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Analytical–numerical investigation of bubble-type solutions of nonlinear singular problems

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Abstract

In this work we are concerned about a singular boundary value problem for a second-order nonlinear ordinary differential equation, arising in hydrodynamics and nonlinear field theory, when centrally symmetric bubble-type solutions are sought. We are interested on solutions of this equation which are strictly increasing on the positive semi-axis and have finite limits at zero and infinity. Necessary conditions for the existence of such solutions are obtained in the form of a restriction on the equation parameters. The asymptotic behavior of certain solutions of this equation 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. Based on the analytic study, an efficient numerical method is proposed to compute approximately the needed solutions of the above problem. Some results of the numerical experiments are displayed and their physical interpretation is discussed.

Keywords: Nonlinear ordinary differential equation; Singular boundary value problem; One-parameter families of solutions; Stable shooting method; Bubble-type solutions

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1. Introduction

The Cahn–Hillard theory has been developed to study the behavior of nonhomogeneous 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 ρ (see, e.g., [4,6] and references therein). Hence, the total volume free energy of a nonhomogeneous fluid can be written as

$$E(\rho, |\nabla\rho|^2) = E_0(\rho) + \frac{\gamma}{2}|\nabla\rho|^2, \quad \gamma > 0. \tag{1.1}$$

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

$$L(\rho, \nabla\rho, \vec{v}) = \rho\frac{|\vec{v}|^2}{2} - E(\rho, |\nabla\rho|^2) \tag{1.2}$$

with a natural constraint: the law of conservation of mass has to be true in the domain $\Omega \subset R^N$. Let

$$J(\rho, \vec{v}) = \int_{t_1}^{t_2}\int_{\Omega} L(\rho, \nabla\rho, \vec{v})\,\mathrm{d}\omega\,\mathrm{d}t. \tag{1.3}$$

By using the D'Alembert–Lagrange principle, to find a solution of $\delta J = 0$, with the above-mentioned constraint, the following system of differential equations has been deduced (see, e.g., [4,6]), describing the behavior of the considered nonhomogeneous fluid:

$$\rho_t + \operatorname{div}(\rho\vec{v}) = 0, \quad \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} + \nabla(\mu(\rho) - \gamma\triangle\rho) = 0. \tag{1.4}$$

Here $\mu(\rho) = \mathrm{d}E_0/\mathrm{d}\rho$ is the chemical potential of the fluid and

$$\mathrm{d}\vec{v}/\mathrm{d}t = \partial\vec{v}/\partial t + (\vec{v}\cdot\nabla)\vec{v}.$$

Let us assume that the motion of the fluid in the domain is potential, i.e. $\vec{v} = \nabla\phi$, and stationary; then system (1.4) can be rewritten as

$$\operatorname{div}(\rho\nabla\phi) = 0, \quad \frac{|\nabla\phi|^2}{2} + \mu(\rho) - \gamma\triangle\rho \equiv \mu_0, \quad \vec{v} = \nabla\phi. \tag{1.5}$$

Here μ_0 is a suitable constant. When the motion of the fluid is absent ($\nabla\phi = 0$), the system is reduced just to one equation

$$\gamma\triangle\rho = \mu(\rho) - \mu_0. \tag{1.6}$$

In fact, this equation can describe the formation of microscopical bubbles in a nonhomogeneous fluid, in particular, vapor inside one liquid. With this purpose, we have to add to Eq. (1.6) the boundary conditions for the bubbles. Let us now introduce in $\mathbb{R}^N$ the polar system of coordinates and search for a solution which depends only on the radial variable r. Due to central symmetry, the derivative of ρ with respect to r vanishes at the origin:

$$\rho'(0) = 0. \tag{1.7}$$

Since the bubble is surrounded by a liquid, the following condition holds at infinity:

$$\lim_{r\to\infty} \rho(r) = \rho_l > 0, \tag{1.8}$$

where ρ_l is the density of the external liquid. From (1.8) it follows that $\mu_0 = \mu(\rho_l)$. Whenever a strictly increasing solution to problem (1.6)–(1.8) exists, for some $\rho(0) = \rho_v$, with $0 < \rho_v < \rho_l$, then ρ_v is the density of the gas at the center of the bubble and the solution ρ determines an *increasing mass density profile*. In the case of plane or spherical bubbles Eq. (1.6) takes the form

$$\gamma\left(\rho'' + \frac{N-1}{r}\rho'\right) = \mu(\rho) - \mu(\rho_l), \quad r \in (0,\infty), \tag{1.9}$$

where $N = 2$ or $N = 3$, respectively, and is known as the density profile equation (DPE) [4,8].

