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Shift invariance and surface growth

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Abstract. The invariance of equations for self-affine surface growth to reparametrization under the Abelian group of shift transformations $h(x,t) \to h(x,t) + l$ is used to bound the form of nonlinear terms and related kinetic coefficients in relaxational surface growth equations. For conserved growth small but relevant diffusive terms second-order in the driving can always be expected. It is also shown that the asymptotic growth distributions in $d > 2$ can be expected to be skew and are not derivable from a Hamiltonian description.

1. Introduction

Interest in surface growth far from thermal equilibrium [1, 2] and the scaling behaviour of the resulting self-affine surfaces has spread to such varied fields as thin film growth by molecular beam epitaxy [3–5]; fluid dynamics at both low Reynolds numbers, such as those observed at the interface of fluid flow in porous media [6, 2], and at high Reynolds numbers such the boundary layers of turbulence [7]; propagating flame fronts in combustion [8, 9]; and the interfaces related to self-organized critical phenomena [10] such as the surface structure of sandpiles [11] and other granular flows. All these phenomena are nonlinear, anisotropic, and involve the interaction of a large number of degrees of freedom. The main tools developed to study their dynamics and conformation have been simulations of simple models, together with the derivation and analysis of local Langevin-like equations believed to incorporate the symmetries and conservation laws of the long-wavelength physics.

The most renowned of such equations for surface growth is probably the Kardar–Parisi–Zhang (KPZ) equation [12] describing the non-conserved height fluctuations $h(x, t)$ in an interface without overhangs growing with a velocity λ normal to the interface

$$\partial h/\partial t = \nu\nabla^2 h + \lambda/2(\nabla h)^2 + \eta(x,t) \tag{1}$$

where $\langle\eta(x,t)\eta(x',t')\rangle = Q\delta(x-x')\delta(t-t')$. This is, however, but one example in a veritable zoo of equations used to describe different aspects of surface growth including the Sun–Guo–Grant (SGG) equation [13] for the surface height of a driven interface with a conservation law

$$\partial h/\partial t = -\nabla^2[\nu\nabla^2 h + \lambda/2(\nabla h)^2] + \eta(x,t) \tag{2}$$

where $\langle\eta(x,t)\eta(x',t')\rangle = -Q\nabla^2\delta(x-x')\delta(t-t')$; the fourth-order Villain–Wolf [3, 4], and Lai–Das Sarma [5] (VWLS) equation

$$\partial h/\partial t = -D_4\nabla^4 h + \lambda_4\nabla^2(\nabla h)^2 + \eta(x,t) \tag{3}$$

with $\langle\eta(x,t)\eta(x',t')\rangle = Q\delta(x-x')\delta(t-t')$ believed to describe relaxation in MBE growth via surface diffusion; the deterministic Kuramoto–Sivashinsky (KS) equation [8, 9]

$$\partial h/\partial t = D_2\nabla^2 h - D_4\nabla^4 h + \lambda/2(\nabla h)^2 \tag{4}$$

which, though having growth terms in common with both the KPZ and VWLS equations is fundamentally different from both as the diffusion coefficient $D_2 < 0$ is negative—this ensures the existence, without forcing, of chaotic fluctuations capable of describing the intrinsic instabilities in flame propagation; and the Nozieres–Gallet (NG) equation [14]

$$\partial h/\partial t = v + \nu\nabla^2 h + y \sin(2\pi h/a) + \eta(x, t) \tag{5}$$

sometimes modified by the nonlinear term [15] $\lambda/2(\nabla h)^2$, and used to describe dynamic roughening of layered growth.

These equations have self-affine solutions which obey a form of dynamic scaling: [16]

$$W(L, t) \sim \begin{cases} t^\beta & \text{if } t \ll t_L \\ L^\alpha & \text{if } t \gg t_L \end{cases} \tag{6}$$

where $W(L, t)$ is a measure of the width of the surface at time t on a length scale L, and $t_L \sim L^z$ with $z = \alpha/\beta$. As these nonlinear equations are in general insoluble, however, most of the efforts have involved determining the scaling exponents using methods such as the dynamic renormalization group [17], direct numerical integration [18, 19], or non-equilibrium scaling arguments [20].

