ANALYTICAL-NUMERICAL APPROACH TO A SINGULAR BOUNDARY VALUE PROBLEM

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Abstract. In this work we are concerned about the following second order nonlinear ordinary differential equation:

\[ \rho''(r) + \frac{2}{r}\rho'(r) = 4\lambda^2(r-r_1)(r-r_2)(r-r_3), \quad 0 < r < \infty, \quad (1) \]

where \( \lambda, r_1, r_2, r_3 \) are real numbers, \( r_1 < r_2 < r_3 \). We search for a strictly increasing solution of this equation which satisfies the following boundary conditions:

\[ \lim_{r \to 0^+} \rho(r) < \infty, \quad \lim_{r \to 0^+} r\rho'(r) = 0, \quad (2) \]

\[ \lim_{r \to \infty} \rho(r) = r_3, \quad \lim_{r \to \infty} \rho'(r) = 0. \quad (3) \]

This boundary value problem arises in the mathematical modeling of such physical phenomena as the formation of gas bubbles in a liquid media (Dell’Isola et al., 1996). (Gouin and Rotoli, 1997). The same kind of problems arise in some models of nonlinear field theory (see (Rubakov, 1999)). The asymptotic behavior of certain solutions of equation (1) is analyzed near the two singularities (when \( r \to 0^+ \) and \( r \to \infty \)), where the considered boundary conditions define one-parameter families of solutions. In the case of \( r \to 0^+ \), these solutions are holomorphic and can be represented in the form of convergent power series. When \( r \to \infty \), the needed solutions can be developed as convergent exponential Lyapunov series. Based on the asymptotic behavior, an efficient numerical method is proposed to compute approximate solutions of the above problem. As it is well-known, the analysis of boundary value problems with singularities at both ends, like this one, is a difficult task, even in the linear case. Note that, although equation (1) satisfies the conditions of the theorems presented in (Baxley, 1995), the existence of at least one strictly monotone solution of (1), (2), (3) does not follow from those theorems. The obtained numerical results show that such a solution exists if the right-hand side of (1) satisfies some conditions.

Keywords: nonlinear ordinary differential equation, singular boundary value problem, one-parameter families of solutions, stable shooting method
1. INTRODUCTION

The Cahn-Hillard theory has been developed to study the behavior of non-homogeneous fluids (fluid - fluid, fluid - vapor, fluid - gas, etc.). In this theory, an additional term, depending on the gradient of density $\nabla \rho$, is added to the classical expression $E_0(\rho)$ for the volume free energy, depending on the density of the medium $\rho$. Hence, the total free energy of a non-homogeneous fluid can be written as

$$E(\rho,|\nabla \rho|^2) = E_0(\rho) + \frac{\gamma}{2}|\nabla \rho|^2, \quad \gamma > 0.$$  \hspace{1cm} (4)

Let $\vec{v} = \vec{v}(\vec{x},t)$ denote the vector-velocity of the particles of the medium. Under isothermal process, our non-homogeneous fluid is characterized by the Lagrangian

$$L = \rho \frac{|\vec{v}|^2}{2} - E_0(\rho,|\nabla \rho|^2)$$  \hspace{1cm} (5)

with a natural constraint: the law of conservation of mass has to be true in the domain $\Omega \subset R^N$. By using the D’Alambert - Lagrange principle, to find a solution of $\delta J = 0$, where

$$J = \int_{t_2}^{t_1} \int_{\Omega} L \, dx \, dt,$$

we deduce the following system of differential equations, describing the behavior of our non-homogeneous fluid

$$\rho_t + div(\rho \vec{v}) = 0,$$

$$\frac{d\vec{v}}{dt} + \nabla (\mu(\rho) - \gamma \Delta \rho) = 0.$$  \hspace{1cm} (7)

Here $\mu(\rho) = E_0'(\rho)$ is the chemical potential of the fluid and $\frac{d\vec{v}}{dt} = \frac{\partial \vec{v}}{\partial t} + (\nabla \cdot \vec{v}) \vec{v}$.

