MATHEMATICAL ANALYSIS AND NUMERICAL SOLUTION OF A SINGULAR PROBLEM IN NONLINEAR PHYSICS

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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. Based on the analytic study, an efficient numerical method is proposed to compute approximately the needed solutions of the above problem. Results of the numerical experiments are displayed and their physical interpretation is discussed.

1. Introduction

To study the motion of non-homogeneous fluids (fluid - vapour, fluid - gas, etc.), in which the internal energy depends on the density ρ of the fluid and the gradient of the density $\nabla\rho$, in [3] the following system of differential equations has been deduced, describing the behavior of non-homogeneous fluid in the stationary case, under isothermal conditions

$$\nabla(\mu(\rho) - \gamma\Delta\rho) = 0, \tag{1.1}$$

where $\mu(\rho) = E_0'(\rho)$ is the chemical potential and $E_0 = E_0(\rho)$ is the free energy of the fluid. The system (1.1) is equivalent to one equation

$$\gamma\Delta\rho = \tilde{\mu}(\rho) \tag{1.2}$$

with $\tilde{\mu}(\rho) = \mu(\rho) - \mu_0$, μ_0 is a suitable constant.

This equation can be applied to describe microscopical bubbles in a non-homogeneous fluid, for instance: vapour inside one liquid. In the case of plane or spherical bubbles the equation (1.2) takes the form

$$\gamma\left(\rho'' + \frac{N-1}{r}\rho'\right) = \tilde{\mu}(\rho), \quad r \in (0,\infty), \tag{1.3}$$

where $N = 2$ or $N = 3$, respectively; this lat equation is known as the density profile equation (DPE) [2], [5]. Equation (1.3) is to be supplemented with appropriate boundary conditions: the derivative of ρ vanishes at the origin

$$\rho'(0) = 0, \tag{1.4}$$

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view of central symmetry, and since the bubble is surrounded by a liquid, the following condition holds at infinity

$$\rho(\infty) = \rho_l > 0, \tag{1.5}$$

where ρ_l is the density of the external liquid. Whenever a strictly increasing solution $\rho = \rho(r)$ to problem (1.3)-(1.5) exists, the solution ρ determines an increasing mass density profile for the bubble.

In the simplest models for non-homogeneous fluids, the free energy E_0 is a fourth-degree polynomial on ρ, with two minima and one maximum. Then $\tilde{\mu}$ is a third degree polynomial on ρ with three distinct real roots and since $\tilde{\mu}(\rho_l) = 0$, we can write

$$\tilde{\mu}(\rho) = 4\alpha(\rho - \wp_1)(\rho - \wp_2)(\rho - \rho_l), \quad 0 < \wp_1 < \wp_2 < \rho_l, \alpha > 0. \tag{1.6}$$

Introducing the variable substitution

$$\tilde{\rho} = \frac{\rho - \wp_2}{\wp_2 - \wp_1} \tag{1.7}$$

and the positive constants λ, ξ by

$$\lambda = \sqrt{\frac{\alpha}{\gamma}}(\wp_2 - \wp_1), \ \xi = \frac{\rho_l - \wp_2}{\wp_2 - \wp_1} > 0,$$

without loss of generality, instead of (1.3)-(1.5) we have to investigate the equation

$$\left(r^{N-1}\rho'(r)\right)' = 4r^{N-1}\lambda^2(\rho + 1)\rho(\rho - \xi), \quad 0 < r < \infty, \tag{1.8}$$

with the boundary condition (1.4) and

$$\rho(\infty) = \xi > 0. \tag{1.9}$$

We are interested in solutions, different from the constant solution $\rho(r) \equiv \xi$, which have exactly one zero in $\mathbf{R}_+$. If such solutions exist, we can give important physical properties of the bubbles: the value of density inside the bubble, the bubble radius, etc.. Over the last thirty years a lot of different approaches have been developed to solve the equation (1.8) (see, references in [1]in [4]). From the results of a recent paper [4], it follows that a sufficient condition for the existence of at least one strictly increasing solution for (1.8), (1.4), (1.9) is the following :

$$0 < \xi < 1.$$

Returning back to the initial system (1.3)-(1.5), physically this condition means that the formation of the bubble in the fluid is possible only for such values of the external pressure $p_l = \rho_l \mu(\rho_l) - E_0(\rho_l)$, for which the roots of the polynomial (1.6) satisfy the inequality

$$0 < \rho_l - \wp_2 < \wp_2 - \wp_1.$$

In [8], it was shown that this condition is also necessary for the existence of such solution.