In the simplest models for nonhomogeneous fluids, the free energy E_0 is a fourth-degree polynomial on ρ, with two minima and one maximum. Then μ is a third-degree polynomial on ρ with three distinct real roots. For the sake of simplicity, let us assume that $\mu(\rho_l) = 0$ (different values of $\mu(\rho_l)$ may be considered by changing the form of μ). Then we can write

$$\mu(\rho) = 4\alpha(\rho - \wp_1)(\rho - \wp_2)(\rho - \rho_l), \quad 0 < \wp_1 < \wp_2 < \rho_l, \quad \alpha > 0. \tag{1.10}$$

In order to diminish the number of parameters, we introduce the variable substitution

$$\tilde{\rho} = \frac{\rho - \wp_2}{\wp_2 - \wp_1}$$

and the positive constant λ, such that $\lambda = \sqrt{\alpha/\gamma}(\wp_2 - \wp_1)$, and denote $\xi = (\rho_l - \wp_2)/(\wp_2 - \wp_1) > 0$. Then, without loss of generality, instead of (1.9) we can investigate the equation

$$(r^{N-1}\rho'(r))' = 4r^{N-1}\lambda^2(\rho+1)\rho(\rho-\xi), \quad 0 < r < \infty, \tag{1.11}$$

and replace the boundary condition (1.8) by

$$\lim_{r\to\infty} \rho(r) = \xi > 0. \tag{1.12}$$

Note that the nonlinear boundary value problem (1.11), (1.7), (1.12) has at least the solution

$$\rho(r) \equiv \xi. \tag{1.13}$$

We are interested in solutions different from (1.13), which have exactly one zero in $\mathbb{R}_+$. If such solutions exist, many important physical properties of the bubbles depend on them (in particular, the gas density inside the bubble, the bubble radius and the surface tension).

Singular boundary value problems for second-order ODEs on the positive semi-axis arise in several fields and have been the subject of research for many authors, who obtained existence results under rather general conditions (see, e.g., [2,3,7] and references therein). In particular, the results of [7] are applicable to the problem (1.11), (1.7), (1.12) and from them it follows that a sufficient condition for the existence of at least one nonconstant solution to the problem is the following:

$$0 < \xi < 1. \tag{1.14}$$

In Section 3 of the present work we will show that this condition is also necessary. It is also interesting to remark that boundary value problems of the same kind arise in nonlinear field theory, in particular, when describing the bubbles generated by scalar fields of the Higgs type in the Minkowski spaces [12], which can be treated as the classical patterns of elementary particles [5]. The case of hyperspherical bubbles in the $(N+1)$-dimensional Minkowski spaces, with $N>3$, has special interest for modern models of the field theory.

One of the most important aspects of the analysis of this boundary value problem is the correct formulation of the boundary conditions (1.7) and (1.12), in such a way that each of them defines a one-parameter family of solutions. Since $r=0$ and $r=\infty$ are singular points of the considered equation, the boundary conditions (1.7) and (1.12) deserve a detailed analysis. This will be the subject of the next section.

2. Associated singular Cauchy problems and their one-parameter families of solutions

2.1. The singularity at zero

The point $r=0$ is a regular singularity for Eq. (1.11) (see, e.g., [14]). Therefore, we subject this equation to the following boundary conditions:

$$\lim_{r\to 0+} \rho(r)=\rho_0, \qquad \lim_{r\to 0+} r\rho'(r)=0, \tag{2.1}$$

where ρ_0 is a real parameter. Linearizing Eq. (1.11) in the neighborhood of $r=0$ and taking (2.1) into account, we obtain a linear equation whose characteristic exponents at $r=0$ are $v_1=0$, $v_2=2-N$. As it follows from Theorem 5 in [9], $\forall \rho_0 \in \mathbb{R}$, $N \geqslant 2$, the singular Cauchy problem (1.11), (2.1) has an unique solution; moreover, this solution is a holomorphic function at the point $r=0$ and can be represented in the form:

$$\rho(r)=\rho_0+\sum_{k=1}^{\infty} \rho_{2k}(\rho_0) r^{2k}, \quad 0 \leqslant r \leqslant \delta, \quad \delta>0, \tag{2.2}$$

where ρ_{2k} are coefficients, which depend on ρ_0 and can be determined by recurrence formulae. For example, if we substitute (2.2) into (1.11), we obtain

$$\rho_2(\rho_0)=(2\lambda^2/N)\rho_0(\rho_0+1)(\rho_0-\xi). \tag{2.3}$$

Analogously, we can derive the formulae for ρ_{2k}:

$$\rho_{2k}(\rho_0)=\frac{2\lambda^2}{k(2k+N-2)}\left(\sum_{m=1}^{k-1}\left(\sum_{l=0}^{m} \rho_{2l}\rho_{2m-2l}\rho_{2k-2m-2}+(1-\xi)\rho_{2m}\rho_{2k-2m-2}\right)-\xi\rho_{2k-2}\right), \quad k=2,3,\ldots\,. \tag{2.4}$$

The above results may be expressed in the following form.

