Anomaly in numerical integrations of the Kardar-Parisi-Zhang equation

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We demonstrate that conventional finite difference schemes for direct numerical integration do *not* approximate the continuum Kardar-Parisi-Zhang equation. The effective diffusion coefficient is found to be inconsistent with the nominal one. This is explained by the existence of microscopic roughness in the resulting surfaces. [S1063-651X(98)11106-6]

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I. INTRODUCTION

The Kardar-Parisi-Zhang (KPZ) equation [1] has been very successful in describing a class of dynamic nonlinear phenomena. It is applied to a wide range of topics including vapor deposition, bacterial colony growth, directed polymers, and flux lines in superconductors [2,3]. Computational studies have mostly concentrated on simulations of discrete models such as ballistic deposition models, solid-on-solid models, Eden model, directed polymer simulations, and so on. They allow very efficient simulations by capturing only the essential features in the physical processes. Another important approach is direct numerical integration. This in general involves more intensive computations. Amar and Family first conducted large-scale numerical integrations of the KPZ equation and verified the universality with discrete models [4]. The accuracy was further improved by the subsequent works of Moser *et al.* [5,6]. Properties of various numerical integration approaches are still being investigated [7–10]. Similar techniques are not only applied to the KPZ equation but also to many related nonlinear phenomena such as growth with correlated noise [11] or quenched noise in anisotropic media [12], reaction-diffusion systems with multiplicative noise [13], Kuramato-Shivashisky equation for flame front propagation [14,15], epitaxial growth [9,16], etc.

Numerical integration is in general considered to be a more direct approach for the investigation of growth equations. Ideally, it should allow full control on the precise form of the equation to be investigated. The parameters involved may also be chosen at will. Unfortunately, many obscure properties of the conventional numerical integration scheme are reported. For example, Newman and Bray [8] identified an unphysical fixed point and an associated instability in the deterministic version of the discrete equation used in the numerical integration of the KPZ equation. They further argue that the stochastic discrete equation and hence the conventional integration method cannot capture the strong coupling behavior of the continuum equation. In another work, Dasgupta, Das Sarma, and Kim [9] reported that numerical instability can occur even for very small time steps used in the numerical integration. They suggest that the instability is an intrinsic property and inferred that the discretized KPZ equation may have very different behavior from that of the continuum version. In an earlier work, Amar and Family [17] integrated a related equation with a generalized nonlinear term. Contrary to predictions from the continuum equation, they quite surprisingly found KPZ scaling behavior in most cases. They explained their observation by the generation of the characteristic KPZ nonlinear term due to the combined effects of noise and nonlinearity. It is thus evident that results from direct numerical integration may not always agree with predictions from the continuum equations.

In this work, we provide a detailed study of the conventional direct numerical integration approach for the KPZ equation in $1+1$ dimensions. We aim at studying quantitatively differences between properties of the continuum growth equation and those of its discretizations. In Sec. II we review the conventional numerical integration techniques used in this study. Section III discusses numerical results on surface width and correlation function measurements on surfaces simulated by numerical integration. Section IV presents results on the coarse-grained dynamics of the surfaces extracted using an inverse method. We conclude in Sec. V with some further discussions.

II. DIRECT NUMERICAL INTEGRATION

The KPZ equation gives the local growth rate of the height profile $h(x,t)$ of a surface at substrate position x and time t [1]:

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

where ν and λ are the diffusion coefficient and the nonlinear parameter, respectively, and c is related to the average growth rate. There is an implicit lower wavelength cutoff so that fluctuations of shorter length scales are truncated. The noise η has a Gaussian distribution and mean 0 and a correlator

$$\langle \eta(x,t)\,\eta(x',t')\rangle = 2D\,\delta(x-x')\,\delta(t-t'). \tag{2}$$

