Numerical simulation of the Kardar-Parisi-Zhang equation

Matteo Beccaria
Dipartimento di Fisica, Università di Pisa, Piazza Torricelli 2, I-56100 Pisa, Italy
and Istituto Nazionale di Fisica Nucleare, Sezione di Pisa Via Livornese 582/a, I-56010 Santo Piero a Grado (Pisa), Italy

Giuseppe Curci
Istituto Nazionale di Fisica Nucleare, Sezione di Pisa Via Livornese 582/a, I-56010 Santo Piero a Grado (Pisa), Italy
and Dipartimento di Fisica, Università di Pisa, Piazza Torricelli 2, I-56100 Pisa, Italy
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We simulate the Kardar-Parisi-Zhang equation [Phys. Rev. Lett. **46**, 889 (1986)] in $2+1$ dimensions. It is a nonlinear stochastic differential equation that describes driven growing interfaces. The Hopf-Cole transformation is used in order to obtain a stable numerical scheme. The two relevant critical exponents are precisely measured.

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I. INTRODUCTION

Growing surfaces exhibit a nonequilibrium critical dynamics with scaling properties similar to those of equilibrium critical phenomena. Many models have been proposed to describe the universal features of the growth process. The first numerical investigations [1] showed that the critical behavior of the surface is described by two exponents z and χ. The interface roughness W (to be defined later) grows with time t as

$$W \sim L^{\chi} f\left(t\, L^{-z}\right), \tag{1}$$

where L is the system size. Among the possible systems possessing such a scaling law, we mention, for instance, lattice ballistic deposition models, lattice stacking models, or Eden clusters. In principle, the exponents χ and z are model dependent. In [2], Kardar, Parisi, and Zhang (KPZ) proposed a nonlinear stochastic differential equation to describe growing interfaces. Nonlinearity was related to lateral growth of the interface. A dynamic renormalization group analysis [2–4] determined the time evolution of the effective nonlinearity parameter λ related to the deposition speed. The exponents χ and z are defined asymptotically and depend on the particular fixed-point λ^* which is reached; the nonasymptotic behavior is not universal and may be rather complicated. Dimensionality of space is *a priori* relevant. If $\lambda^* \neq 0$, the hyperscaling relation $\chi + z = 2$ holds perturbatively. In $d = 1$ (growth on a line), exact exponents can be computed and they are also supported by several numerical simulations on the various models listed above. This favors the possibility that all these discrete models may be in the same dynamical universality class. In $d = 2$, the perturbative renormalization group analysis breaks down, the flow is toward a strong coupling fixed point which determines the exponents, and numerical simulation becomes very interesting. Kardar, Parisi, and Zhang conjectured [2] the χ, z exponents to be superuniversal, namely independent on d, but they did not give analytical arguments. Successive works on the subject can be roughly divided into three groups. The first one deals with Eden cluster growth [5] and off lattice aggregation models with possible readjustement mechanisms [6]. The second group studies directed polymers [7] and restricted solid on solid (RSOS) models [8] which are related to the KPZ equation. Finally, the third group simulates directly the KPZ equation by discretizing space and time and averaging over the realizations of the noise [9–12].

Apart from the direct simulations of the KPZ equation, the information on the exponents extracted from the other models is problematic. Indeed, directed polymers have been studied only in the zero temperature limit whereas the other models have not been shown rigorously to be in the same universality class of the KPZ equation. On the other hand, the direct simulation of the stochastic equation is hampered by great crossover effects which are relevant on the time scale actually explored in the simulations. Numerical instabilities are also potentially harmful.

A summary of the situation in $d = 2$ is the following: (i) the hyperscaling relation has strong numerical support and (ii) the exponents seem to rule out the superuniversality hypothesis and agree reasonably well with the empirical prediction of [13].

Up until now, the most precise data on $\beta = \chi/z$ and χ coming from direct simulations of the KPZ equation are those of Moser *et al.* [12] who however did not check $\chi + z = 2$. The authors of [12] complain about numerical instabilities arising at large nonlinearity: this unpleasant situation forced them to utilize very small integration steps not required in order to reduce the systematic error due to finite integration step. In this work we propose the simulation of the KPZ equation after the Hopf-Cole transformation which improves numerical stability due to the elimination of the nonlinear term. We measure β and χ with high statistics and confirm the results of [12].

