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Singular perturbation analysis for unstable systems with convective nonlinearity

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We use a singular perturbation method to study the interface dynamics of a nonconserved order parameter (NCOP) system, of the reaction-diffusion type, for the case where an external bias field or convection is present. We find that this method, developed by Kawasaki, Yalabik, and Gunton [Phys. Rev. A **17**, 455 (1978)] for the time-dependant Ginzburg-Landau equation and used successfully on other NCOP systems, breaks down for our system when the strength of convective nonlinearity gets large enough.

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I. INTRODUCTION

The study of nonequilibrium systems where interfaces are present is a challenging problem. The challenge often arises due to the interfaces being diffuse on a molecular scale, yet appearing as discontinuities on the mesoscopic length scale of growing domains, thereby generating a mesoscopic description with two disparate length scales. To approximately solve the nonlinear Langevin-type partial differential equation (PDE) used to model one such system—the time-dependent Ginzburg-Landau (TDGL) equation—an analytic method was developed by Kawasaki, Yalabik, and Gunton (KYG) [1]. This singular perturbation method (SPM) was subsequently applied to many other systems where the order parameter is nonconserved [1–3] conserved [4], coupled with long range repulsive interactions [5], etc., all exhibiting strong nonlinear behavior at late times. However, the KYG method has not yet been applied, to our knowledge, to a system with a nonlinear convective derivative of the form $(\mathbf{v}\cdot\boldsymbol{\nabla})\psi^n$, where ψ is the relevant order parameter field in the system. This nonlinearity occurs in hydrodynamics or when an external bias field $\mathbf{E}$ is present [6]. In this case $\mathbf{E}$ plays the role of $\mathbf{v}$. Hence it is of some interest to examine the predictions of singular perturbation theory in this context.

We will consider in particular a system where mechanical transport competes with diffusive transport and dissipation. A mean-field model of such a system is the Fisher equation to which a convective nonlinearity, describing mechanical transport, is added and whose strength can be tuned with a parameter μ. We call this new equation FEC [for Fisher equation with convective nonlinearity; cf. Eq. (1)]. The Fisher equation has been extensively studied in literature [7–9], originally in the context of population dynamics, and its treatment by the KYG analysis yielded good results [7]. For FEC with $\mu \ll 1$, the KYG SPM gives results very similar to those found for the Fisher equation. But when $\mu \sim \mathcal{O}(1)$ or greater, the result breaks down at early times, due to mechanical transport dominating over diffusive processes, imposing a serious limitation to singular perturbation results for the type of system considered here.

Before we proceed to describe our results, some general remarks about the validity and utility of the KYG technique are in order. This technique is not meant to be a means of obtaining a solution to the initial-value problem for a reaction-diffusion equation. Rather, it should be interpreted as a way of obtaining an analytic form, which may replicate the important features of the true solution, thereby enabling one to obtain statistically important quantities.

For the TDGL equation with a scalar order parameter, the analytic solution obtained by KYG is in disagreement on one important point with the real (obtained numerically) solution [7], in that it has infinitesimally thin walls at late times, whereas the real solution always has walls of nonzero thickness. However, the analytic solution does reasonably reproduce the defect (interface) distribution of the real solution, starting from random initial conditions. Also the time-dependent structure factor calculated from the analytic solution of KYG [1] is identical to the better-known result of Ohta *et al.* [10], which is derived using interface dynamics. The next application of the SPM was to the d-dimensional Fisher equation [7,11]. As in the TDGL case, the interfacial profile of the

KYG analytic solution (which is a traveling wave front) is artificially sharp compared to that for the real solution. However, the (traveling wave) analytic solution has the correct asymptotic velocity, even though the approach to this asymptotic velocity is incorrect in one dimension, where the exact result is known [9]. In the case where long-range interactions are also present, these statistics and defect dynamics are actually incorrectly given by the KYG method [12]. We find similar limitation for our *non*-conserved order-parameter system described by the FEC equation, in contrast to other nonconserved systems.

In Sec. II, we extend our earlier applications of the KYG method to the FEC, and follow the formalism described in detail by Puri [7]. Because the KYG analysis can be applied to FEC with only small differences as compared to that done for the Fisher equation, only an outline of the method is given here, emphasizing these differences, and the reader is referred to [7] and [1] for further details. In Sec. III, we compare the analytical solution with numerical results and summarize.

