Coarsening of Surface Structures in Unstable Epitaxial Growth

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Abstract

We study unstable epitaxy on singular surfaces using continuum equations with a prescribed slope-dependent surface current. We derive scaling relations for the late stage of growth, where power law coarsening of the mound morphology is observed. For the lateral size of mounds we obtain $\xi \sim t^{1/z}$ with $z \geq 4$. An analytic treatment within a self–consistent mean–field approximation predicts multiscaling of the height–height correlation function, while the direct numerical solution of the continuum equation shows conventional scaling with $z = 4$, independent of the shape of the surface current.

1 Introduction

On many crystal surfaces step edge barriers are observed which prevent interlayer (downward) hopping of diffusing adatoms [1, 2]. In homoepitaxy from a molecular beam this leads to a growth instability which can be understood on a basic level: Adatoms form islands on the initial substrate and matter deposited on top of them is caught there by the step edge barrier. Thus a pyramid structure of islands on top of islands develops.

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At late stages of growth pyramids coalesce and form large “mounds”. Their lateral size $\xi$ is found experimentally to increase according to a power law in time, $\xi \sim t^{1/z}$ with $z \simeq 2.5 - 6$ depending on the material and, possibly, deposition conditions used. A second characteristic is the slope of the mounds’ hillsides $s$, which is observed to either approach a constant (often referred to as a “magic slope” since it does not necessarily coincide with a high symmetry plane) or to increase with time as $s \sim t^\alpha$ \cite{magic_slope_ref1, magic_slope_ref2}. The surface width (or the height of the mounds) then grows as $w \sim s\xi \sim t^\beta$ with $\beta = 1/z + \alpha$, where $\alpha = 0$ for the case of magic slopes.

On a macroscopic level these instabilities can be understood in terms of a growth-induced, slope-dependent surface current \cite{growth_current_ref1, growth_current_ref2}. Since diffusing adatoms preferably attach to steps from the terrace below, rather than from above, the current is uphill and destabilizing. The concentration of diffusing adatoms is maintained by the incoming particle flux; thus, the surface current is a nonequilibrium effect.

The macroscopic view is quantified in a continuum growth equation, which has been proposed and studied by several groups \cite{continuum_theory_ref1, continuum_theory_ref2, continuum_theory_ref3, continuum_theory_ref4, continuum_theory_ref5, continuum_theory_ref6, continuum_theory_ref7}. The goal of the present contribution is to obtain analytic estimates for the scaling exponents and scaling functions of this continuum theory. To give an outline of the article: In the next section we briefly introduce the continuum equations of interest. A simple scaling ansatz, presented in Section 3, leads to scaling relations and inequalities for the exponents $1/z$, $\alpha$ and $\beta$. In Section 4 we present a solvable mean-field model for the dynamics of the height–height correlation function. Up to logarithmic corrections, the relations of Section 3 are corroborated. Finally, in the concluding Section 5 the mean–field correlation functions are compared to numerical simulations of the full growth equation, and the special character of the mean–field approximation is pointed out.

2 Continuum equation for MBE

Under conditions typical of molecular beam epitaxy (MBE), evaporation and the formation of bulk defects can be neglected. The height $H(x,t)$ of the surface above the substrate plane then satisfies a continuity equation,

$$\partial_t H + \nabla J_{\text{surface}} = F,$$  \hspace{1cm} (1)
where $F$ is the incident mass flux out of the molecular beam. Since we are interested in large scale features we neglect fluctuations in $F$ (“shot noise”) and in the surface current (“diffusion noise”). In general, the systematic current $J_{\text{surface}}$ depends on the whole surface configuration. Keeping only the most important terms in a gradient expansion\[1\] subtracting the mean height $H = Ft$, and using appropriately rescaled units of height, distance and time \[13\], Eq. (1) attains the dimensionless form

$$\partial_t h = - (\nabla^2)^2 h - \nabla \cdot f(\nabla h^2) \nabla h.$$  

(2)

The linear term describes relaxation through adatom diffusion driven by the surface free energy \[13\], while the second nonlinear term models the nonequilibrium current \[3, 8\]. Assuming in-plane symmetry, it follows that the nonequilibrium current is (anti)parallel to the local tilt $\nabla h$, with a magnitude $f(\nabla h^2)$ depending only on the magnitude of the tilt. We consider two different forms for the function $f(\nabla h^2)$:

