Renormalization-group theory for the phase-field crystal equation

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We derive a set of rotationally covariant amplitude equations for use in multiscale simulation of the two-dimensional phase-field crystal model by a variety of renormalization-group (RG) methods. We show that the presence of a conservation law introduces an ambiguity in operator ordering in the RG procedure, which we show how to resolve. We compare our analysis with standard multiple-scale techniques, where identical results can be obtained with greater labor, by going to sixth order in perturbation theory, and by assuming the correct scaling of space and time.

I. INTRODUCTION

A fundamental theoretical and computational challenge in materials modeling is that of simultaneously capturing dynamics occurring over a wide range of length and time scales, under processing conditions. A classic example of such a multiscale problem is dendritic growth, a phenomenon seen in the solidification of undercooled melts, which involves the capillary length $\sim 10^{-9}$ m, the scale of the pattern $\sim 10^{-6}$ m, and the diffusion length $\sim 10^{-4}$ m, which together span length scales over five orders of magnitude, and heat and solute transport through diffusion which occurs on time scales of $\sim 10^{-3}$ s. Only recently, after considerable advances in computing technology, and through the use of sophisticated computational techniques [1–3], has this problem become tractable in three dimensions. Although a number of computational approaches [4,5] including quasicontinuum methods [6–9], the heterogeneous multiscale method [10,11], multiscale molecular dynamics [12–15], multigrid variants [16], and extensions of the phase-field model [17] have been proposed, they all appear to have significant limitations. Developing a "handshake" algorithm, to seamlessly integrate the transition between scales, is a common problem. Also, most models appear to be capable of handling only a limited number of crystallographic orientations, with a few isolated defects.

Elder *et al.* [18,19] recently proposed a continuum, nonlinear partial differential equation, which they called the phase-field crystal (PFC) model, for realistically describing materials processing phenomena in polycrystalline materials. The PFC equation describes the evolution of the time-averaged density field in the material, subjected to the essential constraint of mass conservation. While averaging the density makes it possible for the model to capture phenomena over diffusive time scales (not possible with molecular dynamics), the spatially periodic variations, with a wavelength on the order of the interatomic spacing, allow it to incorporate lattice defects such as vacancies. These rapid spatial variations, however, are also the bane of the model, as they necessitate the use of a uniformly fine computational mesh whose grid spacing approaches the interatomic separa-

tion. Thus the PFC model is computationally expensive for mesoscale problems (such as dendritic growth), although still considerably better than a molecular dynamics calculation.

We have recently described a theoretical approach to this difficulty [20,21], presenting a heuristic renormalization-group (RG) [22] method to coarse-grain the PFC equation and obtain equations of motion for the amplitude and phase of the periodic density field. Using these variables, it is possible to reconstruct the original field to a certain order of approximation. The main advantage of such a description is that the amplitude and phase of the density field vary on length scales much larger in comparison to those of the field itself, which enables us to use a coarser mesh to speed up calculations (see [20] for details on accuracy and speedup). Furthermore, the relative uniformity of these variables permits solution of the equations governing them on an adaptive grid which, we anticipate, will further improve computational efficiency. We emphasize that the RG procedure is more than a naive coarse graining in real space of the density, because it uses the dynamics inherent in the underlying equation to project out the long-wavelength, small-frequency behavior. The essential effect of this distinction is that valuable aspects of the phase-field crystal model, such as its native inclusion of elasticity, are preserved. In [20,21] we verified explicitly, by numerical calculation, how the RG equations are able to accomplish this, and thus are suitable for dealing with polycrystalline systems.

The main purpose of the present paper is to present full details of the systematic calculation to derive such coarse-grained equations from the PFC equation. A secondary goal is to compare and contrast the variety of techniques that are available to derive coarse-grained equations of motion. A rather surprising finding of our work was that when we followed naively the "cookbook recipe" for each method, our results were not identical, with the RG methods yielding a form of the amplitude equation slightly different from that derived by the classical method of multiple scales. The PFC equation obeys a local conservation law, and while this by itself can lead to a variety of interesting features [23], it also brings to the fore an ambiguity with the usual implementation of the renormalization procedure, something that is not unique to conservation laws. This ambiguity is essentially an

operator ordering one, and can be remedied in a straightforward way. Once done, all methods yield the same amplitude equation, even though the technical details are quite distinct in the different methods. As a pedagogical exercise, we present the analysis for the Van der Pol oscillator in the Appendix, once again obtaining consistent results from all methods when using the approach described herein. Our main conclusion is that the renormalization-group method is still considerably easier to implement than competing approaches, and in particular requires no knowledge of the scaling relationship between space and time while achieving full rotational covariance at lowest order in perturbation theory.

In the remainder of this introduction, we review the main conceptual developments leading up to the techniques described in this paper. It is now relatively standard in nonlinear pattern formation problems to use amplitude equations to uncover universal features of pattern forming systems. The formalism, first introduced by Newell, Whitehead, and Segel (NWS) [24,25] to describe periodic patterns in Rayleigh-Bénard convection, offers a way to extract the spatiotemporal envelope of these patterns, which then allows one to predict the dynamics qualitatively with very little information about microscopic details. Unfortunately, however, the NWS equation, as originally constructed, can only describe the dynamics of patterns oriented along the same fixed direction, everywhere in space, whereas physical systems often produce complex mosaics of patterns with no particular orientational preference. Such mosaics arise in real systems which are invariant under rotations, and hence any equation which is used to study them must also have the crucial property of rotational covariance, something that is lacking in the NWS equation. Equations with an orientational bias can be very difficult to implement numerically, especially on systems with arbitrarily oriented patterns. Nevertheless, the NWS equation embodies the important notion of coarse graining, which has played a significant role in shaping the modern day theory of pattern formation [26], and also forms the basis of our approach to multiscale modeling with the PFC equation.

Gunaratne *et al.* [27] first derived a rotationally covariant form of the NWS equation using the method of multiple scales [28–31], where they assumed isotropic scaling of the spatial variables. They showed that the spatial operator in the NWS equation could be *symmetrized*, by systematically extending the calculation to higher orders in the perturbation parameter ϵ, the reduced Rayleigh number. They explained that the finite truncation of the perturbation series destroyed the rotational symmetry of the operator, which could, however, be recovered at a higher order. Another important conclusion of their work was that the qualitative behavior of pattern formation remained unchanged if one ignored higher-order corrections, provided the equation itself was rotationally covariant. A drawback of their calculation, however, was (as with any application of the method of multiple scales) the need to guess *a priori* the correct scaling of space-time variables. In addition, their calculation required gradual accumulation of operators and terms up to $O(\epsilon^4)$, before a rotationally covariant equation emerged.

A more systematic approach emerged shortly after. Chen *et al.* showed how to perform reductive perturbation theory using RG methods [32], and obtained the NWS equation for the Swift-Hohenberg equation [33] by renormalizing the leading secular divergences at each order. Graham [34] subsequently showed that, in fact, this method gave the fully rotational covariant equations, if all secular terms are renormalized and a careful choice of operator splitting is used. Calculations involving the RG typically produce elegant and accurate uniformly valid approximations for ordinary differential equations (ODEs), starting from simple perturbation series where no knowledge of the scaling present in the system is exercised [32]. For partial differential equations (PDEs), the same approach is successful, but generates a tedious number of perturbation terms at higher orders. This difficulty arises from the need to explicitly construct secular solutions of the highest possible order, at every order in ϵ, and from a practical standpoint equals (if not outweighs) the advantage of requiring no prior insight into the problem. For this reason, calculations employing this method for PDEs have rarely gone beyond $O(\epsilon)$. The key advantage of the RG method, however, is that when carefully performed, the calculation yields a rotationally covariant amplitude equation at a much lower order in ϵ compared to the method of multiple scales, as was shown by Graham [34].

Nozaki *et al.* [35,36] have developed a more abstract version of the perturbative RG for weakly nonlinear PDEs, called the "proto-RG" scheme. They argue that if one is willing to sacrifice some of the purely mechanical aspects of the conventional RG by taking cognizance of the system's properties, such as those exhibited by the governing differential equation, one can obtain a rotationally covariant amplitude equation to $O(\epsilon)$ without having to construct any secular solutions. By computing minimal particular solutions, usually obtained by a straightforward inspection, one can even obtain $O(\epsilon^2)$ corrections with only a little more algebra. They illustrated the relative simplicity of this method by deriving the rotationally covariant form of the NWS equation to $O(\epsilon^2)$, as previously derived by Gunaratne *et al.* [27]. Shiwa [37] further demonstrated the efficacy of this scheme by obtaining the well-known Cross-Newell phase equation [38,39], which describes phase dynamics of patterns generated by the Swift-Hohenberg equation. A drawback of this approach is in the selection of the so-called proto-RG operator, which turns out to be nonunique in general. Nozaki *et al.* show, however, that the operator *is* uniquely specified, provided we insist on the lowest-order differential operator possible.

As the reader will have no doubt realized from this synopsis, several methods and variants exist for deriving envelope equations from order parameter equations (OPEs) that produce predominantly periodic patterns. Although one may argue that some of these methods are essentially variants of perturbative RG theory for PDEs, they are structurally very different. It is thus a very instructive exercise to compare the defining properties of each of these methods in the context of a single microscopic OPE. We present such a detailed study in this paper using the PFC equation, which unlike the Swift-Hohenberg model, has not been extensively studied.

The paper is organized as follows. To set the context for our work, we briefly introduce the PFC model in Sec. II. In Sec. III we present a detailed derivation of an amplitude

equation from the PFC model using a heuristic approach. In Sec. IV, we use the proto-RG method to derive the amplitude equation more systematically. We attempt to verify these calculations independently in Sec. V using the method of multiple scales. A one-dimensional (1D) derivation via the conventional RG method is presented for completeness in Sec. VI. We find that while the proto-RG and RG results are consistent, they do not agree with the other calculations, due to an operator ordering ambiguity not previously noticed. We remedy this in Sec. VII, and conclude with some remarks in Sec. VIII.

