k(s))^2} + \frac{\pi^2}{16C^2(Q(s))^2} \tag{5.36}$$

The corresponding function $y(s, R)$ can be then obtained by iterating the relation

$$y(s, R) = \frac{1}{2} + \frac{1}{s+R+1}\, y\left(\ln\left(1+\frac{s}{R+1}\right), \ln(R+1)\right)$$

that follows from (5.5)–(5.9). It is then easily seen that

$$\begin{aligned} y(s, R) = {} & \frac{1}{2}\left[1 + \sum_{k=0}^{N} \frac{1}{g_0(s+R)\cdots g_k(s+R)}\right] \\ & + \frac{1}{g_0(s+R)\cdots g_{N+1}(s+R)}\, y(\ln(g_{N+1}(s+R)) \\ & - \ln(g_{N+1}(R)), \ln(g_{N+1}(R))) \end{aligned}$$

and, taking the limit $N \to \infty$, the series converges by (5.23). We now compute

$$\begin{aligned} \lim_{N\to\infty} & \left[\frac{1}{g_0(s+R)\cdots g_{N+1}(s+R)}\, y(\ln(g_{N+1}(s+R)) \right. \\ & \left. - \ln(g_{N+1}(R)), \ln(g_{N+1}(R)))\right] \equiv J(s, R) \end{aligned}$$

Using (5.23) and the approximation (5.34) we deduce

$$\begin{aligned} J(s, R) &= -\lim_{N\to\infty} \frac{\pi(N/2)^2}{Ce^{2\gamma}N^2} \tan\left(\pi\left(\frac{(\mu(s+R)-\mu(R))(1/N^2)}{C(2/N)^2} - \frac{1}{2}\right)\right) \\ &= -\frac{\pi}{4Ce^{2\gamma}} \tan\left(\pi\left(\frac{(\mu(s+R)-\mu(R))}{4C} - \frac{1}{2}\right)\right) \end{aligned}$$

where $\mu(R)$ is as in (5.23). we then have

$$\begin{aligned} y(s, R) = {} & \frac{1}{2}\left[1 + \sum_{k=0}^{\infty} \frac{1}{g_0(s+R)\cdots g_k(s+R)}\right] \\ & - \frac{\pi}{4Ce^{2\gamma}} \tan\left(\pi\left(\frac{(\mu(s+R)-\mu(R))}{4C} - \frac{1}{2}\right)\right) \end{aligned} \tag{5.37}$$

It is not hard to check by direct computation that (5.31), (5.37) is a solution of the differential Eq. (5.1). On the other hand, if $R > 0$, the series in (5.37) is bounded for $s = 0$, whence (5.2) holds. To verify (5.3), we just need to check that with the choice of $T(R)$ given in (5.30), there holds

$$(\mu(T(R) + R) - \mu(R)) = 4C \tag{5.38}$$

The proof of (5.38) will be given in Appendix B.

Summarizing, we have obtained a solution of (5.1)–(5.3) with $T(R)$ given in (5.30). We now study the problem (5.1)–(5.3) with the choice of $T(R)$ that corresponds to the original problem (5.4). The solution that will be obtained here is not an exact solution as in the previous case, but just an asymptotic solution as $R \to \infty$. However, the main idea is very close to the analysis performed for (5.30). Indeed, the asymptotic behaviours (5.28) in Theorem 5 are very different for small variations of C. Among the asymptotic behaviours (5.28), the "closest" to the one in (5.4) is the corresponding to $C = 1/2$, in the sense that the asymptotics (5.28) for $C > 1/2$ grows faster than any exponential, and for $C < 1/2$ the behaviour (5.28) is much smaller than any exponential. Under the iteration S in (5.13), the function $T(R)$ given in (5.4) approaches very fast to the curve $T = f_1(R)$, since otherwise repeated application of the inverse map S^{-1} would contain points in regions with the asymptotics (5.28) with $C \neq 1/2$, but those points are very different from the function (5.4), this gives a contradiction. It is important to remark that the application S^{-1} amplifies small differences extremely fast, whence the convergence to the curve $T = f_1(R)$ is very fast as well.

We now make this argument more precise. If we apply N times the iteration S in (5.13) to the function (5.4), we obtain a function that we denote as $T_N(R_N)$, where R_N gives the transformed R coordinate under N iterations of S. There is a simple way of writing R_N by means of the function H defined in Theorem 4. Indeed, by (5.24) it actually holds that

$$R_N = H(H^{-1}(R) - N)$$

On the other hand repeated iteration of S implies

$$T_N(R_N) = p^N(1 + R + e^{\beta R}) - R_N$$

where p is as in (5.20), and p^N denotes N iterations of this mapping acting over the function $1 + R + e^{\beta R}$. If we write $\xi = H^{-1}(R)$, it then follows that

$$\frac{T_N(R_N)}{(R_N)^2} = \frac{p^N(1 + H(\xi) + e^{\beta H(\xi)}) - H(\xi - N)}{(H(\xi - N))^2} \tag{5.39}$$