(i) Within a Burton-Cabrera-Frank-type theory \[4, 12, 14\], for small tilts the current is proportional to $|\nabla h|$, and in the opposite limit it is proportional to $|\nabla h|^{-1}$. This suggests the interpolation formula \[7\] $f(s^2) = 1/(1 + s^2)$. Since we are interested in probing the dependence on the asymptotic decay of the current for large slopes, we consider the generalization

$$f(s^2) = 1/(1 + |s|^{1+\gamma}) \ [\text{model (i)}].$$

(3)

Since $\gamma = 1$ also in the extreme case of complete suppression of interlayer transport \[12, 16\], physically reasonable values of $\gamma$ are restricted to $\gamma \geq 1$.

(ii) Magic slopes can be incorporated into the continuum description by letting the nonequilibrium current change sign at some nonzero tilt \[6, 9, 10\]. A simple choice, which places the magic slope at $s^2 = 1$, is

$$f(s^2) = 1 - s^2 \ [\text{model (ii)}];$$

(4)

a microscopic calculation of the surface current for a model exhibiting magic slopes has been reported by Amar and Family \[17\].

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\(^1\)We follow the common practice and disregard contributions to the current which are even in $h$, such as $\nabla(\nabla h)^2$, though they may well be relevant for the coarsening behavior of the surface \[8, 14\].
The stability properties of a surface with uniform slope $m$ are obtained by inserting the ansatz $h(x, t) = m \cdot x + \epsilon(x, t)$ into (2) and expanding to linear order in $\epsilon$. One obtains

$$\partial_t \epsilon = [\nu_\parallel \partial_\parallel^2 + \nu_\perp \partial_\perp^2 - (\nabla^2)^2] \epsilon, \quad (5)$$

where $\partial_\parallel (\partial_\perp)$ denotes the partial derivative parallel (perpendicular) to the tilt $m$. The coefficients are $\nu_\parallel = -(d/d|m|)\|m|/f(m^2)$ and $\nu_\perp = -f(m^2)$. If one of them is negative, the surface is unstable to fluctuations varying in the corresponding direction: Variations perpendicular to $m$ will grow when the current is uphill (when $f > 0$), while variations in the direction of $m$ grow when the current is an increasing function of the tilt. Both models have a change in the sign of $\nu_\parallel$, model (i) at $|m| = \gamma^{-1/(1+\gamma)}$, model (ii) at $|m| = 1/\sqrt{3}$. For model (i) $\nu_\perp < 0$ always, corresponding to the step meandering instability of Bales and Zangwill [13, 18]. In contrast, for model (ii) the current is downhill for slopes $|m| > 1$, and these surfaces are absolutely stable.

In this work we focus on singular surfaces, $m=0$, which are unstable in both models; coarsening behavior of vicinal surfaces has been studied elsewhere [13]. The situation envisioned in the rest of this article is the following: For solutions of the PDE (2) we choose a flat surface with small random fluctuations $\epsilon(x)$ as initial condition. Mostly the initial fluctuations will be uncorrelated in space, though the effect of long range initial correlations is briefly addressed in Section 4. The fluctuations are amplified by the linear instability, and eventually the surface enters the late time coarsening regime that we wish to investigate.

### 3 Scaling Relations and Exponent Inequalities

In this section we assume that in the late time regime the solution of (3) is described by a scaling form, namely that the surface $h(x, t)$ at time $t$ has the same (statistical) properties as the rescaled surface $\tau^{-\beta} h(x/\tau^{1/z}, \tau t)$ at time $\tau t$. The equal time height–height correlation function $G(x, t) \equiv \langle h(x, t) h(0, t) \rangle$ then has a scaling form

$$G(x, t) = w(t)^2 g(|x|/\xi(t)), \quad (6)$$

where the relevant lengthscales are the surface width $w(t) = \langle h(x, t)^2 \rangle^{1/2} \sim t^{\beta}$, i.e. the typical height of the mounds, and their lateral size $\xi(t) \sim t^{1/z}$, given by the first zero of $G$. These choices correspond to $g(0) = 1$ and $g(1) = 0$. Moreover
they lead to a definition of the typical slope of mounds as \( s \equiv w/\xi \sim t^\alpha \) with \( \alpha = \beta - 1/z \).