Euler's method is the most widely used approach for direct numerical integration of the KPZ equation [4–6,9]. It is based on the finite difference equation:

$$h_i^{n+1} = h_i^n + \frac{\Delta t}{\Delta x^2}[\nu_0(h_{i+1}^n + h_{i-1}^n - 2h_i^n) + (\lambda_0/8)(h_{i+1}^n - h_{i-1}^n)^2] + \sqrt{\frac{2D_0\Delta t}{\Delta x}}\xi_i^n, \tag{3}$$

where h_i^n approximates the surface height $h(x_i,t_n)$ at the ith lattice point and the nth time step. The constants Δx and Δt are the spatial and temporal step size, respectively. The subscripted parameters ν_0, λ_0, and D_0 denote nominal values used in the discrete equation to be distinguished from the continuum values in Eq. (1). We have set the nominal value of c to be zero for convenience. Every ξ_i^n is an independent random variable with zero mean and unit variance following a uniform distribution. Using Gaussian deviates will not alter the result. The spatial discretization implies that Δx becomes effectively the lower wavelength cutoff.

Accurate numerical integration involving finite differencing in general requires small values of both Δt and Δx. For the current problem, one ensures that Δt is sufficiently small by verifying that further decreasing its value will not alter the results. In contrast, Δx is usually fixed at 1, very often after some trivial rescaling of the equation [4,5,9]. In fact, decreasing Δx is not a valid way to improve the accuracy but is simply equivalent to diminishing the nonlinear parameter λ. This is because any value of Δx can be rescaled back to 1 through the transformation $x\rightarrow(\Delta x)^{-1}x$, $t\rightarrow(\Delta x)^{-2}t$, $h\rightarrow(\Delta x)^{-1/2}h$ which leaves Eq. (1) invariant except that λ is now replaced by $\lambda\Delta x$. In general, maintaining sufficient nonlinearity of the system is essential to exhibit any relevant properties of the KPZ class. It is most convenient to fix $\Delta x=1$ and adjust the nonlinearity using λ, although tuning the nonlinearity with Δx has also been done [6].

In the main computation in this work, we follow the conventional approach of taking $\Delta x=1$ and a small Δt. We will focus mostly on the case $\nu_0=D_0=1$ and $\lambda_0=3$. This value of λ_0 corresponds to a moderate nonlinearity. It is large enough to drive the system quickly into the characteristic nonlinear KPZ scaling regime without much crossover effect while it is also sufficiently small for reasonable numerical stability.

III. SURFACE WIDTH AND CORRELATION MEASUREMENTS

A widely used approach to investigate the scaling properties of rough surfaces is to measure the rms surface width W defined as

$$W=\left\langle \frac{1}{L}\sum_{i=1}^{L}(h_i-\overline{h})^2\right\rangle^{1/2}, \tag{4}$$

where L is the lattice size used in the numerical integration and $\overline{h}$ is the mean surface height given by

$$\overline{h}=\frac{1}{L}\sum_{i=1}^{L}h_i. \tag{5}$$

The brackets $\langle\ \rangle$ denote ensemble averaging, which is equivalent to averaging over time when steady state is being considered. Consider growth from an initially flat surface. At small time t, W is independent of L and scales with time as $W\sim t^{\beta}$. At large t, W saturates and scales with the lattice size as $W\sim L^{\alpha}$. The exponents α and β are called the roughness and the early time exponent, respectively [18]. In $1+1$ dimensions, they are given exactly by $\alpha=1/2$ and $\beta=1/3$ [19].

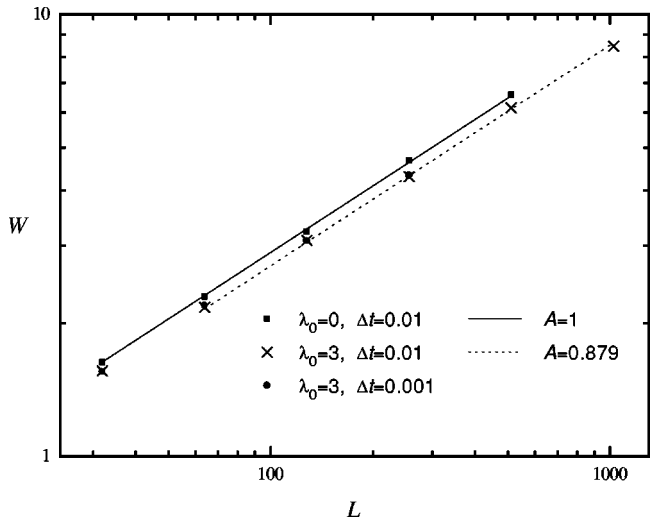

FIG. 1. Log-log plot of saturated surface width W against lattice size L from the Edward-Wilkinson equation ($\lambda_0=0$) and the KPZ equation ($\lambda_0=3$) numerically integrated with time step Δt. The data are respectively compared to the two lines in the form $W=(A/12)^{1/2}L^{1/2}$.

