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Dynamical renormalization group analysis of fourth-order conserved growth nonlinearities

S. Das Sarma and Roza Kotlyar

Department of Physics, University of Maryland, College Park, Maryland 20742-4111

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A nonlinear stochastic fourth-order conserved growth equation $\partial h/\partial t = -\nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \lambda_{13} \nabla (\nabla h)^3 + \eta$ has been studied analytically, using the perturbative dynamical renormalization group approach. One-loop calculation generates long-wavelength scaling properties of the known Edwards-Wilkinson universality class which has the corresponding equation $\partial h/\partial t = \nu_2 \nabla^2 h + \eta$. Our result agrees with the recent numerical result of Kim and Das Sarma (unpublished) based on direct numerical integration. A two-loop calculation validates our conclusion, and we argue that our result holds to all orders in perturbative expansion.

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Considerable progress in our understanding of nonequilibrium surface growth phenomenon has been achieved in the last ten years by using coarse-grained continuum partial differential equations which describe the temporal developments of long-wavelength fluctuations in the local surface height as matter is added to the growing interface from outside [1]. In particular, kinetic roughening of growing interfaces due to the shot noise inherently present in the incident flux may be classified into various universality classes (in the renormalization group-critical phenomena sense) in accordance with the applicability of various continuum equations in determining the critical exponents of the growth dynamics. One type of continuum growth equation has attracted much recent attention because of its possible relevance to the molecular beam epitaxial growth process. This is the conserved growth equation with nonconserved noise where after deposition the mass and the volume of the deposit remain conserved and, consequently, growth must obey a current continuity equation of the type [2]

$$\frac{\partial h}{\partial t} = -\nabla \cdot \mathbf{j} + \eta, \quad (1)$$

where $h(\mathbf{x}, t)$ is the dynamical surface height fluctuation at time t above the substrate point \mathbf{x} , \mathbf{j} is the surface particle current, ∇ is the divergence operator along the substrate (i.e.,

$\nabla \equiv \partial/\partial \mathbf{x}$), and $\eta(\mathbf{x}, t)$ is the nonconserved random shot noise (in both space and time) associated with the deposition flux. (We have subtracted out the uniform growth part of the growing interface concentrating entirely on the fluctuations.) Expressing the current \mathbf{j} in terms of a leading-order gradient expansion consistent with all the symmetries of the problem we arrive [2] at the following conserved continuum growth equation:

$$\frac{\partial h}{\partial t} = \nu_2 \nabla^2 h - \nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \lambda_{13} \nabla (\nabla h)^3 + \eta. \quad (2)$$

When $\nu_2 \neq 0$, clearly it dominates the long-wavelength critical properties of the growth process, and all the other terms (i.e., $\nu_4, \lambda_{22}, \lambda_{13}$) in Eq. (2) are irrelevant from the renormalization group viewpoint. The resulting equation (i.e., $\nu_2 \neq 0$, but $\nu_4 = \lambda_{22} = \lambda_{13} = 0$) in Eq. (2) is the Edwards-Wilkinson (EW) equation [3], which has been well studied and, being linear, is easy to solve.

Our interest in this paper is studying the dynamical critical properties of the fourth-order conserved growth continuum equation obtained by putting $\nu_2 \equiv 0$ in Eq. (2):

$$\frac{\partial h}{\partial t} = -\nu_4 \nabla^4 h + \lambda_{22} \nabla^2 (\nabla h)^2 + \lambda_{13} \nabla (\nabla h)^3 + \eta. \quad (3)$$

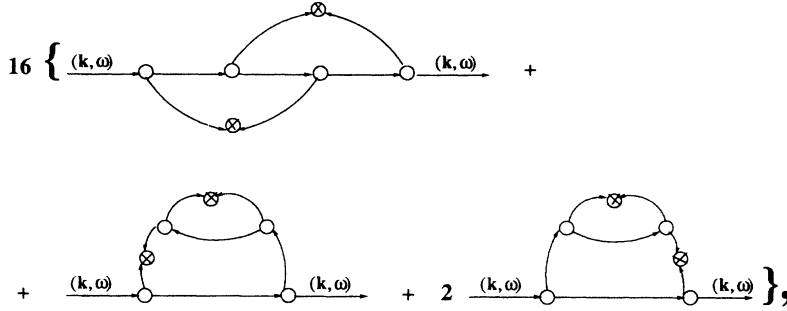


FIG. 1. The relevant irreducible self-energy corrections for the $\lambda_{22}\nabla^2(\nabla h)^2$ nonlinearity in the two-loop order.