Let us assume that the motion of the fluid in the domain is potential, i.e. $\vec{v} = \nabla \phi$, and stationary; then the system (7) can be rewritten as

$$div(\rho \nabla \phi) = 0,$$

$$\frac{|\nabla \phi|^2}{2} + \mu(\rho) - \gamma \Delta \rho \equiv \mu_0$$  \hspace{1cm} (8)

and $\vec{v} = \nabla \phi$. Here $\mu_0$ is a suitable constant. When the motion of the fluid is absent ($\phi = 0$), the system is reduced just to one equation

$$\gamma \Delta \rho = \mu(\rho) - \mu_0.$$  \hspace{1cm} (9)

In fact, this equation can describe the formation of microscopical bubbles in a non-homogeneous fluid, in particular, vapor inside one liquid. With this purpose, we have to add to the equation (9) the boundary conditions for the bubbles: because of spherical symmetry, the derivative of $\rho$ vanishes at the origin

$$\rho'(0) = 0$$  \hspace{1cm} (10)

and since the bubble is surrounded by a liquid, the same condition holds at infinity

$$\rho(\infty) = \rho_t.$$  \hspace{1cm} (11)
Under the conditions (10), (11) the equation (9) uniquely determines the value of the density at the center of the bubble $\rho_r$ and an increasing mass density profile. In the case of spherical bubbles the equation (9) takes the form

$$\gamma (\rho_{rr} + \frac{N - 1}{r} \rho_r) = \mu (\rho) - \mu (\rho_r), \quad r \in (0, \infty)$$

(12)

and is known as the density profile equation (DPE) (Dell’Isola et al., 1996). In the simplest models for non-homogeneous fluids, the free energy $E_0$ is a fourth-degree polynomial on $\rho$, with two minima and one maximum; hence, the chemical potential $\mu$ is a third degree polynomial on $\rho$, with three distinct real roots. Therefore, in the present paper, we consider the case where the right-hand side of the equation (12) has the form

$$4\alpha (\rho - r_1)(\rho - r_2)(\rho - r_3),$$

where $\alpha$ is a positive constant. In particular, from this form of the right-hand side it follows that $\rho_1 = r_3$. We shall restrict ourselves to the three-dimensional case ($N = 3$) and for commodity we introduce the positive constant $\lambda$, such that $\lambda^2 = \alpha / \gamma$.

Then we can rewrite equation (12) in the form (1), which will be analyzed in the next section. The boundary value problem (12), (10), (11) plays a very important role in the analysis of the formation of bubbles, since many important physical properties depend on its solution (in particular, the gas density inside the bubble, the bubble radius and the surface tension). Although numerical simulations have been carried out and reported in (Dell’Isola et al., 1996), there are still many open questions concerning the mathematical analysis of this equation.

One of the most important aspects of this analysis is the correct formulation of the boundary conditions (10) and (11), in such a way that each of them defines a one-parameter family of solutions. As we shall see in the next section, the boundary condition (10) should be rewritten as (2) and (11) as (3). Since $r = 0$ and $r = \infty$ are singular points of this equation, these conditions deserve a detailed analysis. This will be the subject of the next section.

2. ONE-PARAMETER FAMILIES OF SOLUTIONS SATISFYING THE BOUNDARY CONDITIONS

2.1 The singularity at $r = 0$

Let us consider equation (1), subject to the boundary conditions (2), which we rewrite as

$$\lim_{r \to 0^+} \rho(r) = \rho_0, \quad \lim_{r \to 0^+} r \rho'(r) = 0,$$

(13)

where $\rho_0$ is a real parameter. First of all, we should note that (1) has a regular singularity at $r = 0$ (see, e.g., (Wasow, 1965)). If (1) is linearized at $r = 0$, its characteristic exponents satisfy the equation

$$\nu (\nu - 1) + 2\nu = 0.$$  

(14)

