Finite resolution effects in the analysis of the scaling behavior of rough surfaces

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We investigate the influence of finite spatial resolution in the analysis of the scaling behavior of rough surfaces. We analyze such an effect for two usual measurement methods: the local width and the height-height correlation function. We show that while the correlation function is insensitive to finite resolution effects for practical purposes, the local width presents correction terms to the scaling law, leading to an effective value of the local roughness exponent smaller than the theoretically expected. We also show that a functional scaling relation can only be properly formulated in terms of the height-height correlation function.

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To characterize the roughness of a surface is an important issue in science and technology. Mechanical problems concerning friction, wear, or adhesion show a crucial dependence on the smoothness of the surfaces that get into contact. It is also known that surface roughness affects dramatically the electrical and optical properties of thin films, which makes the development of better controlled surface growth techniques an important line of research. Many of these techniques show growth regimes with common spatiotemporal features, as for instance the appearance of scale invariant rough surfaces. Natural processes such as the infiltration of water in porous rocks or the growth of bacterial colonies also show scale invariant behavior [1].

Scale invariance is revealed by scaling exponents and functions that may be measured to classify the growth processes into universality classes. To characterize experimental results or numerical simulations, it is necessary to study the scaling properties of some functions related to the surface profile. One of the most widely used is the so-called *local interface width*, $W_l^2(t)$, defined as the rms fluctuations of the interface height $h(\mathbf{x},t)$, i.e., $W_l^2(t)=\langle[h(\mathbf{x},t)-h_l(\mathbf{x},t)]^2\rangle_{\mathbf{x},l}$, where l is the size of a measurement window, $h_l(\mathbf{x},t)$ is the mean height in the window, and $\langle\cdot\rangle_{\mathbf{x},l}$ indicates averages within a window and over the windows of the same size (there is also an implicit average over realizations when this is needed). After a saturation time that scales as $t_{\mathrm{sat}}\sim l^z$ (z is the dynamic exponent), the local width saturates, and a power law can be defined for small l such that $W_l^2(t\gg t_{\mathrm{sat}})\sim l^{2\alpha_l}$, where α_l is the local roughness exponent. Other relevant quantities, both in experiments and simulations, are the height-height correlation function (HHCF), $G_l^2(t)=\langle[h(\mathbf{x}+l)-h(\mathbf{x})]^2\rangle_{\mathbf{x}}$, which scales in the same way as the local width assuming that any possible overall slope in the interface has been removed, and the power spectrum of the interface, $S(q,t)$ [1].

A common characteristic in experiments and numerical simulations is the finite spatial resolution in the data. In this paper we analyze the limitations introduced in the analysis of scale invariant growth regimes by that unavoidable finite resolution when measuring the local roughness exponent. By considering various scaling behaviors, we show that the local width depends on the spatial resolution in a relevant way, introducing corrections to $W_l^2(t)$ that may lead to wrong values for the local roughness and preclude the possibility of formulating a functional scaling relation in terms of the local width. Moreover, we also show that the corrections to the HHCF can be neglected for practical purposes, and therefore we claim that in experiments and numerical simulations this technique is more adequate to study the scaling properties of rough surfaces.

To put our work in a proper context, we briefly review some of the concepts used in the analysis of growth processes. The usual way to theoretically formulate the scaling properties of rough interfaces is in terms of the global width, $W_L^2(t)$, where L is the system size. The functional behavior of the global width is summarized in the Family-Vicsek (FV) scaling relation [2], $W_L^2(t)\sim L^{2\alpha_g}f(L/t^{1/z})$, where $f(u)\sim$const for $u\ll 1$, and $f(u)\sim u^{-2\alpha_g}$ for $u\gg 1$. The dynamic exponent z reflects the lateral correlation length dependence on time, and α_g is the global roughness exponent. In an experimental situation, the system size is usually a fixed parameter, whereas in numerical simulations changing the system size is not the optimal way to compute the roughness exponent. Therefore, other ways of measurement, not showing these limitations, have to be considered. One possibility is to compute the power spectrum, $S(q,t)$, so that when FV scaling is satisfied it behaves as $S(q,t)=q^{-(2\alpha_g+d)}g(q^{-1}t^{-1/z})$, where $g(u)\sim$const for $u\ll 1$ and $g(u)\sim u^{-(2\alpha_g+d)}$ for $u\gg 1$, and where d denotes the spatial dimension of the interface. However, there are models in the literature for which $S(q,t)$ does not show this scaling behavior. It is known that if the noise is not renormalized (NRN), $g(u)$ behaves as u^{-z} for $u\gg 1$ [3], whereas in some cases, named intrinsic anomalous (IA), $g(u)\sim u^{-2(\alpha_g-\alpha_l)}$ for $u\ll 1$ [4,5]. However, the power spectrum technique is not free of problems. In experiments where the primary data are the topography of the interfaces, the power spectrum is obtained through a Fourier transformation which is usually rather noisy. On the other hand, experiments that yield directly the power spectrum must be cross-checked with other complementary methods giving the topography of the interfaces, because a spurious q decay behavior, which would yield an incorrect α_g value, might be introduced in several ways [6]. Therefore, it is common to focus on the local width function $W_l^2(t)$ or on the height-height correlation function $G_l^2(t)$, that, as already said, scale for $t\gg t_{\mathrm{sat}}$ as $l^{2\alpha_l}$. For the global