II. THE PHASE-FIELD CRYSTAL EQUATION

The phase-field crystal model proposes a sixth-order nonlinear partial differential equation for describing the space-time evolution of the time-averaged, conserved density variable $\psi(\mathbf{x},t)$, of a material. As has been shown [18,19], this equation has the potential to accurately model a variety of key materials processing phenomena, including heterogeneous nucleation and grain growth, liquid phase epitaxial growth, ductile fracture mechanics, dislocation mechanics [40], and plasticity. An important feature that differentiates it from another popular continuum material model, the phase-field model [17], is its incorporation of elasticity in the free-energy functional through terms that guarantee gradients in the equilibrium density field, for certain values of the control parameters. Crucial to the construction of this free energy, is the observation that elasticity is a natural property of a system which is characterized by periodic fields. We refer the reader to the exhaustive article by Elder and Grant [19] for a detailed description of the model and its applications.

From the point of view of pattern formation theory, the PFC equation is the conserved analog of the simplest form of the Swift-Hohenberg equation (with only the cubic nonlinearity), and is written as

$$\partial_t \psi = \nabla^2 \{[(1+\nabla^2)^2 - \epsilon]\psi + \psi^3\} + \zeta. \tag{1}$$

Here, ϵ is the scaled undercooling, a parameter akin to the modified Rayleigh number, controlling the stability of the uniform phase $\bar{\psi}$ (liquid) to the appearance of either a periodic striped phase or a periodic hexagonal phase (both crystalline solids), and ζ is the conserved Gaussian noise which accounts for thermal fluctuations in the system. A phase diagram illustrating the phase boundaries and coexistence curves in $\epsilon - \bar{\psi}$ space is given in [19].

For present purposes we will concern ourselves only with the uniform to hexagonal phase transition (but we are not in any way restricted to it), and will disregard ζ in view of its relative unimportance in describing phase transition kinetics. In a single-mode approximation, a hexagonal pattern is described by

$$\psi(\mathbf{x},t) = \sum_{j=1}^{3} A_j(t)e^{i\mathbf{k}_j \cdot \mathbf{x}} + \bar{\psi} + \text{c.c.}, \tag{2}$$

where $\mathbf{k}_1 = k_0(-\vec{i}\sqrt{3}/2 - \vec{j}/2)$, $\mathbf{k}_2 = k_0\vec{j}$ and $\mathbf{k}_3 = k_0(\vec{i}\sqrt{3}/2 - \vec{j}/2)$ are the reciprocal lattice vectors, k_0 is the wave number of

the pattern, $\vec{i}$ and $\vec{j}$ are unit vectors in the x and y directions, A_j are the complex amplitude functions, and c.c. denotes the complex conjugate. We point out that a striped pattern, with the stripes parallel to the x axis, can be represented by the same equation above with $A_1 = A_3 = 0$ and $A_2 \neq 0$. As shown in Fig. 1 however, the PFC equation describes the evolution of several such hexagonally patterned crystals of arbitrary orientation, that collide to form grain boundaries. While the pattern remains periodic within each crystal, there is a break in the periodicity across the boundaries. Equation (2) can be made to describe such a system by allowing the A_j to be spatially varying, i.e., $A_j(\mathbf{x},t)$. Our goal is then to derive evolution equations for $A_j(\mathbf{x},t)$, which along with Eq. (2) can be used to reconstruct $\psi(\mathbf{x},t)$ in a one-mode approximation. Note that $A_j(\mathbf{x},t)$ now contains information about both the envelope function (amplitude modulus) as well as the orientation (phase angle) of each grain, but varies on a much larger length scale.

In order to proceed with our analysis, which is essentially perturbative, we identify ϵ as a small parameter, in powers of which we shall expand ψ about the steady-state solution. We point out that the PFC model stipulates no such restrictions on the value of ϵ, other than $\epsilon \geq 0$, whereas it is natural to expect our treatment to restrict the validity of the amplitude equations so derived to small values of $\epsilon \ll 1$.

III. HEURISTIC RG CALCULATION

We now present a derivation of the amplitude equation from Eq. (1) using linear stability analysis and a shortcut motivated by experience. An idea along these lines was previously implemented by Bestehorn and Haken [41] to derive an OPE (similar to the Swift-Hohenberg equation) for modeling traveling waves and pulses in two-dimensional systems, but not for deriving amplitude equations.

We pose Eq. (1) in a more convenient form by scaling ψ by $\sqrt{\epsilon}$, and calling this new variable ψ. In this manner, Eq. (1) becomes

$$\partial_t \psi = \nabla^2 (1+\nabla^2)^2 \psi + \epsilon \nabla^2 (\psi^3 - \psi). \tag{3}$$

Let us now consider the stability of the uniform phase solution $\bar{\psi}$ to the formation of the hexagonal pattern by adding to it a small perturbation $\tilde{\psi}$, so that $\psi = \bar{\psi} + \tilde{\psi}$. Substituting in Eq. (3) and linearizing about $\bar{\psi}$ we obtain

$$\partial_t \tilde{\psi} = \nabla^2 [\epsilon(3\bar{\psi}^2 - 1) + (1+\nabla^2)^2]\tilde{\psi}. \tag{4}$$

If $\tilde{\psi}$ is a hexagonal instability in the form given by the spatially dependent part of Eq. (2), then using $A_j(t) = A_{0j}\exp(\omega_j t)$, where A_{0j} are complex constants, and substituting in Eq. (4), we obtain the discrete dispersion relation

$$\omega_j = -|\mathbf{k}_j|^2 [\epsilon(3\bar{\psi}^2 - 1) + (1-|\mathbf{k}_j|^2)^2], \tag{5}$$

after applying orthogonality conditions. Here ω_j predicts the growth or decay rate of a hexagonal instability in the spatially uniform system. Note that for real values of $\bar{\psi}$, ω_j is always real. Thus, a necessary condition for the instability to
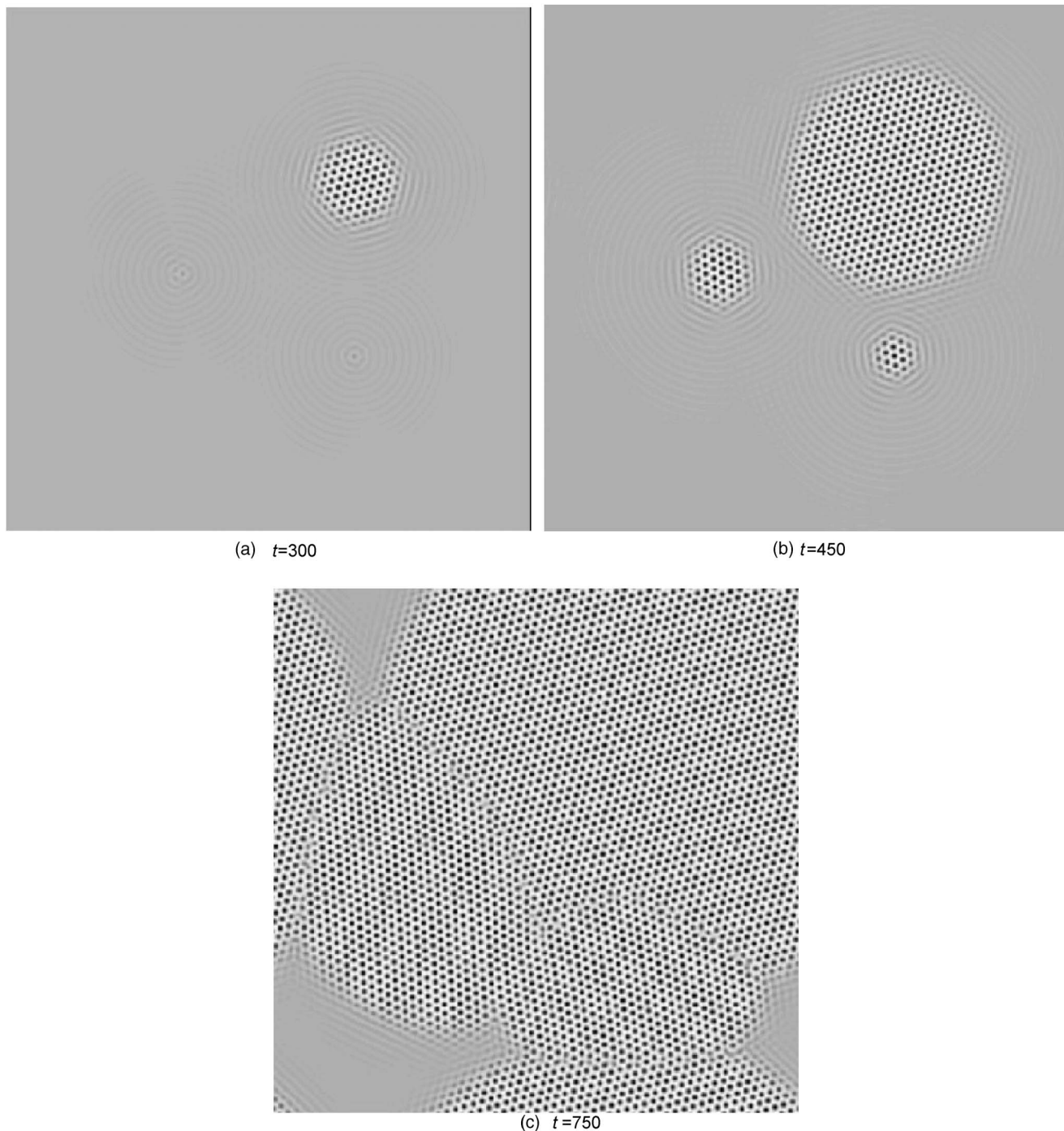
(a) $t=300$

(b) $t=450$

(c) $t=750$

FIG. 1. Heterogeneous nucleation, crystal growth, and formation of grain boundaries in a 2D film from three randomly oriented seeds, as simulated by the PFC model. The field plotted is the density variable $\psi(\mathbf{x},t)$. Note that the pattern is periodic inside each grain.

grow, i.e., for ω_j to take on positive values, is $3\bar{\psi}^2-1<0$, or equivalently $3\bar{\psi}^2-\epsilon<0$ in original variables. The most dangerous wave number is the locus $|\mathbf{k}_j|=k_0=1$.

