

## Improved discretization of the Kardar-Parisi-Zhang equation

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We propose a spatial discretization of the Kardar-Parisi-Zhang (KPZ) equation in 1+1 dimensions. The exact steady state probability distribution of the resulting discrete surfaces is explained. The effective diffusion coefficient, nonlinearity, and noise strength can be extracted from three correlators, and are shown to agree exactly with the nominal values used in the discrete equations. Implications on the conventional method for direct numerical integration of the KPZ equation are discussed. [S1063-651X(98)15011-0]

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### I. INTRODUCTION

The Kardar-Parisi-Zhang (KPZ) equation is one of the most important models for growth of fractal surfaces [1,2]. It gives the local growth rate of a profile  $h(x,t)$  at substrate position  $x$  and time  $t$  [3]:

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

where  $\nu$  and  $\lambda$  are the diffusion coefficient and the nonlinear parameter, respectively. The noise  $\eta$  has a Gaussian distribution and mean zero and a correlator

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

The profile  $h(x,t)$  is assumed to have been coarse grained up to some implicit lower wavelength cutoff.

Direct numerical integration has been an important approach for the investigation of the KPZ equation. Most studies are based on the discrete equation

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

or its simple variants [4–7]. The surface height  $h_i^n$  approximates  $h(x_i, t_n)$  at the  $i$ th lattice point and the  $n$ th time step. The lattice constant  $\Delta x$  has been taken as 1, without loss of generality while the time step  $\Delta t$  must be small enough to ensure convergence. Every  $\xi_i^n$  is an independent random variable with mean zero and unit variance following the Gaussian distribution. The subscripted parameters  $\nu_0$ ,  $\lambda_0$ , and  $D_0$  denote nominal values used in the discrete equation to be distinguished from the effective values which can be different due to numerical errors.

Despite being widely used as a means of numerical integration, Eq. (3) admits certain properties which appear to be fundamentally different from those of its continuum origin [7,8]. Recently, we reported a detailed study of surfaces generated from numerical integrations using Eq. (3) at  $\nu_0 = D_0 = 1$  and  $\lambda_0 = 3$  [9]. In brief, the values of the effective parameters  $\lambda$ ,  $\nu$ , and  $D$  were measured. Using an inverse method [10], it was found that  $\lambda \approx \lambda_0$  and  $D \approx D_0$ , as ex-

pected, but quite surprisingly  $\nu \approx 1.14 \neq \nu_0$ . The parameters  $D$  and  $\nu$  were computed at a short time limit to avoid any renormalization. These values imply a scaling amplitude  $A = D/\nu \approx 0.877$  which agrees nicely with independent estimates of  $A \approx 0.879$  and  $0.876$  taken, respectively, from saturated surface width and correlation function measurements. The discrepancy between  $\nu$  and  $\nu_0$  cannot be rectified by decreasing  $\Delta t$  or  $\Delta x$ . It has thus been concluded in Ref. [9] that the conventional discretization is not a genuine approximation of the continuum KPZ equation, although universality does imply many common properties. The problem has been attributed to microscopic roughness in the surfaces, which leads to inaccuracy in the finite difference expressions in Eq. (3).

This work aims at a better understanding of the relationship between the KPZ equation and its discretizations. This is made possible by studying a spatial discretization of the KPZ equation in 1+1 dimensions. Unlike conventional schemes, these discrete equations can be studied analytically and their properties can thus be compared with those of the continuum counterpart. By calculating analytically the values of three correlators, we found that the effective parameters  $\lambda$ ,  $\nu$ , and  $D$  all agree with the nominal values. We emphasize that we have only investigated three correlators out of infinitely many possible ones, and have not shown that effective parameters extracted from other correlators all give consistent values.

The rest of the paper is structured as follows. In Sec. II, we define the discretization. Section III explains an exact steady state distribution of the discrete surfaces following from the equations. In Sec. IV we extract the continuum parameters in the KPZ description of their dynamics. Section V discusses implications of our results on the conventional discretization scheme, and we conclude in Sec. VI with some further discussion.