The question arises, given this catalogue, what constraints exist on the existence of higher-order terms in such Langevin equations, and what are the magnitudes of their *associated kinetic coefficients? This is important in real experiments where the asymptotic* regimes lie beyond experimental observation. Here we show that the demand that the equations of motion for self-affine surface growth be invariant under the reparametrization

$$h(x, t) \to h(x, t) + l \tag{7}$$

where l is an arbitary global displacement of the whole surface, greatly constrain the form these terms can take. The reason is that these shifts form a group which together with the demand that any fluctuations be relaxational is sufficient to specify the allowed growth law.

2. Global shift invariance and surface growth

In this section we examine the constraints that global shift invariance puts on the form of Langevin equations that describe surface growth obeying non-conserved relaxational dynamics, conserved relaxational dynamics, and layered dynamics.

2.1. *Non-conserved dynamics*

Consider a non-conserved relaxational dynamics of the form

$$\partial h/\partial t = -\Gamma\delta F/\delta h + \eta(x, t) \tag{8}$$

where Γ is the relaxation rate, the driving force has the correlation $\langle\eta(x, t)\eta(x', t')\rangle = Q\delta(x - x')\delta(t - t')$, and the free energy is given by $F = \int dx^{d-1}\mathcal{F}(h, \nabla h)$. Equation (8) which is model A of Hohenberg and Halperin [21] is relaxational as $dF/dt = -\Gamma\int dx^{d-1}(\delta F/\delta h)^2$, and therefore the free energy is a Lyapunov function controlling the global stability. In addition (8) yields the asymptotic equilibrium probability distribution given by the functional $P(\{h\}) = Z^{-1}\exp[-\beta F(\{h\})]$, where $Z = \int \mathcal{D}h \exp[-\beta F(\{h\})]$, and $\{h\}$ is used to represent a configuration of the entire surface. The fluctuation–dissipation theorem is obeyed by such growth in the form $\beta = 2\Gamma/Q$.

The additional demand of shift invariance implies, however, as the transport coefficient Γ is a constant, that the free energy density cannot depend explicitly on h but must be a scalar function of gradients of the height fluctuation $\mathcal{F}((\nabla h)^2)$. To lowest order in the expansion of the free energy density we regain the capillary Hamiltonian $F = (\sigma/2)\int \mathrm{d}x^{d-1}(\nabla h)^2$, with the resulting dynamics given by the diffusion equation.

Equation (8) is not, however, the most general form for a non-conserved relaxational dynamics. Consider allowing the relaxation rate to be an explicit local function of the surface configuration $\Gamma(h, \nabla h)$. For such models provided $\Gamma(h, \nabla h) \geqslant 0$, the free energy would still retain its role as a Lyapunov function, but the asymptotic probability distribution would no longer be governed by the free energy alone—it would take up a form also controlled by the configurationally dependent relaxation rate.

It would appear that we have broken our own demand for shift invariance with this generalization. The equations of motion will still, however, remain invariant provided that the free energy density is also generalized to allow for a specific dependence on the surface height $\mathcal{F}(h, \nabla h)$, and the new free energy density $\mathcal{F}$ and the relaxation rate Γ transform in pairs as

$$\mathcal{F}(h+l, \nabla h) = K(l)\mathcal{F}(h, \nabla h) \qquad \Gamma(h+l, \nabla h) = K(l)^{-1}\Gamma(h, \nabla h) \tag{9}$$

under a shift l. The renormalization due to the shifts form an Abelian group obeying $K(l)K(l') = K(l+l')$ which have the solution $K(l) = \exp sl$ where s is the generator of the group, and consequently for shift invariance we require the the free energy density and relaxation rate have the related forms

$$\mathcal{F}(h, \nabla h) = \exp(sh)\mathcal{F}_1((\nabla h)^2) \qquad \Gamma(h, \nabla h) = \exp(-sh)\Gamma_1((\nabla h)^2)\,. \tag{10}$$

