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Stability of Soft Quasicrystals in a Coupled-Mode Swift-Hohenberg Model for Three-Component Systems

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Abstract. In this article, we discuss the stability of soft quasicrystalline phases in a coupled-mode Swift-Hohenberg model for three-component systems, where the characteristic length scales are governed by the positive-definite gradient terms. Classic two-mode approximation method and direct numerical minimization are applied to the model. In the latter approach, we apply the projection method to deal with the potentially quasiperiodic ground states. A variable cell method of optimizing the shape and size of higher-dimensional periodic cell is developed to minimize the free energy with respect to the order parameters. Based on the developed numerical methods, we rediscover decagonal and dodecagonal quasicrystalline phases, and find diverse periodic phases and complex modulated phases. Furthermore, phase diagrams are obtained in various phase spaces by comparing the free energies of different candidate structures. It does show not only the important roles of system parameters, but also the effect of optimizing computational domain. In particular, the optimization of computational cell allows us to capture the ground states and phase behavior with higher fidelity. We also make some discussions on our results and show the potential of applying our numerical methods to a larger class of mean-field free energy functionals.

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Key words: Quasicrystals, coupled-mode Swift-Hohenberg model, variable cell method, projection method, phase diagram.

1 Introduction

Since the first discovery of quasicrystal in a rapidly-quenched Al-Mn alloy in 1980s [1], hundreds of metallic quasicrystals, whose building blocks are on the atomic scale, are

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found both in syntheses in the laboratory [2–7] and in nature [8]. More recently, a growing number of mesoscopic quasicrystalline orders are reported in soft-matter systems [9–12]. These soft quasicrystals exhibit distinct properties from their solid-state counterparts. For example, dodecagonal or even higher order symmetry are possible in the soft-matter systems [9, 10, 13], while dodecagonal solid-state quasicrystals are rarely seen [5]. Hence, soft quasicrystals are thought to have essentially different source of stability.

Theoretical studies on the origin and stability of an order pattern, including periodic and quasiperiodic crystals, often involve minimizing a suitable free energy functional of the system, and comparing free energies of different candidate phases [14, 15]. Therefore a systematic investigation of the stability of quasicrystals requires the availability of appropriate free energy functionals and accurate methods of evaluating free energies of quasicrystals. Several microscopic models have been studied over the years to explore the formation of quasicrystals arising from pair potentials with more than one microscopic length scales. Among them, Denton and Löwen [16] obtained stable colloidal quasicrystals within one-component system. On the other hand, phenomenological models based on coarse-grained free energy functionals are widely applied and particularly useful to the study of the stability of soft quasicrystals [17–22, 25]. The earliest one can trace back to Alexander and McTague [17]. They showed the possibility of stabilizing icosahedral quasicrystal using a Landau-type free energy functional with one order parameter. Related works include Bak [18], Jarić [19], Kalugin *et al.* [20] and Gronlund and Mermin [21]. Mermin and Troian [22] followed Alexander and McTague's theory, but introduced a second order parameter to obtain stable icosahedral quasicrystal. Swift and Hohenberg [23] added a positive-definite gradient term into the free energy functional to represent the effect of characteristic length scale. From the viewpoint of Fourier space, the gradient term is small only near the critical wave number $k_c = 1$, thus suppressing the growth of any instabilities with wave numbers away from this value. Their model can be used to describe the supercritical instability transition from a homogeneous state to one-mode patterns. After that, Müller [24] used a set of two coupled partial differential equations; the pattern of a primary field is stabilized by a secondary coupled field which provides an effective space-dependent forcing. Two-dimensional quasicrystals, consisting of 8- and 12-fold orientational order have been obtained in their models. Later, Dotera [25] extended Mermin-Troian model to ABC star copolymer systems with incompressible condition; several ordered two-dimensional phases were investigated, including quasicrystals with decagonal and dodecagonal symmetry and an Archimedean tiling pattern named (3.3.4.3.4).

Beyond the study of soft quasicrystals, Lifshitz and Petrich [26] investigated quasicrystalline patterns arising in parametrically-excited surface waves. Although motivated by different physical phenomena, the free energy functional of their model is in a similar form with those in the preceding Landau-type models. They used only one order parameter describing the amplitude of the standing-wave pattern, yet an additional differential term characterizing multiple-frequency forcing in the free energy functional. They successfully stabilized dodecagonal quasicrystalline pattern by introducing