In order to solve the problem (5.1)–(5.4), we iterate the transformation S. Arguing as in the case of (5.30), we would obtain

$$\delta(s)=\frac{1}{4}\sum_{k=0}^{\infty}\frac{1}{(g_0(s)\,g_1(s)\cdots g_k(s))^2}+\lim_{N\to\infty}\left[\frac{\delta_N(\ln(g_N(s)))}{(\prod_{k=0}^{N}g_k(s))^2}\right] \tag{5.40}$$

where δ_N is the transformed δ after N iterations of the discrete group (5.5)–(5.9). We need to compute in this case $\lim_{N\to\infty}[\delta_N(\ln(g_N(s)))/(\prod_{k=0}^{N}g_k(s))^2]$. Notice that the function $T_N(R_N)$ approaches near the origin to the function $f_1(R)$, and it is then natural to obtain δ_N as a perturbation of the function δ near the origin obtained in the analysis of the case (5.30).

Notice further that $T_N(R_N)/(R_N)^2$ depends on R. Let us compute the asymptotic behaviour of this function as $R\to\infty$. In this limit, using the formula of p in (5.20) we obtain to the lowest order in the Taylor expansion

$$p(1+H(\xi)+e^{\beta H(\xi)})\approx\beta H(\xi)+1+\frac{1+H(\xi)}{\beta H(\xi)}$$

as $\zeta\to\infty$. Using (5.24) we can write to the lowest order

$$p^2(1+h(\xi)+e^{\beta H(\xi)})\approx H(\xi-1)+\log(\beta)+\left[\frac{e^{-\beta H(\zeta)}}{\beta}-\frac{(\beta-1)}{\beta(1+H(\xi))}\right]$$

and iterating $(N-2)$ times more we obtain

$$p^N(14+H(\xi)+e^{\beta H(\xi)})$$
$$\approx H(\xi-N+1)+\frac{[\log(\beta)+[e^{-\beta H(\zeta)}/\beta-(\beta-1)/\beta(1+H(\xi))]]}{\prod_{k=1}^{N-2}[1+H(\xi-k)]}$$

as $\zeta\to\infty$. If we just keep the dominant terms as $\zeta\to\infty$, recalling (5.39) we obtain the following approximation

$$\frac{t_N(R_N)}{(R_N)^2}\approx\frac{H(\xi-N+1)-H(\xi-N)}{(H(\xi-N))^2}+\frac{\log(\beta)}{(H(\xi-N))^2\prod_{k=1}^{N-2}[1+H(\xi-k)]}$$

As in the previous case we assume that $\delta_N(s+R_N)\approx\delta_N(s)$. By (5.25) and (5.20) we obtain in the limit $N\to\infty$

$$\frac{T_N(R_N)}{(R_N)^2} \approx \frac{1}{2} + \frac{\log(\beta)}{(R_N)^2 \prod_{k=1}^{N-2} g_k(R)}$$

$$= \frac{1}{2} + \frac{\log(\beta)(1+R)}{(R_N)^2 \prod_{k=0}^{N-2} [g_k(R)\, e^{2/k+1}] \prod_{k=0}^{N-2} (e^{2/k+1})}$$

$$\approx \frac{1}{2} + \frac{\log(\beta)(1+R)}{4Q(R)}$$

where $Q(R)$ is as in (5.19). It then follows that

$$\delta_N(R_N) \approx \frac{\pi^2}{(R_N)^4} \left(\frac{1}{2} + \frac{\log(\beta)(1+R)}{4Q(R)\, e^{2\gamma}}\right)^{-2} \approx \frac{4\pi^2}{(R_N)^4} \left(1 - \frac{\log(\beta)(1+R)}{2Q(R)}\right)$$

as $R \to \infty$, $N \to \infty$. Notice that $R_N = g_N(R)$. It then follows that

$$\delta_N(\ln(g_N(R))) \approx \delta_N(g_N(R)) \approx \frac{4\pi^2}{(R_N)^4} \left(1 - \frac{\log(\beta)(1+R)}{2Q(R)}\right)$$

whence using (5.40) we deduce

$$\delta(s) \approx \frac{1}{4} \sum_{k=0}^{\infty} \frac{1}{(g_0(s)\, g_1(s) \cdots g_k(s))^2} + \frac{\pi^2}{4(Q(s))^2} \left(1 - \frac{\log(\beta)(1+s)}{2Q(s)}\right) \qquad (5.41)$$

as $s \to \infty$. Notice that in (5.41) we obtain the dependence of the precise form of the function $T(R)$ (in particular the exponent β), that appears "beyond all the orders" of the series. If $\beta = 1$, we recover the series (5.36) with $C = 1/2$. When $\beta > 1$, the correction obtained in (5.41) is negative, as it should be expected from (5.1), since in this case we are requiring the solutions of (5.1) to stay longer near the critical line than in the case in which $T(R)$ is given by (5.30). If $\beta < 1$ we obtain in (5.41) a positive correction for δ.

It is clear that the procedure described here allows to solve the problem (5.1)–(5.3) asymptotically as $R \to \infty$ for a large class of functions $T(R)$.