### II. IMPROVED DISCRETIZATION

Equation (3) results from both spatial and temporal discretizations of the KPZ equation. We now suggest a scheme involving only a spatial discretization denoted symbolically as

$$\frac{dh_i(t)}{dt} = \nu_0 \Gamma_i + \frac{\lambda_0}{2} \Psi_i + \eta_i(t). \quad (4)$$

Any further temporal discretization for conducting numerical integrations is straightforward, but will be omitted in our discussion. In the equation,  $h_i(t) = h(x_i, t)$  is the surface height at the  $i$ th lattice point and time  $t$ . We take a spatial discretization  $\Delta x = 1$ . Both the diffusive term

$$\Gamma_i = h_{i+1} + h_{i-1} - 2h_i \quad (5)$$

and the noise  $\eta_i$  with mean zero and a correlator,

$$\langle \eta_i(t) \eta_j(t') \rangle = 2D_0 \delta_{ij} \delta(t - t'), \quad (6)$$

are the conventional choices. The uniqueness of this discretization comes from a nonlinear term  $\Psi_i$  defined as

$$\Psi_i = \frac{1}{3} [(h_{i+1} - h_i)^2 + (h_{i+1} - h_i)(h_i - h_{i-1}) + (h_i - h_{i-1})^2]. \quad (7)$$

This finite difference approximation for  $(\nabla h)^2$  has an error of order  $\Delta x^2$ , as can be easily shown by standard Taylor expansions. The reason for this rather unusual choice is that it enables elegant analytical treatments which will become apparent in subsequent sections.

On the other hand, if  $\Psi_i$  is replaced by the usual choice

$$\Psi_i^0 = \frac{1}{4} (h_{i+1} - h_{i-1})^2, \quad (8)$$

a further temporal discretization of Eq. (4) immediately leads to the conventional discretization in Eq. (3). The error of  $\Psi_i^0$  in approximating  $(\nabla h)^2$  is proportional to  $\Delta x^2$  as well. If  $h_i$  represents some smooth profile,  $\Psi_i$  or  $\Psi_i^0$  will only lead to a small difference in the numerical accuracy. However, since  $h_i$  is in fact rough at all scales [9], they lead to significantly different results.

### III. STEADY STATE DISTRIBUTION

The main advantage of our discretization is that the steady state probability distribution of the corresponding discrete surfaces can be solved exactly. This is in fact a direct consequence of analogous properties of the continuum KPZ equation, which will first be summarized. Let  $P[h(x), t]$  be the time dependent probability functional of a surface described by the KPZ equation. A Fokker-Planck equation

$$\begin{aligned} \frac{\partial P[h(x), t]}{\partial t} = & - \int dx \frac{\delta}{\delta h} \left\{ \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 \right\} P \\ & + D \int dx \frac{\delta^2}{\delta h^2} P \end{aligned} \quad (9)$$

follows, from which we can obtain the well-known steady state solution

$$P[h(x)] = \exp \left[ - \frac{1}{2A} \int dx (\nabla h)^2 \right], \quad (10)$$

where  $A = D/\nu$  [1].

While the KPZ equation is a partial differential equation, the spatial discretization in Eq. (4) denotes a set of coupled ordinary differential equations. Consider periodic boundary

conditions and a lattice of size  $L$ . The probability distribution  $P[h_i, t]$  of the discretized surface  $h_i$  follows a similar Fokker-Planck equation

$$\frac{\partial P[h_i, t]}{\partial t} = - \sum_{i=1}^L \frac{\partial}{\partial h_i} \left[ \left( \nu_0 \Gamma_i + \frac{\lambda_0}{2} \Psi_i \right) P \right] + D_0 \sum_{i=1}^L \frac{\partial^2 P}{\partial h_i^2}. \quad (11)$$