and local roughness exponents we have that if $\alpha_g > 1$, and either FV or NRN is satisfied for the power spectrum (super-roughening), then $\alpha_l = 1$, while if $\alpha_g < 1$ and either FV or NRN holds, then $\alpha_l = \alpha_g$ (self-affinity). Finally if $S(q,t)$ behaves as IA, $\alpha_l \neq \alpha_g$ irrespective of whether α_g is larger or smaller than 1. It is worth pointing out that in all cases $\alpha_l \leqslant 1$ because of a geometrical property [7].

We now study the effect of the spatial resolution on these techniques. We first analyze the effect for the local width, showing that this method depends on it in a crucial way. Then, we show that when analyzing the scaling behavior with the height-height correlation function, the finite spatial resolution effects are negligible. We will restrict the analysis to $1+1$ dimensions, but a generalization to higher spatial dimensions is straightforward (assuming there is a scaling behavior).

Let us call $h(x_j,t)$ the interface height at time t, for a given $x_j = j\Delta x$ where $0 \leqslant j \leqslant N-1$. Recalling that the Fourier decomposition is $\tilde{h}_q(t) = (1/N)\Sigma_j h(x_j,t) e^{-iqx_j}$, we may write for the local surface width

$$W_l^2(L,t;\Delta x) = \sum_{q>0} 2S(q,t;\Delta x)\Phi(q,l;\Delta x) \simeq \sum_{q>0} 2S(q,t;0)\Phi(q,l;\Delta x), \tag{1}$$

where

$$\Phi(q,l;\Delta x) = 1 - \left[\frac{\Delta x}{(l+\Delta x)} \frac{\sin\left(\frac{q(l+\Delta x)}{2}\right)}{\sin\left(\frac{q\Delta x}{2}\right)} \right]^2, \tag{2}$$

and we have replaced the discrete power spectrum by its continuous expression, an approximation fully justified because the corrections to the power spectrum in terms of the spatial resolution begin to be relevant at large q, and those modes do not contribute significantly to the total sum in Eq. (1). Useful analytical expressions can be obtained transforming the sum in Eq. (1) into an integral. Assuming that the system size is finite but large ($L \gg \Delta x$), the limits for the integral are $2\pi/L$ and $\pi/\Delta x$. If, moreover, $\Delta x \ll 1$, the upper limit can be set to ∞. Note also that for $t \gg t_{\rm sat}$ the power spectrum behaves as $S(q,t;0) \sim q^{-(2\chi+1)}$, where $\chi = \alpha_g$ if FV or NRN holds and $\chi = \alpha_l$ if $S(q,t;0)$ behaves as IA. Making a Taylor expansion in Eq. (1), we finally obtain the following expression for the local width at those time scales,

$$W_l^2(L,t;\Delta x) \sim l^{2\chi}\left[f_\chi\left(1 + \frac{2\Delta x \chi}{l}\right) + \sum_{k=2}^{\infty} g_{k,\chi}(l)\left(1 + \frac{2\Delta x(k-1)}{l}\right)\right] + \mathcal{O}(\Delta x^2), \tag{3}$$

where

$$f_\chi = \cos[\pi(\chi+1)]\Gamma(-2(\chi+1)),$$

$g_{k,\chi}(l) = \frac{1}{2}[(-1)^{k+1}/(2k)!(k-\chi-1)](l/l_c)^{2(k-\chi-1)}$, Γ is the usual Gamma function, and $l_c = L/2\pi$ is the characteristic length that separates the small and large length scales. Notice that in the sum in Eq. (3), terms with $k < \chi+1$ are relevant at small length scales ($l < l_c$), i.e., for the scaling properties, and that this is only possible if $\chi > 1$, producing that $W^2_{l<l_c}(L,t;\Delta x)$ scales as $l^2 + 2\Delta x l$. On the other hand, terms with $k > \chi+1$ are important at large length scales ($l > l_c$). We can then write the relation of the local width with the spatial resolution at small length scales as