6. CONCLUDING REMARKS

In this paper a Fokker–Planck equation has been analyzed whose solutions approach for long times to the classical Lifshitz–Slyozov model of coarsening. This model, that it is derived as a limit case of the classical Becker–Döring equations, contains information about the nucleation that takes place by kinetic effects. In particular, a detailed analysis of the critical sizes of the clusters where the transition between the region dominated by nucleation (for clusters of supercritical size) and the region that can be described by the LS theory (subcritical size) has been given. The region near the critical size is approximately invariant under a discrete group of transformations. The structure of the solution of the Fokker–Planck equation may be described by means of a renormalization procedure associated to the discrete group of transformations. The properties of this group of transformations have been studied in detail in this paper. In particular this invariance predicts for the "oversaturation" a behaviour

$$\delta(t)=\frac{B}{t^{1/3}}\left[\frac{1}{4}+\frac{1}{4t}+\frac{1}{4t\ln(t)}+\frac{1}{4t\ln(t)\ln(\ln(t))}+\cdots\right], \qquad t\to\infty \tag{6.1}$$

A precise meaning of this series has been given. The theory developed in this paper is self-consistent, since the main approximation that has been made consist in neglecting the nucleation effects near the critical line. If Φ is a rescaled concentration of clusters and ξ is the corresponding rescaled size of the clusters, the nucleation terms are of order $e^{-2\tau/3}\Phi_{\xi\xi}$. This theory predicts this last term to be bounded by $e^{-2\tau/3}\tau\alpha\Phi$, that it is much smaller that some of the terms kept in the model, whence the selfconsistence of the theory follows.

APPENDIX A

In this Appendix the local well-posedness of model (2.10), (2.11), (2.13), (2.14) is proved.

Theorem 6. For any $\Phi_0(\cdot)\geqslant 0$ such that

$$I=\int_0^\infty \xi\Phi_0(\xi)\,d\xi+\sup_{\xi>0}\,[\xi^{-2/3}\Phi_0(\xi)]<\infty$$

there exists $T=T(\Phi_0)>0$ and a unique solution $(\Phi(\cdot,\cdot),\lambda(\cdot))$ of (2.10), (2.11), (2.13), (2.14) defined in the interval $[\tau_0,\tau_0+T]$ that satisfies

$$\int_0^\infty \xi\Phi(\xi,\tau)\,d\xi+\sup_{\xi>0}\,[\xi^{-2/3}\Phi(\xi,\tau)]<\infty$$

$$\lambda(\cdot)\in L^\infty[\tau_0,\tau_0+T] \tag{A.1}$$

for $\tau\in[\tau_0,\tau_0+T]$.

Proof of Theorem 6. Using the variables (2.9) we can transform (2.10), (2.11), (2.13), (2.14) into the problem (2.7), (2.8) with the boundary condition

$$c(0, t) = 0 \tag{A.2}$$

and the initial data

$$c(l, 0) = \Phi_0(\cdot) \tag{A.3}$$

We introduce a new spatial variable ϑ by

$$\zeta = l^{5/6}$$

and a new dependent variable $W(\zeta, t)$ by means of

$$W(\zeta, t) = \zeta^{-4/5} \cdot c(\zeta, t) \tag{A.4}$$

Then, the problem (2.7) becomes

$$\begin{aligned}\frac{\partial W}{\partial t} = \frac{25}{36}\frac{\partial^2 W}{\partial \zeta^2} + \left[\frac{55}{36}\frac{1}{\zeta} + \frac{5q}{6}(\zeta^{-1/5} - \zeta^{1/5})\right]\frac{\partial W}{\partial \zeta} \\ + \left[\frac{2q}{3\zeta}(\zeta^{-1/5} - \zeta^{1/5}) - \frac{\eta(t)}{3\zeta^{4/5}}\right] W\end{aligned} \tag{A.5}$$

Notice that in this set of variables the integral condition (2.8) reads

$$\int_0^\infty \zeta^{11/5} W(\zeta, t)\, d\zeta = \frac{5\theta}{6} \tag{A.6}$$

Multiplying (2.7) by l and integrating in the l variable, and using (2.14), we formally obtain after some integrations by parts the formula

$$\eta(t) = \frac{q \int_0^\infty c(l, t)\, dl}{\int_0^\infty (l)^{1/3} c(l, t)\, dl} = \frac{q \int_0^\infty W(\zeta, t)\, \zeta\, d\zeta}{\int_0^\infty (l)^{1/3} c(l, t)\, dl} = \frac{q \int_0^\infty W(\zeta, t)\, \zeta\, d\zeta}{\int_0^\infty W(\zeta, t)\, \zeta^{7/5}\, d\zeta} \tag{A.7}$$

where we have used the condition (A.1). We then prove existence and uniqueness of solutions of (2.10), (2.11), (2.13), (2.14) by means of a standard fixed point argument. We write the problem (A.5) as

$$W_t = AW + F[W] \tag{A.8}$$

where the operator A is the unique self-adjoint Friedrichs extension (cf. [10]) in the space of functions $\{W: \int_0^\infty |W(\zeta)|^2 \zeta^{11/5} d\zeta\}$ of the operator that is defined in $C_0^\infty(\mathbb{R}^+)$ by