Numerical simulations have been carried out in [2] and [8]. In this last paper, some interesting properties of the solution have been proved. In particular, it was shown that if ρ is a non-constant solution of the problem (1.4),(1.8),(1.9), with N≥2, then $-1 < \rho(r) < \xi$, for all positive r.

In the next section, we shall obtain asymptotic expansions of some solutions of (1.8) which satisfy the prescribed conditions (1.4) and (1.9).

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

2.1. The singularity at zero

Let us consider equation (1.8), subject 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. From Theorem 5 in [6], $\forall \rho_0 \in \mathbf{R}, N \geq 2$ it follows that this singular Cauchy problem has an unique solution; moreover this solution is a holomorphic function at the point $r = 0$ and can be represented in the form:

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

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 (1.8), 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} :

$$\rho_{2k}(\rho_0) = \frac{2\lambda^2}{k(2k+N-2)} \times$$

$$\times \left(\sum_{m=1}^{k-1} \left(\sum_{l=0}^{m} \rho_{2l}\rho_{2m-2l}\rho_{2k-2m-2} + (1-\xi)\rho_{2m}\rho_{2k-2m-2} \right) - \xi\rho_{2k-2} \right), \quad k = 2,3,\dots . \tag{2.4}$$

The above results may be expressed in the following form.

Proposition 1. *For each $N \geq 2$ and $\rho_0 \in \mathbf{R}$, the singular Cauchy problem (1.8),(2.1) has a unique solution. This solution is holomorphic at the point $r = 0$ and may be expanded in the form of the series (2.2), whose coefficients are given by (2.3) and (2.4).*

Corollary 1. *For each $N \geq 2$, equation (1.8) has a one-parameter set of solutions having finite limits as $r \to 0$ and satisfying condition (1.4). Each solution of this set is a holomorphic function represented by the series (2.2).*

For each $\rho_0 \in \mathbf{R}$ we can compute the approximate value of the corresponding solution and its derivative at a certain δ , such that $0 < \delta << 1$, 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 the equation (1.8). Such problems can be solved by standard numerical methods. In our computations we have used the *NDSolve* command of the *Mathematica* software [10] with this purpose. For details about the one-parameter family of solutions (2.2), please see [8].

2.2. The singularity at infinity

Let us now focus our attention on the boundary condition (1.9). In order to analyse the asymptotic behavior of the solutions of (1.8) as $r \to \infty$, the boundary condition (1.9) 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, the equation (1.8) becomes

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

The equation (2.7) has an irregular singularity at infinity. On the other hand, since $z(r)$ 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 $N > 1$, the equation (2.7) is asymptotically autonomous, i.e. as $r \to \infty$, we obtain the linear autonomous equation

$$z''_\infty = 4\lambda^2(\xi + 1)\xi\, z_\infty. \tag{2.9}$$

The characteristic roots of (2.9) are

$$\tau_{1,2} = \pm\tau, \qquad \tau = 2\lambda\sqrt{\xi(\xi + 1)}. \tag{2.10}$$

Hence the critical point (0,0) is a saddle point and the equation (2.9) possesses a one-parameter family of solutions which satisfy (2.8). These solutions can be written in the form

$$z_\infty(r) = be^{-\tau r}, \tag{2.11}$$

where b is a real constant.

From classical results for ordinary differential equations (see, e.g. [9]), it follows that, for $N > 1$, the solution of the singular Cauchy problem (2.7), (2.8) can be represented as a convergent exponential Lyapunov series in powers of the quantity (2.11):

$$z(r,b) = C_1(r)be^{-\tau r} + \sum_{k=2}^{\infty} C_k(r)b^k e^{-\tau k r}, \qquad r \ge r_\infty, \tag{2.12}$$

where b is a parameter, such that $|be^{-\tau r_\infty}|$ is small, and $C_k(r)$ are coefficients that don't depend on b. The main result about the behaviour of the solution of the considered problem at infinity is given by the following proposition.

Proposition 2. *The singular Cauchy problem (1.8), (2.5) has a one-parameter family of solutions. This family may be represented as a convergent exponential Lyapunov series:*

$$\rho(r,b) = \xi + \frac{1}{r^{(N-1)/2}} + \sum_{k=1}^{\infty} C_k(r) b^k e^{-\tau k r}, \qquad r \ge r_\infty \tag{2.13}$$

where τ *is defined as above and* b *is the considered parameter. This series converges if* $|be^{-\tau r_\infty}|$ *is sufficiently small . The* C_k *coefficients satisfy certain linear differential equations that may be obtained by substituting (2.7) into (2.12).*

For the proof of Proposition 2 and details about the computation of the series coefficients, please see [8].

