Determining exponents in models of kinetic surface roughening

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One of the central objectives when simulating models of kinetic surface roughening is the calculation of the scaling exponents that describe the roughness of the surface and its temporal evolution. This can generally be done by studying various correlation functions. In this paper it is shown that in models that exhibit a crossover at large length scales the choice of the correlation function is crucial: Using the two-dimensional Wolf-Villain model as an example, it is shown that the exponents obtained from the scaling behavior of the width or the height-height correlation function can be almost twice as large as the correct values. Reliable estimates are obtained using the structure factor or the time-time autocorrelation function.

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I. INTRODUCTION

In the past ten years, starting with the discovery of Kardar, Parisi, and Zhang [1] that moving surfaces are generically rougher than equilibrium surfaces, a huge variety of models of kinetic surface roughening have been proposed and investigated in numerical simulations [2]. Typically, the late stages of these growth processes are characterized by generic scale invariance of the correlation functions that is reflected in power-law behavior in space and time. Since the corresponding exponents do not depend on the microscopic details of the system under investigation it is possible to divide growth processes into kinetic universality classes according to the values of these characteristic exponents. The association with one particular class depends only on a few properties of the growth dynamics such as conservation laws and the importance of defects in the growing film. Thus the determination of the scaling exponents allows conclusions about the physical processes that dominate the dynamics and is therefore of primary interest in Monte Carlo simulations.

Exponents are usually determined by exploiting the scaling behavior [3] of correlation functions such as the height-height correlation function

$$G(\mathbf{r},t) = L^{-d} \sum_{\mathbf{x}} \left\langle \left[h(\mathbf{r} + \mathbf{x}, t) - h(\mathbf{x}, t) \right]^{2} \right\rangle$$
$$= r^{2\zeta} g(r/\xi(t)), \tag{1}$$

where $h(\mathbf{r},t)$ is the local position of the moving surface and L^d is the size of system under investigation with d being the dimension of the substrate. The correlation length $\xi \sim t^{1/z}$ that appears in the argument of the scaling function g corresponds to the wavelength of a typical fluctuation. For late times so that $r \ll \xi(t)$, the correlation function becomes time independent, whereas on scales much larger than the correlation length the surfaces appears to be smooth, i.e., the correlation function does not depend on the distance r. Thus the correlation length separates these two regimes

$$g(x) \sim x^{-2\zeta}$$
 for $x \gg 1$ (2a)

and

$$g(x) = \text{const for } x \ll 1 ,$$
 (2b)

which can be used to extract the roughness exponent ζ [from (2b)] and the exponent ζ/z [from (2a)]. Alternatively, the structure factor, which is related to the Fourier transform of the height-height correlation function, can be used

$$S(\mathbf{k},t) = \langle \widehat{h}(\mathbf{k},t)\widehat{h}(-\mathbf{k},t)\rangle = \frac{1}{2} \sum_{\mathbf{r}} \left(\delta_{\mathbf{k},\mathbf{0}} - e^{i\mathbf{k}\cdot\mathbf{r}}\right) G(\mathbf{r},t)$$
$$= k^{-\gamma} s(k^z t), \tag{3}$$

with $\gamma = 2\zeta + d$ and $\widehat{h}(\mathbf{k},t) = L^{-d/2} \sum_{\mathbf{r}} [h(\mathbf{r},t) - \overline{h}(t)] e^{i\mathbf{k}\cdot\mathbf{r}}$, where $\overline{h}(t)$ is the spatial average of $h(\mathbf{r},t)$. In this case the asymptotics of the scaling function are

$$s(x) \sim \begin{cases} x^{\gamma/z}, & \gamma > z \\ x, & \gamma \le z \end{cases}$$
 (4a)

for $x \ll 1$ and

$$s(x) = \text{const for } x \gg 1$$
. (4b)

The limiting behavior (4a) follows from the fact that the noise is not renormalized for $\gamma \leq z$ as can be shown by power counting. Thus the k modes with $k < 2\pi/\xi(t)$ propagate in an uncorrelated fashion $S(\mathbf{k},t) \sim tk^{z-\gamma}$. For $\gamma > z$ this is no longer possible since $S(\mathbf{k},t)$ must not have a singularity in the limit $k \to 0$ at finite times. Hence, the noise is renormalized as, for example, in the Kardar-Parisi-Zhang equation [1].