We start our reasoning with the time dependence of the width

\[
\frac{1}{2} \partial_t w^2(t) = -\langle (\Delta h(x,t))^2 \rangle + \langle \nabla h(x,t)^2 f(\nabla h(x,t)^2) \rangle \equiv -I_1 + I_2. \tag{7}
\]

Clearly \( I_1 \geq 0 \). Since we expect the width to increase with time, we obtain the inequalities

\[
0 \leq \frac{1}{2} \partial_t w^2(t) \leq I_2 \tag{8}
\]

and

\[
I_1 \leq I_2. \tag{9}
\]

The first conclusion can be drawn even without the scaling assumption: For model (ii) and model (i) with \( \gamma \geq 1 \), \((\nabla h)^2 f(\nabla h^2)\) has an upper bound, and so has \( I_2 \). Therefore \( \partial_t w^2 \leq \text{const} \). We conclude that the increase of the width \( w(t) \) cannot be faster than \( t^{1/2} \) if it is caused by a destabilizing nonequilibrium current on a surface with step edge barriers.

Assuming scaling we estimate \( I_1 \sim (s/\xi)^2 \) and \( \partial_t w^2 \sim w^2/t \sim (s\xi)^2/t \). For model (i) we further have \( I_2 \sim s^2 f(s^2) \sim s^{1-\gamma} \). In terms of the scaling exponents \( \alpha \) and \( 1/z \) inequality (8) yields \( 2(\alpha + 1/z) - 1 \leq \alpha(1 - \gamma) \), while the second inequality (9) leads to \( 2\alpha - 2/z \leq \alpha(1 - \gamma) \). Combining both inequalities we have

\[
\frac{1 + \gamma}{2} \alpha \leq \frac{1}{z} \leq \frac{1}{2} - \frac{1 + \gamma}{2} \alpha. \tag{10}
\]

To proceed we note that an upper bound on the lateral mound size \( \xi \) can be obtained from the requirement that the mounds should be stable against the Bales-Zangwill step meandering instability [13, 18]: Otherwise they would break up into smaller mounds. From (5) it is easy to see that, for the large slopes of interest here, fluctuations of a wavelength exceeding \( 2\pi/\sqrt{|\nu_\perp|} \) are unstable. Since \(-\nu_\perp = f(s^2) \sim s^{-(1+\gamma)} \), we impose the condition \( \xi \leq 2\pi/\sqrt{|\nu_\perp|} \sim m^{(1+\gamma)/2} \) or, in terms of scaling exponents,

\[
\frac{1}{z} \leq \frac{1 + \gamma}{2} \alpha. \tag{11}
\]

Hence the first relation in (10) becomes an equality (which was previously derived for the one-dimensional case [4]), and the second relation yields

\[
z \geq 4, \quad \alpha = \frac{2}{z(1+\gamma)} \leq \frac{1}{2(1+\gamma)}, \quad \beta \leq \frac{3 + \gamma}{4(1+\gamma)}. \tag{12}
\]

[Model (i)]
For model (ii) we assume that the slope $s$ approaches its stable value $s = 1$ as $s \sim 1 - t^{-\alpha'}$ with $\alpha' > 0$. The estimate of the last term in (7) then becomes $I_2 \sim s^2(1 - s^2) \sim 1 - s^2 \sim t^{-\alpha'}$. Thus inequality (8) yields $2/z - 1 \leq -\alpha'$, and from (9) it follows that $-2/z \leq -\alpha'$. As for model (i) the next estimation uses $\xi \leq 2\pi/\sqrt{|\nu_\perp|}$ with $|\nu_\perp| = 1 - s^2 \sim t^{-\alpha'}$. Again we obtain the inverse of the second of the above inequalities, viz. $1/z \leq \alpha'/2$. Altogether this yields

$$\frac{1}{z} = \frac{\alpha'}{2} = \beta \leq \frac{1}{4}. \quad \text{[model (ii)]}$$

To summarize the general results obtained in this section: In addition to the bound on the temporal increase of the surface width, $w(t) < \text{const. } t^{1/2}$, the scaling ansatz yields an upper bound on the increase of the lateral length scale, $\xi(t) < \text{const. } t^{1/4}$, valid for both models. A more elaborate approximation, to be presented in the next section, predicts the above inequalities (12, 13) to hold as equalities (up to logarithmic corrections).