This equation has two roots: $\nu_1 = 0$ and $\nu_2 = -1$. Therefore, as it follows from Theorem 5 in (Konyukhova, 1983), we obtain that for any $\rho_0 \in R$ the Cauchy problem (1), (13) has an unique solution; moreover this solution is a holomorphic function at the point $r = 0$ and can be represented in the form:

$$\rho(r) = \rho_0 + \sum_{k=1}^{\infty} \rho_{2k} (\rho_0) r^{2k},$$

(15)
where \( \rho_0 \leq \delta \), \( \delta > 0 \) and \( \rho_{2k} \) are coefficients, which depend on \( \rho_0 \) and can be determined by recurrence formulae. This means also that the Cauchy problem (1), (2) has a one-parameter family of solutions.

In order to derive the formulae for \( \rho_{2k} \), we differentiate the series on the right-hand side of (15). If we substitute the obtained expressions into (1), we obtain:

\[
\sum_{k=1}^{\infty} \rho_{2k}(\rho_0)(2k+1)2k \, r^{2k} = 4 \lambda^2 \, r^2 \, \omega \left( \rho_0 + \sum_{k=1}^{\infty} \rho_{2k}(\rho_0) \right),
\]

where \( \omega(\rho) = (\rho - r_1)(\rho - r_2)(\rho - r_3) \). By comparing the terms with \( r^2 \) on both sides of (16) we get

\[
\rho_2(\rho_0) = \frac{2}{3} \lambda^2 \, \omega(\rho_0).
\]

Analogously, if we compare the terms with \( r^4 \) on both sides of (16) we have

\[
\rho_4(\rho_0) = \frac{\lambda^2}{5} \left( (r_1 r_3 + r_2 r_3 + r_1 r_2) \rho_2 + 3 \rho_2 \rho_0^2 - 2 (r_1 + r_3 + r_2) \rho_0 \rho_2 \right).
\]

The formulae for the remaining coefficients \( \rho_{2k} \), with \( k = 3, 4, \ldots \) can be derived in a similar way.

Since the solution to our problem must satisfy \( \rho'(0) > 0 \) (otherwise it would not be increasing in any neighborhood of \( r = 0 \)), we must have \( \rho_2 > 0 \) and therefore \( \rho_0 \) has to satisfy

\[ r_1 < \rho_0 < r_2. \]

For \( \rho_0 = r_1 \) or \( \rho_0 = r_2 \), we have just constant solutions.

For each \( \rho_0 \in (r_1, r_2) \) we can then compute the approximate value of the corresponding solution at a certain \( \delta \), such that \( 0 < \delta << 1 \), by considering only the first terms of the series on the right-hand side of (15). In our computations, we have used:

\[
\rho(\delta) \approx \rho_0 + \rho_2(\rho_0) \delta^2 + \rho_4(\rho_0) \delta^4,
\]

with \( \rho_2 \) and \( \rho_4 \) given by (17) and (18), respectively. In the same way, the value of \( \rho'(\delta) \) is approximated by

\[
\rho'(\delta) \approx 2 \rho_2(\rho_0) \delta + 4 \rho_4(\rho_0) \delta^3.
\]

Then we can solve a regular Cauchy problem for the equation (1), taking (19) and (20) as initial conditions. Such problems can be solved by standard numerical methods. In our computations we have used the \texttt{NDSolve} command of the \texttt{Mathematica} software (Wolfram, 1996) with this purpose. In Fig. 1, the graphics of some solutions of the considered Cauchy problem are displayed. These solutions have been computed for a particular case of the equation (1), with \( r_1 = -1, r_2 = 0, r_3 = 0.7, \lambda = 1 \), using \( \delta = 0.0001 \) for different values of \( \rho_0 \in (r_1, r_3) \).