The surface width W can be obtained as the sum over either of the two correlation functions $G(\mathbf{r},t)$ or $S(\mathbf{k},t)$,

$$W^{2}(t,L) \equiv L^{-d} \sum_{\mathbf{r}} \langle [h(\mathbf{r},t) - \overline{h}(t)]^{2} \rangle$$

$$= L^{-d} \sum_{\mathbf{k}} S(\mathbf{k},t) = \frac{1}{2L^{d}} \sum_{\mathbf{r}} G(\mathbf{r},t), \qquad (5a)$$

with

$$W(t,L) \sim \frac{t^{\zeta/z}}{L^{\zeta}} \text{ for } \xi(t) \ll L$$
 (5b)

In principle, any of the scaling laws (2), (4), and (5b) can be used to determine the two exponents ζ and z. It is the purpose of this paper to show that the use of Eqs. (2) and (5b) can lead to results that grossly deviate from the asymptotic values if the model exhibits a crossover at some intermediate length scale l_c . In fact, it will be shown that the most accurate estimate of the dynamic exponent z is obtained from the steady-state time-time autocorrelation function

$$\Phi(\mathbf{k},t) = \lim_{\tau \to \infty} \langle \hat{h}(\mathbf{k},t+\tau) \hat{h}(-\mathbf{k},\tau) \rangle / S(\mathbf{k},\tau) = \varphi(k^z t),$$
(6)

which depends on the single scaling argument $k^z t$.

II. FINITE-SIZE AND DISCRETENESS EFFECTS

There are two major differences in which Monte Carlo simulations deviate from a continuum description of a growth process through Langevin equations that belong to the same universality class. First, the space variable r is restricted to a discrete lattice and, second, r is limited by the system size. The latter restriction requires the introduction of boundary conditions that are usually taken to be periodic. These two deviations from the ideal continuum description have opposite effects on the correlation functions in real and momentum space: The discreteness of the lattice has basically no effect on the height-height correlation function; it merely restricts the evaluation to the lattice points. However, the finite lattice constant introduces an upper cutoff in k space. As a consequence, $S(\mathbf{k},t)$ becomes a periodic function of the components of **k**. This leads to a distortion of $S(\mathbf{k},t)$ for $k \lesssim \pi \text{ since } \partial S(\mathbf{k},t)/\partial k_i|_{k_i=\pi} = 0, i = 1,2, \text{ whereas}$ such a roundoff is not obtained from the corresponding Langevin equation. In contrast, periodic boundary conditions restrict the **k** values to $\mathbf{k} = \frac{2\pi}{L}(n, m)$, $n, m = 0, \dots, L-1$, but have only minor effects on the form of the structure factor. However, periodic boundary conditions lead to a rounding of the height-height correlation function at $r \lesssim L/2$. These deviations from the ideal power-law behavior complicate the determination of the scaling exponents from the scaling laws (2) and (4). To illustrate this point let us look at the linear Langevin equation

$$\partial_t h(\mathbf{r}, t) = \nu_2 \nabla^2 h(\mathbf{r}, t) - \nu_4 \nabla^2 \nabla^2 h(\mathbf{r}, t) + \eta(\mathbf{r}, t) ,$$
 (7)

where η represents shot noise with

$$\langle \eta(\mathbf{r},t) \rangle = 0, \quad \langle \eta(\mathbf{r},t) \eta(\mathbf{r}',t') \rangle = 2D\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

and $\nu_2, \nu_4 > 0$. To include discreteness effects the Laplace operator is replaced by its lattice equivalent, e.g., $\nabla^2 h(\mathbf{r},t) = \sum_{\langle \mathbf{r}' \rangle} [h(\mathbf{r}',t) - h(\mathbf{r},t)]$, where \mathbf{r}' denotes the

nearest-neighbor sites of site **r**. The structure factor is easily calculated for Eq. (7). In the steady state, i.e., in the limit $t \to \infty$, it becomes

$$S(\mathbf{k}) = \frac{D}{\nu_4} \frac{1}{\lambda^2(\mathbf{k})[q_s^2 + \lambda^2(\mathbf{k})]},\tag{8}$$