$$AW = \frac{25}{36}\frac{\partial^2 W}{\partial \zeta^2} + \frac{55}{36}\frac{1}{\zeta}\frac{\partial W}{\partial \zeta}$$

where

$$F[W] \equiv \frac{5q}{6}(\zeta^{-1/5} - \zeta^{1/5})\frac{\partial W}{\partial \zeta} + \left[\frac{2q}{3\zeta}(\zeta - 1/5 - \zeta^{1/5}) - \frac{\eta(t)}{3\eta^{4/5}}\right] W \quad \text{(A.9)}$$

and $\eta(t)$ is as in (A.7). It is not hard to check that the semigroup e^{At} has the following representation formula

$$(e^{At}\phi)(x) = \left(\frac{18}{25t}\right)^{8/5} \int_0^\infty e^{-9\xi^2/25t} \cdot \Lambda\left(\frac{18\xi x}{25t}\right) \xi^{11/5} \, d\xi \quad \text{(A.10)}$$

where

$$\Lambda(y) = y^{-3/5} I_{3/5}(y)$$

where $I_\nu(y)$ denotes the modified Bessel function of order ν (cf. [1]). Using the variation of constants formula, (A.8) can be written as

$$W(\cdot, t) = e^{A(t-t_0)} W(\cdot, t_0) + \int_{t_0}^{t} e^{A(t-s)} F[W](\cdot, s) \, ds \quad \text{(A.11)}$$

that reduces the original problem to a fixed point argument.

Using the asymptotic formulae for the modified Bessel functions (cf. [1]) it follows that

$$|\Lambda(y)| + |\Lambda'(y)| \leqslant \frac{C}{y^{11/10} + 1} e^y, \qquad 0 \leqslant y < \infty \quad \text{(A.12)}$$

$$|\Lambda'(y) - \Lambda(y)| \leqslant \frac{C}{y^{21/10} + 1} e^y, \qquad 0 \leqslant y < \infty \quad \text{(A.13)}$$

for some suitable constant $C > 0$. From now on, C will denote a generic positive constant, possibly changing from line to line. Using (A.10), (A.12) and (A.13) it is not difficult to obtain the estimates

$$\sup_{x>0}\left|e^{At}\left(\zeta^{-1/5}\frac{\partial\phi}{\partial\zeta}\right)(x)\right|\leqslant\frac{C}{t^{3/5}}\sup_{x>0}|\phi| \tag{A.14}$$

$$\sup_{x>0}\left|e^{At}\left(\zeta^{1/5}\frac{\partial\phi}{\partial\zeta}\right)(x)\right|\leqslant\frac{C}{t^{2/5}}\sup_{x>0}|\phi| \tag{A.15}$$

$$\sup_{x>0}|e^{At}(\zeta^{-4/5}\phi)(x)|\leqslant\frac{C}{t^{2/5}}\sup_{x>0}|\phi| \tag{A.16}$$

$$\sup_{x>0}|e^{At}(\zeta^{-6/5}\phi)(x)|\leqslant\frac{C}{t^{3/5}}\sup_{x>0}|\phi| \tag{A.17}$$

where (A.16), (A.17) are obtained directly from (A.10) and (A.12), and in (A.14), (A.15) integration by parts is used in order to pass the derivatives of ϕ to the kernel of the semigroup. It readily follows from (A.9) and (A.14)–(A.17) that the last term in (A.11) can be estimated as follows

$$\begin{aligned}\sup_{x>0}&\left|\int_{t_0}^{t}e^{A(t-s)}F[W](\cdot,s)\,ds\right|\\ &\leqslant C\int_{t_0}^{t}\frac{\sup_{\xi>0}|W(\xi,s)|}{(t-s)^{3/5}}(1+\eta(s))\,ds\\ &\leqslant C(t-t_0)^{2/5}\sup_{\xi,t}|W(\xi,t)|\,[1+\sup_t\eta]\end{aligned}$$

On the other hand, given a solution of (A.5) (not necessarily satisfying (A.6)) the following identity holds

$$\frac{\partial}{\partial t}\left[\int_0^\infty\zeta^{11/5}W(\zeta,t)\,d\zeta\right]=\int_{t_0}^{t}\left[\int_0^\infty\zeta^{11/5}F[W](\zeta,s)\,d\zeta\right]ds$$

that implies, using (A.9)

$$\begin{aligned}&\left|\frac{\partial}{\partial t}\left[\int_0^\infty\zeta^{11/5}W(\zeta,t)\,d\zeta\right]\right|\\ &\qquad\leqslant C\max\left\{\sup_{\xi,t}|W(\xi,t)|,\int_0^\infty\zeta^{11/5}W(\zeta,t)\,d\zeta\right\}[1+\sup_t\eta]\end{aligned} \tag{A.18}$$

A standard fixed point argument in the class of functions $W\in L^\infty([t_0,t_0+\delta],L^\infty(\mathbb{R}^+))\cap\{W:\int_0^\infty\zeta^{11/5}W(\zeta,t)\,d\zeta<\infty\},\eta\in L^\infty[t_0,t_0+\delta]$ with $\delta>0$ small enough allows then to conclude the proof of Theorem 6.

