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Asymptotic and effective coarsening exponents in surface growth models

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Abstract. We consider a class of unstable surface growth models, $\partial_t z = -\partial_x \mathcal{J}$, developing a mound structure of size λ and displaying a perpetual coarsening process, i.e. an endless increase in time of λ. The coarsening exponents n, defined by the growth law of the mound size λ with time, $\lambda \sim t^n$, were previously found by numerical integration of the growth equations [A. Torcini, P. Politi, Eur. Phys. J. B **25**, 519 (2002)]. Recent analytical work now allows to interpret such findings as finite time effective exponents. The asymptotic exponents are shown to appear at so large time that cannot be reached by direct integration of the growth equations. The reason for the appearance of effective exponents is clearly identified.

PACS. 81.10.Aj Theory and models of crystal growth; physics of crystal growth, crystal morphology, and orientation – 02.30.Jr Partial differential equations

1 Introduction

In this manuscript we are interested in studying a class of one dimensional growth equations, having the conserved form $\partial_t z = F - \partial_x \mathcal{J}$: the dynamics of the local height $z(x,t)$ of the surface is determined, apart from a trivial constant term F describing the deposition flux, by the processes occuring at the surface, which are all included in the surface current $\mathcal{J}$ [1,2]. Possible noise sources, shot noise first, will be neglected.

The current $\mathcal{J}$ may have a plethora of different forms, depending on the details of the atomistic processes [3]. For Molecular Beam Epitaxy [4,5], a widely used technique for growing metal and semiconductor thin films with nanoscale control, one of the most studied equations has the form [1,5]

$$\partial_t z = -\partial_x (u_{xx} + j(u)) \tag{1}$$

where the constant term F has been included in the left hand side by redefining $z = z - Ft$, and $u = z_x = \partial_x z$ is the slope of the surface. It is worth noting that taking the spatial derivative of both sides, we get $u_t = -\partial_{xx}(u_{xx} + j(u))$, i.e. a generalized Cahn-Hilliard equation [6]. Without the double derivative ($-\partial_{xx}$) we get the corresponding non-conserved models, called generalized real Ginzburg-Landau (or Allen-Cahn) equation [6]. In summary, we are considering the two classes of equations

$$u_t = -\partial_{xx}(u_{xx} + j(u)) \quad \text{conserved} \tag{2}$$
$$u_t = u_{xx} + j(u) \quad \text{non-conserved.} \tag{3}$$

The linear stability analysis of the flat interface, $z = z_0 + \epsilon \exp(\omega t + iqx)$, can be easily applied to equations (2, 3) giving

$$\omega = j'(0)q^2 - q^4 \quad \text{conserved} \tag{4}$$
$$\omega = j'(0) - q^2 \quad \text{non-conserved,} \tag{5}$$

so that an instability appears (i.e. $\omega(q) > 0$ for some q) if $j'(u=0) > 0$. Without loss of generality, we may assume $j'(0) = 1$. The steady states are determined by the equation $u_{xx} = -j(u)$ both in the conserved (2) and non-conserved (3) case. The solutions $u(x)$ correspond to the trajectories of a fictitious particle moving in the symmetric potential $V(u) = \int du\, j(u) = \frac{1}{2}u^2 +$ *higher order terms*. The oscillations in the potential well correspond to periodic steady states of the variable u, with wavelength λ and amplitude A.

The study of the stationary periodic solutions is of great importance for the dynamics as well. In reference [7], for equations (2, 3) and other classes of models, it has been shown that the surface undergoes a coarsening process if and only if $d\lambda/dA > 0$. In simple words, the wavelength of the mound structure (emerging from the linear instability) increases in time if the wavelength $\lambda(A)$ of the periodic steady state increases with the amplitude A. Even

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more importantly, the knowledge of the stationary periodic solutions allows to determine [6] the coarsening law $\lambda(t)$ (see the next section for more details).

2 Numerics vs. analytics

In the following we are focusing on a class of models defined by the currents

$$j(u) = \frac{u}{(1+u^2)^\alpha}, \tag{6}$$

which correspond to the potentials

$$V(u) = -\frac{1}{2(\alpha-1)}\frac{1}{(1+u^2)^{\alpha-1}}. \tag{7}$$

They were introduced in a previous paper on this journal [8] and were called $\alpha-$models.