### 4 Spherical Approximation

We consider the time dependence of the equal time height-height correlation function defined above:

$$\partial_t G(x, t) = -2 \Delta^2 G(x, t) - 2 \nabla \cdot \langle h(0, t) f(\nabla h(x, t)^2) \nabla h(x, t) \rangle,$$

where $\Delta = \nabla^2$ is the Laplace operator. In order to obtain a closed equation for $G(x, t)$ we replace $f(\nabla h^2)$ by $f(\langle \nabla h^2 \rangle)$ in the second term on the right hand side. This approach is inspired by the spherical ‘large $n$’ limit of phase ordering kinetics [19], and will be referred to as the spherical approximation. The argument of $f$ is then easily expressed in terms of $G$:

$$\langle \nabla h(x, t)^2 \rangle = -\Delta \langle h(x, t)^2 \rangle = -\Delta G(0, t),$$

and the closure of (14) reads

$$\partial_t G(x, t) = -2 \Delta^2 G(x, t) - 2 f(|\Delta G(0, t)|) \Delta G(x, t).$$

Since we consider dynamics which are isotropic in substrate space, and also isotropic distributions of initial conditions, $G(x, t)$ will only depend on $|x|$ and
Consequently we consider the structure factor \( S(k, t) \) as a function of \( k = |k| \) and \( t \), which satisfies

\[
\partial_t S(k, t) = -2 \left[ k^4 - f(a(t))k^2 \right] S(k, t).
\]  
(17)

Here we have defined the function \( a(t) \) through

\[
a(t) = \frac{(2\pi^{d/2}/\Gamma(d/2))}{\ell_D} \int_0^{\infty} dk \ k^{d+1} S(k, t),
\]  
(18)

and \( d \) denotes the surface dimensionality \( (d = 2 \text{ for real surfaces}) \). The formal solution of (17) then reads

\[
S(k, t) = S_0(k) \exp \left[ -2tk^4 + 2k^2 \int_0^t ds \ f(a(s)) \right].
\]  
(19)

The initial condition \( S_0(k) \) reflects the disorder in the initial configuration of Eq. (1). It consists of fluctuations at early times, i.e. the first nucleated islands, from which mounds will later develop. Simulations of microscopic models for MBE on singular surfaces at submonolayer coverages [20] indicate the following shape of \( S_0(k) \): From a hump at some finite wavenumber, corresponding to the typical distance \( \ell_D \) between island nuclei, it falls off to zero for \( k \to \infty \). For \( k \to 0 \) it goes down to a finite value \( c > 0 \).

At late times the hump in \( S(k, t) \) persists, situated at some \( k_{\text{max}} \) near the maximum of the exponential in (19). It belongs to a lateral lengthscale \( \xi \), denoting the typical distance of neighboring mounds. For late times \( k_{\text{max}} \) will go to zero, so we need only consider \( S_0(k) \) near \( k = 0 \). In fact for the leading contribution to \( k_{\text{max}} \) (and the leading power in \( \xi \)) we only need \( S_0(k) \equiv c \). More detailed remarks on the case \( \lim_{k \to 0} S_0(k) = 0 \) and on the presence of long range correlations in the initial stage can be found at the end of this section. The particular value of \( c \) has no influence on the coarsening exponent, so we take \( S_0(k) = (2\pi)^{-d/2} \) which corresponds to \( G(\mathbf{x}, t=0) = \delta(\mathbf{x}) \).