In addition, the probability distribution functional of the surface at steady state is also known exactly [2]. In particular, the surface width is given by [20]

$$W=\left(\frac{A}{12}\right)^{1/2}L^{\alpha}, \tag{6}$$

where A is the scaling amplitude defined as $A=D/\nu$. Periodic boundary conditions are assumed. Note that W and indeed the full distribution of the steady state surface are both independent of the nonlinear parameter λ [2].

We first tested Euler's method of numerical integration in Eq. (3) for the linear $\lambda_0=0$ case so that Eq. (1) reduces to the Edward-Wilkinson equation [2,3]. We set $\nu_0=D_0=1$ and the nominal value of A is thus $A_0=D_0/\nu_0=1$. The time step was taken to be $\Delta t=0.01$. Starting from an initially flat surface, the height profile at later time was obtained by iterating Eq. (3). After steady state was attained, we measured the surface width W averaged over a long period of time. Figure 1 shows W as a function of the lattice size L in a log-log plot. It shows good agreement with the expected relation in Eq. (6) with $A=A_0=1$ and $\alpha=1/2$ which is also shown in Fig. 1.

We then applied the conventional integration scheme similarly to the KPZ equation with $\lambda_0=3$ and $\nu_0=D_0=1$. We measured W for L in the range from 32 to 1024. For $L=1024$ the computation was most intensive and we observed that the surface width had long been saturated at $t=2\times10^5$. The value W reported is averaged over the period $2\times10^5\lesssim t\lesssim10^6$ involving about 10^8 iterations since $\Delta t=0.01$. The result is also plotted in Fig. 1. Recall that according to the exact results for the continuum equation, a different value of λ_0 should not alter the surface width W. However, the values of W clearly deviate from the expected relation in sharp contrast to the linear case. The slope in the log-log plot is 0.491, in agreement with the expected value $\alpha=1/2$. A fit to Eq. (6)

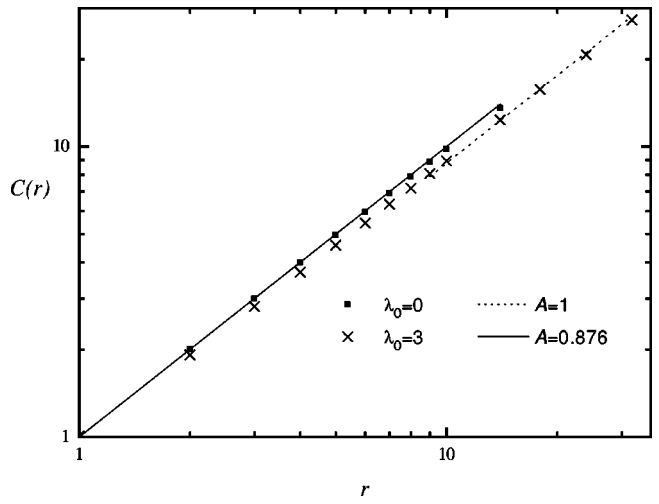

FIG. 2. Log-log plot of correlation function of surfaces from the Edward-Wilkinson equation ($\lambda_0=0$) and the KPZ equation ($\lambda_0=3$). The data are compared to the two lines in the form $C(r)=Ar$.

with α fixed at 1/2, also shown in Fig. 1, gives $A\simeq 0.879$. This estimate is significantly different from the nominal value $A_0=1$.