Note that any strictly monotone solution \( \rho \) to the problem (1), (2), (3) must satisfy

\[
r_1 < \rho(r) < r_3, \forall r \in R^+.
\]

Actually, if \( \rho \) belongs to the family (15), with \( r_1 < \rho_0 < r_2 \), and, for a certain \( r > 0 \), we have \( \rho(r) = r_3 \) (resp. \( \rho(r) = r_1 \)) the solution will increase (resp. decrease) for \( r' > r \). Moreover, it can be shown that in this case the solution will have a pole (it will tend to \( \infty \), if \( \rho(r) > r_3 \), or to \( -\infty \), if \( \rho(r) < r_1 \).
2.2 The singularity at infinity

Let us now focus our attention on the boundary conditions (3). In order to analyze the asymptotic behavior of the solutions as $r \to \infty$ let us represent the equation (1) as

$$(r^2 \rho'(r))' = 4 \lambda^2 r^2 (\rho - r_1)(\rho - r_2)(\rho - r_3), \ 0 < r < \infty.$$  \hspace{1cm} (22)

We introduce the following variable substitution:

$$z = r(\rho - r_3).$$  \hspace{1cm} (23)

In the new variable, the equation (22) becomes

$$z'' = 4 \lambda^2 (z/r + r_3 - r_1)(z/r + r_3 - r_2)z, \ 0 < r < \infty.$$  \hspace{1cm} (24)

The equation (24) has an irregular singularity at $r = \infty$. On the other hand, since $z(r)$ tends to 0 faster than $1/r$ (as it will be shown below), the boundary conditions (3) in the new variable take the form

$$\lim_{r \to \infty} z(r) = \lim_{r \to \infty} z'(r) = 0.$$  \hspace{1cm} (25)

The equation (24) is asymptotically autonomous, i.e. as $r \to \infty$, we obtain the linear autonomous equation

$$z'' = 4 \lambda^2 (r_3 - r_1)(r_3 - r_2)z, \ 0 < r < \infty.$$  \hspace{1cm} (26)

The characteristic roots of (26) are

$$\nu_{1,2} = \pm 2 \lambda \sqrt{(r_3 - r_2)(r_3 - r_1)}.$$  \hspace{1cm} (27)
Hence the critical point \((0, 0)\) is a saddle point and the equation (26) possesses a one-parameter family of solutions which satisfy (25). These solutions can be written in the form

\[ z(r) = \rho_\infty e^{-(\tau r_f)\sqrt{r_3 - r_2}} \]

where \(\rho_\infty\) is a real constant, which must be positive, since \(\rho\) must be less than \(r_3\). Writing (28) in terms of the initial variable, we have the asymptotic expansion

\[ \rho(r, \rho_\infty) = r_3 - \frac{\rho_\infty e^{-\tau r_f}}{r} (1 + o(1)), \quad r \to \infty \]

where

\[ \tau = 2\lambda \sqrt{(r_3 - r_2)(r_3 - r_1)}. \]

From classical results for ordinary differential equations (see, e.g. (Lyapunov, 1947)), it follows that the solution of the Cauchy problem (24), (25) can be represented as a convergent exponential Lyapunov series in powers of the quantity (28).

We can now use the equation (29) to approximate the boundary condition (3). Let \(r_\infty\) be a positive number, such that \(\rho_\infty e^{-\tau r_f} / r_\infty\) is small. Then we deduce from (29) the approximate equalities

\[ \rho(r_\infty, \rho_\infty) \approx r_3 - \rho_\infty e^{-\tau r_f} / r_\infty \]

and

\[ \rho'(r_\infty, \rho_\infty) \approx \rho_\infty \frac{e^{-\tau r_f} + \tau r_\infty e^{-\tau r_f}}{r_\infty^2} \]

The equations (31) and (32) can be used as initial conditions for a regular Cauchy problem, which will be an approximation of the initial value problem (1), (3).

In Fig. 2 the graphics of some solutions of the problem (1), (3) are displayed. They have been computed choosing (31) and (32) as initial conditions and solving the Cauchy problem leftwards, starting from \(r_\infty = 10\) and with different values of \(\rho_\infty\).