Notice that (A.18) controls the variation of the function $\int_0^\infty \zeta^{11/5} W(\zeta, t)\, d\zeta$, and then that of the function $\eta(t)$ by (A.7).

APPENDIX B

In this Appendix we prove many of the results described in Section 5. It is convenient to show these facts in an order different as that in which they were stated.

Proof of Theorem 4. Notice that it is enough to prove the existence of a monotonically increasing function H satisfying (5.24), (5.25) and (5.27), since (5.26) can be obtained by making a translation of the origin to a new position ζ_0.

In order to obtain such a function, we define a sequence of functions $H_N(\zeta) = -2/\zeta - 3\ln(|\zeta|)/4\zeta^2 - 1/\zeta^2$ for $\zeta \in (-N, -N+1)$, $N = 1, 2,...$ and make then use of (5.24) to extend the definition of $H_N(\zeta)$ to the whole line. Notice that, as long as $|H_N(\zeta)| \leqslant 1$, (5.24) implies

$$\left| H_N(\zeta+1) - H_N(\zeta) - \frac{(H_N(\zeta))^2}{2} - \frac{(H_N(\zeta))^3}{6} \right| \leqslant \frac{e}{24} (H_N(\zeta))^4 \tag{B.1}$$

Let us write $X_{k,N} = \sup_{\zeta \in (-k, -k+1)} [H_N(\zeta)]$. Then (B.1) gives

$$X_{k+1,N} \leqslant X_{k,N} + \frac{(X_{k,N})^2}{2} + \frac{1}{6}(X_{k,N})^3 + \frac{e}{24}(X_{k,N})^4 \tag{B.2}$$

and by definition of $H_N(\zeta)$ it follows that $X_{-N,N} \leqslant 2/N + 3\ln(N)/4N^2 - 1/N^2$. Let us define

$$Z_k = -\frac{2}{k} + \frac{3\ln(|k|)}{4k^2} - \frac{A}{|k|^{5/2}} \tag{B.3}$$

It is a simple computation to verify that selecting $A > 0$ large enough, there holds

$$Z_{k+1} \geqslant Z_k + \frac{(Z_k)^2}{2} + \frac{1}{6}(Z_k)^3 + \frac{e}{24}(Z_k)^4 \tag{B.4}$$

for $k < 0$, $|k|$ large enough but independent on N. Notice that since

$$X_{-N,N} \leqslant Z_{-N}$$

we can argue by induction (using (B.2) and (B.4)) to obtain

$$X_{k,N} \leqslant Z_k$$

for $-N \leqslant k \leqslant -k_0$, where k_0 is a fixed positive number independent on N. An analogous argument with $Y_{k,N} = \inf_{\zeta \in (-k, -k+1)}[H_N(\zeta)]$ and the sequence

$$Z_k = -\frac{2}{k} + \frac{3\ln(|k|)}{4k^2} - \frac{2}{k^2} + \frac{A}{|k|^{5/2}}$$

with $A > 0$ large, yields

$$Z_k \leqslant Y_{k,N}$$

We then have the estimates

$$\frac{2}{|\zeta|} + \frac{3\ln(|\zeta|)}{4\zeta^2} - \frac{3}{\zeta^2} \leqslant H_N(\zeta) \leqslant \frac{2}{|\zeta|} + \frac{3\ln(|\zeta|)}{4\zeta^2} + \frac{3}{\zeta^2} \tag{B.5}$$

for $\zeta \leqslant -k_0$, and using (5.24) we obtain that the functions $H_N(\zeta)$ are uniformly bounded (in N) in compact sets of ζ. Differentiating in (5.24), we obtain

$$H'_N(\zeta+1) = eH_N(\zeta)H'_N(\zeta) \tag{B.6}$$

Using (B.5), it now follows that

$$\left| H'_N(\zeta+1) - H'_N(\zeta) + \frac{2}{\zeta} H'_N(\zeta) \right| \leqslant \frac{1}{|\zeta|^{3/2}} |H'_N(\zeta)|$$

for $\zeta \leqslant -k_0$. The choice of $H_N(\zeta)$ implies that $\sup_{\zeta \in (-N, -N+1)}[H_N(\zeta)] \leqslant C/N^2$. Arguing as in the previous case it follows the estimate

$$|H'_N(\zeta)| \leqslant \frac{C}{|\zeta|^2}$$

for $\zeta \leqslant -k_0$. Using then (B.6) it is deriveded that H'_N is uniformly bounded in compact sets of ζ uniformly on N. The procedure can be continued for higher order derivatives in a similar way. A classical compactness argument (using Ascoli–Arzela Theorem) allows then to pass to the limit on the functions $H_N(\zeta)$, as well as in (5.24), to obtain the existence of a solution of

(5.24), (5.25). The strict monotonicity of $H_N(\zeta)$ follows from the fact that (B.6) implies the lower bound

$$H'_N(\zeta) \geqslant \frac{\eta}{|\zeta|^2}$$

for $|\zeta| \leqslant -k_0$, where $\eta > 0$ is independent on N.