We now consider spatial modulations in the amplitude about this preferred wave number, i.e.,

$$A_j(t) \mapsto A_{Rj}(\mathbf{x},t) = A_{0j}e^{\omega_j(\mathbf{Q})t}e^{i\mathbf{Q}\cdot\mathbf{x}}, \qquad (6)$$

where $\mathbf{Q}=Q_x\vec{i}+Q_y\vec{j}$ is a perturbation vector, and A_{Rj} is the renormalized amplitude, whose implication will be clarified

below. Consistent with Eq. (5), we can now write the exponent controlling growth rate along each lattice vector as

$$\omega_j(\mathbf{Q}) = |\mathbf{Q}+\mathbf{k}_j|^2[\epsilon(1-3\bar{\psi}^2) - (1-|\mathbf{Q}+\mathbf{k}_j|^2)^2]. \qquad (7)$$

We now replace the Fourier space variables in the above equation by their real space counterparts so that

$$\omega_j \equiv \partial_t, \quad Q_x \equiv -i\partial_x, \quad Q_y \equiv -i\partial_y, \qquad (8)$$

thus obtaining

$$|\mathbf{Q} + \mathbf{k}_j|^2 \equiv 1 - \nabla^2 - 2i\mathbf{k}_j \cdot \nabla = 1 - \mathcal{L}_{\mathbf{k}_j}. \tag{9}$$

Combining Eqs. (7) and (9), the space-time amplitude variations along each lattice vector is given by the sixth-order linear partial differential equation

$$\partial_t A_{Rj} + (1 - \mathcal{L}_{\mathbf{k}_j})\mathcal{L}_{\mathbf{k}_j}^2 A_{Rj} + \epsilon(1 - 3\bar{\psi}^2)\mathcal{L}_{\mathbf{k}_j} A_{Rj} = \epsilon(1 - 3\bar{\psi}^2)A_{Rj}. \tag{10}$$

We also need nonlinear terms, which play a vital role in pattern dynamics near onset of the instability, to complement the above set of equations. There are a couple of different ways to obtain these terms. One can directly look for the nonlinear part in the normal form equations [42] for the dynamics of A_j in a hexagonal basis [27,43,44]. These equations have been widely used to study the dynamics and stability of *exactly* periodic rolls and hexagonal patterns originating from the static conducting state in Rayleigh-Bénard convection. Alternatively, one can derive these terms to a particular order in ϵ through a renormalization-group (or multiple-scale) analysis of the governing differential equation. Here, we choose the latter approach, starting from Eq. (3), but only going far enough in the RG analysis to identify the correct form of the terms.

We start with a perturbation series in ϵ,

$$\psi = \psi_0 + \epsilon\psi_1 + \epsilon^2\psi_2 + \epsilon^3\psi_3 + \cdots, \tag{11}$$

where ψ_0 is a steady-state solution and $\psi_{j(\neq 0)}$ are the higher-order corrections. As we are interested in amplitude variations in the hexagonal pattern, we pick ψ_0 to be the steady *hexagonal* solution, i.e., Eq. (2) with $A_j(t)$ replaced by $A_j(t \to \infty)$. Substituting in Eq. (3), we obtain the following equation at $O(\epsilon)$:

$$[\partial_t - \nabla^2(1 + \nabla^2)^2]\psi_1 = (\partial_t - \mathcal{L}_\mathcal{P})\psi_1 = \nabla^2(\psi_0^3 - \psi_0), \tag{12}$$

where

$$\nabla^2(\psi_0^3 - \psi_0) = (1 - 3\bar{\psi}^2)\sum_{j=1}^3 A_j e^{i\mathbf{k}_j \cdot \mathbf{x}}$$

$$- 3A_1(|A_1|^2 + 2|A_2|^2 + 2|A_3|^2)e^{i\mathbf{k}_1 \cdot \mathbf{x}}$$

$$- 3A_2(2|A_1|^2 + |A_2|^2 + 2|A_3|^2)e^{i\mathbf{k}_2 \cdot \mathbf{x}}$$

$$- 3A_3(2|A_1|^2 + 2|A_2|^2 + |A_3|^2)e^{i\mathbf{k}_3 \cdot \mathbf{x}}$$

$$- 6A_2^* A_3^* \bar{\psi} e^{i\mathbf{k}_1 \cdot \mathbf{x}} - 6A_1^* A_3^* \bar{\psi} e^{i\mathbf{k}_2 \cdot \mathbf{x}} - 6A_1^* A_2^* \bar{\psi} e^{i\mathbf{k}_3 \cdot \mathbf{x}}$$

$$+ (\text{other terms}) + \text{c.c.} \tag{13}$$

The asterisk denotes complex conjugation. To this order, the "other terms" are functions of complex exponentials that do not lie in the null space of the linear differential operator in Eq. (12), i.e., they are nonresonant terms. Therefore, they do not contribute to unbounded growth in ψ_1. The terms listed in Eq. (13) are, however, resonant with the operator, and their coefficients need to be renormalized in order to bound the solution obtained by truncating the perturbation series at $O(\epsilon)$. The renormalization procedure allows the amplitude A_j, previously constant, to now have space-time variations that absorb secular divergences. We assert that the nonlinear

terms in the amplitude equation to $O(\epsilon)$ must be the *renormalized* coefficients of the exponential terms in resonance with the differential operator. For example, the terms complementing the space-time operator along basis vector $\mathbf{k}_1$ must be

$$\epsilon(1 - 3\bar{\psi}^2)A_{R1} - 3\epsilon A_{R1}(|A_{R1}|^2 + 2|A_{R2}|^2 + 2|A_{R3}|^2)$$

$$- 6\epsilon A_{R2}^* A_{R3}^* \bar{\psi}, \tag{14}$$

where the A_{Rj} are the renormalized amplitude functions (no longer constants). Note that these terms are completely identical to those predicted by normal form theory for a hexagonal basis [27,44]. Combining Eqs. (10) and (14) we write the amplitude equation as

$$\partial_t A_1 = -(1 - \mathcal{L}_{\mathbf{k}_1})\mathcal{L}_{\mathbf{k}_1}^2 A_1 - \epsilon(1 - 3\bar{\psi}^2)\mathcal{L}_{\mathbf{k}_1}A_1 + \epsilon(1 - 3\bar{\psi}^2)A_1$$

$$- 3\epsilon A_1(|A_1|^2 + 2|A_2|^2 + 2|A_3|^2) - 6\epsilon A_2^* A_3^* \bar{\psi}, \tag{15}$$

for lattice vector $\mathbf{k}_1$, and permutations thereof for $\mathbf{k}_2$ and $\mathbf{k}_3$, where we have replaced the variables A_{Rj} by A_j.

We observe that the leading term in Eq. (14) is consistent with the right-hand side of Eq. (10), thereby providing a natural overlapping link about which to match the linear stability and perturbation results. In a more abstract sense, we draw a parallel between this method and the technique of matched asymptotic expansions in singular perturbation theory, where inner and outer asymptotic solutions are matched over a common region of validity in the solution space, to obtain a globally valid solution. This completes our derivation of the amplitude equation via a heuristic or "quick and dirty" approach. For future reference, we will call Eq. (15) the quick and dirty RG (QDRG) equation, and the method used to obtain it the QDRG (or heuristic) method. As we have already demonstrated the remarkable accuracy with which the QDRG equation mimics the PFC equation in a previous paper [20], we will refrain from presenting any new evidence to that effect here.

To summarize the procedure, we first conducted a linear stability analysis of the scaled PFC equation about the uniform state to obtain a linear differential operator controlling the space-time evolution of the complex amplitude A_j of the hexagonal pattern. We superimposed on this dispersion relation periodic modulations of the amplitude, and from the dispersion relation in terms of these latter modulations, identified the gradient terms in the amplitude equation. We then carried out the first step in a conventional RG analysis to obtain the form of the nonlinear terms that should accompany this differential operator, and combining the two results, we wrote down the amplitude equation for the hexagonal pattern. In this respect, our approach lacks the full mathematical rigor of a conventional RG reduction or a multiple-scale derivation, which gives it a somewhat dirty appearance. However, we made no assumptions about the scaling of the space-time variables in the system, nor did we have to construct any secular solutions so far. We will comment on extending this method systematically to higher orders in ϵ in the following section.