Proposition 1. *For each $N \geqslant 2$ and $\rho_0 \in \mathbb{R}$, the singular Cauchy problem* (1.11), (2.1) *has a unique solution* (*at least*, *for sufficiently small r*). *This solution is holomorphic at the point $r=0$ and may be expanded in the series* (2.2), *whose coefficients are given by* (2.3) *and* (2.4).

Corollary 1. *For each* $N \geqslant 2$, *Eq.* (1.11) *has a one-parameter set of solutions having finite limits as* $r \to 0$ *and satisfying condition* (1.7). *Each solution of this set is a holomorphic function represented by series* (2.2).

For each $\rho_0 \in \mathbb{R}$ we can compute the approximate value of the corresponding solution and its derivative at a certain δ, such that $0 < \delta \ll 1$, by considering only some of the first terms of the series on the right-hand side of (2.2). Then we can solve a regular Cauchy problem for Eq. (1.11). Such problems can be solved by standard numerical methods. In our computations we have used the *NDSolve* command of the *Mathematica* software [15] with this purpose.

2.2. The singularity at infinity

Let us now focus our attention on the boundary condition (1.12). In order to analyze the asymptotic behavior of the solutions of (1.11) as $r \to \infty$, the boundary condition (1.12) may be written in a more precise way as

$$\lim_{r\to\infty} (\rho(r) - \xi) = \lim_{r\to\infty} \rho'(r) = 0. \tag{2.5}$$

We introduce the following variable substitution:

$$z = r^{(N-1)/2}(\rho - \xi). \tag{2.6}$$

In the new variable, Eq. (1.11) becomes

$$z'' = 4\lambda^2 (z/r^{(N-1)/2} + \xi + 1)(z/r^{(N-1)/2} + \xi)z + \frac{(N-1)(N-3)z}{4r^2}. \tag{2.7}$$

Eq. (2.7) has an irregular singularity at infinity (see, e.g., [14]). On the other hand, since $\rho(r) - \xi$ tends to 0 faster than $1/r^{(N-1)/2}$, the boundary condition (2.5) in the new variable takes the form

$$\lim_{r\to\infty} z(r) = \lim_{r\to\infty} z'(r) = 0. \tag{2.8}$$

For any $N > 1$, Eq. (2.7) is asymptotically autonomous, i.e., as $r \to \infty$, we obtain a linear autonomous equation whose characteristic exponents are

$$\tau_{1,2} = \pm\tau, \quad \tau = 2\lambda\sqrt{\xi(\xi+1)}. \tag{2.9}$$

From classical results for ordinary differential equations (see [11]), it follows that, for $N > 1$, the singular Cauchy problem (2.7), (2.8) has a parameter set of solutions that can be represented as a convergent exponential Lyapunov series in powers of the quantity $b\mathrm{e}^{-\tau r}$:

$$z(r, b) = C_1(r) b \mathrm{e}^{-\tau r} + \sum_{k=2}^{\infty} C_k(r) b^k \mathrm{e}^{-\tau k r}, \quad r \geqslant r_\infty, \tag{2.10}$$

where b is a parameter, $|b\mathrm{e}^{-\tau r_\infty}|$ is small and $C_k(r)$ are coefficients that do not depend on b, $k = 2, 3, \ldots$. By formally substituting series (2.10) into Eq. (2.7) we can obtain the differential equations for these coefficients. In particular, C_1 satisfies the equation

$$C_1''(r) - 2\tau C_1'(r) = \frac{(N-1)(N-3)}{4r^2} C_1(r), \quad r \geqslant r_\infty. \tag{2.11}$$

We are interested in such a solution of (2.11), which tends to a finite number when r tends to infinity. Since our arbitrary constant is b, we impose to C_1 the following conditions:

$$\lim_{r\to\infty} C_1(r)=1, \quad \lim_{r\to\infty} C_1'(r)=0. \tag{2.12}$$

The solution of the singular Cauchy problem (2.11), (2.12) exists, is unique and may be expanded in the form of an asymptotic series of negative integer powers of r. In particular, the leading terms of this series may be written as

$$C_1(r)=1+(N-1)(N-3)/(8r\tau)+\mathrm{O}(1/r^2), \quad r\to\infty. \tag{2.13}$$

As it follows from (2.11) and (2.12), in the cases $N=1$ and $N=3$, $C_1\equiv 1$. Moreover, in the case $N=1$, all the C_k coefficients are constant (in this case Eq. (2.7) is autonomous).

