



# Investigating the stability of the phase field solution of equilibrium droplet configurations by eigenvalues and eigenvectors



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## ABSTRACT

Phase field models have recently been used to investigate the physical behavior of droplets in static as well as dynamic situations. As those models are often driven by an Allen-Cahn evolution equation, their stationary solution is given by the first order optimality condition of an energy functional. This includes the possibility of computing saddle points and maxima rather than minima of the energy functional. The present work shows the post-processing of eigenvalues and eigenvectors of the system matrix of the phase field model in order to investigate the stability of equilibrium droplet configurations. This post-processing can easily be ported to other evolution equations. The underlying phase field model is described and the resulting discrete finite element eigenvalue problem is stated. The investigation of eigenvalues and eigenvectors is illustrated by examples.

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## 1. Introduction

Understanding how droplets interact with each other as well as the ability to predict wetting phenomena is highly important in a variety of applications, e.g. pyrometallurgical processes [1] or inkjet printing [2]. Phase field simulations in which the presence of a phase is described by a continuous order parameter are capable of gaining this knowledge not only for a two-phase system but also for systems with multiple phases [3–5].

Depending on the case of application, some phase field models examine the static equilibrium [3] of droplets while others investigate the dynamics of (possibly) multicomponent fluid flows [2]. Phase field models offer a straightforward way to consider dynamic as well as static wetting scenarios on a variety of surface geometries. Especially in the case of microstructured surface wetting a profound knowledge of the static equilibrium wetting state of droplets is relevant and can serve as a starting point for a deeper understanding of the underlying effects. Regarding dynamic wetting of microstructured surfaces makes it harder to distinguish

between the different effects due to a greater number of parameters.

The fact that there is often a large difference between the initialization state of the phase field calculation and the final solution brings the necessity of using an evolution equation in order to gradually relax the phase field towards the static solution. Most commonly, an Allen-Cahn [6,3,7] or Cahn-Hilliard (see for instance [2] and the references therein) type evolution equation is chosen.

In order to give the phase field models a physical relevance, molecular simulations can provide a link to the required input parameters for the phase field model and interaction potentials [8]. Phase field studies that obtain their input parameters from molecular simulations can, for instance, be found in [8–11]. Crucial input parameters for phase field models investigating droplet behavior, like the contact angle or the width of the transition zone between the liquid and the gas phase, could, for example, be derived from [12].

When using a phase field model to compute the static equilibrium configuration of a droplet that is in contact with a solid surface the solution is given by the first order optimality condition of an energy functional. As this can lead to a computation of saddle points and maxima rather than minima of the energy functional, a closer investigation of the obtained solution becomes necessary in order to determine the stability of the solution and if a minimum

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energy configuration is attained. While much work has been done on the stability analysis of droplets on a variety of different substrates, see e.g. [13–22], the investigation of the static solution state of a phase field model in order to determine the character of the obtained solution needs (to the best of the authors' knowledge) yet to be done and is the main purpose of the present work.

The basic framework of computing the solution of a phase field model by solving the first order optimality condition of an energy functional is commonly used in a variety of different phase field models. Therefore, the presented post-processing can easily be adapted to a wide range of phase field models and is not limited to the specific case presented in this paper.

The following sections will first give an introduction to the underlying phase field model. Subsequently, an investigation of the eigenvalues and eigenvectors of the system matrix and thereby of the stability of droplet shapes is undertaken. In order to illustrate the stability analysis three examples are presented.

## 2. Phase field model

The present work incorporates a phase field model for a two-phase droplet system (liquid/gas) that is capable of regarding the contact angle between the liquid and a solid surface as well as preserving a specified droplet volume. Since the static solution of small-scale droplets is considered, the influence of gravity is neglected. After a description of the phase field model some details of the numerical implementation are given and the considered eigenproblem is formulated.

### 2.1. Model description

Based upon a continuous order parameter  $\varphi(\mathbf{x}, t)$  that indicates whether the gas or the liquid phase is present at a certain location

$$\varphi = \begin{cases} 0, & \text{for gas} \\ 1, & \text{for liquid} \end{cases} \quad (1)$$

the free energy  $F$  is defined as

$$F = \int_{\Omega} \left[ 12 \frac{\gamma_{GL}}{\kappa} f(\varphi) + \frac{3}{4} \gamma_{GL} \kappa |\nabla \varphi|^2 \right] dV + \lambda \left( \int_{\Omega} h(\varphi) dV - V_0 \right) + \int_{\partial\Omega_s} [h(\varphi) \gamma_{SL} + (1 - h(\varphi)) \gamma_{SG}] dA. \quad (2)$$