IV. PROTO-RENORMALIZATION-GROUP DERIVATION

With the proto-RG method, our starting point is Eq. (3) with the perturbation series Eq. (11). Thus, to $O(\epsilon)$ we obtain Eq. (12), whereas to $O(\epsilon^2)$ we get

$$(\partial_t - \mathcal{L}_\mathcal{P})\psi_2 = \nabla^2(3\psi_0^2\psi_1 - \psi_1). \tag{16}$$

The structure of Eq. (12) allows us to infer that its simplest particular solution will take the form

$$\psi_1 = \sum_{j=1}^3 P_{1j}(\mathbf{x},t)e^{i\mathbf{k}_j\cdot\mathbf{x}} + \sum_{j=1}^3 Q_{1j}e^{2i\mathbf{k}_j\cdot\mathbf{x}} + \sum_{j=1}^3 R_{1j}e^{3i\mathbf{k}_j\cdot\mathbf{x}}$$
$$+ \sum_{j=1}^3 S_{1j}e^{i\mathbf{s}_j\cdot\mathbf{x}} + \sum_{j=1}^2 T_{1j}e^{i\mathbf{t}_j\cdot\mathbf{x}} + \sum_{j=1}^2 U_{1j}e^{i\mathbf{u}_j\cdot\mathbf{x}} + \sum_{j=1}^2 V_{1j}e^{i\mathbf{v}_j\cdot\mathbf{x}}$$
$$+ \text{c.c.}, \tag{17}$$

where

$$\mathbf{s}_1 = -\vec{i}\frac{\sqrt{3}}{2} - \vec{j}\frac{3}{2}, \quad \mathbf{s}_2 = \vec{i}\frac{\sqrt{3}}{2} - \vec{j}\frac{3}{2}, \quad \mathbf{s}_3 = \mathbf{s}_2 - \mathbf{s}_1,$$

$$\mathbf{t}_1 = -\vec{i}\frac{3\sqrt{3}}{2} - \vec{j}\frac{1}{2}, \quad \mathbf{t}_2 = \vec{i}\frac{3\sqrt{3}}{2} - \vec{j}\frac{1}{2},$$

$$\mathbf{u}_1 = -\vec{i}\frac{\sqrt{3}}{2} - \vec{j}\frac{5}{2}, \quad \mathbf{u}_2 = \vec{i}\frac{\sqrt{3}}{2} - \vec{j}\frac{5}{2},$$

$$\mathbf{v}_1 = -\vec{i}\sqrt{3} - \vec{j}2, \quad \mathbf{v}_2 = \vec{i}\sqrt{3} - \vec{j}2 \tag{18}$$

are nonresonant modes generated by the cubic term. Note that we have explicitly denoted the space-time dependence of the secular coefficients $P_{1j}(\mathbf{x},t)$, which are polynomials in x, y and t, whereas by inspection, the other coefficients Q_{1j}, R_{1j}, S_{1j}, T_{1j}, U_{1j}, and V_{1j} can be complex constants. Specifically, P_{11} satisfies

$$(\partial_t - \mathcal{L}_\mathcal{P})P_{11}e^{i\mathbf{k}_1\cdot\mathbf{x}} = (1 - 3\bar{\psi}^2)A_1 e^{i\mathbf{k}_1\cdot\mathbf{x}} - 3A_1(|A_1|^2 + 2|A_2|^2$$
$$+ 2|A_3|^2)e^{i\mathbf{k}_1\cdot\mathbf{x}} - 6A_2^*A_3^*\bar{\psi}e^{i\mathbf{k}_1\cdot\mathbf{x}}$$

$$\Rightarrow[\partial_t + (1 - \mathcal{L}_{\mathbf{k}_1})\mathcal{L}_{\mathbf{k}_1}^2]P_{11} = (1 - 3\bar{\psi}^2)A_1 - 3A_1(|A_1|^2 + 2|A_2|^2$$
$$+ 2|A_3|^2) - 6A_2^*A_3^*\bar{\psi} \equiv L_{\mathbf{k}_1}P_{11}, \tag{19}$$

where $L_{\mathbf{k}_j}$ is the proto-RG operator for lattice vector $\mathbf{k}_j$. From the above equation it is quite obvious that P_{11} cannot be constant for any nontrivial solutions, and likewise for P_{12} and P_{13}.

As P_{1j} are secular, we now renormalize [32] ψ about arbitrary regularization points $\mathbf{X}$ and T, as in the conventional RG method, to get

$$\psi = \bar{\psi} + \sum_{j=1}^3 A_{Rj}(\mathbf{X},T)e^{i\mathbf{k}_j\cdot\mathbf{x}} + \epsilon\sum_{j=1}^3 [P_{1j}(\mathbf{x},t) - P_{1j}(\mathbf{X},T)]e^{i\mathbf{k}_j\cdot\mathbf{x}}$$
$$+ \cdots + \text{c.c.}, \tag{20}$$

where A_{Rj} is now the renormalized amplitude that absorbs secular divergences. Since ψ must be independent of these regularization points, we have

$$L_{\mathbf{k}_1}^{\mathbf{X},T}\psi = 0$$

$$\Rightarrow L_{\mathbf{k}_1}^{\mathbf{X},T}A_{R1}(\mathbf{X},T) = \epsilon L_{\mathbf{k}_1}^{\mathbf{X},T}P_{11}(\mathbf{X},T) + \epsilon^2 L_{\mathbf{k}_1}^{\mathbf{X},T}P_{21}(\mathbf{X},T)$$
$$+ \epsilon^3 L_{\mathbf{k}_1}^{\mathbf{X},T}P_{31}(\mathbf{X},T) + \cdots \tag{21}$$

after applying orthogonality conditions. This is the general form of the proto-RG equation for weakly nonlinear oscillators [36]. $L_{\mathbf{k}_1}^{\mathbf{X},T}$ is the proto-RG operator $L_{\mathbf{k}_1}$ in Eq. (19), with variables $\mathbf{x}$ and t replaced by $\mathbf{X}$ and T, respectively. Changing back from $(\mathbf{X},T)\rightarrow(\mathbf{x},t)$ and $A_{Rj}\rightarrow A_j$, and using Eqs. (19) and (21), we can write the amplitude equation along lattice vector $\mathbf{k}_1$ to $O(\epsilon)$ explicitly as

$$\partial_t A_1 = -(1 - \mathcal{L}_{\mathbf{k}_1})\mathcal{L}_{\mathbf{k}_1}^2 A_1 + \epsilon(1 - 3\bar{\psi}^2)A_1 - 3\epsilon A_1(|A_1|^2 + 2|A_2|^2$$
$$+ 2|A_3|^2) - 6\epsilon A_2^*A_3^*\bar{\psi}, \tag{22}$$

with appropriate permutations for A_2 and A_3. Note that in using Eq. (19), we have replaced A_j by their renormalized counterparts A_{Rj} as is consistent with the proto-RG procedure, before reverting to the former notation for amplitude. Upon comparing the two amplitude equations obtained so far, Eqs. (15) and (22), we note that the QDRG-derived equation carries the extra term $\epsilon(1-3\bar{\psi}^2)\mathcal{L}_{\mathbf{k}_1}A_1$. Evidently, the QDRG and the proto-RG methods produce different amplitude equations when applied to the PFC equation, the extent of this difference being controlled by the parameter $\epsilon(1-3\bar{\psi}^2)$.

As mentioned earlier, the principal advantage of using the proto-RG method is the relative ease with which one can progress to higher-order calculations. Let us now extend this calculation to $O(\epsilon^2)$. We need ψ_1 in order to evaluate the right-hand side of Eq. (16), which means that we additionally need to evaluate Q_{1j}, R_{1j}, S_{1j}, T_{1j}, U_{1j}, and V_{1j}. The constant values of these terms can be determined by inspection. For example, by analogy with P_{11}, we see that Q_{11} must satisfy

$$(\partial_t - \mathcal{L}_\mathcal{P})Q_{11}e^{2i\mathbf{k}_1\cdot\mathbf{x}} = -12(A_1^2\bar{\psi} + 2A_1A_2^*A_3^*)e^{2i\mathbf{k}_1\cdot\mathbf{x}}$$

$$\Rightarrow [\partial_t + (4 - \mathcal{L}_{2\mathbf{k}_1})(\mathcal{L}_{2\mathbf{k}_1} - 3)^2]Q_{11}$$

$$= -12(A_1^2\bar{\psi} + 2A_1A_2^*A_3^*). \tag{23}$$

Unlike Eq. (19), however, we see that Eq. (23) permits a constant solution for Q_{11}, which in turn is determined to be

$$Q_{11} = -\frac{1}{3}(A_1^2\bar{\psi} + 2A_1A_2^*A_3^*). \tag{24}$$

Similarly, constant solutions for the other coefficients are

$$Q_{12} = -\frac{1}{3}(A_2^2\bar{\psi} + 2A_1^*A_2A_3^*),$$

$$Q_{13} = -\frac{1}{3}(A_3^2\bar{\psi} + 2A_1^*A_2^*A_3),$$

$$R_{1j} = -\frac{A_j^3}{64},$$

$$S_{11} = -\frac{3}{4}(A_1^2A_3 + 2A_1\bar{\psi}A_2^* + A_2^{*2}A_3^*),$$

$$S_{12} = -\frac{3}{4}(A_1A_3^2 + 2A_2^*\bar{\psi}A_3 + A_2^{*2}A_1^*),$$

$$S_{13} = -\frac{3}{4}(A_2A_3^2 + 2A_1^*\bar{\psi}A_3 + A_1^{*2}A_2^*),$$

$$T_{11} = -\frac{A_1^2A_3^*}{12},$$

$$T_{12} = -\frac{A_3^2A_1^*}{12},$$

$$U_{11} = -\frac{A_1A_2^{*2}}{12},$$

$$U_{12} = -\frac{A_3A_2^{*2}}{12},$$

$$V_{11} = -\frac{A_1^2A_2^*}{12},$$

$$V_{12} = -\frac{A_3^2A_2^*}{12}. \tag{25}$$

We know that the particular solution to Eq. (16) has the form

$$\psi_2 = \sum_{j=1}^{3} P_{2j}(\mathbf{x},t)e^{i\mathbf{k}_j\cdot\mathbf{x}} + \cdots + \text{c.c.} \tag{26}$$

where we have shown only the resonant part of the solution. The terms on the right-hand side of Eq. (16), resonant with lattice vector $\mathbf{k}_1$, evaluate to

$$\Phi = \{[1 - 3\bar{\psi}^2 - 6(|A_1|^2 + |A_2|^2 + |A_3|^2)](1 - \mathcal{L}_{\mathbf{k}_1})P_{11} - 3A_1^2(1$$