The equations of motion defined by (8) and (10) are thus still local, shift invariant, and relaxational, but the price to be paid is that the 'free energy density' and 'relaxation rate' have lost their individual identities—if each term is examined individually then it does not make sense that they should depend on the local value of $h(x, t)$ but should depend only on its gradients. The point, however, is that when taken together the resulting dynamics does indeed remain invariant as can be seen by direct substitution of (10) into (8) which yields the general form for equations of motion for surface growth obeying non-conserved relaxational dynamics

$$\partial h/\partial t = \Gamma_1[2\mathcal{F}_1'\nabla^2 h + 2\mathcal{F}_1''\nabla((\nabla h)^2)\cdot\nabla h] - s\Gamma_1[\mathcal{F}_1 - 2\mathcal{F}_1'(\nabla h)^2] + \eta(x, t)\,. \tag{11}$$

In (11) we have used the notation $\mathcal{F}_1' = \mathrm{d}\mathcal{F}_1/\mathrm{d}(\nabla h)^2$, while $\mathcal{F}_1'' = \mathrm{d}^2\mathcal{F}_1/\mathrm{d}((\nabla h)^2)^2$.

If we now expand $\mathcal{F}_1((\nabla h)^2) = \mathcal{F}_{10} + \mathcal{F}_{11}(\nabla h)^2 + \cdots$ and $\Gamma_1((\nabla h)^2) = \Gamma_{10} + \cdots$ in (11) in powers of $(\nabla h)^2$, then to linear order in the expansion we recover the KPZ equation. Higher powers $\mathcal{F}_1((\nabla h)^2) = \mathcal{F}_{10} + \mathcal{F}_{11}(\nabla h)^2 + \mathcal{F}_{12}(\nabla h)^4$, $\Gamma_1((\nabla h)^2) = \Gamma_{10} + \Gamma_{11}(\nabla h)^2$ will renormalize both transport coefficients into functions of the curvature $\lambda((\nabla h)^2)$ and $\nu((\nabla h)^2)$ and generate new terms, which to next lowest order result in the equation

$$\partial h/\partial t = \nu[\nabla^2 h + s/2(\nabla h)^2] + g[3s(\nabla h)^4 + 4\nabla\cdot[(\nabla h)^2\nabla h]] + \eta(x, t)\,. \tag{12}$$

Note that we have not only recovered the KPZ equation as the relevant asymptotic terms in an expansion of the Langevin equation in powers of s, but the driving velocity $\lambda = s\nu$ is directly proportional to the shift invariance generator; or conversely the driving velocity can be used to find the magnitude of the generator directly as $s = \lambda/\nu$. The higher order kinetic coefficients will also be proportional to various powers of s and their magnitudes can therefore also be estimated.

2.2. Conserved dynamics

If the height of the interface $h(x, t)$ is a locally conserved order parameter we can expect its rate of growth to be controlled by an equation of continuity $\partial h/\partial t = -\nabla \cdot j$, and if the current is diffusive then the growth will be controlled by a nonlinear diffusion equation (a generalization of model B of Hohenberg and Halperin [21]) of motion of the form

$$\partial h/\partial t = \nabla \cdot [\Gamma(h, \nabla h)\nabla \delta F/\delta h] + \eta(x, t)\,. \tag{13}$$

Once again we demand shift invariance for the conserved growth equation and once again this leads to constraints on the relationship between the free energy and a transport coefficient given by (9). The resulting equation of motion for conserved dynamics (dropping all terms involving more than fourth-order derivatives) is of the form

$$\begin{aligned}\partial h/\partial t = \gamma_2 s^2 \nabla^2 h - D_4\{\nabla^4 h + (s/2)[\nabla^2(\nabla h)^2 + 2\nabla\cdot[\nabla^2 h \nabla h]] \\ +(s^2/2)\nabla\cdot[(\nabla h)^2 \nabla h]\} + \eta(x, t)\,.\end{aligned} \tag{14}$$