where

$$\overrightarrow{(k, \omega)} = G_0(k, \omega),$$

$$\overrightarrow{(k, \omega)} \otimes \overrightarrow{(-k, -\omega)} = 2D,$$

$$\circlearrowleft(k, \omega) = \lambda k^2,$$

$$\begin{array}{l} k_1 \\ \diagdown \\ k_2 \end{array} = k_1 \bullet k_2.$$

The relevance of the situation with $\nu_2=0$ (i.e., no EW term) to surface diffusion driven epitaxial growth in a chemical bonding environment has been much discussed and debated in the recent literature. Several discrete conserved growth models, which mimic aspects of molecular beam epitaxy, are known to have vanishing (or, in some cases, almost-vanishing) values of ν_2 , making Eq. (3) the leading-order conserved continuum growth equation. We do not further discuss in this paper the motivation and rationale for putting $\nu_2=0$ because we have nothing to add to the existing literature. In the rest of this paper we present theoretical results for the dynamical critical properties of Eq. (3). Our results are based on both one-loop and two-loop dynamical renormalization group (DRG) calculations for both the nonlinearities in Eq. (3). The motivation for our DRG analysis comes from the recent direct numerical integration study of Eq. (3) carried out by Kim and Das Sarma [4], who found the unanticipated and seemingly surprising result that while the λ_{22} nonlinearity produces critical growth exponents consistent with an earlier DRG analysis [2] (as well as Flory-type dimensional arguments [5]) of the $\nabla^2(\nabla h)^2$ nonlinearity, the $\lambda_{13}\nabla(\nabla h)^3$ nonlinearity produces precisely the EW exponents consistent with the $\nabla^2 h$ linear term and totally inconsistent with a Flory-type dimensional scaling analysis [2]. Since the $\nabla(\nabla h)^3$ nonlinearity is the most relevant term in Eq. (3), as can be easily verified by a power-counting analysis of the three conserved fourth-order terms, the fact that it belongs to the linear $\nabla^2 h$ EW universality class is obviously of considerable significance. In particular, this implies that conserved epitaxial growth (i.e., no evaporation, no overhangs or vacancies) generically belongs to EW universality independent of whether $\nu_2=0$ or not (except in the very special circumstances of ν_2 and λ_{13} both being zero). In this paper we derive this potentially important result of Kim and Das Sarma [4] based on what we believe to be essentially exact DRG arguments.

We first consider the $\lambda_{13}=0$ case when Eq. (3) in Fourier space can be written as

$$\begin{aligned} h(k, \omega) &= G_0(k, \omega) \eta(k, \omega) + \lambda_{22} k^2 G_0(k, \omega) \\ &\times \iint \mathbf{q} \cdot (\mathbf{k} - \mathbf{q}) h(q, \omega_q) \\ &\times h(|\mathbf{k} - \mathbf{q}|, \omega - \omega_q) \frac{d^d \mathbf{q}}{(2\pi)^d} \frac{d\omega_q}{2\pi}, \end{aligned} \quad (4)$$

where

$$G_0(k, \omega) = (\nu_4 k^4 - i\omega)^{-1}. \quad (5)$$

The one-loop DRG calculation for the $\nabla^2(\nabla h)^2$ nonlinearity has been carried out by Lai and Das Sarma [2] with the dynamical critical exponents z , α , and β being given by $z=(8+d)/3$, $\alpha=(4-d)/3$, and $\beta=(4-d)/(8+d)$, where d is the substrate dimension. One important feature of the lowest-order calculation is that there is no vertex correction to the nonlinearity λ_{22} because the leading-order vertex diagrams exactly cancel out. Similarly, the noise remains unrenormalized because all corrections to the noise propagator are higher orders in k , and are therefore irrelevant. While the nonrenormalization of the noise spectrum is a generic feature of *all* conserved growth models to all orders in perturbation theory (irrespective of whether the noise is nonconserved, as it is in our case, or not, as in [6]), the nonrenormalization of the “interaction” term λ_{22} is a more interesting finding, because, in general, one expects perturbation corrections to the vertex function unless there is a symmetry in the problem. While the leading-order vertex correction explicitly vanishes, a question naturally arises whether this is valid to all orders in perturbation theory. There have been arguments both in favor of vertex renormalization vanishing to all orders [2,6] and against it [5,7]. We, therefore, carried out a two-loop DRG calculation of Eq. (4). We find that the two-loop critical exponents for the λ_{22} nonlinearity remain the same as in [2] in the one-loop order. Our two-loop calculation (Fig. 1) clearly supports the view [8] that the one-loop results of Lai

and Das Sarma for the $\lambda_{22}\nabla^2(\nabla h)^2$ nonlinearity are valid to all orders in the perturbative DRG theory. We believe that the reason for the nonrenormalization of λ_{22} is the exact symmetry discovered in Ref. [6], which acts as a pseudo-Galilean invariance making the hyperscaling relation $\alpha+z=4$ exact.