$$- \mathcal{L}_{\mathbf{k}_1})P_{11}^* - 6A_1A_2(1 - \mathcal{L}_{\mathbf{k}_1})P_{12}^* - 6A_1A_3(1 - \mathcal{L}_{\mathbf{k}_1})P_{13}^*$$

$$- 6\bar{\psi}A_3^*(1 - \mathcal{L}_{\mathbf{k}_1})P_{12}^* - 6\bar{\psi}A_2^*(1 - \mathcal{L}_{\mathbf{k}_1})P_{13}^* - 6A_1A_2^*(1$$

$$- \mathcal{L}_{\mathbf{k}_1})P_{12} - 6A_1A_3^*(1 - \mathcal{L}_{\mathbf{k}_1})P_{13} - 6A_2\bar{\psi}S_{11} - 3A_2^2U_{11}$$

$$- 6A_3A_1^*T_{11} - 6A_2A_1^*V_{11} - 6A_1^*A_3^*S_{11} - 3A_3^{*2}S_{12} - 3A_2^{*2}S_{12}^*$$

$$- 6A_3\bar{\psi}S_{13}^* - 6A_1^*A_2^*S_{13}^* - 3A_3^2T_{12}^* - 6A_2A_3^*Q_{12}^* - 6A_3A_2^*Q_{13}^*$$

$$- 3A_1^{*2}R_{11} - 6A_2A_3Q_{11} - 6\bar{\psi}A_1^*Q_{11}\}e^{i\mathbf{k}_1\cdot\mathbf{x}}. \tag{27}$$

Thus P_{21} satisfies

$$L_{\mathbf{k}_1}P_{21} = \Phi. \tag{28}$$

The nonconstant terms in Φ (terms containing P_{1j}) are now ignored [35,36] while the remaining terms are determined from their constant solutions Eqs. (24) and (25). Thus, using Eq. (21) we can write the amplitude equation along lattice vector $\mathbf{k}_1$ to $O(\epsilon^2)$ as

$$\partial_t A_1 = -(1 - \mathcal{L}_{\mathbf{k}_1})\mathcal{L}_{\mathbf{k}_1}^2 A_1 + \epsilon(1 - 3\bar{\psi}^2)A_1 - 3\epsilon A_1(|A_1|^2 + 2|A_2|^2$$

$$+ 2|A_3|^2) - 6\epsilon A_2^*A_3^*\bar{\psi} + 11\epsilon^2\bar{\psi}A_1^2A_2A_3 + \epsilon^2\bar{\psi}^2A_1(2|A_1|^2$$

$$+ 9|A_2|^2 + 9|A_3|^2) + 11\epsilon^2\bar{\psi}(2|A_1|^2 + |A_2|^2 + |A_3|^2)A_2^*A_3^*$$

$$+ \frac{27}{2}\epsilon^2 A_1^*A_2^{*2}A_3^{*2} + 5\epsilon^2 A_1|A_1|^2(|A_2|^2 + |A_3|^2)$$

$$+ 12\epsilon^2 A_1|A_2|^2|A_3|^2 + \frac{3}{64}\epsilon^2 A_1|A_1|^4 + \frac{5}{2}\epsilon^2 A_1|A_2|^4$$

$$+ \frac{5}{2}\epsilon^2 A_1|A_3|^4, \tag{29}$$

with cyclic permutations for lattice vectors $\mathbf{k}_2$ and $\mathbf{k}_3$.

We can in principle extend the QDRG method also to higher orders by performing the same steps above, until the point where we identify the resonant terms on the right-hand side of Eq. (16), i.e., Φ. Combining this result with Eqs. (10) and (14) we can then obtain the amplitude equation (29), but with an extra term $\epsilon(1 - 3\bar{\psi}^2)\mathcal{L}_{\mathbf{k}_1}A_1$.

In summary, both the proto-RG and the QDRG can be calculated including terms of $O(\epsilon^2)$, and the results differ by a small but nonzero term. Which, if either, of these calculations is correct? And what is the origin of the discrepancy between the two methods? Is the QDRG result not to be trusted, being derived heuristically? Faced with two seemingly incompatible, although very similar, results, it is natural to attempt an independent test of the analysis, which we did using the standard method of multiple scales. This calculation is presented below, but owing to technical complications arising from the interference of modes and the need to go to sixth order of perturbation theory, we found it only feasible to perform the calculation for the case of one dimension. Nevertheless, we will see that, in fact, the QDRG result Eq. (15) is more correct. The small discrepancy between this result and the proto-RG result is finally resolved in Sec. VII.

V. MULTIPLE-SCALE DERIVATION

We now rederive the amplitude equation using the traditional method of multiple scales. As the primary purpose of this derivation is to verify the previous calculations via an independent method, we stick to a one-dimensional analysis here that considerably simplifies the algebra. For convenience we use $\delta^2 = \epsilon$, and write Eq. (3) in 1D as

$$[\partial_t - \partial_x^2(1 + \partial_x^2)^2]\psi = \delta^2\partial_x^2(\psi^3 - \psi). \qquad (30)$$

The basic premise of the multiple-scale analysis is that while the pattern itself varies on the scale of its wavelength $(2\pi/k_0)$, its amplitude varies on much larger length and time scales. It is then appropriate to introduce slowly varying arguments

$$X = \delta x, \quad T = \delta^2 t \qquad (31)$$

for the envelope function $A(X,T)$. This scaling was previously applied by Gunaratne *et al.* [27] to the Swift-Hohenberg equation with success (based on the form of the discrete dispersion relation), and as the PFC equation is essentially a conserved analog of the Swift-Hohenberg equation we anticipate that the same scaling holds here.

Derivatives scale as follows:

$$\partial_x \rightarrow \partial_x + \delta\partial_X,$$

$$\partial_x^2 \rightarrow \partial_x^2 + 2\delta\partial_X\partial_x + \delta^2\partial_X^2,$$

$$\partial_t \rightarrow \delta^2\partial_T, \qquad (32)$$

whereas the operator

$$\partial_x^2(1 + \partial_x^2)^2 \rightarrow \sum_{j=0}^{6} \delta^j\mathcal{L}_j \qquad (33)$$

such that

$$\mathcal{L}_0 = \partial_x^2(1 + \partial_x^2)^2,$$

$$\mathcal{L}_1 = 4\partial_X\partial_x^3(1 + \partial_x^2) + 2\partial_X\partial_x(1 + \partial_x^2)^2,$$

$$\mathcal{L}_2 = 4\partial_X^2\partial_x^4 + 10\partial_X^2\partial_x^2(1 + \partial_x^2) + \partial_X^2(1 + \partial_x^2)^2,$$

$$\mathcal{L}_3 = 12\partial_X^3\partial_x^3 + 8\partial_X^3\partial_x(1 + \partial_x^2),$$

$$\mathcal{L}_4 = 13\partial_X^4\partial_x^2 + 2\partial_X^4(1 + \partial_x^2),$$

$$\mathcal{L}_5 = 6\partial_X^5\partial_x,$$

$$\mathcal{L}_6 = \partial_X^6. \qquad (34)$$

We now expand ψ in a perturbation series in δ to get

$$\psi = \psi_0 + \delta\psi_1 + \delta^2\psi_2 + \delta^3\psi_3 + \cdots. \qquad (35)$$

Using Eq. (32) and the above series, the δ expansion of the nonlinear term in Eq. (30) can be written as

$$\partial_x^2(\psi^3 - \psi) = \partial_x^2(\psi_0^3 - \psi_0) + \delta[\partial_x^2(3\psi_0^2\psi_1 - \psi_1) + 2\partial_X\partial_x(\psi_0^3 - \psi_0)] + \delta^2[\partial_x^2(3\psi_0\psi_1^2 + 3\psi_0^2\psi_2 - \psi_2) + 2\partial_X\partial_x(3\psi_0^2\psi_1 - \psi_1) + \partial_X^2(\psi_0^3 - \psi_0)] + \delta^3[\partial_x^2(\psi_1^3 + 6\psi_0\psi_1\psi_2 + 3\psi_0^2\psi_3 - \psi_3) + 2\partial_X\partial_x(3\psi_0\psi_1^2 + 3\psi_0^2\psi_2 - \psi_2) + \partial_X^2(3\psi_0^2\psi_1 - \psi_1)] + \delta^4[\partial_x^2(3\psi_1^2\psi_2 + 3\psi_0\psi_2^2 + 6\psi_0\psi_1\psi_3 + 3\psi_0^2\psi_4 - \psi_4) + 2\partial_X\partial_x(\psi_1^2$$

$$+ 6\psi_0\psi_1\psi_2 + 3\psi_0^2\psi_3 - \psi_3) + \partial_X^2(3\psi_0\psi_1^2 + 3\psi_0^2\psi_2 - \psi_2)] + O(\delta^5). \qquad (36)$$

Substituting Eq. (35) in Eq. (30), and using the scaled operators in Eqs. (32)–(34), we can write equations satisfied by the ψ_m at each $O(\delta^m)$. At $O(1)$ we obtain,

$$\mathcal{L}_0\psi_0 = 0$$

$$\Rightarrow \psi_0 = \bar{\psi} + A_{01}(X,T)e^{ix} + \text{c.c.} \qquad (37)$$

where A_{mn} is the complex amplitude of mode n at $O(\delta^m)$. At $O(\delta)$ we get

$$\mathcal{L}_0\psi_1 + \mathcal{L}_1\psi_0 = 0$$

$$\Rightarrow \psi_1 = A_{11}(X,T)e^{ix} + \text{c.c.} \qquad (38)$$

where (and henceforth) we neglect the constant term in view of its inclusion in Eq. (37). At the next order we have

$$\mathcal{L}_0\psi_2 = \partial_T\psi_0 - \mathcal{L}_1\psi_1 - \mathcal{L}_2\psi_0 - \partial_x^2(\psi_0^3 - \psi_0). \qquad (39)$$

For $\psi_2(x,t)$ to remain bounded we have to guarantee that the right-hand side of Eq. (39) does not have a projection in the null space of $\mathcal{L}_0$, which yields a solvability condition [30,31] (also known as the Fredholm alternative). Applying the alternative imposes the following condition on the amplitude at $O(\delta^2)$:

$$\partial_T A_{01} = 4\partial_X^2 A_{01} + (1 - 3\bar{\psi}^2)A_{01} - 3A_{01}|A_{01}|^2. \qquad (40)$$

Thus,

$$\psi_2 = A_{21}e^{ix} + A_{22}e^{2ix} + A_{23}e^{3ix} + \text{c.c.} \qquad (41)$$

where $A_{22} = A_{01}^2\bar{\psi}/3$ and $A_{23} = A_{01}^3/64$.