Remark. By means of the variable substitutions

$$C_1(r)=\sqrt{\frac{2\tau r}{\pi}}\mathrm{e}^{\tau r}y(\tau r), \quad t=\tau r,$$

Eq. (2.11) may be reduced to the form

$$t^2y''(t)+ty'(t)-(t^2+v^2)y(t)=0, \tag{2.14}$$

where $v=N/2-1$. Since (2.14) is a modified Bessel equation it possesses a solution which tends to 0 at infinity and in the case $N\neq 1$, $N\neq 3$ has the following asymptotic expansion (see [1, 9.7.2]):

$$y(t)=\sqrt{\frac{\pi}{2t}}\mathrm{e}^{-t}\left(1+\frac{4v^2-1}{8t}+\mathrm{O}\left(\frac{1}{t^2}\right)\right). \tag{2.15}$$

Writing (2.15) in terms of the variables C_1 and r, we obtain again the asymptotic expansion (2.13).[1]

Concerning the coefficients C_k, with $k\geqslant 2$ and $N>1$, they can be obtained in a similar way, recursively, by solving a sequence of singular Cauchy problems. The solutions of these problems must tend to zero as r tends to infinity and it may be shown that under this condition each singular Cauchy problem has an unique solution that can be expanded in a series of integer or half-integer negative powers of r. Here, we shall not go into details concerning these coefficients, since in our computations we have used only C_1 (for such details, see [9]). Now we give a proposition which summarizes the main results concerning the asymptotic expansion of the solution at infinity.

Proposition 2. *For any* $N>1$, *the singular Cauchy problem* (1.11), (2.5) *has a one-parameter family of solutions. This family may be represented as a convergent exponential Lyapunov series*:

$$\rho(r,b)=\xi+\frac{1}{r^{(N-1)/2}}\sum_{k=1}^{\infty}C_k(r)b^k\mathrm{e}^{-\tau kr}, \quad r\geqslant r_\infty, \tag{2.16}$$

[1] The authors would like to thank the referee for his comments about the connection between the solutions of Eq. (2.11) and the Bessel functions, which gave rise to this remark.

where τ is defined as above and b is the considered parameter. This series converges if $|b\mathrm{e}^{-\tau r_\infty}|$ is sufficiently small. The C_1 coefficient is the solution of the singular Cauchy problem (2.11), (2.12) *and the leading term of its asymptotic expansion is given by* (2.13).

Let $r_* \geqslant r_\infty$ be a sufficiently large positive number. Then, we can use (2.16) to approximate the values of $\rho(r_*, b)$ and $\rho'(r_*, b)$. These values can be used as initial conditions for a regular Cauchy problem, which will be an approximation of the initial value problem (1.11), (2.5).

The original boundary value problem (1.11), (1.7), (1.12) can now be formulated as two equivalent problems

- From the set of solutions of (1.11) satisfying (2.16) find a particular one which also satisfies (2.1).
- From the set of solutions of (1.11) satisfying (2.2) find a particular one which additionally fulfills (2.5).

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 ∞, any numerical method becomes unstable as r grows, because the solution tends to an unstable saddle point. If we start from r_* 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 Section 4, we shall propose a simple and efficient numerical algorithm to overcome these difficulties.

3. Parameter estimates and necessary conditions for the existence of strictly increasing solutions

First of all, the solution to our problem must satisfy $\rho''(0) > 0$; therefore, we must have $\rho_2 > 0$, from (2.3), ρ_0 has to satisfy

$$-1 < \rho_0 < 0. \tag{3.1}$$

For $\rho_0 = -1$ or $\rho_0 = 0$, we have just constant solutions of the singular Cauchy problem (1.11), (2.1). For $-1 < \rho_0 < 0$, we can have solutions of different kinds (oscillatory, monotone or even unbounded).

The results of Section 2.1 about the one-parameter family of solutions of the singular Cauchy problem (1.11), (2.1) give us also some information about upper and lower bounds of these solutions. We shall now resume this information in the form of a proposition.

Proposition 3. *If ρ is a nonconstant solution to the BVP* (1.11), (2.1), (2.5), *with $N \geqslant 2$, then $-1 < \rho(r) < \xi$, for $r > 0$.*

In order to prove this proposition we shall need the following lemmas, whose proof is elementary.