II. MODEL: KYG METHOD ON FEC

The FEC in one space dimension is

$$\frac{\partial u}{\partial t} + \mu u \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial x^2} + u - u^2, \tag{1}$$

where the order parameter field u, the position x, and the time t have been rescaled to dimensionless units. The dimensionless quantity μ is the ratio of convective to diffusive strengths in the equation of motion for u and cannot be scaled out. This equation is equivalent to Burgers's equation [13] in which one would add a linear source term u (providing the instability) and a quadratic sink term u^2 (providing the damping). Burgers's equation is itself *analytically solvable*. It often appears as a limiting case in more complicated problems in hydrodynamics, usually in the context of turbulence. Its main feature, due to the convective term, is that it yields shocks, also observed in the FEC. Note that $\mu = 0$ is the Fisher equation itself.

The solution, in Fourier space, of the *linearized* equation (1) is $\tilde{u}_k^0(t) = e^{\gamma_k t}\tilde{u}_k(0)$ with $\gamma_k = 1 - k^2$. Thus for $k < 1$, $\tilde{u}_k^0(t)$ grows exponentially in time with rate γ_k, a signature of linear instability. In what follows, the tilde denotes Fourier space and the superscript zero denotes the solution to the linearized PDE.

The *non*linear equation (1) can be rewritten in an integral form in terms of the linear solution as

$$\tilde{u}_k(t) = \tilde{u}_k^0(t) - \frac{1}{(2\pi)^2}\int_0^t \int_{k_1,k_2} e^{\gamma_k (t-t')}\delta(k - k_1 - k_2) \times g(k_1)\tilde{u}_{k_1}(t')\tilde{u}_{k_2}(t') dk_1 dk_2 dt', \tag{2}$$

where $g(k) = 1 - i\mu k$ and δ represents a Dirac δ function. The effect of convection is totally included in $g(k)$, which would be identically 1 for the Fisher equation. In applying the KYG technique, this modification creates no major difficulty. Note, however, that if the nonlinear damping term had been a u^3 instead of a u^2, $g(k)$ would actually be a functional of u, so that the KYG analysis would be impossible to carry out.

The essential idea of the KYG method is to generate an infinite order perturbative expansion around $\tilde{u}_k^0(t)$, approximate the nth order term in a suitable manner and resum the resulting infinite series to get an approximate, yet analytic, closed form result [14]. The only difference between the Fisher equation (FE) and the FEC is that $g(k)$ is not identically 1. In spite of this difference, the early part of the KYG analysis can be carried out for (2), yielding for the nth-order term

$$C_n^{\mathrm{FEC}} = \left[g\left(\frac{k}{n+1}\right)\right]^n C_n^{\mathrm{FE}}, \tag{3}$$

where the superscripts FEC and FE refer to the respective equations, and

$$C_n^{\mathrm{FE}} \simeq \frac{(-1)^n}{n!\prod_{i=1}^n \left(1 + \frac{i+1}{(n+1)^2}k^2\right)} \times \prod_{i=1}^n \left[\int_{k_i} \tilde{u}_{k_i}^0(t)\right] \tilde{u}^0_{k-\sum_1^n k_j}(t), \tag{4}$$

with $\tilde{u}_k(t) = \sum_{n=0}^\infty n! C_n^{\mathrm{FEC}}(k,t)$. Even with this much simpler form, the power series for $\tilde{u}_k(t)$ is still not summable analytically. To do this and also be able to Fourier transform back to real space, one approximates the *coefficient* of the multiple integrals in (4) to first order in k, since the major contribution to the Fourier transform comes from k near 0. For $\mu = 0$ this is a very good approximation. But for $\mu \neq 0$, $g(k)$ is complex, so that a phase error is also introduced. Because the singular perturbation expansion contains an infinite number of terms which must partly cancel each other to give a convergent sum, this phase error, although small, could introduce cancellation effects whose consequences can be judged only *a posteriori.*

With this further approximation, one can analytically resum the power series for $\tilde{u}_k(t)$ and invert the Fourier transform to get [15]

$$u(x,t) \simeq \left(1 + \mu\frac{\partial}{\partial x}\right)\left(\frac{u^0(x,t)}{1 + u^0(x,t)}\right). \tag{5}$$