We have repeated the simulation at a much smaller time step $\Delta t=0.001$ for L from 32 to 256. The result, also shown in Fig. 1, is indistinguishable from the previous one within our numerical precision. Therefore the discrepancy between the measured A and the nominal A_0 is not due to a finite time step. Furthermore, one cannot improve the method by decreasing Δx as has been explained in Sec. II.

To further confirm our result, we calculated the amplitude A independently from the correlation function

$$C(r)=\langle[h(x+r)-h(x)]^2\rangle. \tag{7}$$

It follows from the KPZ equation in $1+1$ dimensions that [20]

$$C(r)=Ar^{2\alpha} \tag{8}$$

for $\Delta x\ll r\ll\xi$. The correlation length ξ specifies the scale below which fluctuations have saturated and its value is limited either by time or the system size. We integrated the KPZ equation similarly using Eq. (3) with the same parameters $\lambda_0=3$, $\nu_0=D_0=1$, and $\Delta t=0.01$ starting from flat surfaces of size $L=65\,536$ until $t\simeq 5200$. The correlation $C(r)$ was then calculated and averaged over seven independent realizations. The result is shown in Fig. 2 in a log-log plot. We only show data points corresponding to r well within the correlation length so that the values have become time independent. The slope of the linear region at $9\leqslant r\leqslant 32$ when compared to Eq. (8) gives $\alpha\simeq 0.480$. It is slightly smaller than the exact value $\alpha=1/2$, probably due to the rather small r considered. The same data were fitted to Eq. (8) with α fixed at 1/2 and are shown in Fig. 2. We obtained $A\simeq 0.876$ in good agreement with the previous estimate from surface width measurements. Figure 2 also shows the result for the linear $\lambda_0=0$ case in which $A=A_0=1$ as expected from the continuum equation.

IV. INVERSE METHOD RESULTS

We have shown numerically that the measured value of the amplitude A differs from the nominal A_0. This implies that at least one of the continuum parameters ν and D must disagree with their nominal values. To measure ν and D independently, we apply an inverse method proposed by Lam and Sander [21]. This approach computes all the parameters in the KPZ equation from realizations of simulated surfaces. The parameters are those which enable the growth equation to give the best prediction on the evolution of a surface.

Our procedure follows from Ref. [21]. We consider the KPZ equation coarse grained up to length l and discretized with a time step τ:

$$\frac{\Delta h(x,t)}{\tau}\simeq \mathbf{a}\cdot\mathbf{H}(x,t)+\eta(x,t), \tag{9}$$

where the parameter vector $\mathbf{a}$ and the surface derivative vector $\mathbf{H}$ are given, respectively, by

$$\mathbf{a}=\left[c,\nu,\frac{\lambda}{2}\right], \tag{10}$$

$$\mathbf{H}(x,t)=\left[1,\frac{\partial^2 h}{\partial x^2},\left(\frac{\partial h}{\partial x}\right)^2\right]. \tag{11}$$

Unlike Ref. [21], we do not consider any higher order terms. To calculate $\mathbf{H}(x,t)$, the surface at time t is first coarse grained by truncating the Fourier components with wavelength smaller than l. Subsequent differentiations and multiplications are carried out in the Fourier and the real spaces, respectively. An additional coarse graining is then carried out to maintain the cutoff which is shifted by the nonlinearities. We then grow the surface further for a period τ to obtain $h(x,t+\tau)$. The surface advance $\Delta h(x,t)$ is computed by similarly coarse graining $h(x,t+\tau)-h(x,t)$ up to length l. It can be shown easily that the noise correlator follows from

$$D=\frac{\tau}{2}\left\langle\left[\frac{\Delta h(x,t)}{\tau}-\mathbf{a}\cdot\mathbf{H}(\mathbf{x},\mathbf{t})\right]^2\right\rangle \tag{12}$$

once $\mathbf{a}$ is computed as to be explained below. The averaging can be performed over both x and t. Minimizing this expression of D with respect to $\mathbf{a}$ gives the main equation of the inverse method, from which $\mathbf{a}$ can be solved:

$$\mathcal{A}\mathbf{a}=\mathbf{b}, \tag{13}$$

where the matrix $\mathcal{A}$ and the vector $\mathbf{b}$ are defined, respectively, by

$$\mathcal{A}=\langle\mathbf{H}(x,t)\otimes\mathbf{H}(x,t)\rangle, \tag{14}$$

$$\mathbf{b}=\left\langle\frac{\Delta h(x,t)}{\tau}\ \mathbf{H}(x,t)\right\rangle. \tag{15}$$

The symbol $\otimes$ denotes the vector outer product. All the growth parameters c, ν, λ, and D thus obtained depend on both the spatial and temporal resolutions l and τ, respectively.