Note the relationships the shift invariance introduces among the various terms generated by the non-equilibium driving. For example it appears that at second order in the driving s^2 a diffusive term with diffusion constant $D_2 = \gamma_2 s^2$ is generated. This term will always appear even for a constant free energy (as $\gamma_2 \propto \mathcal{F}_{10}$), and it may be the cause of the Edwards–Wilkinson-like regime [22] observed by Kessler *et al* [23] in a model for molecular beam epitaxy and surface diffusion. Also note that the magnitude of the coefficients for the nonlinear terms are proportional to the equilibrium fourth-order diffusion coefficient D_4. A comparison of (14) with both the SGG and VWLS equations, which differ mainly in whether the noise fluctuations are conserved or not, appears to suggest that both these equations need to be modified to lowest nonlinear order if global shift invariance is a required symmetry of the dynamics—for the nonlinear term $D_4 s\nabla\cdot[\nabla^2 h \nabla h]$ appears in addition to the term $(D_4 s/2)\nabla^2(\nabla h)^2$ and they are both of equal relevance from a scaling viewpoint.

2.3. *Layered and generalized dynamics*

Our approach can be extended to generate growth equations with lower symmetry requirements. One particularly important field where this lower symmetry requirement holds may be in studies of layered growth. In this situation, it is to be expected that the equations of motion will only be invariant under shifts of a specified length scale a. In this case we may use Bloch's theorem to demand

$$\mathcal{F}(h, \nabla h) = \exp(sh) T_1(h) \mathcal{F}_1((\nabla h)^2) \qquad \Gamma(h, \nabla h) = \exp(-sh) T_2(h) \Gamma_1((\nabla h)^2) \tag{15}$$

where $T_1(h + a) = T_1(h)$ and $T_2(h + a) = T_2(h)$ are periodic functions of the required periodicity. The additional demand that purely diffusive motion is unaffected by the layering leads to the additional requirement $T_1(h) = T_2(h)^{-1} = T(h)$ and (11) is transformed into

$$\begin{aligned}\partial h/\partial t = -\Gamma_1\{(s + (\mathrm{d}\ln T/\mathrm{d}h))[\mathcal{F}_1 - 2\mathcal{F}_1'(\nabla h)^2] - 2\mathcal{F}_1'\nabla^2 h \\ -2\mathcal{F}_1''\nabla[(\nabla h)^2]\cdot\nabla h\} + \eta(x, t)\,.\end{aligned} \tag{16}$$

In consequence, the KPZ equation is transformed into a generalization of the Nozieres–Gallet (NG) equation [14]

$$\partial h/\partial t = v(h) + \nu\nabla^2 h + (\lambda(h)/2)(\nabla h)^2 + \eta(x, t) \tag{17}$$

where both $v(h + a) = v(h)$ and $\lambda(h + a) = \lambda(h)$ are proportional periodic functions of a with the amplitude of the periodic fluctuation to the average driving velocity being of order $(as)^{-1}$, and therefore the periodic variations in layered growth being most observable at small driving rates.

More general shift invariant relaxational growth can be found by allowing for higher derivative dependence for both the free energy density and its associated relaxation rate

$$\mathcal{F}(h, \nabla h, \nabla^2 h) = \exp(sh)\mathcal{F}_1((\nabla h)^2, \nabla^2 h)$$
$$\Gamma(h, \nabla h, \nabla^2 h) = \exp(sh)\Gamma_1((\nabla h)^2, \nabla^2 h)\,. \tag{18}$$

The $\nabla^2 h$ dependence of the free energy in (18) will generate terms such as the $\nabla^4 h$ term in the Kurumoto–Sivashinsky equation. For example if the free energy density is a function of $\nabla^2 h$ alone, $\mathcal{F}_1(\nabla^2 h)$, then to lowest nonlinear order the Kuramoto–Sivashinshy equation will be directly generated and keeping one higher set of nonlinear terms we find

$$\partial h/\partial t = \gamma_2 s \nabla^2 h + D_4 \nabla^4 h + \gamma_2 s^2 (\nabla h)^2$$
$$+ D_4[(3s/2)(\nabla^2 h)^2 + s^2 (\nabla h)^2 \nabla^2 h + 2s \nabla h \cdot \nabla^2 \nabla h] \tag{19}$$