It is straightforward to check that $V(u)$ has a minimum in $u = 0$ and goes to zero for large u, as $V(u) \sim -1/|u|^{2(\alpha-1)}$. The curves $\lambda(A)$ can be found numerically, but the sign of $d\lambda/dA$ can be easily deduced from the behavior of $V(u)$ at small and large u. At small u, $V(u) \approx V(0) + \frac{1}{2}u^2 - \frac{\alpha}{4}u^4$, so that the quartic term is negative. At large u, $V(u)$ increases and goes to a constant value. Both these features are signatures [10] for a positive $d\lambda/dA$, i.e. for a perpetual coarsening.

2.1 Old results

In reference [8] we studied the coarsening exponent n ($\lambda(t) \sim t^n$) for the $\alpha-$models. The non-conserved version, equations (3, 6), allowed for an analytical treatment which followed an approach due to Langer [9]: it consists in evaluating the most unstable eigenvalue of the linear operator describing perturbations of the periodic stationary solution. This method gave the results

$$n = \begin{cases} \frac{1}{2} & \alpha < 2 \\ \frac{\alpha}{3\alpha-2} & \alpha > 2 \end{cases} \quad \text{non-conserved (Ref. [8])} \tag{8}$$

The conserved version, equations (2, 6), of $\alpha-$models did not allow for an equally rigorous approach. Therefore, we integrated numerically [8] the growth equations $\partial_t z = -\partial_x \mathcal{J}$: it appeared that coarsening exponents agreed fairly well with the relations

$$n = \begin{cases} \frac{1}{4} & \alpha < 2 \\ \frac{\alpha}{5\alpha-2} & \alpha > 2 \end{cases} \quad \text{conserved (Ref. [8])}. \tag{9}$$

These results were interpreted by doing the following ansatz: "*as for the coarsening exponent, passing from the non-conserved to the conserved models is equivalent to replace* $(-\partial_{xx})$ *in equation (2) with* $1/\lambda^2$." This recipe allows to get the conserved coarsening exponents (9) from the non-conserved ones (8) in a straightforward manner. The previous picture appeared to be reasonably correct until a more general analytical approach [6] has been recently developed.

2.2 New results

This new theory relies on the observation that the coarsening law $\lambda(t)$ can be extracted from the so-called phase diffusion coefficient, which describes the dynamics of the local phase, when the periodic stationary solution is perturbed. This approach is applicable to large classes of models, both conserved and non-conserved. As for the $\alpha-$models, $\lambda(t)$ is deduced from the relations [6]

$$\frac{j(A)}{I\,\lambda'(A)} \sim \frac{1}{t} \quad \text{conserved models} \tag{10}$$

$$\frac{j(A)}{J\,\lambda'(A)} \sim \frac{1}{t} \quad \text{non-conserved models.} \tag{11}$$

In equations (10, 11), all the quantities refer to the periodic steady states, $u(x+\lambda) = u(x)$, satisfying the equation $u_{xx} + j(u) = 0$: A is the amplitude (the maximal positive value of $u(x)$); λ is the oscillation period (i.e. the wavelength) and $\lambda'(A)$ is its derivative with respect to A; J is the action variable, defined by $J = \oint dx\, u_x^2$; finally, $I = \oint dx\, u^2$.

For large A, we can split the motion of the fictitious particle in the potential $V(u)$ in a region close to the origin, $|u| < A_0$, and in the complementary regions $A_0 < |u| < A$. A_0 is chosen so that in the regions $|u| > A_0$, $j(u)$ and $V(u)$ can be approximated by their asymptotic expressions $j(u) \simeq 1/|u|^{2\alpha-1}$ and $V(u) \simeq -\frac{1}{2(\alpha-1)}|u|^{-2(\alpha-1)}$.

Since $V(A)$ goes to a constant for diverging A, the motion of the particle in the small u region ($|u| < A_0$) does *not* depend on A. Therefore, every integral quantity (λ, I, J) is the sum of a constant term, coming from the integration in the small u region, and an asymptotic $A-$dependent term, coming from the integration in the large u region. In all cases (with one exception, see below) the asymptotic contribution diverges with A and therefore dominates. Such contribution can be evaluated by dimensional arguments and, more rigorously, using the law of mechanical similarity [11]. For example, $\lambda(A)$ can be simply deduced equating the 'acceleration' A/λ^2 to the 'force' $j(A) \sim 1/A^{2\alpha-1}$, therefore getting $\lambda \sim A^\alpha$. Similarly, we get $I \sim \lambda A^2$.

As for J, the asymptotic contribution amounts to $\lambda(A/\lambda)^2 \sim A^{2-\alpha}$, which diverges for $\alpha < 2$ only. For $\alpha > 2$ (this is the exception mentioned above) the asymptotic contribution of J vanishes, indicating that the small u region, giving a constant contribution, dominates. In conclusion, $J \sim A^{2-\alpha}$ for $\alpha < 2$ and $J \sim 1$ for $\alpha \geq 2$.