To prove uniqueness of the function H, let us assume that there exist two functions H_1, H_2 satisfying (5.24), (5.25), (5.26). Local analysis of the asymptotics of the functions H_1, H_2 (using comparison sequences as before) yields

$$H_i(\zeta) = -\frac{2}{\zeta} + \frac{4\ln(|\zeta|)}{3\zeta^2} + \frac{A_i}{\zeta^2} + o\left(\frac{1}{\zeta^2}\right), \qquad i = 1, 2 \tag{B.7}$$

as $\zeta \to -\infty$. Let us consider the function

$$W(\zeta) = H_1(\zeta) - H_2(\zeta)$$

that solves the equation

$$\begin{aligned} W(\zeta+1) &= e^{H_2(\zeta)}[W(\zeta) + O((W(\zeta))^2)] \\ &= W(\zeta)\left[1 - \frac{2}{\zeta} + O\left(\frac{1}{|\zeta|^{3/2}}\right)\right] + O((W(\zeta))^2) \end{aligned}$$

Assume that $A_l \neq A_2$. Then local analysis of this equation implies

$$\left| W(\zeta) - \frac{A_1 - A_2}{\zeta^2} \right| \leqslant \frac{|A_1 - A_2|}{2\zeta^2} \tag{B.8}$$

if $\xi \leqslant -k_0$. Using (5.24), we then easily obtain $H_1(0) \neq H_2(0)$, that contradicts (5.26). Then $A_1 = A_2$ and (B.8) yields $W(\zeta) = 0$.

In order to conclude the proof of Theorem 4, it only remains to verify (5.27). Passing to the limit in (B.6) as $N \to \infty$, it follows that

$$H'(\zeta+1) = e^{H(\zeta)} H'(\zeta) \tag{B.9}$$

and differentiating in (B.9) we obtain

$$H''(\zeta+1) = e^{H(\zeta)} H''(\zeta) + e^{H(\zeta)} (H'(\zeta))^2 \tag{B.10}$$

Using (5.24) and (5.26) we now deduce

$$\lim_{\zeta \to \infty} H(\zeta) = \infty$$

Taking ζ large enough, we then have

$$H'(\zeta + 1) \geqslant eH'(\zeta)$$

that by iteration implies

$$H'(\zeta) \geqslant Ce^{\zeta} \tag{B.11}$$

for some constant $C > 0$. The formulae (B.10) and (5.25) imply that H is convex. Then, using (5.24), (B.9), (B.11), it follows that

$$\begin{aligned} H(\zeta + a) &\geqslant H(\zeta) + H'(\zeta)\, a \geqslant e^{H(\zeta - 1)} H'(\zeta - 1)\, a \\ &\geqslant Ca(H(\zeta) + 1)\, e^{\zeta - 1} \gg H(\zeta) \end{aligned}$$

whence (5.27) follows.

Proof of Theorem 3. The function p defined in (5.20) satisfies $p(x) - 1 < x - 1$ if $x > 1$. It then follows that the sequence $g_k(R)$ is decreasing for fixed R, and $\lim_{k \to \infty}(g_k(R)) = 1$. Taylor Theorem then gives

$$g_{k+1}(R) - 1 = g_k(R) - 1 + \tfrac{1}{2}(g_k(R) - 1)^2 + O((g_k(R) - 1)^3) \tag{B.12}$$

as $g_k(R) - 1 \to 0$. Standard analysis of difference equations (cf. [4]) implies in turn (5.23). It then follows that the product that defines $Q(R)$ in (5.19) converges. A simple computation reveals that function $Q(R)$ satisfies (5.17). In order to prove Theorem 3 it is convenient to make the change of variables

$$R = H(\zeta)$$

that transforms Eq. (5.17) in

$$\Psi(\zeta + 1) = H(\zeta) + \Psi(\zeta) \tag{B.13}$$

where $\Psi(\zeta) = \log(f(H(\zeta)))$. Using the expansion (B7), we can show as in the proof of Theorem 4 the existence of a solution of this equation such that

$$\Psi(\zeta) \sim -2\ln(|\zeta|) + \ln(4C) + o(1) \tag{B.14}$$

as $\zeta \to -\infty$. It is then easy to check that the corresponding function $f(R)$ satisfies

$$f(R) \sim CR^2$$

as $R \to 0$. Iterating (B.13) we obtain an expression for this function, namely

$$\Psi(\zeta) = \sum_{k=1}^{N} H(\zeta - k) + \Psi(\zeta - N)$$

For each fixed value of ζ, we now take the limit as $N \to \infty$. Using (B.14), we see that

$$\Psi(\zeta) = \lim_{N \to \infty} \left[\sum_{k=1}^{N} \left(H(\zeta - k) - \frac{2}{k} \right) \right] + \lim_{N \to \infty} \left[\sum_{k=1}^{N} \left[\frac{2}{k} \right] - 2 \ln(N) \right] + \ln(4C)$$

that after some simple computations gives

$$f(R) = 4e^{2\gamma} \prod_{k=0}^{\infty} \left[g_k(R)\, e^{-2/k+1} \right]$$

This concludes the proof of (5.21).