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with $\lambda^2(\mathbf{k}) = 4[\sin^2(k_1/2) + \sin^2(k_2/2)]$ and $q_c^2 = \nu_2/\nu_4$. Due to the crossover at $k \simeq q_c$ the asymptotic behavior $S(\mathbf{k}) \sim k^{-2}$ is found only at small $k \ll q_c$. But, provided that $q_c \gg 2\pi/L$, the extraction of the exponent $\gamma = 2$ is not affected by the periodic boundary conditions or by discreteness effects since they only influence the behavior at large k. The determination of the scaling exponents from the height-height correlation function $G(\mathbf{r})$ is more complicated, since the exponent ζ must be calculated from the large-distance behavior $r \gg 2\pi/q_c$, the same regime that is distorted due to the periodic boundary conditions. Thus one is forced to choose an intermediate interval for the determination of ζ so that $2\pi/q_c \ll r \ll L/2$. The extent of this interval may not be very well defined, as we will see in the next section. The same difficulty does not exist for the structure factor since the exponent γ is always determined from the small k limit of $S(\mathbf{k})$.

III. THE TWO-DIMENSIONAL WOLF-VILLAIN MODEL

The Wolf-Villain (WV) model [4] was the first model introduced to investigate kinetic surface roughening in the absence of desorption in order to model dynamics of surfaces under conditions typical for molecular-beam epitaxy. At each time step a particle is added to a randomly chosen site of the substrate and the particle relaxes instantaneously to one of the nearest-neighbor sites by maximizing the number of horizontal bonds. Subsequently it was found [5,6] that this simple relaxation rule oversimplifies the diffusion dynamics and that so-called full-diffusion models are required to get a more realistic picture of the surface evolution. Nevertheless, the WV model has inspired much research on kinetic roughening phenomena. The two-dimensional variant of the model was introduced by Kotrla et al. [7]. In both one and two dimensions it was found that the surface is extremely rough with $\zeta \simeq 1.4$ [4] and $\zeta \simeq 0.7$ [7], respectively. Based on these results it was concluded that the model belongs to universality classes described by Eq. (7) with $\nu_2 = 0$. For two-dimensional substrates the data indicated that an additional term [8] $\sim \nabla^2(\nabla h)^2$ should be included in the equation of motion [7]. All these conclusions were reached by studying exclusively the scaling behavior of the width (5b). These classifications were seriously questioned by the work of Krug et al. [9], who measured surface diffusion currents as a function of the tilt $m = |\nabla h|$. Whereas the results for the one-dimensional WV model were inconclusive because of severe finite size effects, in d=2 they found a small negative surface current j(m) < 0 for m > 0. Since the coefficient ν_2 in Eq. (7) can be determined as $\nu_2 = -j'(m=0)$ it was

concluded that the two-dimensional (d = 2) WV model in fact belongs to the Edwards-Wilkinson (EW) [10] universality class. However, the measured coefficient ν_2 is so small that the crossover to EW behavior was estimated to occur on time scales larger than $t_c = 2 \times 10^4$ deposited monolayers. Subsequently it was found [11] that the one-dimensional WV model does not obey the standard scaling assumptions (2), (4), and (5b) due to an anomalous time dependence of the average step size $a(t) \sim t^{\kappa}$, $a^{2}(t) \equiv G(1,t)$ that persists up to $t = t^{\star} \simeq 10^{6}$ deposited monolayers. Only for $t \gg t^*$ the step size saturates and conventional scaling is recovered. Since it is impossible to distinguish between anomalous and conventional scaling by looking at the scaling properties of the width (5a) alone, all classifications based on an investigation of only the width must be regarded with great care, especially in one dimension, where anomalous scaling has been found in many different models [12,13].

From the preceding paragraph it has become clear that the asymptotic behavior of the WV model can only be determined if late times and therefore large system sizes are investigated. This has been done [14] for system sizes as large as $L = 40\,000 \ (d = 1)$ and $L = 1000 \ (d = 2)$. By studying the scaling properties of the width and the height-height correlation function some indications of a crossover to EW behavior were indeed found. In the remainder of this paper it will be shown that the asymptotic scaling behavior can convincingly be established already for much smaller systems (L = 256 for d = 2)if the structure factor (3) and the time-time autocorrelation function (6) are investigated, whereas the width (5a) and the height-height correlation (1) function still give misleading results for these system sizes. Recently [15], the WV model was modified in an attempt to reduce the crossover length and time, and logarithmic dependences $W(t), G(r,t) \sim \log t$ were obtained, although only within a very small regime. Furthermore, these models with only instantaneous relaxation are quite sensitive to changes in the algorithm, e.g., the slight differences between the WV model and the model of Das Sarma and Tamborenea [16] already lead to significant differences in the asymptotic behavior [9].