The original boundary value problem (1), (2), (3) can now be formulated as follows: we must find from the set of solutions of (1) which satisfy (29) a particular solution which also satisfies (2). Alternatively, we can look for a particular solution of the set (15) which additionally fulfills (3). However, the usual shooting method does not work properly for such problems. For example, if we "shoot" from the left end of the interval to \(\infty\), any numerical method becomes unstable as \(r\) grows, because the solution will tend to a saddle point, which is unstable. If we start from \(r_\infty\) to the left, the numerical solutions will also have large errors near 0 and it is not possible to obtain an accurate approximation of the true solution. In the following section, we shall propose a simple and efficient numerical algorithm to overcome these difficulties.

In order to complete the analysis of the behavior of the solutions of (1), as \(r \to \infty\), we introduce the variable substitution \(u = r(\rho - r_2)\). Then the equation (1) takes the form

\[ u'' = 4\lambda^2 u(u/r - r_1 + r_2)(u/r - r_3 + r_2), \quad 0 < r < \infty. \]

As \(r \to \infty\), the equation (33) is asymptotically autonomous and tends to

\[ u'' = 4\lambda^2 u(-r_1 + r_2)(-r_3 + r_2), \quad 0 < r < \infty. \]
Figure 2: Solutions of the equation (1) belonging to the family (29) in the case $r_3 = 0.7$, $\lambda = 1$ with different values of $\rho_\infty$.

Since $(-r_1 + r_2)(-r_3 + r_2) < 0$, the critical point $(0, 0)$ is a centre for the equation (33). Therefore, we can assure that the equation (1) has a two-parameter family of solutions which can be written, in the linear approximation, as:

$$
\rho(r, C_1, C_2) = r_2 + [C_1 \sin(\sigma r) + C_2 \cos(\sigma r)] r^{-1} + o(1/r),
$$

where $C_1$ and $C_2$ are arbitrary constants, $\sigma = 2\lambda \sqrt{-(r_2 - r_1)(r_2 - r_3)}$.

Such solutions belonging also to the family (15) are displayed in Fig. 1. They are oscillatory and tend to $r_2 = 0$ at the infinity; therefore they cannot fulfill the conditions of our boundary value problem.

3. Numerical methods

Our main goal is to approximate monotone solutions of the equation (1) subject to the conditions (2) and (3). According to their physical meaning, which was discussed in the introduction, such solutions are called bubbles. In principle, there may exist non-monotone solutions which satisfy the same conditions, but they are out of the scope of the present paper.

Without loss of generality, we can consider only the case $r_1 = -1, r_2 = 0$, since for any choice of $\omega(\rho)$ the problem can be reduced to this case by means of the variable substitution $\tilde{\rho} = \frac{\rho - r_2}{r_1}$. Moreover, it is enough to consider the case $\lambda = 1$, since the equation can be reduced to this case by the substitution of the independent variable $\tilde{r} = r/\lambda$. In particular, if we have $\rho(r_0, 1) = 0$, then we also have $\rho(r_0/a, a) = 0$, where $r_0 > 0$ and $\rho(r, a)$ denotes the solution of (1) with $\lambda = a$ and any $a > 0$. On the other hand, since $\rho(0, a) = \rho(0, 1) = \rho_0$ for any $a > 0$, we can conclude that $\rho_0$ does not depend on $\lambda$.

We begin by fixing a certain $r_0 > 0$ and dividing the set $[0, r_\infty]$, where we want to approximate the solution, into two subintervals: $[0, r_0]$ and $[r_0, \infty]$. Then we consider the boundary conditions

$$
\lim_{r \to 0^+} \rho(r) = \rho_0, \quad \lim_{r \to 0^+} r\rho'(r) = 0, \quad \rho(r_0) = 0.
$$
Suppose that the equation (1) with \( \lambda = a \) has a monotone solution \( \rho_-(r, a) \) on \( (0, r_0) \) that satisfies (36) and (37). Then any function with the form \( \rho_-(cr, a) \) will be also a solution of (1) with \( \lambda = ac \). Obviously, this solution satisfies (37) with \( r_0 \) replaced by \( r_0/c \). In other words, it is equivalent to solve the equation (1) with \( \lambda = a \) on the interval \( (0, r_0) \) or with \( \lambda = ac \) on the interval \( (0, r_0/c) \).

