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Efficient Numerical Methods for Computing Stationary States of Spherical Landau-Brazovskii Model

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Abstract. In this paper, we develop a set of efficient methods to compute stationary states of the spherical Landau-Brazovskii (LB) model in a discretization-then-optimization way. First, we discretize the spherical LB energy functional into a finite-dimensional energy function by the spherical harmonic expansion. Then five optimization methods are developed to compute stationary states of the discretized energy function, including the accelerated adaptive Bregman proximal gradient, Nesterov, adaptive Nesterov, adaptive nonlinear conjugate gradient and adaptive gradient descent methods. To speed up the convergence, we propose a principal mode analysis (PMA) method to estimate good initial configurations and sphere radius. The PMA method also reveals the relationship between the optimal sphere radius and the dominant degree of spherical harmonics. Numerical experiments show that our approaches significantly reduce the number of iterations and the computational time.

AMS subject classifications: 20C35, 35Q74, 49M37

Key words: Spherical Landau-Brazovskii model, stationary states, spherical harmonic expansion, optimization methods, principal mode analysis.

1 Introduction

Landau models are powerful tools for studying the microscopic behavior of structures in physics and materials science, such as symmetry breaking [20], pattern formation [10, 30, 40] and phase transitions [33, 38]. These models utilize order parameter functions to

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characterize the degree of order in the system. One specific Landau model of interest is the Landau-Brazovskii (LB) model [10], which has proven valuable in describing periodic crystals and phase transitions in Euclidean space [33, 38, 40]. Recently, the spherical LB model has been widely employed to explore pattern formation [23, 29], block copolymer assembly [39], and viral capsids [13] on a spherical surface. Compared with the Swift-Hohenberg model without three-body interaction terms [1–3, 5, 6, 14, 24, 30], the LB model can describe the first-order phase transition [10, 16, 38]. In this work, we focus on the development of efficient methods of finding equilibrium ordered structures of spherical LB model instead of studying quasi-equilibrium dynamical phase behavior.

The presence of multiple solutions and non-linearity poses a challenge in designing fast and efficient methods for quickly finding stationary states. Efficient computation of stationary states of the Landau free energy functional, corresponding to ordered structures, is essential due to their significance in determining material properties. Generally, existing numerical approaches for computing stationary states of the Landau free energy functional can be divided into three categories. The first category involves solving the Euler-Lagrange equation, the first-order variation of free energy functional. The second category comprises gradient flow approaches, such as general semi-implicit methods [3, 24, 39], stabilized factor methods [15, 27], exponential time difference schemes [29], convex splitting [28, 32], operator splitting [21, 37] and auxiliary variable methods [26, 35, 36]. Except the time discretization methods, spatial discretization techniques are important to numerically solve gradient flow equations, including the finite difference method [34], the finite volume method [31], the finite element method [2, 3, 6] and the spectral method [24, 39]. Gradient flow approaches primarily focus on the dynamic evolution of ordered structures. The third approach treats the problem as an optimization task, directly computing stationary states of free energy functional using optimization algorithms based on proper spatial discretization methods. A relevant study concerning spherical Landau models is the calculation of multi-component lipid vesicles on a spherical surface [22]. This study discretizes the modified Landau-Ginzburg free energy using spherical harmonics and directly obtains stationary states using the Broyden-Fletcher-Goldfarb-Shanno algorithm. Furthermore, a similar idea has been shown to be more efficient than the second category approach for finding stationary states of single- and multi-component phase field models in Euclidean space [7, 8, 18]. Motivated by this, our work aims to efficiently compute stationary states of the spherical LB model using the third type of numerical approach.

This work has two main contributions. The first contribution is to develop a set of optimization algorithms to directly compute stationary states of discretized spherical LB free energy based on the spherical harmonics discretization. The optimization approaches include the accelerated adaptive-Bregman proximal gradient (AA-BPG), Nesterov, adaptive Nesterov (ANesterov), adaptive gradient descent (AGD) and adaptive nonlinear conjugate (ACG) methods. Theoretically, we give the convergence properties of these algorithms for the spherical LB model. Besides the efficient algorithms, good initial values can greatly speed the convergence to stationary structures. Inappropri-