Lemma 1. *Let ρ be a nonconstant solution of Eq.* (1.11). *If ρ has a maximum at $s > 0$, then either $0 < \rho(s) < \xi$ or $\rho(s) < -1$.*

Lemma 2. *Let ρ be a nonconstant solution of Eq.* (1.11). *If ρ has a minimum at $s > 0$, then either $-1 < \rho(s) < 0$ or $\rho(s) > \xi$.*

Proof of Proposition 3. Let us first show that, if ρ is a solution of the singular Cauchy problem (1.11), (2.1), with $-1<\rho_0<\xi$, then there is at most one value $\bar{r}\in\mathbb{R}$ such that $\rho(\bar{r})=\xi$. Suppose that $\bar{r}$ is the least value of r, for which $\rho(\bar{r})=\xi$. Then, since $\rho(0)<\xi$, ρ must be increasing at $r=\bar{r}$, that is, $\rho'(\bar{r})\geqslant 0$. On the other hand, if $r>\bar{r}$, we have $\rho'(r)>0$, because otherwise ρ would have a maximum at a certain r, with $\rho(r)>\xi$, which contradicts Lemma 1. Hence, if $\rho(\bar{r})=\xi$, we have $\rho(r)>\xi$, for $r>\bar{r}$, and $\bar{r}$ is the only value of r such that $\rho(\bar{r})=\xi$.

In the same way, using Lemma 2, it may be shown that here is at most one value $\tilde{r}\in\mathbb{R}$ such that $\rho(\tilde{r})=-1$; if such a value exists, then $\rho(r)$ is decreasing, for $r>\tilde{r}$.

Therefore, if we have $\rho(\bar{r})\geqslant\xi$, for some $\bar{r}>0$, or $\rho(\tilde{r})\leqslant -1$, for some $\tilde{r}>0$, the condition $\lim_{r\to\infty}\rho(r)=\xi$ cannot be satisfied (except in the case $\rho(r)\equiv\rho_0=\xi$). This concludes the Proof of Proposition 3. □

In Section 1, we have remarked that we are interested only on strictly increasing solutions of the considered boundary value problem, since nonmonotone solutions have no physical meaning. In [5], a necessary condition for the existence of at least one monotone solution of a general boundary value problem is obtained from a variational approach (see also [13]). We shall now show how this result may be applied to the problem (1.11), (1.7), (1.12). Eq. (1.11) may be considered as the Lagrange–Euler equation for the functional

$$J(\rho)=\int_0^\infty\left(\frac{1}{2}\left(\frac{\mathrm{d}\rho}{\mathrm{d}r}\right)^2+W(\rho)\right)r^{N-1}\,\mathrm{d}r, \tag{3.2}$$

where $W(\rho)$ is given by

$$W(\rho)=4\lambda^2\int_\xi^\rho(s+1)s(s-\xi)\,\mathrm{d}s. \tag{3.3}$$

Then the boundary value problem (1.11), (1.7), (1.12) is equivalent to the following problem: find a solution of (1.11), different from the constant ξ, for which the integral (3.2) converges.

In [5], using a variational principle, it was shown, in the case $N=3$, that a necessary condition for the existence of at least one solution to the considered problem is that, for some ρ, we have $W(\rho)<0$. Let us recall the main idea of this proof, which is true, not only for $N=3$, but for any $N\geqslant 2$. Let $\rho(r)$ be a solution of (1.11), for which the integral (3.2) converges, and denote $\rho_\mu(r)=\rho(\mu r)$, where μ is a positive parameter. Let us replace ρ by ρ_μ in (3.2) and introduce the variable substitution $r_{\text{new}}=\mu r$. Then we obtain

$$I(\mu)\equiv J(\rho_\mu)=\int_0^\infty\left(\frac{1}{2}\left(\frac{\mathrm{d}\rho_\mu}{\mathrm{d}r}\right)^2+W(\rho_\mu)\right)r^{N-1}\,\mathrm{d}r=\frac{I_1(\rho_1)}{\mu^{N-2}}+\frac{I_2(\rho_1)}{\mu^N}, \tag{3.4}$$

where I_1 and I_2 do not depend on μ:

$$I_1(\rho_1)=\int_0^\infty\frac{1}{2}\left(\frac{\mathrm{d}\rho_1}{\mathrm{d}r}\right)^2r^{N-1}\,\mathrm{d}r,\quad I_2(\rho_1)=\int_0^\infty W(\rho_1)r^{N-1}\,\mathrm{d}r$$