We now turn to the situation $\lambda_{13} \neq 0$ in Eq. (3). We now take $\lambda_{22}=0$ without any loss of generality since $\lambda_{13}\nabla(\nabla h)^3$ is more relevant than $\lambda_{22}\nabla^2(\nabla h)^2$. Dimensional analysis of Eq. (3) with $\lambda_{13} \neq 0$ gives [2] $z=(4+d)/2$; $\alpha=(4-d)/4$, and $\beta=(4-d)/2(4+d)$. The corresponding Fourier space equation [$\lambda_{13} \neq 0$, $\lambda_{22}=0$ in Eq. (3)] is given by

$$h(k, \omega) = G_0(k, \omega) \eta(k, \omega) + \lambda_{13} G_0(k, \omega) f(k, \omega), \quad (6)$$

where

$$f(k, \omega) = \iiint \frac{d^d \mathbf{k}'}{(2\pi)^d} \frac{d\omega_{k'}}{2\pi} \frac{d^d \mathbf{k}''}{(2\pi)^d} \frac{d\omega_{k''}}{2\pi} g(\mathbf{k}, \mathbf{k}', \mathbf{k}'') \times h(|\mathbf{k}-\mathbf{k}'|) h(k'') h(|\mathbf{k}'-\mathbf{k}''|), \quad (7)$$

with

$$g(\mathbf{k}, \mathbf{k}', \mathbf{k}'') = [\mathbf{k} \cdot (\mathbf{k} - \mathbf{k}')] [\mathbf{k}'' \cdot (\mathbf{k}' - \mathbf{k}'')]. \quad (8)$$

The self-energy diagrams renormalizing the bare propagator $G_0(k, \omega) = (\nu_4 k^4 - i\omega)^{-1}$ up to two-loop orders are shown in Fig. 2. The leading-order correction comes from the contracted Hartree diagrams in the one-loop order [Fig. 2(a)] which lead to the following one-loop correction to the bare coupling constant ν_4 :

$$\tilde{\nu}_4 = \nu_4 \left[1 - \frac{D\lambda_{13}}{\nu_4^2} \frac{1}{k^2} \frac{S_d}{(2\pi)^d} \frac{d+2}{d} \int dk' k'^{d-3} \right], \quad (9)$$

and the corresponding renormalized propagator $G(k, 0)$ is given up to $O(\lambda_{13})$ by

$$\begin{aligned} G(k, 0) &\equiv (\tilde{\nu}_4 k^4)^{-1} \\ &= \left[\nu_4 k^4 - \frac{D\lambda_{13}}{\nu_4} \frac{S_d}{(2\pi)^d} \left(\frac{d+2}{d} \right) k^2 \int dk' k'^{d-3} \right]^{-1} \\ &= [-\tilde{\nu}_2 k^2 + \nu_4 k^4]^{-1}, \end{aligned} \quad (10)$$

where

$$\tilde{\nu}_2 \equiv \frac{D\lambda_{13} S_d}{\nu_4 (2\pi)^d} \frac{d+2}{d} \int dk' k'^{d-3}. \quad (11)$$

In Eqs. (9)–(11),

$$S_d = \frac{2\pi^{d/2}}{\Gamma\left(\frac{d}{2} + 1\right)}$$

and D is the strength of the white noise η in Eq. (3), i.e.,

$$\langle \eta(1) \eta(2) \rangle \equiv 2D \delta^d(\mathbf{x}_1 - \mathbf{x}_2) \delta(t_1 - t_2).$$

The infrared divergent integral over \mathbf{k}' is handled by the usual DRG procedure. The most striking result, which is al-