The proof of (5.22) is a consequence of the formula

$$\frac{Q'(R)}{Q(R)} = \sum_{k=0}^{\infty} \frac{1}{g_0(R) \cdots g_k(R)}$$

that is obtained on taking the logarithmic derivative of (5.19) and using then (5.20). Integration of the inequality

$$\frac{Q'(R)}{Q(R)} \geqslant \sum_{k=0}^{n+1} \frac{1}{g_0(R) \cdots g_k(R)}$$

readily implies the first estimate in (5.22). The second estimate there follows by integrating the estimate

$$\sum_{k=n+1}^{\infty} \frac{1}{g_0(R) \cdots g_k(R)} \ll \frac{\sigma}{g_0(R) \cdots g_n(R)}$$

as $R \to \infty$ for $\sigma > 0$ small. This formula in turn is a consequence of

$$\sum_{k=n+1}^{\infty} \frac{1}{g_{n+1}(R) \cdots g_k(R)} \ll \sigma$$

as $R \to \infty$, that can be obtained by using the Lebesgue dominated convergence theorem and the monotonicity of the functions $g_k(R)$ on R. The proof of (5.23) is just a consequence of (B.7) and (5.24).

Proof of Theorem 2. It is very similar to the proof of Theorem 4, and therefore only the main ideas will be sketched. Changing variables to $R = H(\zeta)$, and defining $\Psi(\zeta) = f(H(\zeta))$, Eq. (5.15) becomes

$$\Psi(\zeta) = (1 + H(\zeta))[\exp(\Psi(\zeta - 1)) - 1] \tag{B.15}$$

Using (5.25) and Taylor expansion, it follows that

$$\Psi(\zeta) - \Psi(\zeta - 1) = -\frac{2}{\zeta}\Psi(\zeta - 1) + O\left((\Psi(\zeta - 1))^2 + \frac{1}{|\zeta|^{3/2}}\Psi(\zeta - 1)\right)$$

as $\zeta \to -\infty$. Using then local barriers as in the proof of Theorem 4, it can be deduced the existence of an unique solution of (B.15) such that

$$\Psi(\zeta) \sim \frac{4C}{\zeta^2}$$

as $\zeta \to -\infty$. The regularity of $\Psi(\zeta)$ can be proved as in the proof of Theorem 4, whence Theorem 2 follows.

Proof of Theorem 5. Let us define the function

$$f_{N;a}(x) = H(H^{-1}(x) + a) \tag{B.16}$$

for $x \in (H(N), H(N+1))$, and then extend it to the whole line by means of (5.15). We claim that

$$\frac{a}{2} \leqslant \liminf_{x \to 0^+} \frac{f_{N;a}(x)}{x^2} \leqslant \limsup_{x \to 0^+} \frac{f_{N;a}(x)}{x^2} \leqslant \frac{a}{2} + \varepsilon_N \tag{B.17}$$

where $\varepsilon_N > 0$, $\lim_{N \to \infty} \varepsilon_N = 0$.

To prove (B.17) we introduce the new variable $H^{-1}(x) = \zeta$. Notice that the graph of $f_{N;a}$ for $x \leqslant H(N+1)$ is obtained by iterating the transformation S defined in (5.13) over the portion of curve

$$(x, y) = (H(\zeta), H(\zeta + a))$$

where $\zeta \in (N, N+1]$. Let us write

$$S^k(H(\zeta), H(\zeta + a)) = (a_{k;N}(\zeta), b_{k;N}(\zeta))$$

where $\zeta \in (N, N+1]$. As indicated before, the curve obtained in this way is the graph of $f_{N;a}$. Using (5.25) it follows that

$$a_{k;N}(\zeta) = H(\zeta - k)$$

On the other hand, using (5.13) it is easy to obtain by induction that

$$b_{k;N}(\zeta) = h^N[H(\zeta + a) + H(\zeta)] - H(\zeta - N)$$

where $h(\xi) = \log(1 + \xi)$. Taking into account the monotonicity of h and H we now obtain

$$\frac{h^k[H(\zeta+a)] - H(\zeta-k)}{(H(\zeta-k))^2} \leqslant \frac{b_{k;N}(\zeta)}{(a_{k;N}(\zeta))^2} \leqslant \frac{h^k[2H(\zeta+a)] - H(\zeta-k)}{(H(\zeta-k))^2} \tag{B.18}$$

By (5.25) one has that $h^k[H(\zeta+a)] = H(\zeta+a-k)$. Notice that

$$\liminf_{x \to 0^+} \frac{f_{N;a}(x)}{x^2} = \inf_{\zeta \in (N, N+1]} \left\{ \liminf_{k \to \infty} \frac{b_{k;N}(\zeta)}{(a_{k;N}(\zeta))^2} \right\}$$

$$\limsup_{x \to 0^+} \frac{f_{N;a}(x)}{x^2} = \sup_{\zeta \in (N, N+1]} \left\{ \limsup_{k \to \infty} \frac{b_{k;N}(\zeta)}{(a_{k;N}(\zeta))^2} \right\}$$

It then follows that

$$\liminf_{x \to 0^+} \frac{f_{N;a}(x)}{x^2} \geqslant \lim_{k \to \infty} \frac{h^k[H(\zeta+a)] - H(\zeta-k)}{(H(\zeta-k))^2}$$

$$= \lim_{k \to \infty} \frac{H(\zeta+a-k) - H(\zeta-k)}{(H(\zeta-k))^2} = \frac{a}{2}$$

where we have used (5.26). This yields the estimate on the left in (B.17).