$$W^2_{l<l_c}(L,t;\Delta x) \sim l^{2\alpha_l} + 2\alpha_l \Delta x l^{2\alpha_l - 1}, \tag{4}$$

for any of the above described scaling behaviors. If $\alpha_l > 1/2$ the finite resolution effect contributes in a relevant way, since, at very small scales, $l \sim \Delta x$, the correction is larger than $l^{2\alpha_l}$ and so the finite resolution correction increases significantly the local width at those length scales. As a consequence, the measured local roughness exponent, called the *effective* roughness exponent, $\alpha_{\rm eff}$, is smaller than α_l. On the contrary, if $\alpha_l = 1/2$, as in the KPZ equation for example, the correction introduced by the finite resolution increases the local width at small length scales by a very small constant [10], and, therefore, there is no significant change in the scaling behavior.

It is also interesting to point out that the finite spatial resolution does not allow us to have a scaling relation in terms of a unique variable. As an example, the functional behavior of the local width for the IA scaling [11] can now be written as

$$W_l^2(L,t;\Delta x) \sim l^{2\alpha_g} f(l/t^{1/z}, t^{1/z}, \Delta x), \tag{5}$$

where the scaling function $f(u,v,\Delta x)$ is

$$f(u,v,\Delta x) \sim \begin{cases} u^{2(\alpha_l - \alpha_g)}[1 + 2\Delta x \alpha_l (uv)^{1-2\alpha_l}] & (u \ll 1) \\ u^{-2\alpha_g} & (u \gg 1) \end{cases} \tag{6}$$

and no collapse of the local width for different evolution times at small length scales is possible.

Incidentally, Eq. (3) also serves to analyze the existence of a crossover between small and large length scales proposed in Ref. [8] for super-rough interfaces. There it has been claimed that the value $\alpha_l < 1$, obtained in numerical simulations using the local width technique, is due to the convergence of the local and global widths at $l = L$, i.e., that there is a crossover between small and large length scales that leads to an $\alpha_{\rm eff}$ that underestimates α_l. However, the possible corrections to the scaling behavior (4) begin to be relevant for length scales $l \geqslant l_c = L/2\pi$. In this case all terms for $k > \chi+1$ are important, and no scaling behavior can be defined. As a consequence, no crossover effect can explain the values $\alpha_l < 1$.

Some of these analytic results are illustrated in Fig. 1 for the equilibrium linear molecular beam epitaxy (LMBE) model [9], also called the Mullins-Herring model, for which it is known that in $1+1$ dimensions, $\alpha_g = 3/2$, $z = 4$, and $S(q,t)$ obeys the FV scaling (super-roughening). The LMBE model reads

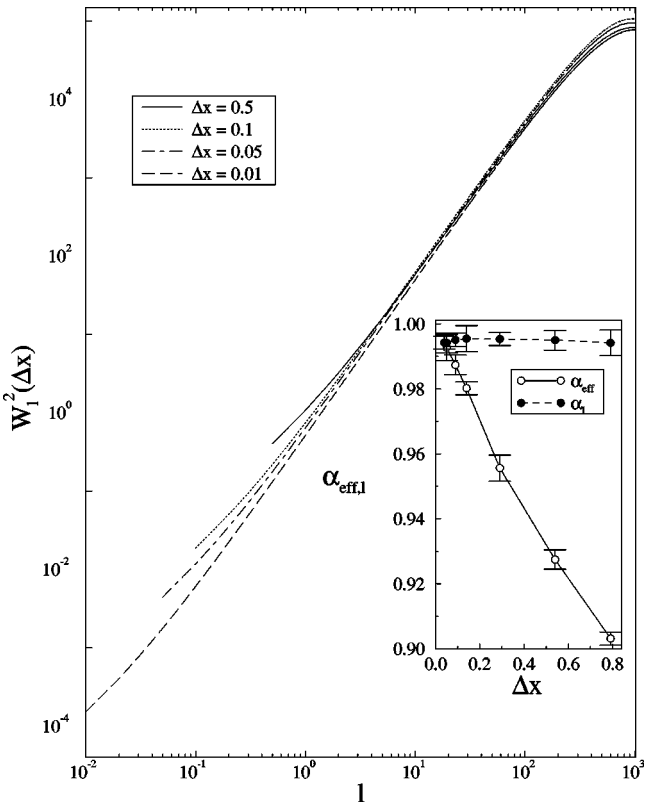

FIG. 1. Discrete local width (1) for different values of the spatial resolution for the LMBE model. The system size is $L=1000$ ($l_c \simeq 160$). The inset plot shows the local and the effective roughness exponents versus the spatial resolution. The average value of α_l is 0.996 ± 0.004.