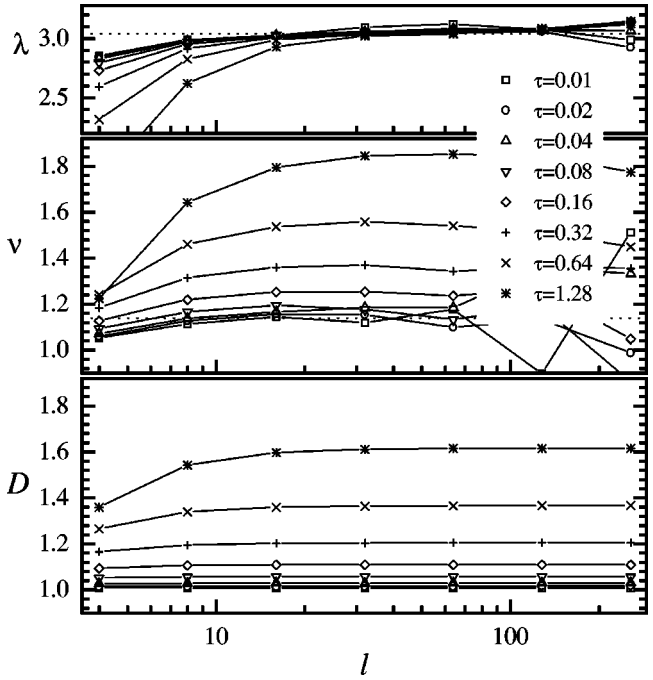

FIG. 3. Inverse method results of the continuum parameters λ, ν, and D as functions of the spatial and temporal resolutions l and τ. The dotted lines are $\lambda=3.04$ and $\nu=1.14$.

We focus on steady state surfaces generated using Euler's integration method with the same parameters $\nu_0=D_0=1$, $\lambda_0=3$, and $\Delta t=0.01$ on a lattice of size $L=32\,768$. To speed up the simulation, a steady state surface is obtained by successively magnifying smaller ones anisotropically utilizing the self-affine property with the known exponent $\alpha=1/2$. Specifically, a fully relaxed surface on a lattice of size L is mapped onto another one of size $2L$. The height is rescaled by a factor 2^{α} and proper interpolation has to be carried out. The resulting surface is then evolved into steady state before another step of magnification. At $L=32\,768$, the surface is evolved further for a period of 100 before data are collected. We have checked that using surfaces relaxed for longer periods does not alter our results.

We then computed $\mathcal{A}$ and **b** using Eqs. (14) and (15) for various values of l and τ. The results were averaged over a period of about 4×10^4 corresponding to 4×10^6 iterations. The parameter vector **a** and hence its components c, ν, and $\lambda/2$ are solved from Eq. (13) and D is then computed from Eq. (12). The results which are qualitatively similar to those in Ref. [21] are shown in Fig. 3, where the continuum parameters λ, ν, and D are plotted as functions of the resolutions l and τ. We now examine the values at large l which should be equivalent to the small τ regime in which the temporal discretization in Eq. (9) is valid. We obtained the nonlinear parameter $\lambda\simeq3.04$ which agrees reasonably well with $\lambda_0=3$. This parameter is known to admit no renormalization [19] and is thus independent of both l and τ for sufficiently large l. For any given τ, the parameters ν and D renormalize at first as l increases corresponding to the elimination of the fast evolving short wavelength Fourier components. Subsequently they converge at larger l since the long wavelength modes with time scales longer than τ evolve too slowly to contribute to any renormalization [21]. The converged values depend only on τ which now dictates the extent of the renormalization. At small τ, there is hardly any renormalization. We can thus obtain the ''bare'' continuum parameters which have not been renormalized by the dynamics although effects due to spatial coarse graining are already taken into account. We found $\nu\simeq1.14$ and $D\simeq1.01$ at the smallest $\tau=0.01$ we investigated. Within our numerical accuracy, we conclude that the bare parameters satisfy $\lambda=\lambda_0$ and $D=D_0$ but $\nu\neq\nu_0$. It is known that ν and D renormalize in the same way due to a fluctuation dissipation theorem so that $A=D/\nu$ is a constant [19]. This is confirmed by our results and we obtained $A\simeq0.877$ independent of τ.