Figure 1 shows the width (5a) of the two-dimensional WV model for three different system sizes as a function of the number of deposited monolayers. For $t \leq 10^4$ monolayers the data obey an almost perfect power law with an exponent $\beta = 0.21 \pm 0.01$. As already noticed by Schroeder et al. [11], the d = 2 WV model shows anomalous scaling for times smaller than $t^* \simeq 10^3$ monolayers. This is also shown in Fig. 1: For $t < t^*$ the average step size $a(t) \equiv G(1,t)$ obeys a power law $a(t) \sim t^{\kappa}$ with $\kappa \simeq 0.048$. This value is in agreement with the results found in Refs. [11,14]. However, since this exponent is so small the data may also be fitted by a logarithm. That fit is shown in the inset of Fig. 1 and is at least as good as the power-law fit. That the time dependence of the average step size is in fact better described by a logarithmic increase is also supported by fitting the average step size to the form $a(t) = a_0(t^{\kappa} - 1)/\kappa + a_1$. Such a fit gives values for κ in the range 0.002-0.01 in agreement

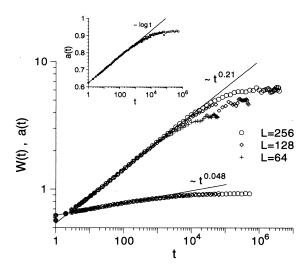


FIG. 1. Time dependence of the width W(t) (upper curves) and average step size a(t). The straight lines correspond to power-law fits with the indicated exponents. The inset shows the same a(t) data in a semilogarithmic plot and the straight line corresponds to $a(t) \sim \log t + \text{const.}$

with a behavior $a(t) = a_0 \log t + a_1$. Therefore, in the following κ is regarded as being zero effectively and no distinction between conventional and anomalous scaling is made. For $t \gtrsim 10^4$ monolayers the average step size, a(t) is basically constant independent of the system size, indicating conventional scaling in that regime. Due to the smallness of κ for d=2 anomalous scaling is much less a problem than it is in one dimension, where it is impossible to infer the universality class of a model from the scaling behavior of the width alone [11].

There is no indication of a crossover to EW behavior in Fig. 1. This remains true when W(t) is plotted on a log-linear scale: There is no extended regime in which $W(t) \sim \log t$. Even if much longer times are simulated [14] it is very hard to establish such a regime since it is difficult to distinguish a crossover to smaller β values from saturation effects due to the finite size of the system. This is, besides the difficulties related to anomalous scaling behavior, an intrinsic problem when calculating exponents using W(t) and makes this method inferior to the methods discussed below.

In Fig. 2 the steady-state height-height correlation function $G(\mathbf{r}) \equiv G(\mathbf{r},t \to \infty)$ is shown. For $r \lesssim 10$ lattice constants the correlation function shows a power-law behavior $G(\mathbf{r}) \sim r^{2\zeta}$, with $\zeta \simeq 0.65 \pm 0.05$. This value coincides within the error bars with the value that is inferred from $\beta = 0.21$, obtained from Fig. 1, and the exponent relation $z = 2\zeta + d$ [4]. It also agrees with previously published results [7,14]. For r > 10 the data do not obey a power law. Again, it is impossible to decide whether this is due to finite-size effects caused by the periodic boundary conditions as explained in Sec. II or due to a crossover to a logarithmic r dependence that would be indicative of EW behavior. If the data are plotted on a semilogarithmic scale there is a regime where the data

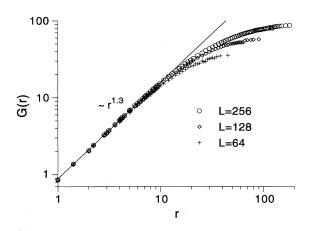


FIG. 2. Steady-state height-height correlation function for three different system sizes. The straight lines correspond to $G(\mathbf{r}) \sim r^{2\zeta}$ with $\zeta = 0.65$.

fall approximately on a straight line, but these intervals do not coincide for the system sizes that are studied in this work. Thus a regime $G(\mathbf{r}) \sim \log r$ cannot be established.