$$\partial_t h(x,t) = -\frac{\partial^4 h(x,t)}{\partial x^4} + \eta(x,t), \tag{7}$$

where $\eta(x,t)$ denotes Gaussian white noise with zero mean value and correlation given by $\langle \eta(x,t)\eta(x',t')\rangle = 2D\delta(t-t')\delta(x-x')$. Figure 1 shows that the effect of the finite resolution is to increase the local width at small length scales. The effective roughness exponents were obtained fitting the local width to a power law as it is usually done in numerical simulations and experiments, $f(l) \propto l^{2\alpha_{\rm eff}}$. From the same plot, it is clear that the larger the lattice spacing the smaller the effective local roughness exponent. On the other hand, the local roughness exponents have been computed fitting the local width with a function $f(l) \propto (l^{2\alpha_l} + 2l\Delta x)$ according to Eq. (4). As one expects, the local roughness exponent does not depend on the finiteness of the spatial resolution once this effect is properly taken into account in the fitting function.

Now we analyze the effect of the spatial resolution on the height-height correlation function. With the same approximation used in Eq. (1), the expression for the correlation function in terms of the power spectrum and the spatial resolution is

$$G_l^2(t;\Delta x) = \sum_{q>0} 4S(q,t;\Delta x)[1-\cos(ql)] \approx G_l^2(t;0), \tag{8}$$

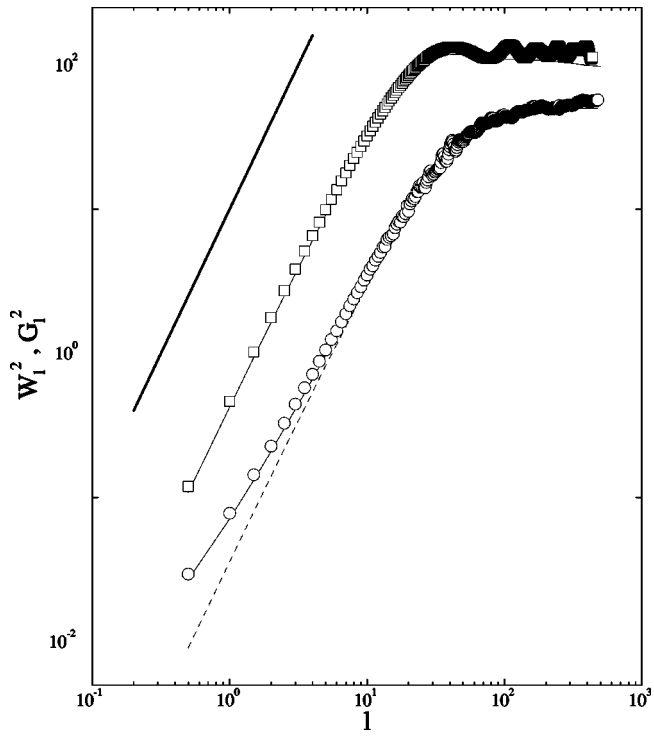

FIG. 2. The local width (circles) and the HHCF (squares) of the LMBE model obtained from numerical simulations using their definition in terms of the interface height. In both cases the solid lines are the discrete versions obtained from Eqs. (1) and (8), respectively. The continuous local width, Eq. (1) in the limit $\Delta x = 0$, is also plotted (broken line). For the HHCF the continuous and the discrete results are indistinguishable. The values of the parameters are $D=0.1$, $\Delta x = 0.5$, $L=500$, and $t=8192$. The short wide solid line has slope 2 and serves to guide the eye.

and, therefore, the corrections introduced by the spatial resolution are negligible for the HHCF (a result already pointed out in [3]). Consequently, the correlation function is a much more adequate method for computing the local roughness than the local width.