Let us now denote \( \rho_+(r, a) \) a monotone solution of (1) on \([r_0, \infty)\), with \( \lambda = a \), which satisfies the boundary condition (37) and

\[
\lim_{r \to \infty} \rho(r) = r_3, \quad \lim_{r \to \infty} \rho'(r) = 0. \tag{38}
\]

Assuming that the solutions \( \rho_-(r, a) \) and \( \rho_+(r, a) \) exist and satisfy the prescribed conditions, let us define

\[
\rho(r, a) = \begin{cases} 
\rho_-(r, a), & \text{if } \delta \leq r \leq r_0; \\
\rho_+(r, a), & \text{if } r_0 < r \leq r_\infty.
\end{cases} \tag{39}
\]

In general, \( \rho(r, a) \) is not a solution of (1) on \([0, \infty]\), because the condition

\[
\lim_{r \to r_0^-} \rho'(r, a) = \lim_{r \to r_0^+} \rho'(r, a) \tag{40}
\]

is not satisfied for \( \lambda = a \). Our goal now is to find such a value \( \hat{\lambda} \in R^+ \) that the condition (40) is true when \( a \) is replaced by \( \hat{\lambda} \). If such a value exists, then \( \rho(r, \hat{\lambda}) \) is a solution of the original boundary value problem (1), (2), (3) with \( \lambda = \hat{\lambda} \). Moreover, from this solution we can obtain the solution to the equation with \( \lambda = a \) for any \( a \). This solution will be given by \( \rho(r, a) = \rho(ra/\hat{\lambda}, \hat{\lambda}) \).

In order to find the needed value of \( \hat{\lambda} \) we use numerical algorithms which solve the following auxiliary problems:

1. **For** a given \( \lambda \in R^+, \delta > 0 \) and \( r_0 > \delta \), approximate \( \rho_-(\lambda, r) \) on \([\delta, r_0]\).

2. **For** a given \( \lambda \in R^+, \) \( r_0 ~ r_\infty > r_0 \), approximate \( \rho_+(\lambda, r) \) on \([r_0, r_\infty]\).

Note that each of these problems can be solved by the usual shooting method, taking into account the asymptotic properties of the solution, discussed in the previous section. More precisely, for the first problem, we must find such a value of \( \rho_0 \), that the corresponding solution of the family (15) satisfies \( \rho(r_0) = 0 \). For the second problem, we must find such a value of \( \rho_\infty \), that the corresponding solution of the set (29) satisfies \( \rho(r_0) = 0 \).

Finally, we use the following algorithm to find the value \( \hat{\lambda} \), such that the condition (40) is satisfied, if \( a \) is replaced by \( \hat{\lambda} \). Let us denote

\[
\Delta(r_0, \lambda) = \lim_{r \to r_0^+} \rho'(r, \lambda) - \lim_{r \to r_0^-} \rho'(r, \lambda). \tag{41}
\]

Given \( \lambda \) and \( r_0 \), the value of \( \Delta(r_0, \lambda) \) can be computed by solving the two auxiliary problems mentioned above (provided that both problems have solution). Suppose that two values \( \lambda_0 \) and \( \lambda_1 \) are given, such that \( \lambda_0 < \lambda_1, \Delta(r_0, \lambda_0) > 0 \) and \( \Delta(r_0, \lambda_1) < 0 \). Then the needed value \( \hat{\lambda} \) satisfies \( \lambda_0 < \hat{\lambda} < \lambda_1 \) and can be found by any iterative method for nonlinear equations. In our computations, we have used the secant method and the value of \( \hat{\lambda} \) has been obtained with 5-6 digits in less than 10 iterations.