At subsequent orders, the following equations are obtained for ψ_m:

$$\mathcal{L}_0\psi_3 = \partial_T\psi_1 - \mathcal{L}_1\psi_2 - \mathcal{L}_2\psi_1 - \mathcal{L}_3\psi_0 - [\partial_x^2(3\psi_0^2\psi_1 - \psi_1) + 2\partial_X\partial_x(\psi_0^3 - \psi_0)] \quad [O(\delta^3)],$$

$$\mathcal{L}_0\psi_4 = \partial_T\psi_2 - \mathcal{L}_1\psi_3 - \mathcal{L}_2\psi_2 - \mathcal{L}_3\psi_1 - \mathcal{L}_4\psi_0 - [\partial_x^2(3\psi_0\psi_1^2 + 3\psi_0^2\psi_2 - \psi_2) + 2\partial_X\partial_x(3\psi_0^2\psi_1 - \psi_1) + \partial_X^2(\psi_0^3 - \psi_0)] \quad [O(\delta^4)],$$

$$\mathcal{L}_0\psi_5 = \partial_T\psi_3 - \mathcal{L}_1\psi_4 - \mathcal{L}_2\psi_3 - \mathcal{L}_3\psi_2 - \mathcal{L}_4\psi_1 - \mathcal{L}_5\psi_0 - [\partial_x^2(\psi_1^3 + 6\psi_0\psi_1\psi_2 + 3\psi_0^2\psi_3 - \psi_3) + 2\partial_X\partial_x(3\psi_0\psi_1^2 + 3\psi_0^2\psi_2 - \psi_2) + \partial_X^2(3\psi_0^2\psi_1 - \psi_1)] \quad [O(\delta^5)],$$

$$\mathcal{L}_0\psi_6 = \partial_T\psi_4 - \mathcal{L}_1\psi_5 - \mathcal{L}_2\psi_4 - \mathcal{L}_3\psi_3 - \mathcal{L}_4\psi_2 - \mathcal{L}_5\psi_1 - \mathcal{L}_6\psi_0 - [\partial_x^2(3\psi_1^2\psi_2 + 3\psi_0\psi_2^2 + 6\psi_0\psi_1\psi_3 + 3\psi_0^2\psi_4 - \psi_4) + 2\partial_X\partial_x(\psi_1^2 + 6\psi_0\psi_1\psi_2 + 3\psi_0^2\psi_3 - \psi_3) + \partial_X^2(3\psi_0\psi_1^2 + 3\psi_0^2\psi_2 - \psi_2)] \quad [O(\delta^6)], \qquad (42)$$

and successive applications of the Fredholm alternative yield

the following amplitude equations at those respective orders:

$$\partial_T A_{11} = -12i\partial_X^3 A_{01} + 4\partial_X^2 A_{11} - (1 - 3\bar{\psi}^2)2i\partial_X A_{01} + (1$$
$$- 3\bar{\psi}^2)A_{11} - 6A_{11}|A_{01}|^2 - 3A_{01}^2 A_{11}^* + 6i\partial_X(A_{01}^2 A_{01}^*),$$

$$\partial_T A_{21} = -13\partial_X^4 A_{01} - 12i\partial_X^3 A_{11} + 4\partial_X^2 A_{21} - (1 - 3\bar{\psi}^2)(2i\partial_X A_{11}$$
$$+ \partial_X^2 A_{01}) + (1 - 3\bar{\psi}^2)A_{21} - 3A_{11}^2 A_{01}^* - 6|A_{01}|^2 A_{21}$$
$$- 6\bar{\psi}A_{22}A_{01}^* - 3A_{23}A_{01}^{*2} - 6A_{01}|A_{11}|^2 - 3A_{01}^2 A_{21}^*$$
$$+ 6i\partial_X(A_{01}^2 A_{11}^* + 2|A_{01}|^2 A_{11}) + 3\partial_X^2(A_{01}^2 A_{01}^*),$$

$$\partial_T A_{31} = 6i\partial_X^5 A_{01} - 13\partial_X^4 A_{11} - 12i\partial_X^3 A_{21} + 4\partial_X^2 A_{31} - (1 - 3\bar{\psi}^2)$$
$$\times(2i\partial_X A_{21} + \partial_X^2 A_{11}) + (1 - 3\bar{\psi}^2)A_{31} - 6A_{11}A_{21}A_{01}^*$$
$$- 6|A_{01}|^2 A_{31} - 6A_{01}A_{21}A_{11}^* - 6A_{23}A_{01}^* A_{11}^*$$
$$- 6A_{01}A_{11}A_{21}^* - 3A_{01}^2 A_{31}^* - 6\bar{\psi}A_{32}A_{01}^* - 3A_{33}A_{01}^{*2}$$
$$- 6\bar{\psi}A_{22}A_{11}^* + 6i\partial_X(2A_{01}|A_{11}|^2 + 2|A_{01}|^2 A_{21} + A_{01}^* A_{11}^2$$
$$+ A_{01}^2 A_{21}^*) + 3\partial_X^2(A_{01}^2 A_{11}^* + 2|A_{01}|^2 A_{21}) + \text{h.o.t},$$

$$\partial_T A_{41} = \partial_X^6 A_{01} + 6i\partial_X^5 A_{11} - 13\partial_X^4 A_{21} - 12i\partial_X^3 A_{31} + 4\partial_X^2 A_{41} - (1$$
$$- 3\bar{\psi}^2)(2i\partial_X A_{31} + \partial_X^2 A_{21}) + (1 - 3\bar{\psi}^2)A_{41} - 3A_{21}^2 A_{01}^*$$
$$- 6A_{11}A_{31}A_{01}^* - 6A_{01}A_{41}A_{01}^* - 6A_{11}A_{21}A_{11}^*$$
$$- 6A_{01}A_{31}A_{11}^* - 3A_{11}^2 A_{21}^* - 6A_{01}|A_{21}|^2 - 6A_{01}A_{11}A_{31}^*$$
$$- 3A_{01}^2 A_{41}^* - 6\bar{\psi}A_{42}A_{01}^* - 3A_{43}A_{01}^{*2} - 6\bar{\psi}A_{32}A_{11}^*$$
$$- 6A_{33}A_{01}^* A_{11}^* - 3A_{23}A_{11}^{*2} - 6\bar{\psi}A_{33}A_{22}^* - 6A_{01}|A_{23}|^2$$
$$+ 6i\partial_X(2A_{11}A_{21}A_{01}^* + 2|A_{01}|^2 A_{31} + A_{11}|A_{11}|^2$$
$$+ 2A_{01}A_{21}A_{11}^* + 2A_{01}A_{11}A_{21}^* + A_{01}^2 A_{31}^*)$$
$$+ 3\partial_X^2(2A_{01}|A_{11}|^2 + A_{01}^* A_{11}^2 + 2|A_{01}|^2 A_{21} + A_{01}^2 A_{21}^*)$$
$$+ \text{h.o.t} \tag{43}$$

Here, "h.o.t." refers to higher-order terms that are functions of A_{01} and its derivatives. The amplitude function for the pattern (e^{ix}) can be written as

$$A(X,T) = A_{01}(X,T) + \delta A_{11}(X,T) + \delta^2 A_{21}(X,T) + \cdots. \tag{44}$$

Using Eqs. (40), (43), and (44), and scaling back to the original variables, i.e., $X \to \delta^{-1}x$ and $T \to \delta^{-2}t$, the amplitude equation to $O(\delta^4)$ can be written as

$$\partial_t A = 4\partial_x^2 A - 12i\partial_x^3 A - 13\partial_x^4 A + 6i\partial_x^5 A + \partial_x^6 A - \delta^2(1 - 3\bar{\psi}^2)$$
$$\times(2i\partial_x + \partial_x^2)A + \delta^2[(1 - 3\bar{\psi}^2)A - 3A|A|^2 + 3(2i\partial_x + \partial_x^2)$$
$$\times(A|A|^2)] - \delta^4\left(\frac{3}{64}A|A|^4 + 2\bar{\psi}^2 A|A|^2\right) + O(\delta^6), \tag{45}$$

or more compactly, after replacing $\delta^2 \to \epsilon$, to $O(\epsilon^2)$

$$\partial_t A = -(1 - \mathcal{L}_{1D})\mathcal{L}_{1D}^2 A - \epsilon(1 - 3\bar{\psi}^2)\mathcal{L}_{1D}A + \epsilon(1 - 3\bar{\psi}^2)A$$
$$- 3\epsilon A|A|^2 + 3\epsilon\mathcal{L}_{1D}(A|A|^2) - \epsilon^2\left(\frac{3}{64}A|A|^4 + 2\bar{\psi}^2 A|A|^2\right)$$
$$+ O(\epsilon^3), \tag{46}$$

where $\mathcal{L}_{1D} \equiv (2i\partial_x + \partial_x^2)$.