where the s dependence of the various coefficients has been made explicit. We can recover the correct sign of the various kinetic coefficients in (4) if $\gamma_2 > 0$ but $D_4 < 0$ and $s < 0$. The contribution of the nonlinear terms to the dynamics is interesting for despite the fact that as $L \to \infty$ the term $\gamma_2 s^2 (\nabla h)^2$ is dominant over the other nonlinearities (provided the exponent $\alpha < 1$), the s^2 dependence of the kinetic coefficient suggests that at small driving rates there may be a cross-over from a regime dominated by the nonlinear terms $D_4 s[(3/2)(\nabla^2 h)^2 + 2\nabla h \cdot \nabla^2 \nabla h]$.

3. Shift invariance and skewness

As the shift invariance generator s has dimensions of an inverse length scale, the question remains as to whether this length scale can be directly extracted from a single image of a growing surface? This seems unlikely, anymore than the Reynolds number can be extracted from a single image of a flow field. The shift invariance generator s is, however, closely related to surface skewness, and we can estimate this length scale as the magnitude of the surface fluctuations $s^{-1} \sim h(t_{\text{skew}})$ at early times t_{skew} at which the skewness of the surface fluctuations reaches its maximum value.

This can be seen by examining (11). If only the first term on the right-hand side of (11) existed then the equation of motion would be invariant under the operation $h \to -h$; the second term proportional to s breaks this symmetry. The magnitude of the second to first term at early times t is $\approx sh_t$. Thus the second term can start to significantly influence surface growth when $sh_t \approx 1$. Surface skewness $S(t, L) = \langle (h(x+L, t) - h(x, t))^3 \rangle / \langle (h(x+L, t) - h(x, t))^2 \rangle^{3/2}$ can thus be expected to grow rapidly from zero $S(0, L) = 0$ for times $t \ll t_{\text{skew}} \sim s^{-1/\beta}$. At long times $t \gg t_L$ the asymptotic fluctuations set in where skewness may or may not exist depending on the properties of the asymptotic fluctuations.

Indeed, there is plenty of evidence for the KPZ equation [24–26] in $d = 2$ dimensions (here we use the convention that the surface on which growth is occuring has dimension $(d-1)$) that in the transient regime the skewness $S(t, L)$ rapidly rises at very early times, reaches a maximum at some time $t \ll t_L$ (which we identify with $t_{\text{skew}}(s)$), and then decays again. For times $t \gg t_L$, because of the Gaussian nature of the asymptotic fluctuations in $d = 2$, the skewness must disappear $S(\infty, L) = 0$. These arguments suggest any scaling form for the skewness involves two timescales $S(t, L) = f_{\text{skew}}(t/t_L, t/t_{\text{skew}}(s))$ rather than the simpler form $S(t, L) = f_{\text{skew}}(t/t_L)$.

To examine skewness in the asymptotic fluctuations of non-conserved dynamics it is useful to study the Fokker–Planck equation related to (8)

$$\partial P(\{h\},t)/\partial t = \int \mathrm{d}x^{d-1}\delta/\delta h\{\Gamma\delta F/\delta h P(\{h\},t) + (Q/2)\delta P(\{h\},t)/\delta h\} \tag{20}$$

where $P(\{h\},t)$ is the probability of observing the surface in configuration $\{h\}$ at time t. Equation (20) has the equilibrium form

$$\int \mathrm{d}x^{d-1}\delta/\delta h\{\Gamma\delta F/\delta h P(\{h\}) + (Q/2)\delta P(\{h\})/\delta h\} = 0\,. \tag{21}$$