In the next section, we shall present some numerical results obtained by the described algorithm.
The proposed method enabled us to compute the needed solutions accurately, within a reasonable computing time, for a large range of values of \( r_3 \). However, it is not applicable to all the cases, in which monotone solutions exist.

Computational difficulties have arisen in the case where \( r_3 < 0.28 \) (as we shall see in the next section, this value of \( r_3 \) is critical in the sense that it corresponds to the minimal bubble radius). The mentioned difficulties can be explained by the fact that, as it is shown by the numerical results, when \( r_3 \) is near the critical value, the derivative of the solution is very close to 0 near \( r_0 \). Therefore, the numerical approximations of the solution and its derivative have very large relative errors near \( r_0 \). In such cases the condition (40) is not a good way to determine the needed solution, since the limits of the derivative cannot be computed accurately.

Hence, we need an alternative computational method to solve our problem, when \( r_3 < 0.28 \). This method, which we now describe, provides accurate solutions for the mentioned values of \( r_3 \). First note that from (29) we obtain the following approximate equality:

\[
\rho'(r) - (\tau + 1/r)(r_3 - \rho(r)) \approx 0, \quad (42)
\]

for sufficiently large values of \( r \). Then we choose a certain value \( r_{\text{max}} \in (r_0, r_\infty) \) and instead of (37) we consider the boundary condition:

\[
\rho'(r_{\text{max}}) - (\tau + 1/r_{\text{max}})(r_3 - \rho(r_{\text{max}})) = 0. \quad (43)
\]

The numerical solution of the boundary value problem with the conditions (36), (43) can be computed by the shooting method, in the same way as in the case of the boundary conditions (36), (37). For the mentioned values of \( r_3 \), this method gives an accurate approximation of the exact solution on \([\delta, r_{\text{max}}]\). Once this solution is computed, we obtain a numerical approximation \( \tilde{\rho}(r_{\text{max}}) \) to \( \rho'(r_{\text{max}}) \). Then, in order to extend the obtained solution to the interval \([r_{\text{max}}, r_\infty]\), we consider the new boundary condition

\[
\lim_{r \to r_{\text{max}}} \rho'(r) = \tilde{\rho}'(r_{\text{max}}). \quad (44)
\]

This condition together with (3) defines a new boundary value problem, which can be solved as in the case of the conditions (37), (3).

When this method is used, we test its accuracy by computing the difference

\[
\lim_{r \to r_{\text{max}}} \rho'(r) - \lim_{r \to r_{\text{max}}} \rho'(r), \quad (45)
\]

which must be close to 0 for an accurate approximation of \( \rho \).

4. Numerical Results

Now we present the numerical results obtained for the problem (1), (2), (3) by the numerical methods proposed in the previous section.

As mentioned in the Introduction, some approximate solutions for this problem have been presented in (Dell’Isola et al., 1996), in the form of graphics. According to the authors, those solution have been constructed by standard numerical methods. Since the numerical values of \( \rho \) were not given there, we cannot compare the results with respect to the accuracy. However, the qualitative behavior of our solutions corresponds to what could be expected, taking into account the mentioned graphics and the physical meaning of the variables.

We should point out here that the main goal of the present paper has been to provide a mathematical analysis of the problem, which enabled us to improve the computational methods.
According to the physical meaning of the problem (1), (2), (3) with $r_1 = -1$ and $r_2 = 0$, the existence of a monotone solution is expected when $0 < r_3 < 1$. In the case $r_3 = r_2 = 0$, the free energy $E_0$ of the fluid has only one maximum at $\rho = -1$ and an inflexion at $\rho = 0$; in physics, this case is called the spinoidal limit. When $r_3 = 1$, we have $r_3 = -r_1$ and the free energy is an even function (it takes the same value at the two minima); this corresponds to the saturation limit.