Let us now compare Eq. (46) with the one-dimensional equivalents of the $O(\epsilon)$ amplitude equations that we have previously derived for hexagonal patterns, i.e., Eqs. (15) and (22). Without rederiving, the one-dimensional equivalents are readily obtained by setting

$$A_2 = A_3 = 0 \quad \text{and} \quad \mathcal{L}_{\mathbf{k}_2} = \mathcal{L}_{1D} \tag{47}$$

in those equations. We observe that Eq. (46) [also truncated to $O(\epsilon)$] contains at least one term that is not present in either of the equations previously derived.

We note that the QDRG result of Eq. (15) is closer to the multiple-scale result compared to the proto-RG result (and the RG result in Sec. VI), in that it fails to capture only the nonlinear derivative term at $O(\epsilon)$, which is actually a higher-order correction to $3A|A|^2$. This is clearly because the spatial operator in the QDRG method is an outcome of a *linear* stability analysis, whereas one would have to perform a non-linear stability analysis to obtain nonlinear spatial derivative terms. The clear advantage of the QDRG calculation however is that it was done with significantly less effort, and in a rotationally covariant manner; perturbation theory to $O(\epsilon)$ was all that was required. The multiple-scale analysis, on the other hand, required a sixth-order perturbation theory treatment, and in order to simplify the algebra, we only worked in one dimension. In higher dimensions, the interference between the modes would have created a huge increase in the complexity at each successively higher order in perturbation theory. The QDRG calculation is only heuristic, but as we will show below, can be justified from a full calculation, albeit with a minor technical modification of the previously published recipe, to take into account the special feature of the conservation law in the PFC model.

We conclude therefore that although the QDRG result of Eq. (15) and the multiple-scale method to $O(\epsilon)$ still do not yield consistent results, the QDRG method is still an improvement over the proto-RG method. In order to track down the source of the discrepancy, we next attempted a full RG calculation without any shortcuts, i.e., systematically calculating explicitly and renormalizing all the divergent terms to $O(\epsilon)$.

VI. RENORMALIZATION GROUP DERIVATION

In this section, we present a derivation of the amplitude equation using the conventional RG method, in one dimension for pedagogical simplicity (just as was done for the method of multiple scales). The calculation is complicated because of the need to obtain explicit formulae for the secular divergences [32,34], but this is possible at the order to which we worked.

Starting from Eq. (30) (with δ^2 replaced by ϵ) and a naive perturbation series in ϵ as in Eq. (11) the zeroth- and first-order solutions can be written as

$$\psi_0 = \bar{\psi} + A e^{ix} + \text{c.c.},$$

$$\psi_1 = P_1(x,t)e^{ix} + Q_1 e^{2ix} + R_1 e^{3ix} + \text{c.c.} \qquad (48)$$

The difficulty in the conventional RG method comes from the need to explicitly determine the form of the secular coefficient P_1. While this is a routine task for ODEs, it is far from trivial for PDEs. A further complication is that the solution for P_1 must be the highest-order polynomial that satisfies the PDE, to be able to eliminate all secular divergences. It turns out that this is critical to obtaining the rotationally covariant operator at a lower order in ϵ. Using the method of undetermined coefficients we find such a solution to be

$$P_1(x,t) = \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A \sum_{j=1}^{6} C_j P_{1j}(x,t), \qquad (49)$$

where

$$P_{11} = t,$$

$$P_{12} = -\frac{1}{720}(-89\,280t^2 + 7680t^3 + 4320ixt - 34\,560ixt^2$$
$$- 4680x^2t + 2880x^2t^2 - 1440ix^3t + 120x^4t + x^6),$$

$$P_{13} = \frac{i}{720}(-5760it^2 - 1560xt + 960xt^2 - 720ix^2t + 80x^3t$$
$$+ x^5),$$

$$P_{14} = \frac{1}{312}(192t^2 - 288ixt + 48xt^2 + x^4),$$

$$P_{15} = -\frac{i}{72}(24xt + x^3),$$

$$P_{16} = -\frac{x^2}{8}, \qquad (50)$$

and the constants C_j satisfy $\Sigma_{j=1}^{6}C_j = 1$.

The RG method proceeds as follows: (1) dummy variables X and T are introduced, (2) the divergent terms in P_{1j} of the form $x^m t^n$ are split to read $x^m t^n = (x^m t^n - X^m T^n) + X^m T^n$, (3) the constant amplitude A is redefined using an ϵ expansion $A = A_R(X,T)(1 + \Sigma_{j=1} \epsilon^j Z_j)$, where A_R is now the renormalized amplitude, and Z_j are the renormalization constants which are chosen order by order in ϵ to absorb the $X^m T^n$ terms, and (4) since the solution ψ is independent of X and T, all derivatives of ψ with respect to X, T, or a combination thereof must be zero. This last condition yields the following RG equations at $O(\epsilon)$:

$$\frac{\partial A_R}{\partial T} = C_1 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A,$$

$$-\frac{\partial^6 A_R}{\partial X^6} = C_2 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A,$$

$$-6i\frac{\partial^5 A_R}{\partial X^5} = C_3 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A,$$

$$13\frac{\partial^4 A_R}{\partial X^4} = C_4 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A,$$

$$12i\frac{\partial^3 A_R}{\partial X^3} = C_5 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A,$$

$$-4\frac{\partial^2 A_R}{\partial X^2} = C_6 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A. \qquad (51)$$

Further, using $\Sigma_{j=1}^{6}C_j = 1$ and replacing $A_R \to A$, $X \to x$, and $T \to t$, the above equations can be combined to read

$$\partial_t A + (1 - \mathcal{L}_{1D})\mathcal{L}_{1D}^2 A = \epsilon(1 - 3\bar{\psi}^2)A - 3\epsilon A|A|^2, \qquad (52)$$

which is also the 1D proto-RG equation.

We close this section with some interesting observations. (i) The equations in (51) do not form a unique set of solvability conditions. Other equations are possible, e.g.,

$$-\frac{1}{16}\frac{\partial^4 A_R}{\partial X^2 \, \partial T^2} = C_2 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A,$$

$$-\frac{3i}{8}\frac{\partial^3 A_R}{\partial X \, \partial T^2} = C_3 \epsilon(1 - 3\bar{\psi}^2 - 3|A|^2)A,$$

$$\vdots \qquad (53)$$

The choice of Eq. (51) is motivated by the observation that it yields a rotationally covariant amplitude equation, and other physical considerations such as the microscopic equation being only first order in time. (ii) The list of possible terms P_{1j} does not include the leading polynomial term Bx, where B is an arbitrary constant, as this term is annihilated by the kernel of the PDE. Thus no constraint is available to fix B. It turns out that unless this term is also renormalized, all secular divergences are not removed. This may explain the absence of certain terms in Eq. (52) that however show up in the multiple-scale analysis. To be certain, the calculation needs to be carried out to higher orders; but we do not attempt this here.

VII. OPERATOR ORDERING AMBIGUITY AND ITS RESOLUTION IN THE RG METHOD

In this section, we resolve the discrepancy between the answers generated by the QDRG method, the RG methods, and the method of multiple scales. Curiously, no such discrepancy was observed in the treatment of the Swift-Hohenberg equation, a nonconservative OPE, by RG methods [32,34,36] and multiple-scale techniques [27]. In fact, it

can also be readily ascertained that the QDRG method will produce the same result as the other methods for this equation, which we leave as a simple exercise for the reader. Why then does a discrepancy arise in the PFC equation? Clearly, the role played by the extra Laplacian, a consequence of the conservation law in this case, must be nontrivial.

Note that this Laplacian operator carries over to the right-hand side of both Eq. (12), the $O(\epsilon)$ equation for the RG methods, and Eq. (39), the $O(\epsilon)$ equation for multiple scales. However, also note that, in the method of multiple scales, in addition to the nonlinear terms, this operator is also subjected to an ϵ expansion. There is no provision in any of the RG methods to allow the same to happen to the Laplacian. In other words, the operator may very well have not existed on the right-hand side at $O(\epsilon)$, and we would have obtained exactly the same result as before.

A clue to the subtlety is to look at the way in which the secular terms are renormalized. The naive way, as followed here, would be to evaluate the right-hand side first, look for secular terms later, and then renormalize these divergent coefficients. However, this will not eliminate secular terms generated by the differential operator. In order to eliminate all secular terms, the amplitude must be renormalized before differentiation, for the simple reason that renormalization and differentiation are noncommutable operations. In other words, there is an operator ordering ambiguity in the implementation of the renormalization-group method, exposed in this problem by the conservation law. Performing the calculation with the operations of renormalization and differentiation reversed is equivalent to performing an ϵ expansion in the differential operator.