Let $r_* \ge r_\infty$ be a sufficiently large positive number. Then we can use (2.13) 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 (1.8), (1.9).

The original boundary value problem (1.8), (1.4), (1.9) can now be formulated as follows: we must find from the set of solutions of (1.8) which satisfy (2.13) a particular solution which also satisfies (2.1). Alternatively, we can look for a particular solution of the set (2.2) which additionally fulfills (2.5), i.e. belongs to the family (2.13). 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 a saddle point, which is unstable. 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 the following section, we shall propose a simple and efficient numerical algorithm to overcome these difficulties.

3. Numerical methods

Our main goal is to compute a monotone solution of the equation (1.8) subject to the conditions (1.4) and (1.9). In section 1, such solutions were called bubbles. The main idea of the numerical method we introduce in this section is to replace the considered boundary value problem (which is singular at the origin and at infinity) by two auxiliary boundary value problems, each of them having only one singularity. A natural way to achieve this is to consider two subdomains: $[0,r_0]$ and $[r_0,\infty]$, where r_0 is such , that $\rho(r_0) = 0$. Thus, we shall use the following property of our problem: if a solution is known, corresponding to a certain $\lambda = \hat{\lambda}$, (let us denote it $\rho(r,\hat{\lambda})$), then the solution for any other value of λ , say $\lambda = a$, can be otained from the former by a simple variable substitution: $r' = r\hat{\lambda}/a$. More precisely, the solution for the new value of λ satisfies

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

From the last equality it follows that, by changing the value of λ we also change the value of r, for which $\rho(r,\lambda) = 0$. Therefore, if we fix any value r_0, there must be such $\hat{\lambda}$, that $\rho(r_0,\hat{\lambda}) = 0$. The algorithm for the computation of the approximate solution we shall now describe is based on this idea.

1st step. We begin by fixing a certain values r_0, δ, r_∞, such that $0 < \delta < r_0 < r_\infty$. Then we divide the set $]\delta, r_\infty[$, where we want to approximate the solution, into two subintervals: $]\delta, r_0]$ and $[r_0, r_\infty[$. Let $\rho_-(r,a)$ be a monotone solution of (1.8) on $[\delta, r_0]$ with $\lambda = a$, which satisfies the boundary conditions

$$\rho(\delta,a) = \sum_{k_1}^{n_1} \rho_{2k}(\rho_0)\delta^{2k}, \tag{3.1}$$

$$\rho(r_0,a) = 0, \tag{3.2}$$

where n_1 depends on δ and on the required accuracy. Let us now denote $\rho_+(r,a)$ a monotone solution of (1.8) on $[r_0,\infty[$ with $\lambda = a$, which satisfies the boundary condition (3.2) and

$$\rho(r_\infty,a) = \xi + \frac{1}{r_\infty^{(N-1)/2}} \sum_{k=1}^{n_2} C_k(r) b^k e^{-\tau k r_\infty}, \tag{3.3}$$

where n_2 depends on r_∞ and on the required accuracy. Assuming that the solutions $\rho_-(r,a)$ and $\rho_+(r,a)$ exist and satisfy the prescribed conditions, let us define

$$\rho(r,a) = \begin{cases} \rho_-(r,a), & \text{if } \delta \le r \le r_0; \\ \rho_+(r,a), & \text{if } r_0 < r \le r_\infty. \end{cases} \tag{3.4}$$

In general, $\rho(r,a)$ is not a solution of (1.8) on $[0,\infty[$, because the condition

$$\lim_{r \to r_o -} \rho'(r,a) = \lim_{r \to r_0 +} \rho'(r,a) \tag{3.5}$$

is not satisfied for $\lambda = a$. Our goal now is to find such a value $\hat{\lambda} \in \mathbf{R}_+$ that the condition (3.5) 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 (1.8), (1.4), (1.9) with $\lambda = \hat{\lambda}$.

2nd step. In order to find the needed value of $\hat{\lambda}$ we use numerical algorithms which solve the following auxiliary problems:

1. For fixed $\lambda \in \mathbf{R}_+$, $\delta > 0$ and $r_0 > \delta$, approximate $\rho_-(r,\lambda)$ on $[\delta, r_0]$.
2. For fixed $\lambda \in \mathbf{R}_+$, r_0 and $r_\infty > r_0$, approximate $\rho_+(r,a)$ on $[r_0, r_\infty]$.