(here and below we write r instead of r_{new}). Differentiating (3.4) with respect to μ, we obtain

$$\frac{\mathrm{d}I}{\mathrm{d}\mu} = -\frac{I_1(N-2)}{\mu^{N-1}} - \frac{I_2 N}{\mu^{N+1}} \tag{3.5}$$

and, since $\rho_1(r) \equiv \rho(r)$ (the solution of the variational problem) we must have $\mathrm{d}I/\mathrm{d}\mu|_{\mu=1} = 0$ and therefore

$$I_2 = -\frac{I_1(N-2)}{N}. \tag{3.6}$$

If $W(\rho) \geqslant 0$, $\forall \rho \in \mathbb{R}$, then I_2 is positive (as well as I_1) and (3.6) is not satisfied, for any $N \geqslant 2$. Hence the existence of at least one solution to the considered variational problem (and to the equivalent boundary value problem) requires that $W(\rho) < 0$, for some real ρ.

In the case of (1.11), it follows from (3.3) that $W(\rho)$ has the form

$$W(\rho) = \lambda^2(\rho - w_1)(\rho - w_2)(\rho - \xi)^2, \tag{3.7}$$

where

$$w_{1,2} = \frac{-(\xi+2) \mp \sqrt{2(\xi+2)(1-\xi)}}{3}. \tag{3.8}$$

From (3.8) it follows that two distinct real roots $w_{1,2}$ exist if and only if $-2 < \xi < 1$. Hence, only for such values of ξ there exist such ρ_-, that $W(\rho_-) < 0$. On the other hand, we must have $\xi > 0$. The restrictions on the value of ξ can be summarized in the following proposition.

Proposition 4. *The restrictions* $0 < \xi < 1$ *are a necessary condition for the existence of a solution to the boundary value problem* (1.11), (1.7), (1.12), *distinct from* $\rho(r) \equiv \xi$.

The integral (3.2) was computed numerically for some solutions of the considered boundary value problem. The numerical results are displayed in Section 5. During the computation of the integral, it was verified that the numerical solution indeed satisfies the equality (3.6) within the expected accuracy (4–5 digits).

4. Numerical methods

The numerical method presented in this section is based on the following idea. First, we replace the considered boundary value problem with two singularities (at the origin and at infinity) by two auxiliary boundary value problems, each of them having only one singularity. Then to construct the solution of the original problem we use the following fact: let $\rho(r, \hat{\lambda})$ be a solution of (1.11), (1.7), (1.12) for a given value $\hat{\lambda}$. Then for an arbitrary value of λ, the corresponding solution can be calculated by the formula

$$\rho(r, \lambda) = \rho(r\lambda/\hat{\lambda}, \hat{\lambda}). \tag{4.1}$$

Let us describe this method in detail.

Step 1: We begin by fixing certain values r_0, δ and r_∞, such that $r_\infty > r_0 > \delta > 0$. Then we divide the set $[\delta, r_\infty[$, where we want to compute the approximate solution, into two subintervals: $[\delta, r_0]$ and

$[r_0, r_\infty]$. Let $\rho_-(r, \lambda)$ be a monotone solution of (1.11) on $[\delta, r_0]$, with fixed λ, which satisfies the boundary conditions

$$\rho(\delta, \lambda) = \rho_0 + \sum_{k=1}^{n_1} \rho_{2k}(\rho_0)\delta^{2k}, \tag{4.2}$$

$$\rho(r_0, \lambda) = 0, \tag{4.3}$$

where n_1 depends on δ and on the required accuracy. Let us now denote $\rho_+(r, \lambda)$ a monotone solution of (1.11) on $[r_0, \infty)$, with the same value of λ, which satisfies the boundary condition (4.3) and

$$\rho(r_\infty, \lambda) = \xi + \frac{1}{r_\infty^{(N-1)/2}} \sum_{k=1}^{n_2} C_k(r_\infty) b^k \mathrm{e}^{-\tau k r_\infty}, \tag{4.4}$$

where n_2 depends on r_∞ and on the required accuracy. Finally, let us define

$$\rho(r, \lambda) = \begin{cases} \rho_-(r, \lambda) & \text{if } \delta \leqslant r \leqslant r_0, \\ \rho_+(r, \lambda) & \text{if } r_0 \leqslant r \leqslant r_\infty. \end{cases} \tag{4.5}$$

Note that the functions ρ_-, ρ_+ are obtained by the shooting method as described above. When applying the shooting method we must take into account that $b < 0$ in (4.4), due to Proposition 3, and ρ_0 in (4.2) satisfies $-1 < \rho_0 < 0$.