To check all the previous analytical results we performed numerical simulations of Eq. (7) using an Euler scheme with periodic boundary conditions. Figure 2 shows unambiguously that the local width obtained in the simulations coincides with the finite resolution local width (1). Numerical values for the local and effective roughness exponents have been obtained by fitting the data to expressions $f(l) \propto (l^{2\alpha_l} + 2l\Delta x)$ and $f(l) \propto l^{2\alpha_{\rm eff}}$, respectively. The values obtained are $\alpha_l = 0.96 \pm 0.01$ and $\alpha_{\rm eff} = 0.81 \pm 0.03$. For the sake of completeness, we have also plotted in Fig. 2 the correlation function. Fitting the data at small length scales to a power law yields $\alpha_l = 0.95 \pm 0.01$. Notice that no relevant correction to the scaling at small scales is observable in contrast with the case of the local width.

Another useful way to look for the scaling exponents is to collapse the local width or the correlation at different times by appropriately rescaling the axis. In Fig. 3 we plot $W_l^2(t)/l^{2\alpha_g}$ and $G_l^2(t)/l^{2\alpha_g}$ versus $l/t^{1/z}$ for two different evolution times. Note that while a good data collapse can be obtained for the correlation function for all length scales, this is not so for the local width at small length scales.

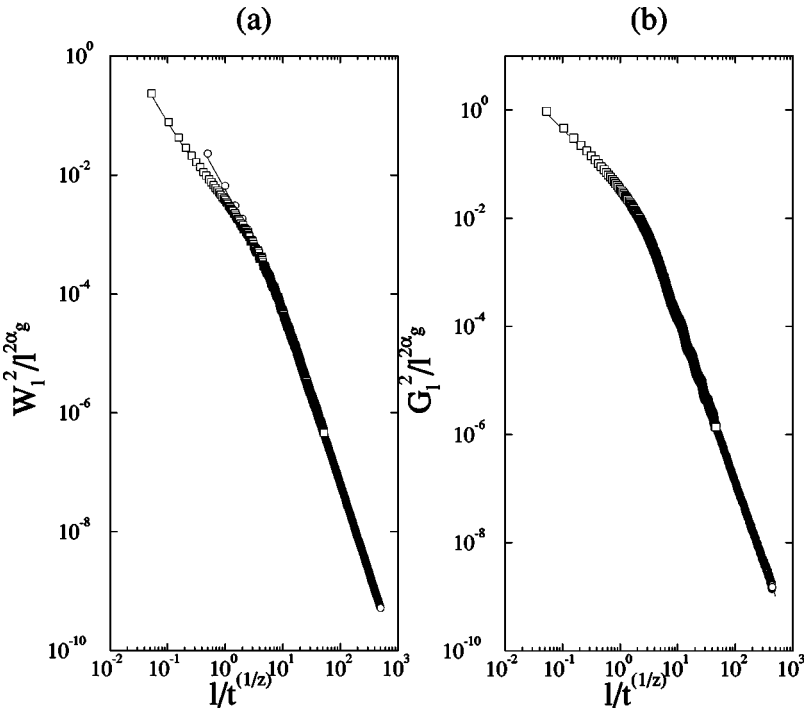

FIG. 3. Simulation and theoretical values of (a) $W_l^2(t)/l^{2\alpha_g}$ and (b) $G_l^2(t)/l^{2\alpha_g}$ vs $l/t^{1/z}$ for $t=1$ (circles) and $t=8192$ (squares). The solid lines indicate the predictions obtained from the discrete versions (1) and (8). Note that at small scales a collapse can only be obtained for the correlation function. The exponents α_g and z are 3/2 and 4 in both cases.

In summary, in this work we have shown for quite general scaling behaviors that, when considering the local width-function, the effects of finite spatial resolution are important and, if not taken into account, they may lead to wrong values for the local roughness exponent. As a consequence, the scaling ansatz cannot be consistently formulated in terms of the local width. These limitations, however, do not apply to the HHCF. These results have several important practical consequences for experiments and numerical simulations. First, and most important, the HHCF should be the preferred tool for the scaling analysis of rough surfaces in situations where the raw data are the topography of the interfaces, whereas if the experimental setup registers directly the power spectrum, the HHCF should be the cross-checking tool for validating the results. Second, the local width can be used properly only if the finite resolution correction to the scaling is included in the analysis. Third, data collapsing according to the scaling ansatz can only be correctly performed with the HHCF.

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[11] Note that setting $\alpha_l=1$ and if FV holds for the power spectrum, this case includes the super-rough scaling.