II. SCALING BEHAVIOR OF THE KARDAR-PARISI-ZHANG EQUATION

The Kardar-Parisi-Zhang equation [2] in d dimensions for the interface height $h(x,\ t)$ is

$$\frac{\partial h}{\partial t} = \nu\ \nabla^2 h + \frac{\lambda}{2}\,(\nabla h)^2 + \eta(x,t),\quad x \in \mathbb{R}^d\ , \tag{2}$$

where η is a Gaussian white noise with constant diffusion D and it can be thought as a suitable limit of a Gaussian colored noise. The relaxation term in Eq. (2) provides the surface tension responsible for molecular readjustment. The nonlinear term is related to lateral growing of the interface. The KPZ equation is actually a truncated gradient expansion and its unbroken symmetry under infinitesimal tilts is ultimately responsible for the hyperscaling relation $\chi + z = 2$. We can rescale time and h in order to reduce the number of independent parameters in the KPZ equation. Its canonical form is thus

$$\frac{\partial h}{\partial t} = \nabla^2 h + \sqrt{\lambda}\,(\nabla h)^2 + \eta(x,t), \tag{3}$$

where η has now unit variance and where we have changed variable

$$\frac{2\lambda^2 D}{\nu^3} \to \lambda. \tag{4}$$

The equation depends thus on only one parameter which determines the degree of nonlinearity. The quadratic term $(\nabla h)^2$ is responsible for numerical instabilities since the typical surface becomes more and more rough. The measure of β, χ is done according to Eq. (1) by looking at the interface roughness W defined as

$$W = \langle h^2 \rangle_c = \langle h^2 \rangle - \langle h \rangle^2, \tag{5}$$

where the average is over the lattice and $W(t,L)$ is averaged over the noise. At the unstable trivial fixed point $\lambda = 0$, the growth is marginal and follows the law [14]

$$W^2 \sim \ln t. \tag{6}$$

Starting from $\lambda \neq 0$, we expect to observe the asymptotic scaling

$$W \sim t^{\beta} \tag{7}$$

in infinite volume. Actually, the determination of β is made difficult by the competition of finite size saturation and crossover. Finite size effects allow the observation of Eq. (7) only as an intermediate regime and at $t \to \infty$ we have saturation with $W \to W_{\rm sat}(L)$. On the other hand, the above scaling is asymptotic and holds only when λ has grown up to its critical point. The evolution from an initial small λ is hampered by a strong crossover effect which results in a fictitious effective value for the β exponent. The solution is to choose the initial λ as large as possible, taking into account that, at large λ, a small time step is needed to keep the systematic error small in the integration of the stochastic equation. In order to reduce the problem of numerical instabilities, we propose to utilize the Hopf-Cole transformation (see [15] for a different application)

$$h = \frac{1}{\sqrt{\lambda}}\ \ln w,\quad w = \exp\left(\sqrt{\lambda} h\right). \tag{8}$$

This gives a diffusion equation with multiplicative noise

$$\dot{w} = \nabla^2 w + \sqrt{\lambda}\ w\ \eta(x,t). \tag{9}$$

We used conventional analysis rules in arriving at Eq. (9) and, consequently, Eq. (9) is to be understood in Stratanovich interpretation. Namely, the noise $\eta(x,t)$ correlates with the field $w(x,t)$ at the same point. The Ito representation of the same equation, which is more suitable for numerical work, is [16]

$$\dot{w} = \nabla^2 w + \sqrt{\lambda}\ w\ \eta(x,t) + \frac{\lambda}{2} w. \tag{10}$$

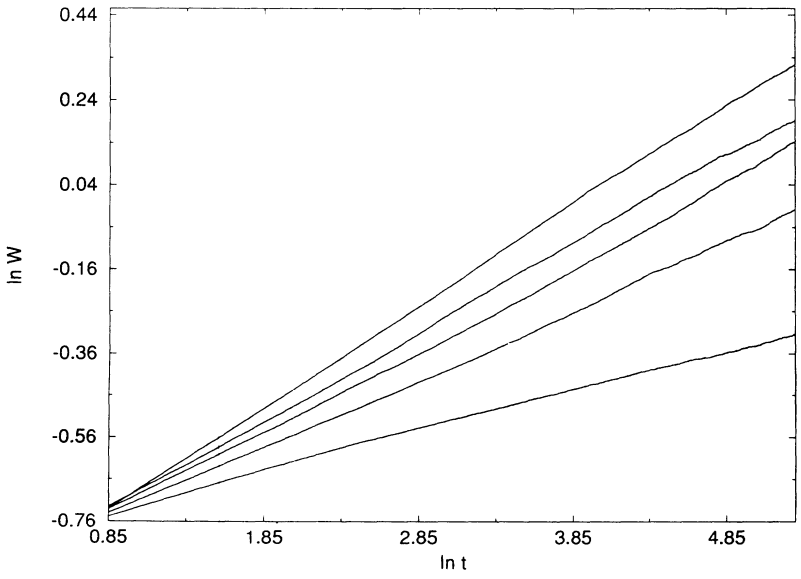

FIG. 1. W versus t at $\lambda = 25, 10, 7.5, 5, 2$.