To follow the analysis, note that \( a(t) \) is a functional (18) of \( S(k, t) \), and on the other hand it is used for the calculation of \( S(k, t) \). This imposes a condition of self consistency on the solution, which we write as follows

\[
\frac{db}{dt} = f \left( 2/(2^{d/2}\Gamma(d/2)) \right) \int_0^{\infty} dk \ k^{d+1} \exp \left( -2tk^4 + 2k^2b(t) \right).
\]  
(20)

We used the initial conditions motivated above, and the shorthand \( b(t) = \int_0^t ds \ f(a(s)) \). The integral can be evaluated, yielding for \( b(t) \) the differential
equation
\[
\frac{db}{dt} = f \left( \frac{d}{2} (4t)^{-(d+2)/4} 2^{-d/2} D_{-d/2}(-b/\sqrt{t}) \exp \frac{b^2}{4t} \right),
\]  
(21)
where \( D \) denotes a parabolic cylinder function [21]. Equation (21) cannot be solved explicitly, but for the late time behavior we can use an asymptotic approximation for \( D \), since its argument \( b/\sqrt{t} \to \infty \) for \( t \to \infty \). To see this, note that (21) is of the form
\[
\frac{db}{dt} = f \left( t^{-(d+2)/4} F\left( \frac{b}{\sqrt{t}} \right) \right).
\]  
(22)
Therefore, if \( b/\sqrt{t} \) remained bounded, for large \( t \) the argument of \( f \) in Eq. (21) would be close to 0, and (21) would approximately be \( db/dt \approx f(0) = 1 \). This is in contradiction to the assumption \( b < \text{const.} \times \sqrt{t} \) which therefore cannot be true.

For large \( t \) (and large \( b/\sqrt{t} \)) we then approximate (21) by
\[
\frac{db}{dt} = f \left( \sqrt{\frac{\pi}{2d-1}} (4t)^{-(d+2)/4}/\Gamma(d/2) \left( \frac{b}{\sqrt{t}} \right)^{d/2} \exp \frac{b^2}{2t} \right).
\]  
(23)
This shows that \( b/\sqrt{t} \) must grow more slowly than any power of \( t \): If \( b \sim t^{1/2+\epsilon} \) then \( db/dt \sim t^{\epsilon-1/2} \), whereas the argument in \( f \) would increase exponentially, dominated by a term \( \exp t^{2\epsilon} \). For both choices (3) and (4) of \( f \) the right hand side of (21) would decrease much faster than the left or even become negative.

Depending on the choice of the current function \( f \) we get different asymptotic behaviors in the leading logarithmic increase of \( B = b^2/(2t) \). We first consider the case (ii), where \( f(s^2) = 1 - s^2 \). Here Eq. (21) reads
\[
\frac{dB}{dt} = -B + \sqrt{2Bt} \left( 1 - C_{\text{ii}} B^{d/4} t^{-(d+2)/4} \exp B \right),
\]  
(24)
where \( C_{\text{ii}} \) is a constant without any interest. None of the terms must increase with time as a power of \( t \). Hence asymptotically the term in brackets must vanish, which requires that \( \exp B \sim t^{(d+2)/4} \). The leading behavior of \( B \) is therefore
\[
B \approx \frac{d + 2}{4} \log t.
\]  
(25)
Similarly we treat case (i), using the asymptotic behavior \( f(s^2) \approx (s^2)^{-\gamma/2} \) for large \( s^2 \). Equation (21) then becomes
\[
\frac{dB}{dt} = -B + C_{\text{i}} t^{-(\gamma/2)(d+2)/2} B^{-(\gamma/2)d/4+1/2} \exp -((\gamma/2))B.
\]  
(26)
Again the powers of $t$ in the last term must cancel, yielding

$$B \simeq \left( \frac{d + 2}{4} + \frac{1}{\gamma} \right) \log t. \quad (27)$$

There is a noteworthy correspondence between models (i) and (ii): The solution of (ii) is the limit $\gamma \to \infty$ of the solution of (i). In this sense, a current which vanishes at a finite slope is equivalent to a positive shape function $f(s^2)$ decreasing faster than any power of $s$. The same correspondence applies also on the level of the inequalities derived in Section 3, as can be seen by letting $\gamma \to \infty$ in (12) and comparing to (13).

The asymptotic form of $b(t)$ gives us the following time dependence of the coarsening surface structure: Inserting $b(t)$ into the expression for the structure factor $S(k, t)$ (19) we obtain for each time $t$ a wavenumber

$$k_m(t) = \left( \frac{1}{2} \left( \frac{d + 2}{8} + \frac{1}{\gamma} \right) \frac{\log t}{t} \right)^{1/4}, \quad (28)$$

which has the maximal contribution to $S(k, t)$. It can be interpreted as the inverse of a typical lateral lengthscale $\xi \sim (t/\log t)^{1/4}$. Up to a logarithmic factor, we obtain lateral coarsening with a power $1/4$ for both choices of $f(s^2)$. This corresponds to $z = 4$, which saturates the bound derived in Section 3.