V. DISCUSSIONS

We have investigated the conventional approach for direct numerical integration of the KPZ equation using Euler's method. We performed the numerical integration with nominal parameters $\nu_0=D_0=1$ and $\lambda_0=3$. The scaling amplitude $A=D/\nu$ is measured from the resulting surfaces. Measurements taken from saturated surface width, correlation function, and the inverse method calculation all give consistent results of $A\simeq0.879$, 0.876, and 0.877, respectively. These estimates are distinctly different from the expected nominal value $A_0=D_0/\nu_0=1$. Using the inverse method, we found that the unrenormalized continuum noise correlator $D=D_0$ and also the nonlinear parameter $\lambda=\lambda_0$ as expected. However, quite surprisingly the diffusion coefficient is given by $\nu\simeq1.14\neq\nu_0$.

We thus conclude that the continuum diffusion coefficient which actually describes the dynamics of the surface is incompatible with the nominal value used in the discrete equation. We have shown that this occurs only for the KPZ equation but not for the linear Edward-Wilkinson version. Our results show that it is an intrinsic property of the method since it cannot be rectified by altering the spatial or temporal discretization steps used in the numerical integration.

There are other discretization methods for the KPZ equation. For example, Beccaria and Curci investigated a numerical integration approach based on the Hopf-Cole transformed KPZ equation in order to achieve improved numerical stability [7]. Newman and Bray also proposed a related discretization which is claimed to be capable of better capturing the strong coupling behavior of the KPZ equation. We have simulated surfaces in $1+1$ dimensions with the same parameters using these discretizations and obtained $A\simeq0.79$ and 0.49, respectively. To arrive at the results, we have conducted both surface width measurements and the inverse method which give consistent results. The discrepancy between A and A_0 is also a consequence of $\nu\neq\nu_0$. Therefore the anomaly seems to be a common feature of discretization schemes for the KPZ equation. Recently, we have successfully constructed a class of discretizations for the KPZ equation such that $\nu=\nu_0$ is followed exactly. This will be reported elsewhere.

The reason behind the anomaly in the diffusion coefficient will be apparent when we examine the geometry of surfaces resulting from direct numerical integration. Figure 4 shows the details of a surface generated using Eq. (3). We have again set $\nu_0=D_0=1$, $\lambda_0=3$, and $\Delta t=0.01$. A smaller Δt and even a vanishing nonlinear parameter λ_0 will not alter

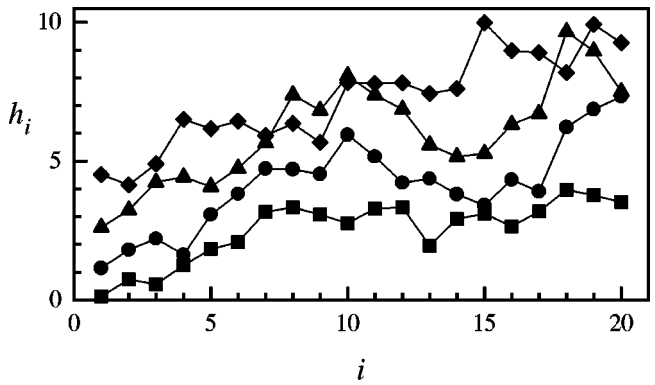

FIG. 4. Snapshots of a segment of an interface generated by numerical integration. The time between two consecutive snapshots is 0.2 corresponding to 20 iterations.

the qualitative features. We see that the surface is rough not only at macroscopic scales but all the way down to the lattice level. In general, for a finite difference equation in the form of Eq. (3), one would expect an $O(\Delta x^2)$ error due to the discretization provided that $h(x,t)$ were smooth. With such a rough solution, the approximation is indeed uncontrolled. For the linear case, it is easy to show explicitly that the discrete equation does agree exactly with the continuum counterpart in the long length scale limit. However, for the KPZ equation there is no *a priori* reason to believe Eq. (3) is a valid approximation.