Note that we recover the KYG solution to the Fisher equation when $\mu = 0$. The $\mu\frac{\partial}{\partial x}$ term induces the same type of asymmetry in (5) as that given to the PDE (1) by the convective term. However, one of the consequences of $\mu\frac{\partial}{\partial x}$ is the development, at large times, of strong peaks in $u(x,t)$ at the interfaces, indicating a breakdown of the singular perturbation result. Furthermore, one can see that this occurs *for any finite order expansion* of $\left[g(\frac{k}{n+1})\right]^n$ in k. Given that higher order C_n^{FE} ($n \to \infty$) will dominate the power series for $\tilde{u}_k(t)$ at large times, and that the k values dominating the dynamics are near zero, a remedy is to approximate $\left[g(\frac{k}{n+1})\right]^n$ with a simpler nonpolynomial function in k, close to it for $k \to 0$ and $n \to \infty$. One possibility which will give tractable summation and a Fourier-transformable diagram is $\exp(-i\mu k)$. This approximation, which is very good for $\mu \ll 1$ (cf. Sec. III) exhibits no peaks at the interfaces even as $t \to \infty$. Then from (3) one now gets, instead of (5),

$$u^{\rm FEC}(x,t) \simeq \exp\left(\mu\frac{\partial}{\partial x}\right)\left(\frac{u^0(x,t)}{1+u^0(x,t)}\right). \qquad (6)$$

Although the $\exp(\mu\frac{\partial}{\partial x})$ operator does not create artificial peaks at the interfaces for any μ and t, it is in effect a translation operator. Hence if the KYG solution to the Fisher equation ($\mu = 0$) is denoted by $u^{\rm FE}(x,t) = u^0(x,t)/[1+u^0(x,t)]$, we have $u^{\rm FEC}(x,t) = u^{\rm FE}(x-\mu,t)$, i.e., the solution to the FEC from this singular perturbation expansion is in fact a translated solution to the Fisher equation. Since the true effect of the convective term cannot be equated to a translation, it is immediately apparent that important characteristics of convection have been lost in this singular perturbation analysis. This will be crucial when μ is sufficiently large. We now briefly discuss and compare these analytic results with those of numerical integrations.

III. DISCUSSION

In Fig. 1 we show the exact numerical integration of the FEC equation, at relatively small values of μ and intermediate times ($t = 20$), for a seed initial condition centered at $x = 0$ [i.e., $u(x,0) = \delta(x)$]. The $\mu = 0$ curve is a numerical solution to the Fisher equation. The standard Euler integration method was used for all numerical integrations, with time and space meshes suitably chosen to insure stability and precision. After a transient time approximately equal to 10, the interface profiles change little and the interface velocity reaches a value within 10% of its asymptotic value. Hence the curves for $t > 20$ are almost identical to those of Fig. 1 but with larger bulk region (where $u = 1$). As for the shock waves found in the solution of the Burgers equation, the effect of the convective term on the spatially symmetric solution of the Fisher equation is to steepen the right interface and broaden the left one, as μ increases. One way of seeing analytically how the convective nonlinearity operates is to look at the PDE $\frac{\partial}{\partial t}u = u\frac{\partial}{\partial x}u$ which has, in implicit form, $u(x,t) = f[x - u(x,t)t]$ as a solution. This is a "wave" with points at height u traveling at speed u, so that higher points travel faster than lower ones.

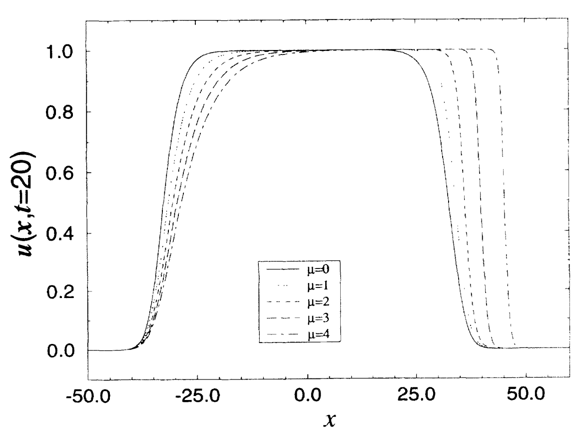

FIG. 1. Numerical solution of FEC at $t = 20$ and several values of μ (cf. figure legend), from a localized initial condition in $x = 0$. The $\mu = 0$ curve is symmetric with respect to the origin. Others get distorted by the convection term ($\mu \neq 0$).

In Fig. 2 we compare the results of a numerical integration for FEC with the analytical results of Eqs. (5) and (6), for $\mu = 0.1$ and $t = 20$. The offset between the interface of either of the approximate solutions and that of the exact numerical one occurs because at early times the front velocity in the exact numerical solution is significantly smaller than in the approximate solutions (always 2). The *asymptotic* velocity of the exact solution, namely 2 (independent of μ for small μ) is correctly given by (5) and (6). Hence, although the profiles of the approximate solutions are too steep, the dynamics of the walls are correctly given.

The interfaces given by our approximate solutions can be softened further by approximating $\prod_{i=1}^{n}\left(1+\frac{i+1}{(n+1)^2}k^2\right)$ in (4) by $\exp(-k^2/2)$ instead of 1, which is an extremely good approximation (less than 1% error) for all $k \leq 1$ and $n \gtrsim 4$ (this softening is analogous to one done by Oono and Puri [16] and Puri [7]). However, one finds that the change induced is very slight, indicating that the hardness of the interfaces of the approximate solutions is deeply buried in the earlier approximations.