If we replace the previous relations in equations (10, 11), we get equations (8) for the non-conserved models, but we get a constant coarsening exponent, $n = \frac{1}{4}$, for the conserved models, in sharp contrast with equation (9). In conclusion, the Langer-type approach and the recent theory based on the phase diffusion coefficient give the same results (8) for the non-conserved $\alpha-$models. For the conserved models, where the Langer-type approach is not applicable, the recent theory seems not to agree with the numerical results (9) found in reference [8] via direct

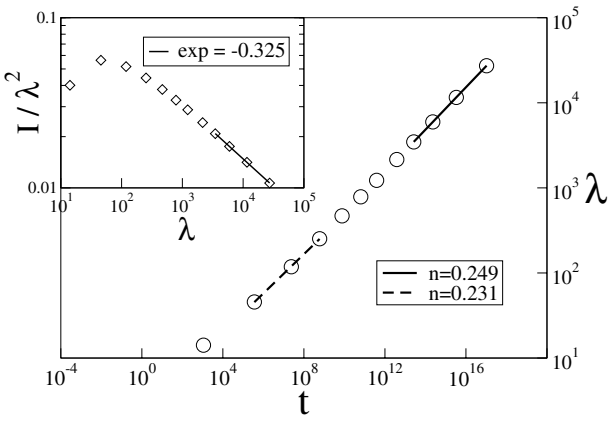

Fig. 1. The coarsening law $\lambda(t)$ for the conserved model $\alpha = 3$, as derived by equation (10) after numerical determination of the steady states $u(x)$. Full and dashed lines refer to the asymptotic fit and to the fit in the region $\lambda \approx 10^2$, respectively. Inset: The quantity I/λ^2 as a function of λ, for the same conserved model.

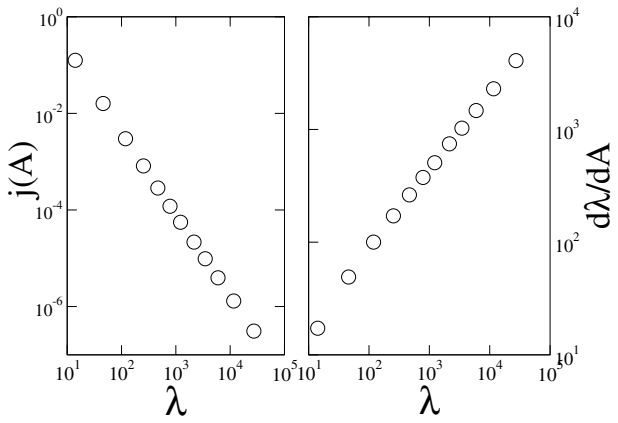

Fig. 2. The scaling of the maximal force $j(A)$ (left) and of the quantity $\lambda'(A)$ (right), as functions of λ.

numerical integration. This disagreement also calls for reconsidering the ansatz $(-\partial_{xx}) \rightarrow 1/\lambda^2$. Next section is devoted to understand the origins of this discrepancy (therefore, we will limit to $\alpha > 2$).

3 The origin of the effective exponents

First of all, let us determine numerically $\lambda(t)$ from equation (10) at all times. Results for $\alpha = 3$ are shown as circles in Figure 1 (main). The direct integration of the growth equation was performed in reference [8] up to $\lambda \approx 10^2$. A numerical fit in this region (dashed line) gives an effective exponent $n = 0.231$, which is in perfect agreement with such simulations and with the relation $n = \alpha/(5\alpha - 2)$. Conversely, a fit in the asymptotic region (full line) gives $n = 0.25$, as expected. The numerical results found in [8] are therefore interpreted as finite-time exponents: formulas (9) are applicable up to $\lambda \approx 10^2$, but the asymptotic exponent for the conserved model is $\frac{1}{4}$.

Let us now discuss the origin of such finite-time exponents. As discussed in the previous Section, formulas (9) are correct insofar as the ansatz $(-\partial_{xx}) \rightarrow 1/\lambda^2$ is correct. Its validity corresponds to say that

$$\left(\frac{1}{t}\right)_{\rm conserved} \sim \frac{1}{\lambda^2}\left(\frac{1}{t}\right)_{\rm non-conserved}. \qquad (12)$$

If we focus on our *exact* relations (10, 11), this relation would imply

$$\frac{j(A)}{I(\partial_A\lambda)} \sim \frac{1}{\lambda^2}\frac{j(A)}{J(\partial_A\lambda)}, \qquad (13)$$

i.e. $I/\lambda^2 \sim J$. Since J is constant for $\alpha > 2$, the formula $n = \alpha/(5\alpha-2)$ would be correct if (I/λ^2) were constant as well. In the inset of Figure 1 we plot the numerical results for I/λ^2 *vs* λ: for very large λ, $I/\lambda^2 \sim \lambda^{-1/3}$ decreases, but for $\lambda \approx 10^2$ it has a *maximum*. In other words, in the region of wavelengths which can be reasonably investigated with the direct integration of the growth equation, the quantity I/λ^2 is approximately constant, which implies $n \approx \alpha/(5\alpha - 2)$.