When  $\lambda_0 = 0$ , i.e., in the linear case, it can be shown easily by direct substitution that a steady state solution is

$$P[h_i] = \exp \left[ - \frac{1}{2A_0} \sum_{i=1}^L (h_{i+1} - h_i)^2 \right], \quad (12)$$

where  $A_0 = D_0/\nu_0$ . A special feature of our discretization is that  $P[h_i]$  given above is also the steady state solution for all values of  $\lambda_0$ . In fact, when  $P[h_i]$  is substituted into Eq. (11), the  $\lambda_0$  dependent term on the right-hand side is proportional to

$$\sum_{i=1}^L \frac{\partial}{\partial h_i} \Psi_i P = - \frac{1}{3} \sum_{i=1}^L \left[ \delta_i - \delta_{i-1} - \frac{1}{A_0} (\delta_i^3 - \delta_{i-1}^3) \right] P, \quad (13)$$

where  $\delta_i = h_{i+1} - h_i$ . It is easy to see that it vanishes due to exact cancellation of terms after applying the periodic boundary conditions. Therefore, the distribution  $P[h_i]$  is not affected by the nonlinearity, and can remain as the steady state solution even for nonzero  $\lambda_0$ . Note that the form of  $\Psi_i$  defined in Eq. (7) has been chosen precisely to allow for this cancellation of terms. Furthermore, our calculations have been based on analogous considerations for the continuum case [1]. In particular, the distribution  $P[h_i]$  is also a discretized form of  $P[h(x)]$  in Eq. (10).

### IV. EXTRACTION OF CONTINUUM PARAMETERS

Using the exact distribution explained above, we now calculate the effective continuum parameters. In contrast to the results for the conventional discretization, all three parameters obtained, including the diffusion coefficient, agree exactly with the nominal values, i.e.,

$$\nu = \nu_0, \quad \lambda = \lambda_0, \quad D = D_0, \quad (14)$$

as will be proved below.

Let us first examine the scaling amplitude  $A = D/\nu$  which admits no renormalization [11], and hence can be extracted relatively easily. Due to the factorized form of the probability distribution  $P[h_i]$  in Eq. (12), every step  $(h_{i+1} - h_i)$  in the discrete surface is an independent Gaussian variable. We have neglected any correlation imposed by the periodic boundary conditions which vanishes for large lattice size  $L$ . It is then easy to show that the two-point correlation function, defined as

$$C(r) = \langle (h_{i+r} - h_i)^2 \rangle, \quad (15)$$

is given by

$$C(r) = A_0 r^{2\alpha} \quad (16)$$

for  $r \ll L$ , and we have used  $A_0 = D_0 / \nu_0$ . The roughness exponent  $\alpha$  is  $\frac{1}{2}$  in 1 + 1 dimensions. It is well known that from the continuum KPZ equation, we have [12]

$$C(r) = \langle [h(x+r) - h(x)]^2 \rangle = Ar^{2\alpha}. \quad (17)$$

Comparing Eqs. (16) and (17), we see that the continuum scaling amplitude agrees with the nominal value, i.e.,  $A = A_0$  implying that  $D/\nu = D_0/\nu_0$ .

To extract  $\lambda$ , we adopt the approach of Krug and Meakin previously applied to a single step model [13]. Consider a screw boundary condition in which the surface has an average slope  $u$ . The steady state probability distribution in Eq. (12) is generalized to

$$P[h_i] = \exp \left[ -\frac{1}{2A_0} \sum_{i=1}^L (h_{i+1} - h_i - u)^2 \right]. \quad (18)$$

Every step  $h_{i+1} - h_i$  is still an independent Gaussian variable as before, but the mean is now  $u$  instead of zero. We can show easily that

$$\langle (h_{i+1} - h_i)(h_{j+1} - h_j) \rangle = A_0 \delta_{ij} + u^2. \quad (19)$$

The average growth velocity  $v(u) = \langle \partial h_i / \partial t \rangle$  now depends on the inclination. Using Eqs. (4) and (19), we obtain

$$v(u) = \frac{\lambda_0 A_0}{3} + \frac{\lambda_0}{2} u^2. \quad (20)$$

The nonlinear parameter  $\lambda$  is given by [13]

$$\lambda = \left. \frac{d^2 v}{du^2} \right|_{u=0} = \lambda_0, \quad (21)$$

which again coincides with the nominal value.