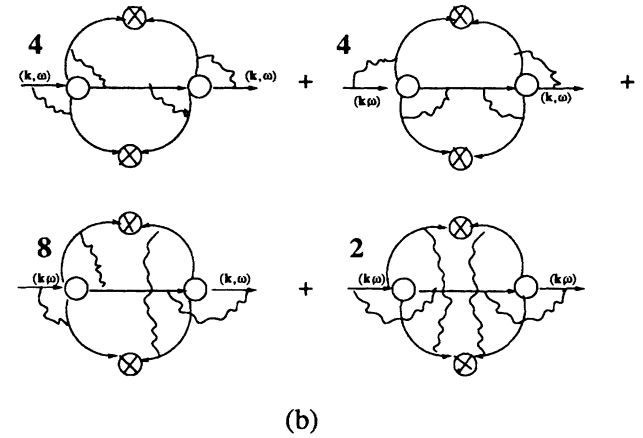
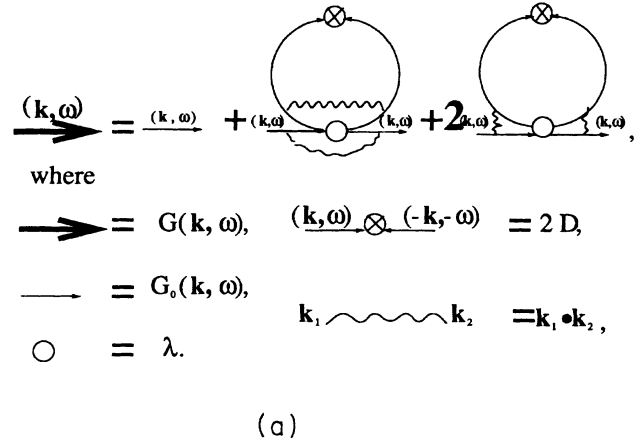


FIG. 2. One- and two-loop order self-energy corrections for the $\lambda_{13}\nabla(\nabla h)^3$ nonlinearity: (a) one-loop calculation; (b) two-loop calculation (only relevant irreducible graphs are shown).

ready apparent at this one-loop order, is the appearance of the more relevant k^2 term renormalizing the higher-order k^4 term of the bare propagator. Thus the long-wavelength critical properties of the $\nabla(\nabla h)^3$ nonlinearity are given by the exact ($k \rightarrow 0$) propagator:

$$G(k, 0) \equiv [-\tilde{\nu}_2 k^2]^{-1}, \quad (12)$$

which, of course, has identical singular properties as the EW propagator [3] corresponding to the $\nu_2 k^2$ term in Eq. (2): $G_{\text{EW}}(k, 0) = [-\nu_2 k^2]^{-1}$. We conclude, therefore, in agreement with Ref. [4] that the most relevant fourth-order conserved nonlinearity in Eq. (3), i.e., $\lambda_{13}\nabla(\nabla h)^3$, belongs to the EW universality class with the dynamical critical exponents given by $z=2$, $\alpha=(2-d)/2$; $\beta=(2-d)/4$. It is obvious that this one-loop result is, in fact, exact to all orders because each Hartree contraction [cf. Fig. 2(a)] would necessarily generate a k^2 term in the propagator upon renormalization, and all higher-order corrections are less relevant in the renormalization group sense than the Hartree self-energy correction. An explicit analysis of the two-loop $O(\lambda_{13}^2)$ diagrams [Fig. 2(b)] manifestly establishes this rather self-evident fact. For the sake of completeness we mention that the noise spectrum remains unrenormalized exactly the same

way as it does for the $\lambda_{22}\nabla^2(\nabla h)^2$ nonlinearity, and the vertex correction terms to the λ_{13} nonlinearity, which are technically nonzero, are all higher-order corrections and are irrelevant for determining the critical exponents. The dynamical critical exponents of Eq. (3) are, therefore, the same as the EW exponents.

We conclude by mentioning a number of salient features of this rather simple but striking result. First, the Flory-type dimensional analysis fails completely for the $\nabla(\nabla h)^3$ nonlinearity because the leading-order Hartree diagrams renormalize the divergent critical properties of the model. Second, the Hamiltonian $H_4 \sim \int d^d x (\nabla h)^4$ produces the $\nabla(\nabla h)^3$ nonlinearity through the nonequilibrium Langevin equation formalism and a simple contraction argument suggests that

the critical properties of H_4 should be identical to the Gaussian model defined by the Hamiltonian $H_2 \sim \int d^d x (\nabla h)^2$ which, of course, leads to the EW growth equation in the nonequilibrium Langevin formalism. Finally, EW universality predicts smooth growth for the physical $d=2$ interface, which implies that epitaxial growth for real surfaces may very well be smooth independent of whether $\nu_2=0$ or not as long as conserved growth conditions (i.e., no evaporation or defect formation) apply. This, as has already been noted [4], by Kim and Das Sarma, has obvious technological implications.

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