Here,  $\Omega$  is the domain in which the gas and the liquid phase exist and  $\partial\Omega_s$  denotes the part of the boundary where  $\Omega$  is bounded by a solid surface. In the following,  $F$  is simply referred to as energy. The first contribution to  $F$  includes the separation and gradient terms which are well known for phase field models. The surface tension between the gas and the liquid phase is given by  $\gamma_{GL}$  and  $f(\varphi)$  is a classical double well potential

$$f(\varphi) = \varphi^2(1 - \varphi)^2. \quad (3)$$

The separation and gradient terms are weighted in such a way that the width of the transition zone between gas and liquid can be adjusted by  $\kappa$ . In order to give  $\kappa$  a physical meaning it can be set to a value that represents the width of the density gradient between liquid and gas (approximately 1 nm). As mentioned this width can be obtained from molecular simulations. However, since the width of the transition zone between gas and liquid needs to be resolved by an adequate number of finite elements, simulations that are not done on a molecular scale require a larger choice of  $\kappa$  in order to limit the numerical cost. For an interpretation of the parameters in phase field simulations, see e.g. [23]. A deeper

discussion of the width of the transition zone and the so called sharp-interface limit beyond which the phase field results do not depend on the width of the transition zone can for instance be found in [24] or [25].

Solely minimizing the energy contributed by the surface tension  $\gamma_{GL}$  would inevitably cause the drop to shrink and vanish. Therefore, an additional volume constraint has to be added in order to prescribe the liquid volume  $V_l$ . Ideas to enforce a volume constraint within a phase field model are presented in [6,4]. In the present work we choose a Lagrange multiplier  $\lambda$  to incorporate the volume constraint (second contribution to (2)). In comparison to a penalty term this adds one global degree of freedom  $\lambda$  which only marginally rises the numerical cost for the finite element implementation. During the simulation, the liquid volume  $V_l = \int_{\Omega} h(\varphi) dV$  is conserved with the target volume  $V_0$  without the need of computing and updating an intermediate solution. Therefore, the volume constraint does not contribute to the free energy of the domain. The value of  $\lambda$  is equivalent to the difference between the pressure inside and outside of a droplet which can also be obtained analytically by the Young-Laplace equation for spherical droplets [26].

The third contribution to (2) adds the energy contributions of the surface tension between the solid surface and the liquid  $\gamma_{SL}$  as well as the surface tension between the solid surface and the gas  $\gamma_{SG}$  and allows for an adjustment of the contact angle  $\Theta$  between a droplet and a solid surface [3]. With these energy contributions the natural boundary conditions read

$$\frac{3}{2} \gamma_{GL} \kappa \nabla \varphi \cdot \vec{n} + h'(\varphi) (\gamma_{SL} - \gamma_{SG}) = 0, \quad (4)$$

for the part of the boundary where  $\Omega$  is bounded by a solid surface  $\partial\Omega_s$  and

$$\nabla \varphi \cdot \vec{n} = 0, \quad (5)$$

for the remaining boundary of  $\Omega$ . Here,  $\vec{n}$  is the outer normal to the boundary. Young's equation for the contact angle

$$\cos \Theta = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma_{GL}} \quad (6)$$

is not explicitly prescribed. However, it can be shown that boundary condition (4) leads to Young's equation. For more details the reader is referred to [27].

For numerical reasons (smoothness and stability) the interpolation function [28]

$$h(\varphi) = \varphi^3(6\varphi^2 - 15\varphi + 10) \quad (7)$$

is introduced in (2). For both, the volume constraint as well as the energy contribution from the contact with the solid, this smooth function brings the advantage that  $h'(0) = 0$  and  $h'(1) = 0$  while satisfying  $h(0) = 0$  and  $h(1) = 1$ .

Cahn-Hilliard type approaches have a stiff numerical behavior due to the fourth order spatial derivatives and (low order) bilinear elements cannot be applied [29]. For their implementation in the FE context techniques like mixed finite element methods, coupled equations, interpolation functions that have a high degree of continuity, or a discontinuous Galerkin method are required [30]. Without claiming completeness we cite [30–32,29]. In the context of explicit finite differences the Cahn-Hilliard type approach requires small time steps thus the identification of equilibrium states is very cumbersome. To bypass these drawbacks an evolution equation of Allen-Cahn [33] type is chosen for the presented FE model as it allows for a simpler and therefore resource efficient implementation [7] and has proven to be useful for the simulation of droplets [3,6,7]. Although the Allen-Cahn evolution equation might follow a different kinetic path to find the static equilibrium state of a droplet it will reach the same stationary solution as the

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