The continuum parameters  $\nu$  and  $D$  admit renormalizations and are scale dependent [11]. To calculate the bare parameters, we consider a short time limit in which the surface is not able to evolve sufficiently to contribute to any dynamical renormalization [9]. We denote the surface advance within a short period  $\Delta t$  by  $\Delta h$ . The KPZ equation implies

$$\Delta h = \left[ \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 \right] \Delta t + \Delta W, \quad (22)$$

where

$$\Delta W = \int_t^{t+\Delta t} \eta(x, t') dt' \propto \Delta t^{1/2}. \quad (23)$$

Since the noise  $\Delta W$  is of lower order in  $\Delta t$ , the deterministic terms can be neglected in the short time limit corresponding to  $\Delta t \rightarrow 0$ . Similarly, the noise term dominates in the discrete equation (4) as well. The two noise terms can therefore be compared directly, disregarding any influence from the deterministic parts. It is then easy to see that the noise terms are equivalent at long length scales if  $D = D_0$ .

The identities  $A = A_0$  and  $D = D_0$  already imply  $\nu = \nu_0$ . However, we can gain some further insights by deriving it directly. We multiply Eq. (22) by  $\nabla^2 h$ , and take an ensemble average at steady state. The noise term, which has a mean zero, vanishes. Furthermore, terms with odd powers in  $h$  including  $\langle \nabla^2 h \rangle$  and  $\langle (\nabla^2 h)(\nabla h)^2 \rangle$  also go to zero due to a reflection symmetry with respect to the transformation  $h \rightarrow -h$ , followed by the distribution  $P[h(x)]$  in Eq. (10). Some further rearrangement of the resulting equation gives

$$\nu = \frac{\langle (\nabla^2 h) \Delta h \rangle}{\Delta t \langle (\nabla^2 h)^2 \rangle}, \quad (24)$$

which will be used to calculate  $\nu$ . Applying the continuum description to the discrete surfaces,  $h$  now represents a smoothed version of  $h_i$ . Coarse graining Eq. (4) gives

$$\Delta h = \left[ \nu_0 \Gamma_c + \frac{\lambda_0}{2} \Psi_c \right] \Delta t + \Delta W_c, \quad (25)$$

where the subscript  $c$  denotes a coarse-grained quantity. The discrete diffusive term  $\Gamma_c$  is equal to the continuum counterpart  $\nabla^2 h$  at long wavelength, as can be easily demonstrated in the Fourier space. Hence, substituting Eq. (25) into Eq. (24) gives

$$\nu = \nu_0 + \frac{\lambda_0}{2} \frac{\langle (\nabla^2 h) \Psi_c \rangle}{\langle (\nabla^2 h)^2 \rangle}. \quad (26)$$

The steady state distribution  $P[h_i]$  in Eq. (12) also follows an analogous up-down reflection symmetry, and hence

$$\langle (\nabla^2 h) \Psi_c \rangle = 0, \quad (27)$$

as  $\Psi_c$  is even in  $h_i$ . Therefore, Eq. (26) reduces to  $\nu = \nu_0$ .

The exact continuum parameters  $\nu$ ,  $\lambda$ , and  $D$  calculated in this section have all been verified numerically using correlation function measurements and an inverse method. The details, including the introduction of a higher order numerical integration algorithm and stability issues, will be reported elsewhere [14].