As shown above, a crossover to EW behavior in the two-dimensional WV model cannot be found for system sizes as large as $L^2 = 256 \times 256$ if real-space correlation functions such as the width (5a) or the heightheight correlation function (1) are studied, although such a crossover was predicted [9] within this regime. On grounds of measurements of surface diffusion currents the crossover time was estimated as $t_c \sim \nu_2^{-2} \simeq 2 \times 10^4$ and the crossover length should be of the order of $l_c = 2\pi/q_c \sim 2\pi\nu_2^{-1/2} \simeq 29$. It will now be shown using the scaling behavior of correlation functions in momentum space that these estimates are in fact fairly accurate. Figure 3 shows the steady-state structure factor. For $k > q_c \simeq 0.11$ the structure factor shows a power law $S(\mathbf{k}) \sim k^{-\gamma}$ with $\gamma = 3.5 \pm 0.2$ corresponding to $\zeta \simeq 0.75$, in agreement with the results obtained from the width and the height-height correlation function. But for smaller $k < q_c$ there is a clear crossover to a regime corresponding to a much smaller surface roughness. If only the five smallest k modes for L=256 of $S(\mathbf{k})$ are fitted to a power law an exponent $\gamma \simeq 2.2$ is obtained in good agreement with EW behavior. As explained in Sec. II, this smaller exponent is not influenced by finite size or discreteness effects. Thus it is exactly the property of the structure factor that the asymptotic regime at small k is separated from the regime that is distorted by finite-size effects that makes it possible to extract the asymptotic behavior from $S(\mathbf{k})$, whereas for the same system size this is impossible using the Fourier transform $G(\mathbf{r})$.

Steady-state correlation functions allow for the most accurate calculation of the roughness exponent, but they contain no information about the dynamical exponent. In principle, one can use the exponent relation $z=\gamma$ to determine the dynamical exponent z, but quite often it is desirable to have an independent measurement of the dynamic properties, at least as a consistency check.

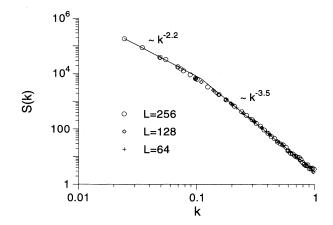


FIG. 3. Steady-state factor for three different system sizes. The straight lines are power-law fits $S(\mathbf{k}) \sim k^{-\gamma}$ with the indicated exponents.

This can be done using the scaling properties of the autocorrelation function $\Phi(\mathbf{k},t)$ [17,6], which allows a direct measurement of the exponent z. The results for the d=2WV model for a system size $L^2 = 256 \times 256$ are shown in Fig. 4 for the five smallest k modes. Since the functional form of the scaling function $\varphi(k^z t)$ is not known [18], the exponent z is determined by adjusting its value so that the best data collapse is obtained. If such a data collapse is attempted for the height-height correlation function, two exponents ζ and z have to be determined and this procedure does not allow for a very reliable determination of the scaling exponents. Since the autocorrelation function $\Phi(\mathbf{k},t)$ depends only on the single exponent z, it can, on the other hand, be determined quite accurately. Figure 4 shows the data collapse for z = 2.1. If only the smallest three k modes are taken into account, the data collapse almost perfectly onto a universal curve. For the larger two k values the data deviate significantly from that curve, indicating already the crossover to the regime

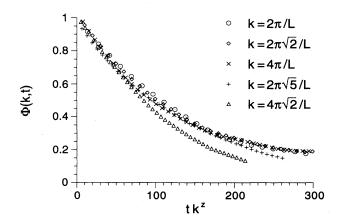


FIG. 4. Steady-state autocorrelation function $\Phi(\mathbf{k},t)$ as a function of the scaling argument $k^z t$ for z=2.1. The system size is $L^2=256\times256$.

with $z=\gamma\simeq 3.5$. The accuracy of the value z=2.1 can be estimated by plotting the same data also for z=2 and z=2.2. In both cases the collapse is slightly worse than the one shown in Fig. 4. Thus the result $z=2.1\pm0.1$ obtained from the autocorrelation function $\Phi({\bf k},t)$ is probably the most convincing evidence of the asymptotic EW behavior of the two-dimensional WV model.

In principle $\Phi(\mathbf{k},t)$ may only be calculated for two different k values to calculate the dynamical exponent z. Thus this method is even more powerful than calculating γ from the steady-state structure factor $S(\mathbf{k})$ and using the exponent relation $z=\gamma$, since in that case a larger spread in k values is needed to establish a convincing power-law fit. In fact, the results from Fig. 4 indicate that the fit for small k shown in Fig. 3 is already influenced by the crossover at smaller length scales. The disadvantage of determining z from the autocorrelation function over the calculation of γ from $S(\mathbf{k})$ is the necessity of running the simulation over a large period of time in the steady state to collect the necessary data.