In $d = 2$ dimensions, even in the presence of the nonlinear symmetry breaking terms in the KPZ equation, the asymptotic fluctuations remain symmetric and indeed Gaussian $P(\{h\}) = Z^{-1}\exp -\beta\int \mathrm{d}x(\mathrm{d}h/\mathrm{d}x)^2$ because the additional nonlinear contributions vanish on integration by parts. In general, however, (21) will only have a Hamiltionian asymptotic fluctuations $P(\{h\}) = Z^{-1}\exp -H(\{h\})$ if the related functional equation $\delta H/\delta h = (2/Q)\Gamma\delta F/\delta h$ has a solution. Even for natural boundary conditions $P \to 0$ as $h(x,t) \to \pm\infty$, however, it is not true in general that this equation can be solved; and in the present case it is easy to show using (10) that $\delta^2 H/\delta h(x)\delta h(x') \neq \delta^2 H/\delta h(x')\delta h(x)$ and consequently no Hamiltonian form exists. It is also easy to see that no new free energy $F_{\mathrm{new}}((\nabla h)^2, s)$ and constant kinetic coefficient $\Gamma_{\mathrm{new}}(s)$ related to the old parameters by $\Gamma(h)\delta F/\delta h = \Gamma_{\mathrm{new}}\delta F_{\mathrm{new}}/\delta h$ can exist which would allow a Hamiltonian asymptotic distribution because the left-hand side of this equation is not invariant under the operation $h \to -h$ for all $s \neq 0$, while the right-hand side is. A direct consequence is that the asymptotic height fluctuations for non-equilibrium surface growth in higher dimensions $d > 2$ can be expected to be fundamentally different from those observed in equilibrium growth or in $d = 2$ dimensions.

Thus despite the fact that the free energy, F, drives the system to some asymptotic distribution, this same free energy does not control the asymptotic fluctuations alone, but they are also intimately dependent on the nonlinear form of the relaxation rate. One consequence is that the fluctuation–dissipation theorem in the form $\Gamma = 2\beta Q$ breaks down. It is possible, however, to recover an approximate equilibrium form for the fluctuations simply by replacing the exact relaxation rate $\Gamma(h, \nabla h) = \exp(-sh)\Gamma_1((\nabla h)^2)$ by the simple but non-unique approximation $\Gamma(\langle h\rangle, 0) = \exp(-s\langle h\rangle)\Gamma_1(0)$, where we argue that at small wavelengths k any gradient dependence (there may be none) of the kinetic coefficient disappears as $|\nabla h| \sim k^{1-\alpha}$, and the local height $h(x)$ is replaced by its global average $\langle h\rangle = L^{-(d-1)}\int \mathrm{d}x^{d-1}h(x)$. In this case we find that the asymptotic fluctuations obey the functional expression

$$P(\{h\}) = Z^{-1}\exp[-(2\Gamma_1(0)/Q)\int \mathrm{d}x^{d-1}\exp[s(h-\langle h\rangle)]\mathcal{F}_1((\nabla h)^2)]\,. \tag{22}$$

It is interesting to note that this asymptotic distribution is skew for all $s \neq 0$, a result that is well known in the study of the fluctuations in both the energies of directed polymers in random media and the height fluctuations in surface growth [27, 28] in $d = 2$ dimensions in the transient regime, but here we argue that even in the asymptotic regime such skewness should be visible in higher dimensions.

4. Discussion

In conclusion, it appears, as though shift invariance combined with other known conservation laws is a powerful tool for generating the possible kinematics of interfacial growth, and finding dependence on driving of the various nonlinear transport coefficients. In lowest nonlinear order in the gradients the equations of motion derived agree with the surface growth equations derived phenomenologically by assuming a constant growth velocity λ normal to the interface for non-conserved dynamics—the KPZ equation. For conserved growth the situation is more complex. It appears that small diffusive terms are always generated of magnitude s^2. In addition, forms valid to all powers in the nonlinear gradients have been derived, which, however, disagree with the assumption of a constant growth velocity normal to the interface.

Three direct consequences of global shift invariance appear: first, the generator of the group s has units of an inverse length scale so that $s^{-1} \approx h(t_{\rm skew})$ defines the height fluctuations and the timescale at which skewness is maximum at early times. Second, we argue that for all $s \neq 0$ there is no Hamiltonian formulation for the asymptotic distribution in $d > 2$ to which these driven surfaces tend at long times $t \gg t_L$; but whatever their form, they can be expected to be skew; third, the magnitude of the shift invariance generator s can be used to estimate whether a particular higher-order term needs to be included in the Langevin equation describing a real rough surface.

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