## V. CONVENTIONAL DISCRETIZATION

We have explained in Sec. III that, for the linear  $\lambda_0 = 0$  case,  $P[h_i]$  in Eq. (12) is a steady state probability distribution of the discrete surfaces. Even when the nonlinear  $\Psi_i$  term is introduced, the distribution is not disturbed, since all the additional terms induced in the Fokker-Planck equation cancel nicely with each other. However, when the nonlinear  $\Psi_0^i$  term is introduced in the conventional discretization, the extra  $\lambda_0$  dependent term is proportional to

$$\sum_{i=1}^L \frac{\partial}{\partial h_i} \Psi_0^i P = \frac{1}{4A_0} \sum_{i=1}^L (\delta_i^3 - \delta_i^2 \delta_{i-1} - \delta_i \delta_{i-1}^2 + \delta_{i-1}) P, \quad (28)$$

which, unlike the analogous expression in Eq. (13), remains nonzero in general. Therefore,  $P[h_i]$  is no longer a steady state solution, and we should have a  $\lambda_0$  dependent probabil-

ity distribution, which we have not been able to solve. Many of the foregoing nice analytic properties thus do not apply to the conventional discretization.

We mentioned in Sec. I that, for the conventional discretization, numerical studies indicate that the continuum and discrete parameters bear the relationships

$$\nu \neq \nu_0, \quad \lambda = \lambda_0, \quad D = D_0 \quad (29)$$

in the short time limit [9]. Due to the same reason of noise domination explained in Sec. IV, it can be shown that  $D = D_0$  is exact. However, without knowing the steady state distribution, we have not been able to prove  $\lambda = \lambda_0$ , and it may only hold approximately.

The result  $\nu \neq \nu_0$  is more interesting. For our discretization, in Sec. IV we proved a definitive relation of  $\nu = \nu_0$ . This equality is a consequence of Eq. (27), which is in turn due to an exact up-down reflection symmetry of the steady state distribution  $P[h_i]$  defined in Eq. (12). However, for the conventional discretization, we have a  $\lambda_0$  dependent distribution. It can be proved numerically that the reflection symmetry does not hold [14], and hence  $\langle (\nabla^2 h) \Psi_c \rangle \neq 0$ . Similar to Eq. (26), we have

$$\nu = \nu_0 + \frac{\lambda_0 \langle (\nabla^2 h) \Psi_c^0 \rangle}{2 \langle (\nabla^2 h)^2 \rangle}, \quad (30)$$

with the correction term now nonvanishing. We are not able to proceed further analytically without the knowledge of the steady state distribution. As summarized in Sec. I, the corrected numerical value of  $\nu$  has been computed using an inverse method [9]. The formula adopted in that approach, after simplifications due to symmetry, is actually equivalent to Eq. (30) derived here.

## VI. DISCUSSION

In most investigations on direct numerical integration of the KPZ equation, the use of finite difference discretization has been taken for granted [4–6]. However, finite difference expressions are accurate only if the surface is smooth microscopically. As suggested previously, this is unfortunately not true, and is evident from simple visual inspection of the surfaces [9]. Furthermore, we have shown in this work that two seemingly equally valid discretizations of the KPZ equation indeed behave very differently. Therefore, we believe that the relationship between continuum growth equations and their discretizations is actually a nontrivial problem. Similar discrete equations are routinely applied in direct numerical integrations of the KPZ equation and other related growth problems [7,15–22]. Our results may provide useful insights into how those continuum growth equations are related to their discretizations.

It is straightforward to generalize our discretization to include higher order terms such as  $(\nabla h)^4$  [15] without affecting the exact solvability. The results will be presented elsewhere [14]. However, generalization to higher dimensions may be difficult if not impossible, since our calculations have been based on exact properties of the KPZ equation in  $1+1$  dimensions, and most of them have no counterpart in higher dimensions.

In summary, we have suggested an analytically tractable spatial discretization of the KPZ equation. The effective parameters  $\nu$ ,  $\lambda$ , and  $D$  extracted from three correlators equal exactly the nominal values. This is irrespective of the fact that the finite difference approximation involved is in general inaccurate due to the presence of microscopic roughness.

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