The anomaly in the diffusion coefficient ν or the scaling amplitude A in our knowledge has not been reported previously even though numerical integration has been routinely applied to the KPZ equation for nearly a decade. This is probably because the study of the scaling exponents instead of the amplitude is predominantly the main focus in most works. The scaling exponents obtained in general agree nicely with the exact values from the continuum KPZ equation available in $1+1$ dimensions. However, this is not necessarily because the discrete equation genuinely approximates the continuum one, which is indeed not true according to our findings. Instead, we believe that the agreement is solely due to universality. The discrete equations are themselves nonlinear local growth equations with translational symmetry. In many cases, this is already sufficient for the discrete equations to be in the KPZ universality class as has been argued for many discrete models [1]. Therefore, although the conventional approach does not provide a genuine numerical integration of the KPZ equation, we have no doubt about the validity of the scaling exponents measured previously because of universality.

For measurements other than the scaling exponents, caution must be taken when applying direct numerical integration. For example, when computing the coupling constant $\overline{\lambda^2}(\tau)=[(\lambda^4 D^2/\nu^5)\tau]^{2/3}=[(\lambda^4 A^2/\nu^3)\tau]^{2/3}$ using the inverse method [21], which actually motivated this work, it must be noted that the continuum A is different from the nominal one used in the discrete equations.

Newman and Bray [8] suggested that a discretization mentioned earlier better capture the strong coupling physics of the KPZ equation. We do not agree with this point. Recall that the scaling amplitude we found with their approach is $A\simeq 0.49$, which is very different from $A_0=1$. Neither this discretization nor the conventional one approximate the continuum equation genuinely. However, both of them are discrete equations in the KPZ class and should exhibit the same physics at long length scales. Therefore, as far as universal properties are concerned, both are equally valid discretizations and their numerical stability may be the only concern when choosing between them for certain applications.

Since there is no guarantee that the parameters in a discrete equation can be inherited directly from the original continuum equation, the same reasoning also implies that the presence or absence of a whole term may not be straightforwardly controlled except under certain symmetry constraints. Amar and Family [17] investigated an equation with a generalized nonlinear term which in one case reduces to

$$\frac{\partial h}{\partial t}=\nu\nabla^2 h+\lambda(\boldsymbol{\nabla} h)^4+\eta(x,t). \tag{16}$$

The $(\nabla h)^4$ term is irrelevant at long length scales and the equation is expected to be in the Edward-Wilkinson universality class. However, they found KPZ exponents. The authors suggested that a $(\boldsymbol{\nabla} h)^2$ term is induced by the combined effects of noise and nonlinearities. From our point of view, which is consistent with theirs, microscopic roughness of the surfaces implies that the discrete equation used in Ref. [17] does not faithfully approximate Eq. (16). Since the equation is nonlinear and there is no special symmetry to forbid a $(\boldsymbol{\nabla} h)^2$ term, it is quite natural that the term should exist and the equation should be in the KPZ universality class.

In conclusion, we have explained that the conventional Euler method does *not* provide a genuine direct numerical integration of the KPZ equation. The continuum diffusion coefficient is indeed incompatible with the nominal one in the discrete equations due to microscopic roughness of the surfaces. Although the scaling exponents are not affected due to universality, caution must be taken when inferring other properties of the continuum equation from their discretized counterparts. Direct numerical integration is also routinely applied to growth in higher dimensions and other related growth equations [9–17]. Analogous anomalies might also exist.

ACKNOWLEDGMENTS

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