For large μ (starting at about 5), both approximate solutions break down, although for different reasons. Equation (5) has peaks appearing at the interfaces, while the asymmetry of the analytical solution Eq. (6) matches in no way that of the real numerical solution. The velocity of the right interface is wrongly given by both analytic solutions, as the real velocity is much greater than 2 (cf. Fig. 3) at all times. Finally, the left interface of the exact numerical result is extremely broad for large μ, something that the SPM seems incapable of describing. Because the breakdown occurs not only in terms of order-parameter profile but of defect dynamics as well, statistical properties (due to random initial conditions, for example) will also be incorrectly given by the SPM.

We can therefore say that KYG SPM gives results very close to the real solution in terms of profile and velocity

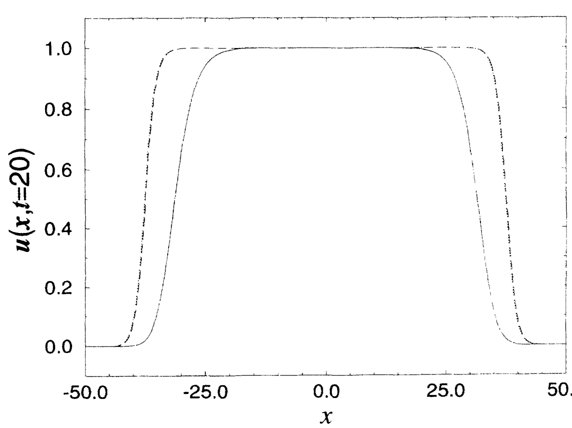

FIG. 2. Order parameter profile for the numerical solution (solid curve), for Eq. (5) (dotted curve), and for Eq. (6) (dashed curve), at $t = 20$ and $\mu = 0.1$.

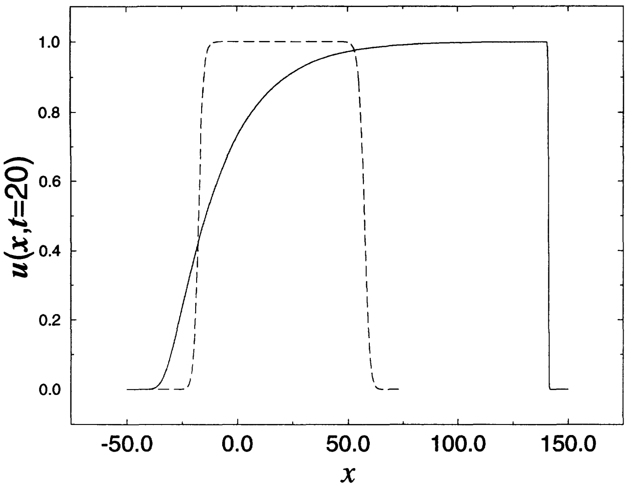

FIG. 3. Numerical solution (solid curve) and Eq. (6) (dashed curve) at $t = 20$ and $\mu = 20$. Again, from initial condition in $x = 0$.

up to $\mu \sim \mathcal{O}(1)$. But as the shock wave nature of the convective nonlinearity manifests itself more and more strongly (as μ increases), the KYG SPM does not manage to capture the essential features of convection, both in profiles and defect dynamics. Several analytical approaches are being investigated by us to make the results more quantitative and insightful. Apparently there is more to the failure of KYG at large μ than just a limitation of the SPM: any type of analysis performed around the *linear* solution, as done here, cannot be expected to work if the (attracting fixed point) solution becomes hyperbolic at some large enough value of μ, while an alternate solution (corresponding to a different asymptotic profile and velocity) becomes stable.

IV. CONCLUSION

The utility of singular perturbation methods lies in the calculation of statistical quantities (e.g., time-dependent structure factors, domain growth laws), which are determined by the qualitative features of the solution. However, we have shown that the singular perturbation approach will not give a reasonable solution to the initial-value problem for a reaction-diffusion equation where convection is strong enough (a precise criterion will be given in a future article) even in terms of such statistical quantities since the defect dynamics are incorrectly predicted. It can be shown [17] that this incorrect defect dynamics is due to the convection term dominating the diffusive transport of perturbations, and is not due only to some intrinsic limitations of the singular perturbation approach itself. Hence approaches which treat the full nonlinear PDE must be sought to study the dynamics of reaction-diffusion systems where an external bias field or convection is present.

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