IV. CONCLUSION

In this paper it has been shown that the choice of the correlation functions that are used to determine the scaling exponents of a specific model of kinetic surface roughening is extremely important. Previously it has been shown [11,12] that using the scaling behavior of the width can lead to totally misleading classifications because of an anomalous time dependence of the average step size, especially in one dimension. But, even the height-height correlation function and the structure factor, although mathematically equivalent since they are related by a Fourier transform, are not equivalent when it comes to the determination of the scaling exponents on finite systems in a numerical simulation. If crossovers at large length scales are present, finite-size effects due to periodic boundary conditions make the determination of, e.g., the roughness exponent from the height-height correlation function less accurate than its determination from the structure factor for the same system size. For the two-dimensional WV model, for example, for a system size of $L^2 = 256 \times 256$ an estimate of the roughness exponent obtained from $G(\mathbf{r})$ yields $\zeta \simeq 0.65$ (see Fig. 2), in agreement with the result obtained from the surface width (see Fig. 1). However, the structure factor shows a power law $S(\mathbf{k}) \sim k^{-\gamma}$ with $\gamma \simeq 2.2$ for $k \lesssim 0.1$. This behavior is in agreement with EW scaling, i.e., $\zeta = 0$ and $G(\mathbf{r}) \sim \log r$, which was predicted for the d=2WV model on the grounds of measurements of the surface diffusion current [9]. Figure 3 also shows that the exponents deduced from the real-space correlation functions correspond to an extensive crossover regime with $S(\mathbf{k}) \sim k^{-3.5}$ for $k \gtrsim 0.1$.

Naturally, there are disadvantages in computing scaling exponents from correlation functions in momentum Most significantly, statistical fluctuations are much more pronounced in $S(\mathbf{k},t)$ and $\Phi(\mathbf{k},t)$ in comparison with $G(\mathbf{r},t)$. Thus many more independent runs are needed to obtain the necessary statistics. Additionally, to obtain the autocorrelation function $\Phi(\mathbf{k},t)$ the simulations must be run in the steady state much longer to access sufficiently large time intervals t: The data for Fig. 4 were generated in runs in which the number of monolayers that were deposited in the steady state are 6 times larger than the number of monolayers that are needed to reach that steady state. Alternatively, one could have computed real-space correlation functions on larger lattice sizes within the same CPU time. If the data shown in Fig. 2 for the system size $L^2 = 256 \times 256$ are plotted on a semilogarithmic scale, one finds a regime 25 < r < 60 where the correlation functions is roughly proportional to $\log r$. In order to establish this behavior unambiguously this interval must be increased to cover at least one order of magnitude. Thus system sizes as large as $L^2 = 1000 \times 1000$ are needed and the simulation still must reach the steady state in order to distinguish between crossover and finite-size effects. The CPU time needed is roughly 256 times larger than the time needed to run the 256² system into saturation. To calculate $\Phi(\mathbf{k},t)$ the simulation was carried out 6 times longer in the steady state and the data were time averaged as well as ensemble averaged over 20 independent runs. Even if we assume that two runs are sufficient to calculate $G(\mathbf{r},t)$, the CPU time required to calculate $\Phi(\mathbf{k},t)$ for L=256 is still smaller by a factor of roughly 4. If only $S(\mathbf{k},t)$ is calculated, this factor is much larger. Therefore, momentum space correlation functions such as the structure factor $S(\mathbf{k})$ and the autocorrelation function $\Phi(\mathbf{k},t)$ are generally superior for obtaining high-precision estimates for the scaling exponents in models for kinetic surface roughening.

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The most convincing data that establish the asymptotic EW behavior of the two-dimensional WV model are obtained from the steady-state autocorrelation function $\Phi(\mathbf{k},t)$. This correlation function allows us to study the temporal correlations of single k modes. Only very few modes with $k < q_c = 2\pi/l_c$, l_c being the crossover length, are necessary to extract the asymptotic dynamic exponent z as demonstrated in Fig. 4. This dynamic exponent differs from the one that is extracted from the width W(t) by a factor larger than 1.6: $z \simeq 2.1$ compared to $z \simeq 3.4$.

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