In order to support the idea that the origin of the effective exponents is indeed the maximum in I/λ^2, in Figure 2 we also plot the two other relevant quantities appearing in equation (10), $j(A)$ and $d\lambda/dA$: none of them has any special behaviour for small λ.

4 Conclusions

In this short note we have reconsidered a class of conserved (2) and non-conserved (3) growth models, in the light of recent theoretical results [6]. These models, defined by the current (6) and termed $\alpha-$models, all display perpetual coarsening, $\lambda(t) \sim t^n$.

For the non-conserved models, n depends on α according to formula (8): therefore, the theory based on the phase diffusion coefficient [6] confirm previous results [8] based on a Langer-type approach [9]. For the conserved models, recent theoretical results [6] give a constant coarsening exponent, $n = \frac{1}{4}$, at odds with our previous numerical results, equation (9). We have explained the effective exponent $n = \alpha/(5\alpha - 2)$ as a finite-time exponent, whose appearance is due to the fact that the quantity I/λ^2, instead of decreasing as a power law, is approximately constant for not too large λ (see Fig. 1, inset). This constant behaviour is equivalent to assume that the operator $(-\partial_{xx})$ in equation (2) can be effectively replaced by $1/\lambda^2$, when n is evaluated.

It is worth noting that the result $n = \frac{1}{4}$ for the conserved models was firstly found by Golubović [12] using some dimensional arguments (see Sect. 7 of Ref. [8] for more details). The main problem with this approach is that it also gives a constant coarsening exponent $n = \frac{1}{2}$ for the non-conserved models, which is wrong. The reason of this failure is clear from Section 2.2, because dimensional analysis can be valid only if the $A-$dependent asymptotic contribution to the integral quantities λ, I, J outnumbers the contribution from the small u region. This is not the

case for the non-conserved models and $\alpha > 2$: exactly the class of equations where dimensional analysis fails.

Similar arguments can be used to understand the failure of the ansatz ($-\partial_{xx} \to 1/\lambda^2$), which has clearly to do with dimensional analysis. The weak point is that this ansatz is applied along with the correct results for the non-conserved models, where dimensional analysis works for $\alpha < 2$ only: therefore, the ansatz gives the final correct result (for the conserved models) for $\alpha < 2$ only.

It is also worth stressing that a more rigorous application of dimensional arguments [13] to the conserved models gives an inequality, $n \leq \frac{1}{4}$, which does not allow to discriminate between $n = \frac{1}{4}$ and $n = \alpha/(5\alpha - 2)$.

We conclude with some remarks on the possibility to access numerically the asymptotic scaling region reported in Figure 1 for the conserved model with $\alpha = 3$. We are going to argue that a direct integration of equation (1) would require astronomically long CPU times.

Since the correct scaling sets in for $\lambda > 2000$ (see Fig. 1), it would be necessary to consider a chain of length $L \sim 10^4$ and to integrate for times $t \sim 10^{15}$. In our numerical results published in reference [8], we integrated equation (1) using a time-splitting pseudo-spectral code, using a spatial resolution $\Delta x = 0.25$, a time step $\Delta t = 0.05$ and a chain of length $L = 1024$. Employing an "Opteron AMD64 Dual Core" machine with a 2 GHz clock, we are *currently* able to reach $\lambda \approx 10^2$ and $t \approx 10^8$ with 20 hours of CPU time. This means that in order to simulate a chain of length $L \sim 10^4$ for a time $t \sim 10^{15}$, we would require (on the same machine) a CPU time of $10 \times 10^7 \times 20$ hours $\approx 2 \times 10^5$ years. The simulation time can be reduced to some extent by lowering the precision of the integration. In particular, we have verified that results of quality comparable with those reported in [8] can still be obtained by increasing the time step up to four times, while the integration scheme becomes rapidly unstable by considering a coarser space grid. As a matter of fact, we cannot expect to lower the CPU time more than a factor $\sim$10, which renders still unfeasible the observation of the asymptotic exponents (by the way, even a lowering up to a factor 10^5 would make it unfeasible).

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