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# Density profile equation with $p$-Laplacian: Analysis and numerical simulation

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ABSTRACT

Analytical properties of a nonlinear singular second order boundary value problem in ordinary differential equations posed on an unbounded domain for the density profile of the formation of microscopic bubbles in a nonhomogeneous fluid are discussed. Especially, sufficient conditions for the existence and uniqueness of solutions are derived. Two approximation methods are presented for the numerical solution of the problem, one of them utilizes the open domain MATLAB code `bvpsuite`. The results of numerical simulations are presented and discussed.



## 1. Introduction

In this paper, we consider second order nonlinear ordinary differential equations (ODEs) arising in the modeling of nonhomogeneous fluids. In the Cahn–Hilliard theory for mixtures of fluids (see, for example, [5]) an additional term involving the gradient of the density $\mathrm{grad}(\rho)$ is added to the classical expression $E_0(\rho)$ for the volume free energy, depending on the density $\rho$ of the medium. Hence the total volume free energy of a non-homogeneous fluid can be written as

$$E(\rho, \mathrm{grad}(\rho)) = E_0(\rho) + \frac{\sigma}{2}(\mathrm{grad}(\rho))^2, \tag{1}$$

where $E_0(\rho)$ is a double-well potential, whose wells define the phases. The potential $E_0(\rho)$ causes an interfacial layer within which the density $\rho$ suffers large variations [10].

Because of the shape of $E_0$, the fluid tends to divide into two phases with densities $\rho = \rho_l$ (liquid) and $\rho = \rho_v$ (vapour) and the term $\frac{\sigma}{2}(\mathrm{grad}(\rho))^2$ tends to turn the interface between them into a thin layer, endowing it with energy (the surface tension) [24].

When the free energy is given by (1) the density profile $\rho(r)$ can be obtained in the stationary case by means of minimization of the functional,

$$J(\rho) = \int_\Omega \left(E_0(\rho) + \frac{\sigma}{2}(\mathrm{grad}(\rho))^2\right) dr, \tag{2}$$

where $\Omega \subset R^N$. This minimization problem leads to a partial differential equation of the form

$$\gamma \nabla \rho = \mu(\rho) - \mu_0, \tag{3}$$

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where $\mu(\rho) = \frac{dE_0}{d\rho}$ is the chemical potential of the considered mixture of fluids. In the case of spherical symmetry, which is the most common in applications, Eq. (3) can be reduced to a second order ODE of the form

$$r^{1-N}(r^{N-1}\rho'(r))' = f(\rho(r)), \quad r > 0, \tag{4}$$

where $N$ is the space dimension and $f$ represents the right-hand side of (4). This function is usually known and depends on the properties of the considered mixture of fluids. Typically it is a cubic polynomial of $\rho$, with three real roots. Choosing an adequate system of units, we may write $f$ as

$$f(\rho) := 4\lambda^2\rho(\rho+1)(\rho-\xi), \tag{5}$$

where $\xi = \rho_v$ (vapour density) and $\lambda$ is a real parameter. Eq. (4) is called the density profile equation and was studied, for example in [6,7]. The authors of those articles show that the density profile ($\rho$) is a monotone solution of Eq. (4) satisfying the boundary conditions,

$$\rho'(0) = 0, \quad \lim_{r\to\infty}\rho(r) = \xi. \tag{6}$$

In [12,18,20], a detailed study of the boundary value problem (BVP) (4), (6) has been provided. In [18,20] the asymptotic properties of the solutions near the singular points, 0 and $\infty$, have been studied. This enables approximate representations of the solution for $r \to 0$ and $r \to \infty$. Based on these representations, stable shooting methods were implemented for the numerical solution of the problem. Moreover, in [12], accurate numerical results were obtained for this problem, using the `bvpsuite` code based on polynomial collocation.

In the present paper, we consider a more general problem, where the energy integral has the form

$$J(\rho) = \int_\Omega \left(E_0(\rho) + \frac{c}{p}(\mathrm{grad}(\rho))^p\right)dr, \tag{7}$$

where $p > 1$ is a given constant.[1] Such models were analyzed in [22,23], where the authors have studied the minimization of the functional (7), which has led them to the analysis of a partial differential equation of the form

$$\Delta_p u := c\,\mathrm{div}(|\mathrm{grad}(\rho)|^{p-2}\mathrm{grad}(\rho)) = \frac{dE_0}{d\rho}. \tag{8}$$

The operator $\Delta_p$ on the left-hand side of (8) is the so called $p$-Laplacian. This operator enables the description of mixtures of fluids of a more general nature when compared to the classical Cahn–Hilliard theory, $p = 2$. In particular, with this formulation we can deal with the case where the surface tension of the fluid is not constant in the region of the interface. As for $p = 2$, we consider here spherical bubbles, and therefore spherical symmetry is used to reduce the dimension of the model. The study of the general case, without spherical symmetry, can be found in [22,23]. Using spherical coordinates and introducing a convenient system of units, the following ODE arises:

$$r^{1-N}(r^{N-1}|\rho'(r)|^{p-2}\rho'(r))' = f_p(\rho), \quad r > 0, \tag{9}$$

where $f_p$ is a function which reduces to $f$, given by (5), in the case $p = 2$. The form of $f_p$ for $p \neq 2$ will be discussed in the next section. We are interested in strictly monotone solutions of (9) satisfying the boundary conditions specified in (6).

It is worth mentioning that a closely related problem was analyzed in the recent papers [8,25], where the authors consider

$$\epsilon^p r^{1-N}(r^{N-1}|\rho'(r)|^{p-2}\rho'(r))' - W'(\rho) = 0, \quad r > 0. \tag{10}$$

Here, the function $W$ is a double-well potential (like $E_0$ in our case), and $\epsilon$ is an unknown parameter which has to be determined. The solution of Eq. (10) has to satisfy the boundary conditions,

$$\rho'(0) = \rho(R) = \rho'(R) = 0, \tag{11}$$

where $R$ is a given constant. Under certain conditions on $W(\rho)$, $p$, and $N$, the existence and uniqueness of solution of the problem (6), (10) is shown in the case when $\epsilon$ belongs to a certain set of the eigenvalues $\epsilon_n, n \in \mathbf{N}$.

In the present paper we analyze the BVP (6), (9) and propose efficient numerical methods for its approximate solution.

The paper is organized as follows. In Section 2, we discuss existence and uniqueness of solutions to the BVP (6), (9). In Section 3, a shooting method based on the asymptotic properties of solutions and a collocation method are introduced. Numerical results are presented in Section 4 and conclusions can be found in Section 5.

## 2. Existence and uniqueness of solutions to the analytical problem

In order to investigate the existence and uniqueness of the solution to problem (6), (9), we exploit the results presented in [9]. Especially, we focus on Corollary 1 [9].

[1] For $p = 2$ we obtain the case (2).