Step 2: In general, the obtained function $\rho(r, \lambda)$ is not a solution of (1.11) on $[0, \infty[$, because the condition

$$\lim_{r \to r_0-} \rho'(r, \lambda) = \lim_{r \to r_0+} \rho'(r, \lambda) \tag{4.6}$$

is not satisfied for the given λ. Let us compute the difference

$$\Delta(r_0, \lambda) = \lim_{r \to r_0-} \rho'(r, \lambda) - \lim_{r \to r_0+} \rho'(r, \lambda). \tag{4.7}$$

Our goal now is to find such a value $\hat{\lambda} \in \mathbb{R}_+$ that $\Delta(r_0, \hat{\lambda}) = 0$. In order to find the needed value of $\hat{\lambda}$ we use the secant method, starting from two values λ_0 and λ_1, such that $\Delta(r_0, \lambda_0) < 0$, $\Delta(r_0, \lambda_1) > 0$.

Step 3: Finally, from this solution we can obtain the solution to the equation with the initial value of λ. This can be done by using the substitution (4.1).

Step 4: In order to extend the approximate solution to the intervals $[0, \delta]$ and $[r_\infty, \infty[$, we use the expansions (2.2), (2.16), with the computed values of ρ_0 and b.

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 ξ. However, it is not applicable to all the cases, in which monotone solutions exist. Computational difficulties have arisen in the case where $\xi < \xi_{\min}$, where $\xi_{\min}$ is the value of ξ, which corresponds to the minimal bubble radius. As we shall see in the next section, in the case $N = 3$, we have $\xi_{\min} \approx 0.28$. The mentioned difficulties can be explained by the fact that, as it is shown by the numerical results, when ξ 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 condition (4.6) 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 $\xi < \xi_{\min}$. This method, which we now describe, provides accurate solutions for the mentioned values of ξ. First note that, taking into consideration the first term of (2.16), we obtain, for $N \geqslant 2$, the following approximate equality:

$$\rho'(r) \approx \left(\tau + \frac{N-1}{2r} - \frac{C_1'(r)}{C_1(r)}\right)(\xi - \rho(r)), \tag{4.8}$$

for sufficiently large values of r, where C_1 is given by (2.13). The numerical solution of the boundary value problem with conditions (4.2), (4.8) can be computed by the shooting method, in the same way as in the case of the boundary conditions (4.2), (4.3). For the mentioned values of ξ, this method gives an accurate approximation of the exact solution on $[\delta, r_\infty]$.

5. Numerical results

Now we present the numerical results obtained for problem (1.11), (1.7), (1.12) by the numerical methods proposed in the previous section. In [4] some approximate solutions of the considered problem have been presented in the case of the van der Waals potential. Comparing our results with those and taking into account the physical meaning of the variables, we can conclude that the behavior of our solutions corresponds to what could be expected. Some of these results were also presented in a previous paper [10]. 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, in particular, to improve the computational methods.

According to Proposition 4, $0 < \xi < 1$ is a necessary condition for the existence of a monotone solution. As follows from [7] and pointed out in the Introduction, this condition is also sufficient. In the case $\xi = 0$, the function W has only one minimum at $\rho = -1$ and an inflexion at $\rho = 0$; in physics, this case is called the spinoidal limit. When $\xi = 1$, W is an even function (it takes the same value at the two minima); this corresponds to the saturation limit. In both mentioned cases problem (1.11), (1.7), (1.12) has no solution, since the necessary condition, formulated in Proposition 4, is not satisfied.

In our computations, we have determined numerical approximations to the solution for different values of ξ in the range [0.1, 0.8]. We used values of δ in the range $[10^{-6}, 10^{-3}]$ and r_∞ in the range [6, 10], depending on the value of ξ. In the case $N = 3$, the value of $\hat{\lambda}$ has been obtained with 9–10 digits in less than 10 iterations of the secant method.

We now describe some properties of the obtained numerical results.

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

In Table 1, the values of ρ_0, $|b|$ and R are displayed for different values of ξ in the case $\lambda = 1$ and $N = 3$. The values of $|b|$ increase and tend very fast to ∞ as $\xi \to 1$. The value of ρ_0 decreases and tends to -1 as $\xi \to 1$. Note that ρ_v (the density of the gas in the centre of the bubble) is connected with ρ_0 by $\rho_v = \rho_0(\wp_2 - \wp_1) + \wp_2$. The integral J is defined by (3.2) and its value increases with ξ.