It is however important to note that the resulting structure factor cannot be written in a simple scaling form $S(k, t) = w^2 k_m^{-d} S(k/k_m)$, as would be expected if $k_m^{-1}$ were the only scale in the problem [19]. Rather, one obtains the multiscaling form [22]

$$S(k, t) = L(t)^{\varphi(k/k_m(t))}, \quad (29)$$

where $\varphi(x) = 2x^2 - x^4$, and $L(t) \sim t^{(d+2)/4 + 1/\gamma}/d$ is a second lengthscale in the system. In contrast to $k_m^{-1}$, the exponent describing the temporal increase of $L(t)$ does depend on the shape of the current function $f$.

Next we discuss the behavior of the typical slope of the coarsening mounds, given by $a(t) = \langle (\nabla h)^2 \rangle$. This is obtained directly from (21). For model (ii) $a(t)$ approaches the stable value ("magic slope") $s^2 = 1$, with a leading correction

$$a(t) = 1 - \dot{b}(t) \simeq 1 - \frac{1}{2} \sqrt{\frac{d + 2}{2} \left( \frac{\log t}{t} \right)^{1/2}}. \quad (30)$$

Note that the approach to the magic slope is very slow, a possible explanation for the common difficulty of deciding whether $a(t)$ attains a final value or grows.
indefinitely in numerical simulations [23]. We further remark that, up to a logarithmic factor, the inequality \( \alpha' \leq \frac{1}{2} \) derived in (13) for the exponent describing the approach to the magic slope becomes an equality within the spherical approximation.

For model (i) the typical slopes diverge as

\[
a(t) \simeq \tilde{b}^{-2/(1+\gamma)} \simeq \left( \frac{8}{d+2} + \frac{1}{\gamma} \right)^{1/(1+\gamma)} \left( \frac{t}{\log t} \right)^{1/(1+\gamma)},
\]

consistent with the value \( \alpha = 1/(2 + 2\gamma) \) derived as a bound in (12). In the limit \( \gamma \to \infty \) the slope does not increase at all, which again is comparable to the presence of a stable slope.

To close this section we briefly comment on the the shape of the structure factor \( S(k, t) \) and the correlation function \( G(x, t) \) obtained within the spherical approximation. Assuming initial correlations as used above, \( S_0(k) \equiv c \), the structure factor is analytical at any time \( t \), as can be seen in equation (19). The corresponding correlation function therefore decays faster than any power of \( |x| \), modulated with oscillations of wavenumber \( k_{\text{max}}(t) \).

We can also predict the further evolution of long range correlations, assuming that they were initially present. A power law decay of \( G(x, t=0) \) corresponds to a singularity in \( S_0(k) \). Suppose the singularity is located at some point \( k_0 > 0 \) (the power decay of \( G \) is then modulated by oscillations). Then the singularity will remain present in \( S(k, t) \), but it will be suppressed as \( \exp -tk_{\text{max}}^4 \) for late times. This implies that \( G(x, t) \) has a very weak power law tail for very large \( |x| \), but up to some \( x_0 \) (which increases with time) it decays faster than any power. However a singularity in \( S_0(k) \) will not be suppressed if it lies at the origin \( k_0 = 0 \), since then in Eq. (19) it is multiplied by unity. In real space, this implies that a power law decay of correlations without oscillations will remain present.

Even if \( S_0(k) \) is singular at \( k = 0 \), the scaling laws derived above remain valid. Suppose for example that \( S_0(k) \sim k^\sigma \) for \( k \to 0 \). In transforming (19) back to real space, such a power law singularity can be absorbed into the phase space factor \( k^{d-1} \) involved in the \( k \)-integration. The result is simply a shift in the dimensionality, \( d \to d + \sigma \), which affects the prefactors of the scaling laws (28), (30) and (31) for \( k_{\text{m}}(t) \) and \( a(t) \) but not the powers of \( t/\log t \).
5 Conclusions

We have presented two approximate ways to predict the late stage of mound coarsening in homoepitaxial growth. To our knowledge this is the first theoretical calculation of coarsening exponents for this problem.