We find that by following this procedure, additional terms in the coefficients of the resonant modes are automatically generated. Specifically, when we evaluate the right-hand side of Eq. (12) after assuming the amplitudes of ψ_0 to have a space-time dependence, the renormalized coefficients of the resonant $\exp(i\mathbf{k}_1 \cdot \mathbf{x})$ forcing term work out to be

$$
\begin{aligned}
&\epsilon[(1 - 3\bar{\psi}^2)A_1 - 3A_1(|A_1|^2 + 2|A_2|^2 + 2|A_3|^2) - 6A_2^* A_3^* \bar{\psi} \\
&\quad - (1 - 3\bar{\psi}^2)\mathcal{L}_{\mathbf{k}_1}A_1 + 6(|A_1|^2 + |A_2|^2 + |A_3|^2)\mathcal{L}_{\mathbf{k}_1}A_1 \\
&\quad + 6A_1^*|\nabla A_1|^2 + 3A_1^2 \mathcal{L}_{\mathbf{k}_1}A_1^* + 6A_1 A_2^* \mathcal{L}_{\mathbf{k}_1}A_2 + 6A_1 A_2 \mathcal{L}_{\mathbf{k}_1}A_2^* \\
&\quad + 6A_1 A_3^* \mathcal{L}_{\mathbf{k}_1}A_3 + 6A_1 A_3 \mathcal{L}_{\mathbf{k}_1}A_3^* + 6\bar{\psi}A_3^* \mathcal{L}_{\mathbf{k}_1}A_2^* \\
&\quad + 6\bar{\psi}A_2^* \mathcal{L}_{\mathbf{k}_1}A_3^* + 12\bar{\psi}\nabla A_2^* \cdot \nabla A_3^* + 12A_1(\nabla A_1 \cdot \nabla A_1^* \\
&\quad + \nabla A_2 \cdot \nabla A_2^* + \nabla A_3 \cdot \nabla A_3^*) + 12A_2 \nabla A_1 \cdot \nabla A_2^* \\
&\quad + 12A_2^* \nabla A_1 \cdot \nabla A_2 + 12A_3 \nabla A_1 \cdot \nabla A_3^* + 12A_3^* \nabla A_1 \cdot \nabla A_3],
\end{aligned}
\tag{54}
$$

which when specialized for the 1D case becomes

$$
\begin{aligned}
&\epsilon\left[(1 - 3\bar{\psi}^2)A - 3A|A|^2 - (1 - 3\bar{\psi}^2)\mathcal{L}_{1D}A + 6|A|^2\mathcal{L}_{1D}A \right.\\
&\quad \left. + 3A^2\mathcal{L}_{1D}A^* + 6A^*\left(\frac{\partial A}{\partial x}\right)^2 + 12A\frac{\partial A}{\partial x}\frac{\partial A^*}{\partial x}\right] \\
&= \epsilon[(1 - 3\bar{\psi}^2)A - 3A|A|^2 - (1 - 3\bar{\psi}^2)\mathcal{L}_{1D}A \\
&\quad + 3\mathcal{L}_{1D}(A|A|^2)].
\end{aligned}
\tag{55}
$$

We note that the above terms are identical to the $O(\epsilon)$ terms on the right-hand side of Eq. (46). Therefore the correct amplitude equation to $O(\epsilon)$ should contain all the terms in Eq. (54). In order to illustrate the generality of this approach, we apply this idea again in the Appendix to the Van der Pol oscillator, another equation for which the previously reported implementation of the RG method, and the method of multiple scales produce different answers.

We wish to point out that the assumption of a constant amplitude in the ψ_0 solution makes it possible for the coefficients of the nonresonant terms in ψ_1 to assume constant values, a fact that is favorably used in extending the proto-RG calculation to the next order. However, with our modification to the proto-RG procedure, it is clear that for the PFC equation at least, nonresonant coefficients cannot have constant values. Thus computing higher-order corrections to the amplitude equations, will require explicit construction of particular solutions, which may limit progress beyond $O(\epsilon)$ by purely analytical methods.

VIII. CONCLUSION

We have presented a detailed illustration of various perturbative techniques to derive amplitude equations from order parameter equations that produce periodic patterns. Amplitude equations serve as powerful analytical tools with which to investigate pattern stability and defect interactions, as well as accurate coarse-grained descriptions of pattern-forming systems, and this calls for practical and reliable mathematical methods for deriving them.

Although our benchmark for accuracy is the widely accepted method of multiple scales, it is critical to note that this method is not fail safe, because it requires *a priori* identification of the way in which space and time scale with the small parameter ϵ. There are many instances where surprising scales emerge that would not easily be identified *a priori* (e.g., see the analysis of the Mathieu equation in [32]).

The method of multiple scales typically involves a very lengthy calculation before a rotationally covariant operator ensues, and involves computation of various higher-order terms which ultimately do not improve the overall result significantly. In the example presented here, a sixth-order calculation was required to get the lowest-order amplitude equation. The reader should bear in mind that the fairly involved calculation shown in this paper was only one dimensional.

On the other hand, the practicality of RG-based methods, where the amplitude equation was obtained very quickly at $O(\epsilon)$ itself, is self-evident. No guesswork was required to determine the scaling of the variables and all calculations

started with naive perturbation expansions in ϵ. In particular, our so-called quick and dirty (QDRG) method and the proto-RG method are attractive techniques, because there is virtually no need to construct explicit solutions. Both methods use only information available from the differential equation and in that sense, are very general ways of building a controlled coarse-grained approximation to the order parameter equation being studied. Furthermore, the QDRG method gives the correct result quickly, apart from a small nonlinear rotationally covariant gradient term which is not captured by the linear stability argument.

At $O(\epsilon)$, we have shown that the QDRG method produces a more accurate amplitude equation compared to the proto-RG method, by capturing certain extra terms that are revealed in the multiple-scale analysis. However, with our corrected order of operators in the way in which the RG is implemented, we find that all methods converge identically at this order.

In conclusion, we have presented a detailed calculation of the coarse-graining of the phase field crystal equation, for small ϵ. Elsewhere [20,21], we have demonstrated the utility of the coarse-grained equation in performing large-scale simulations of materials processing phenomena in two dimensions. Further developments of these techniques are under way, implementing adaptive mesh refinement to solve the amplitude equations obtained here in two and three dimensions, and going beyond the single-mode approximation which has formed the basis of our work and that of Elder and collaborators. We hope to report on these developments at a future date.

ACKNOWLEDGMENTS

APPENDIX: VAN DER POL OSCILLATOR

In this Appendix, we explore the commuting of differentiation and renormalization with a simple ordinary differential equation example: the Van der Pol oscillator. Note that this yet another case in which a differential operator is multiplied by a small parameter [see right-hand side of Eq. (A1)].

The autonomous ODE is given by

$$y'' + y = \epsilon(1 - y^2)y', \qquad (A1)$$

where the prime denotes differentiation with respect to the variable t. As there is a derivative on the right-hand side of this equation we anticipate that the proto-RG amplitude equation will fail to capture certain terms that turn out in the multiple-scale analysis.

It is known that the scaling $\tau = \epsilon t$ works for this problem [30]. Hence,

$$y' \to (\partial_t + \epsilon\partial_\tau)y,$$

$$y'' \to (\partial_t^2 + 2\epsilon\partial_\tau\partial_t + \epsilon^2\partial_\tau^2)y, \qquad (A2)$$

where the subscripts denote partial differentiation. Expanding y in a perturbation series

$$y = y_0 + \epsilon y_1 + \epsilon^2 y_2 + \cdots, \qquad (A3)$$

we obtain

$$(\partial_t^2 + 1)y_0 = 0 \quad [O(1)],$$

$$(\partial_t^2 + 1)y_1 = -2\partial_\tau\partial_t y_0 + (1 - y_0^2)\partial_t y_0 \quad [O(\epsilon)],$$

$$(\partial_t^2 + 1)y_2 = -2\partial_\tau\partial_t y_1 + (1 - y_0^2)\partial_t y_1 - \partial_\tau^2 y_0 - 2y_0 y_1 \partial_t y_0$$
$$+ (1 - y_0^2)\partial_\tau y_0 \quad [O(\epsilon^2)]. \qquad (A4)$$

From this we find

$$y_0 = A_{01}(\tau)e^{it} + \text{c.c.},$$

$$y_1 = A_{11}(\tau)e^{it} + A_{13}(\tau)e^{3it} + \text{c.c.} \qquad (A5)$$

Application of the Fredholm alternative at $O(\epsilon)$ and $O(\epsilon^2)$ yields the following amplitude equations:

$$2i\partial_\tau A_{01} = iA_{01}(1 - |A_{01}|^2),$$

$$\partial_\tau^2 A_{01} + 2i\partial_\tau A_{11} = i(A_{11} - 2A_{11}|A_{01}|^2 - A_{01}^2 A_{11}^*)$$
$$+ \partial_\tau(A_{01} - A_{01}|A_{01}|^2) + \frac{A_{01}|A_{01}|^4}{8},$$
$$(A6)$$

which can be combined after scaling back to the original variables to get

$$\partial_t^2 A + 2i\partial_t A = \epsilon[iA(1 - |A|^2) + \partial_t A(1 - |A|^2)] + O(\epsilon^2). \qquad (A7)$$

Nozaki and Oono [36], on the other hand, have obtained the following equation using the proto-RG method:

$$\partial_t^2 A + 2i\partial_t A = \epsilon iA(1 - |A|^2) + O(\epsilon^2). \qquad (A8)$$

Note that the missing term $\partial_t A(1 - |A|^2)$ can be captured by differentiating the lower-order result, i.e.,

$$2i\partial_t A = \epsilon iA(1 - |A|^2), \qquad (A9)$$

but this does not seem a very general approach. In particular, it is not obvious how this can be extended to PDEs.

The $O(\epsilon)$ equation using the proto-RG method reads

$$y_1'' + y_1 = (1 - y_0^2)y_0', \qquad (A10)$$

where

$$y_0 = Ae^{it} + \text{c.c.},$$

$$y_1 = P(t)e^{it} + Qe^{3it} + \text{c.c.}, \qquad (A11)$$

where A can be a constant while P cannot. Thus, the proto-RG operator turns out to be

$$\mathcal{L} = \partial_t^2 + 2i\partial_t, \qquad (A12)$$

and the proto-RG equation reads

$$\mathcal{L}A = \epsilon \mathcal{L}P + O(\epsilon^2), \qquad (A13)$$

where A is now the renormalized amplitude. When evaluating $\mathcal{L}P$, however, we allow for the possibility that A, which appears on the right-hand side of the equation can also be a function of t, or equivalently renormalize A on the right-hand side before differentiating y_0, which gives us

$$\mathcal{L}P = \epsilon[iA(1 - |A|^2) + \partial_t A(1 - |A|^2)]. \qquad (A14)$$

Therefore the true amplitude equation should read [using Eq. (A13)]

$$\mathcal{L}A = \epsilon[iA(1 - |A|^2) + \partial_t A(1 - |A|^2)] + O(\epsilon^2), \quad (A15)$$

which is identical to the multiple-scale result of Eq. (A7).

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