Each of these problems can be solved by the usual shooting method. If both problems are solved for a given value of λ, then we can compute the difference

$$\Delta(r_0,\lambda) = \lim_{r \to r_0 +} \rho'(r,\lambda) - \lim_{r \to r_0 -} \rho'(r,\lambda). \tag{3.6}$$

Now our problem is reduced to find the value of $\hat{\lambda}$, for which $\Delta(r_0, \hat{\lambda}) = 0$. With this purpose we have used the secant method and in the case $N = 3$ the value of $\hat{\lambda}$ has been obtained with 9-10 digits in less than 10 iterations.

3d step. From this solution we can obtain the solution to the equation with $\lambda = a$ for the considered value of a.This solution will be given by the mentioned above variable substitution.

4th step. Finally, in order to extend the obtained approximate solution to the intervals $[0, \delta]$ and $[r_\infty, \infty[$, we use the asymptotic expansions (3.1) and (3.3), with the computed values of ρ_0 and b.

In the next section, we shall present some numerical results obtained by the described algorithm.

4. Numerical results

Now we present the numerical results obtained for the problem (1.8), (1.4), (1.9) by the numerical methods proposed in the previous section.

As mentioned in the Introduction, some approximate solutions for this problem (in the case $N = 3$) have been presented in [2], in the form of graphics. According to the authors, those solutions have been constructed by standard numerical methods. Since the numerical values of ρ 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. Some of these results were also presented in a previous paper [7]. 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 [4], the existence of a monotone solution is possible if and only if $0 < \xi < 1$. 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. 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.

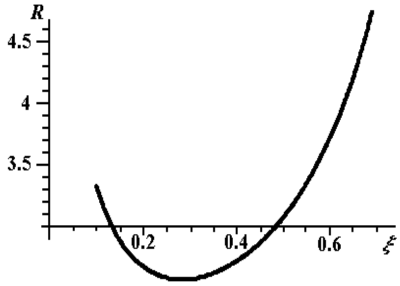

Fig. 1: $R(\xi)$ in the case $\lambda = 1, N = 3$.

Table 1

ξ	ρ_0			R		
	N=2	N=3	N=4	N=2	N=3	N=4
0.1	-0.1429	-0.3048	-0.5476	2.836	3.321	3.786
0.2	-0.2930	-0.5677	-0.8127	2.127	2.685	3.373
0.3	-0.4494	-0.7707	-0.9339	1.871	2.582	3.474
0.4	-0.6092	-0.9031	-0.9823	1.787	2.721	3.827
0.5	-0.7646	-0.9711	-0.9970	1.831	3.070	4.440
0.6	-0.8966	-0.9953	-0.9998	2.035	3.695	5.436
0.7	-0.9765	-0.9997		2.518	4.817	
0.8	-0.9989	-0.9999995		3.626	7.131	

In Table 1, the values of ρ_0 and R are displayed for different values of ξ and N in the case $\lambda = 1$. The value of ρ_0 decreases and tends to -1 as $\xi \to 0$. Note that ρ_v (the density of the gas in the centre of the bubble) is connected with ρ_0 by $\rho_v = \rho_0(\wp_2 - \wp_1) + \wp_2$.

For values of $\xi > \xi_{\min}$ ($\lambda = 1, N = 3$), 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 and its value grows with ξ. These properties are well described by the graphics in Fig. 2.

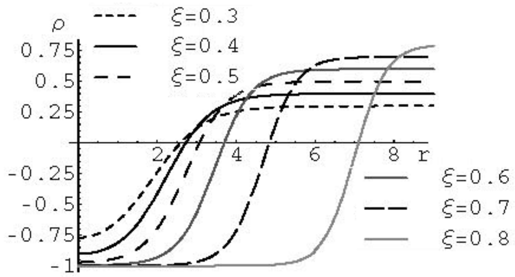

Fig. 2: $\rho(r)$ in the case $\xi > \xi_{\min}$ ($\lambda = 1, N = 3$).

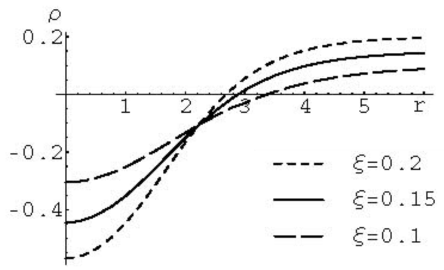

Fig. 3: $\rho(r)$ in the case $\xi < \xi_{\min}$ ($\lambda = 1, N = 3$).

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. Some graphics of the solutions are displayed in Fig. 3.

5. Conclusions

In the present work we have analysed the boundary value problem (1.8), (1.4), (1.9) and the asymptotic properties of some solutions. This analysis enabled us to introduce new numerical methods for the accurate approximation of monotone solutions. 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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