For values of ξ greater than $\xi_{\min}$, 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

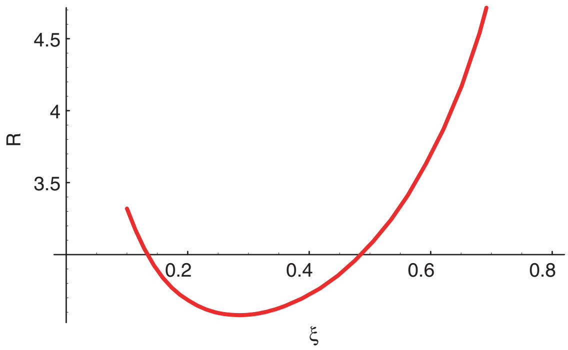

Fig. 1. The bubble radius R, as a function of ξ, in the case $\lambda = 1$, $N = 3$.

Table 1
Values of ρ_0, $|b|$, R and J as functions of ξ

ξ	ρ_0	$\lvert b \rvert$	R	J
0.1	−0.3048	4.0175	3.32	0.06349
0.15	−0.4437	6.3477	2.89	0.12663
0.2	−0.5681	9.857	2.685	0.21340
0.28	−0.7356	22.678	2.580	0.41726
0.3	−0.7707	28.113	2.582	0.48450
0.4	−0.90313	95.980	2.721	0.9691
0.5	−0.97112	491.92	3.068	1.884
0.6	−0.99531	5080.9	3.696	3.775
0.7	−0.99979	207675	4.833	8.315
0.8	−0.9999996	$2.54 \cdot 10^8$	7.128	22.611

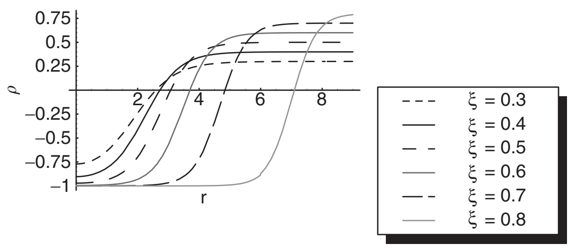

Fig. 2. Graphics of the solutions in the case $\lambda = 1$, $N = 3$ and $\xi > \xi_{\min}$.

and liquid phases. The absolute maximum of the derivative is attained near R and its value grows with ξ. These properties are well described by the graphics in Fig. 2 (solutions) and Fig. 3 (their derivatives).

On the other hand, when $\xi < \xi_{\min}$ the solutions change uniformly along all the domain. The maximum of the first derivative decreases as $\xi \to 0$. The physical meaning of this behavior is a smooth transition between the gaseous and the liquid phase of the fluid.

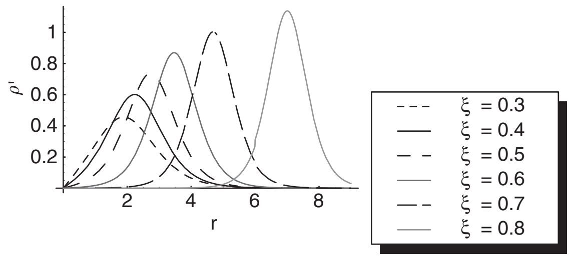

Fig. 3. Graphics of the derivatives of the solutions in the case $\lambda = 1$, $N = 3$ and $\xi > \xi_{\min}$.

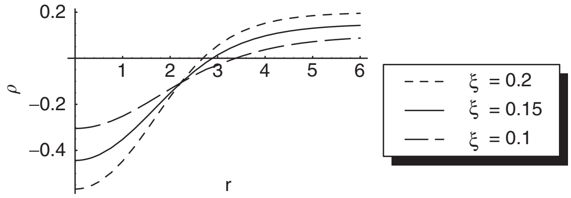

Fig. 4. Graphics of the solutions in the case $\lambda = 1$, $N = 3$ and $\xi < \xi_{\min}$.

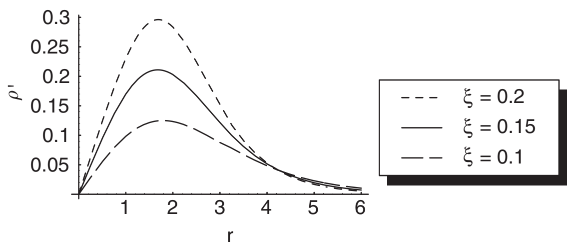

Fig. 5. Graphics of the derivatives of the solutions in the case $\lambda = 1$, $N = 3$ and $\xi < \xi_{\min}$.

Some graphics of the solutions and their derivatives with such properties are displayed in Figs. 4 and 5.

6. Conclusions

In the present work we have analyzed the boundary value problem (1.11), (1.7), (1.12) 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. Although the obtained theoretical results are valid for $N \geqslant 2$, the numerical experiments were carried out so far for the case $N = 3$, when the physical meaning of the problem is well-known. By extending the proposed computational algorithm to other values of N, the authors intend to obtain new numerical results, which may find application in other problems of mathematical physics.

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