In order to conclude the proof of (B.17), we notice that the monotonicity of the function h implies

$$h(2H(\zeta+a)) < \ln(2(1 + H(\zeta+a))) = \ln(2) + H(\zeta+a-1)$$

On the other hand, the concavity of h gives

$$h^2(2H(\zeta+a)) < H(\zeta+a-2) + \frac{\ln(2)}{1 + H(\zeta+a-1)}$$

and by induction it readily follows that

$$h^k(2H(\zeta+a)) < H(\zeta+a-k) + \frac{\ln(2)}{\prod_{l=1}^{k}[1+H(\zeta+a-l)]}$$
$$= H(\zeta+a-k) + \frac{\ln(2)}{\prod_{l=1}^{k}(e2/l)\prod_{l=1}^{k}[(1+H(\zeta+a-l))\,e^{-2/l}]}$$

Using (5.23) it turns out that $\prod_{l=1}^{k}(e^{2/l}) \sim e^{2\gamma}k^2$ as $k \to \infty$. By (5.26), we then obtain from (B.18) that

$$\limsup_{x\to 0^+} \frac{f_{N;a}(x)}{x^2} \leqslant \frac{a}{2} + \sup_{\zeta\in(N,N+1]} \frac{1}{4e^{2\gamma}\prod_{l=1}^{\infty}[g_l(\zeta+a)\,e^{-2/l}]} \equiv \frac{a}{2} + \varepsilon_N$$

where it is easily checked that $\varepsilon_N \to 0$ as $N \to \infty$, since the functions $g_l(\zeta)$ are increasing on ζ and they approach to ∞ as $\zeta \to \infty$. Then (B.17) follows.

We now conclude the proof of the Theorem 5. Notice that (5.16) and (8.17) imply that in a neighbourhood of the origin, there holds

$$f_{N;2C-\delta}(x) \leqslant f_C(x) \leqslant f_{N;C+\delta}(x) \tag{B.19}$$

where C can be chosen arbitrarily small if N is large enough. Taking into account (5.15), it follows that the estimate (B.19) holds for $x \in \mathbb{R}^+$. Then

$$H(H^{-1}(x)+2C-2\delta) \leqslant f_C(x) \leqslant H(H^{-1}(x)+2C+2\delta)$$

if $x \in (H(N), H(N+1))$. Since δ can be selected arbitrarily small, we finally obtain

$$\lim_{x\to\infty} [H^{-1}(f_c(x)) - H^{-1}(x)] = 2C$$

that concludes the proof of Theorem 5.

Proof of (5.38). To conclude this Appendix, we prove the formula (5.38). It readily follows from (5.20) that

$$g_k'(R) = \frac{1}{\prod_{l=0}^{k-1} g_l(R)}$$

We then obtain the asymptotics

$$g_k'(R) \sim \frac{4}{Q(R)\,k^2}$$

as $k \to \infty$, where $Q(R)$ is defined in (5.19). We can then write

$$g_k(R) \sim g_k(1) + \frac{4}{k^2} \int_1^R \frac{d\eta}{Q(\eta)}$$

as $k \to \infty$. Using then (5.23) we obtain

$$\mu'(R) = \frac{4}{Q(R)}$$

that implies

$$\mu(R + T(R)) - \mu(R) = 4 \int_R^{R+T(R)} \frac{d\eta}{Q(\eta)}$$

Making the change of variables $y = \ln(1+\eta)$, we easily deduce that

$$\begin{aligned} \mu(R + T(R)) - \mu(R) &= 4 \int_{\ln(R+1)}^{\ln(R+T(R)+1)} \frac{dy}{Q(y)} \\ &= \mu(\tilde{R} + T(\tilde{R})) - \mu(\tilde{R}) \end{aligned}$$

where $\tilde{R} = \ln(R+1)$, $T(\tilde{R}) = \ln(1 + T(R)/R + 1)$. Let us write

$$S^N(R, T(R)) = (R_N, T_N)$$

where S is as in (5.13). Then

$$\mu(R + T(R)) - \mu(R) = \lim_{N \to \infty} [(\mu(R_N + T_N) - \mu(R_N))]$$

By assumption $T_N \sim C(R_N)^2$. The asymptotic behaviour of $\mu(R)$ as $R \to 0$ can be easily obtained by a local analysis of the iteration that defines the functions g_k. Using (B.12), it follows by standard asymptotic techniques that

$$\mu(R) \sim -\frac{4}{R}$$

as $R \to 0$, whence

$$(\mu(R_N + T_N) - \mu(R_N)) \sim -\frac{4}{R_N + T_N} + \frac{4}{R_N} \sim \frac{4T_N}{(R_N)^2} \sim 4C$$

as $N \to \infty$. This concludes the proof of (5.38).

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