In our computations, we have determined numerical approximations to the solution for different values of $r_3$ in the range $[0.1, 0.8]$. We now describe some properties of the obtained numerical results.

As we have seen in Section 3, the solution always has a root at a certain point $r_0 > 0$. In physics, this value is considered as the radius of the bubble. If we fix a value of $\lambda$, for example $\lambda = 1$, and vary $r_3$, the radius of the bubble changes as shown in Fig. 3. This value increases when $r_3$ tends to 0 or to 1 and attains a minimum at a certain point $r_3 = r_{\text{min}}$, called the minimal nucleation radius. According to our computations, $r_{\text{min}} \in [0.28, 0.29]$ and the corresponding value of the minimal nucleation radius is approximately 2.58.

In Table 1, the values of $\rho_0$ and $\rho_{\infty}$ are displayed for different values of $r_3$ in the case $\lambda = 1$. The values of $\rho_{\infty}$ increase and tend very fast to $\infty$ as $r_3 \to 1$. The value of $\rho_0$ (the density of the gas in the centre of the bubble $\rho_0$) decreases and tends to $-1$ as $r_3 \to 1$.

**Table 1**: Values of $\rho_0$ and $\rho_{\infty}$ as functions of $r_3$

<table>
<thead>
<tr>
<th>$r_3$</th>
<th>$\rho_0$</th>
<th>$\rho_{\infty}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.3048</td>
<td>4.0175</td>
</tr>
<tr>
<td>0.15</td>
<td>-0.4437</td>
<td>6.3477</td>
</tr>
<tr>
<td>0.2</td>
<td>-0.5681</td>
<td>9.857</td>
</tr>
<tr>
<td>0.28</td>
<td>-0.7356</td>
<td>22.678</td>
</tr>
<tr>
<td>0.3</td>
<td>-0.7707</td>
<td>28.113</td>
</tr>
<tr>
<td>0.4</td>
<td>-0.90313</td>
<td>95.980</td>
</tr>
<tr>
<td>0.5</td>
<td>-0.97112</td>
<td>491.92</td>
</tr>
<tr>
<td>0.6</td>
<td>-0.99531</td>
<td>5080.9</td>
</tr>
<tr>
<td>0.7</td>
<td>-0.99979</td>
<td>207675</td>
</tr>
<tr>
<td>0.8</td>
<td>-0.999996</td>
<td>$2.54 \times 10^8$</td>
</tr>
</tbody>
</table>

For values of $r_3$ greater than $r_{\text{min}}$, the solutions increase slowly along almost all the domain,
except a thin zone, where they change very fast. This zone corresponds to the transition between the gaseous and liquid phases. The absolute maximum of the derivative is attained near $r_0$ and its value grows with $r_3$. These properties are well described by the graphics in Fig. 4 (solutions) and Fig. 5 (their derivatives). On the other hand, when $r_3 < r_{\text{min}}$ the solutions change smoothly along all the domain. The maximum of the first derivative decreases as $r_3 \to 0$. The physical meaning of this behavior is a smooth transition between the gaseous and the liquid phase of the fluid.

Some graphics of the solutions and their derivatives with such properties are displayed in Fig. 6 and Fig. 7.

5. Conclusions

In the present work we have analyzed the boundary value problem (1), (2), (3) and the asymptotic properties of some solutions. This analysis enabled us to introduce new numerical methods for the accurate approximation of monotone solutions. However, some important questions remain open and should be the subject of future research. In particular, the existence and uniqueness of monotone solutions has not been proved theoretically. Moreover, a detailed error analysis of the applied numerical techniques must be carried out.
Figure 6: Graphics of the solutions in the case $\lambda = 1$ and $r_3 < r_{\text{min}}$.

Figure 7: Graphics of the derivatives of the solutions in the case $\lambda = 1$ and $r_3 < r_{\text{min}}$.

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