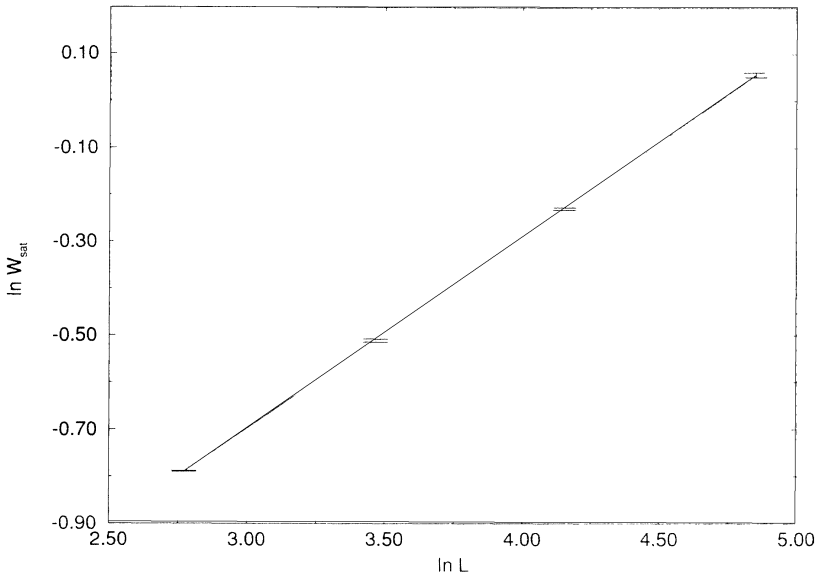

FIG. 2. Determination of χ.

In Eq. (10) the fields $\eta(x,t)$ and $w(x,t)$ do not correlate at the same point. This is exactly what will be assumed in the discrete version of Eq. (10) in the following section. On the other hand, the term $\frac{\lambda}{2}w$ which is left in the numerical scheme rigorously based on Eq. (10) can be easily eliminated by changing the variables $w' = w\exp(\lambda t/2)$.

$$w_{i,j}^{(n+1)} = w_{i,j}^{(n)} + \varepsilon \left(w_{i+1,j}^{(n)} + w_{i-1,j}^{(n)} + w_{i,j+1}^{(n)} + w_{i,j-1}^{(n)} - 4w_{i,j}^{(n)} + \frac{\lambda}{2} w_{i,j}^{(n)} \right) + \sqrt{\varepsilon\lambda}\; w_{i,j}^{(n)}\; \xi_{i,j}^{(n)}. \tag{11}$$

We remark that this discretization follows the Stratanovich interpretation of the stochastic equation and indeed reproduces a discrete version of Eq. (10). We used lattices with size up to $L = 512$. Every integration of the KPZ equation was averaged over 128 realizations of the noise. We used both independent Gaussian random numbers generated by the Box-Muller algorithm [17] and uniform random numbers with zero mean and unit variance as suggested in [10]. Either choices are possible up to the precision of the chosen integration scheme. We checked on trial runs that the average over 128 processes gave the same results with the two choices. Therefore, for the long runs, we have used the uniform random numbers which are considerably faster. The value of the integration step was chosen in order to have irrelevant differences with smaller values. In Fig. 1, we show (from top to bottom) the behavior of W at $\lambda = 25, 10, 7.5, 5, 2$; we have used $\varepsilon = 5\times10^{-4}, 10^{-3}, 2.5\times10^{-3}$ for the first three and $\varepsilon = 5\times10^{-3}$ for the others. At $\lambda = 25$ we have taken data on the $L = 512$ lattice, the other values are at $L = 256$. The crossover effect inducing effective exponents is evident in the figure. Effective increasing values of β are obtained as λ is increased. In order to avoid finite size effects, we determined β over a range where changing L from 256 to 512 was irrelevant. We obtained $\beta = 0.240(1)$ from the upper curve corresponding to $\lambda = 25$. The exponent χ has been obtained by studying the saturation width as a function of L by mean of long runs. The points in Fig. 2 give $\chi = 0.404(1)$. Therefore, the hyperscaling relation is well satisfied. Our results are compatible with [12] and suggest that the empirical conjecture of [13] is incorrect. However, we cannot be sure to have eliminated totally the crossover effects. The common lore is that, due to saturation effects, numerical estimates for β must be considered lower bounds. It is clear that, even if the agreement with RSOS models is encouraging, an analytical upper bound would be desirable.

III. THE SIMULATION

We have simulated the $d = 2$ growth process on a square lattice with periodic boundary conditions. We utilized the following Euler scheme for the integration of the Hopf-Cole diffusion equation:

IV. CONCLUSIONS

The main goal of this paper has been a high statistics simulation of the KPZ equation put in an alternative form after the Hopf-Cole transformation. This change of variables in the stochastic equation does not present any problem from the point of view of the simulations and is numerically stable. Our measures of β and χ satisfy the hyperscaling relation and are compatible with the result of [12]. We do not rule out the conjecture of [13] because of the theoretical uncertainty on the systematic error.

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