Although we have made heavy use of concepts developed in phase-ordering kinetics [19], our results cannot be directly inferred from the existing theories in that field. As was explained in detail by Siegert [10], equation (2) rewritten for the slope \(u \equiv \nabla h\) has the form of a relaxation dynamics driven by a generalized free energy, \(\dot{u} = \nabla \nabla \cdot \delta F(u)/\delta u\). Phase ordering with a conserved vector order parameter \(m\) is described by a similar form, \(\dot{m} = \nabla \cdot \nabla \delta F(m)/\delta m\), however it appears that the interchange of the order of the differential operators, from \(\nabla^2\) to \(\nabla \nabla\cdot\), may lead to a qualitatively different behavior [10].

Nevertheless, the results obtained so far must be refined. Ideally, one would like to derive equalities for the exponents using the scaling ansatz of Section 3. More modestly, it would be desirable to extend the approach so that the effects of current functions without in-plane isotropy [9, 10] and of contributions proportional to \(\nabla (\nabla h)^2\) [8, 14] on the scaling behavior can be assessed.

The main drawback of the spherical approximation in Section 4 is that it does not predict conventional scaling. The experience from phase-ordering kinetics in the \(O(n)\) model suggests that the multiscaling behavior obtained above may be an artefact of the spherical approximation [18, 22]. To address this issue, we have carried out a numerical integration of Equation (2), with weak uncorrelated noise as initial condition. The results indicate conventional scaling behavior in the late stage of growth, with exponents \(z = 4, \alpha = 1/(2 + 2\gamma)\), which saturate the bounds of Section 3.

Figure 1 shows a scaling plot of \(G(|x|, t)\) of model (i) with \(\gamma = 1\) for times \(t = 500, 600, \ldots, 10000\) obtained from the numerical integration of (2). It is compared at times \(t = 1000, 1100, \ldots, 10000\) to the spherical approximation. The first zero and the width at \(|x| = 0\) are rescaled to 1. Initial conditions of the approximation were chosen to coincide with the full dynamics at \(t = 100\). The spherical approximation of \(G\) takes a slightly different shape – its oscillations are more pronounced for larger \(|x|\). We obtained a similar scaling plot for \(\gamma = 3\) and for model (ii).

The inset shows the evolution of the first zero of \(G\): In the full dynamics it is
best approximated by a power law $\xi \sim \tau^{1/z}$ with $z = 3.85$ for the full dynamics, where $\tau = t - t_0$. The spherical approximation deviates from a power law. Here for late times the best fit is $\xi \sim (\tau / \log \tau)^{1/z}$ with $z = 3.87$. The beginning of the time integration $t = 0$ does not coincide with the extrapolated zero of the power laws $t_0$, because the mounds take a finite time to develop out of the initial growth instability. This introduces the additional fitting parameter $t_0$. The steepening of the mounds (not shown in the graph) develops with the power $\alpha = 0.26$. For $\gamma = 3$ in model (i) we obtain $z = 4.18$ and $\alpha = 0.126$. For model (ii) we refer to the integrations of Siegert [10], which indicate $z = 4$.

Note that the multiscaling behavior of $G$ in the spherical approximation is very weak, in the sense that the curves at different times do not differ in shape too much. A more sensitive test of the scaling behavior of Equation (1), in order to pin down the difference to the spherical approximation, would be desirable and can be achieved by extracting the function $\varphi$ (see Eq. (2)) from the data of the numerical integration. Conventional scaling yields $\varphi \equiv \text{const}$. Work in this direction is currently in progress [24].

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Figure 1: Comparison of numerical integration of Eq. (1) and the spherical approximation described in Section 4, both for model (i) with $\gamma = 1$. Main figure shows a scaling plot of the correlation function $G(|x|, t)$ with the first zero and $G(0, t)$ rescaled to unity. For large $|x|$ the approximate solution differs from the full model by more pronounced oscillations. The inset shows the evolution of the first zero of $G$, also indicating best fits to the form $t^{1/z}$ (full dynamics) and $(t/\log t)^{1/z}$ (spherical approximation).
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