Numerical solution of the Kardar-Parisi-Zhang equation with a long-range spatially correlated noise

Minchun Wu
Physics Department, Princeton University, Princeton, New Jersey 08544

K. Y. R. Billah
Department of Civil, Environmental and Coastal Engineering, Stevens Institute of Technology, Hoboken, New Jersey 07030

Masanobu Shinozuka
Department of Civil Engineering and Operations Research, Princeton University, Princeton, New Jersey 08544
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The Kardar-Parisi-Zhang (KPZ) equation for stochastic surface growth is numerically integrated in the presence of a long-range spatially correlated noise and the scaling behavior of the growing surfaces is investigated. A robust methodology for simulating the colored noise directly from uniform random variates is used with the discretized KPZ equation. The sample functions are expressed in terms of harmonic functions and the powerful fast Fourier transform is used. The growth exponents α and β are calculated and the results are compared with the predictions by Medina *et al.* [Phys. Rev. A **39**, 3053 (1989)], Zhang [Phys. Rev. B **42**, 4897 (1990)], and with the numerical results of Amar *et al.* [Phys. Rev. A **43**, R4548 (1991)] and Peng *et al.* [Phys. Rev. A **44**, R2239 (1991)]. The agreement of the present results with the theoretical prediction by Medina *et al.* shows that the current method of colored noise simulation is uniquely effective.

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I. INTRODUCTION

The physical significance of the Kardar-Parisi-Zhang (KPZ) equation [1] has become widely recognized in nonequilibrium statistical mechanics. As a nonlinear generalization of the diffusion equation, it describes many diverse processes, of which the study of stochastically growing surfaces has attracted extensive attention in recent years. The KPZ equation can be applied to the growth of many rough surfaces [2,3] such as crystal growth, vapor deposition, fluid flow in porous media, and biological growth.

The surface is specified by the height $h(\mathbf{r},t)$ at position $\mathbf{r}$ and time t, with the initial condition specified as $h(\mathbf{r},0)=0$. The surface with $w(L,t)$ on length scale L at time t initially increases with time, and without any characteristic length scale, it grows with some power of time, $w(L,t)\sim t^{\beta}$. After the length over which the fluctuations are correlated becomes comparable to the length L, the surface evolves to a steady state with a constant value of its width, which is expected to have a power law dependence on L, $w(L,t\to\infty)\sim L^{\alpha}$. The dependence of $w(L,t)$ on t and L can be combined into the dynamic scaling form [4,5,6,7]:

$$w(L,t)\sim L^{\alpha}f(t/L^{\alpha/\beta}) \tag{1}$$

with the scaling function $f(x)\sim x^{\beta}$ for $x\ll 1$ and $f(x)=\text{const}$ for $x\gg 1$, which suggests that the characteristic time $\tau\sim L^{\alpha/\beta}$. The exponents α and β can also be measured by studying various types of surface correlation functions, such as the height difference correlation function,

$$G(\mathbf{r},t)=\langle\{[h(\mathbf{r},t)-\langle h(t)\rangle_{\mathbf{r}}]-[h(\mathbf{r}+\mathbf{r}',t+t')-\langle h(t+t')\rangle_{\mathbf{r}}]\}^2\rangle_{\mathbf{r},t}^{1/2}\,, \tag{2}$$

where $G(r,0)\sim r^{\alpha}$ for $r\ll L$ and $G(0,t)\sim t^{\beta}$ for $t\ll\tau$.

II. KPZ EQUATION AND ITS NUMERICAL SOLUTION

Kardar, Parisi, and Zhang [1] have proposed a continuous model for the time evolution of the profile of a growing interface, namely

$$\frac{\partial h(\mathbf{r},t)}{\partial t}=\nu\nabla^2 h(\mathbf{r},t)+\frac{\lambda}{2}[\nabla h(\mathbf{r},t)]^2+\eta(\mathbf{r},t)\,. \tag{3}$$

This model takes into account both the relaxation of the surface with a surface tension ν and the lateral growth with the growth velocity proportional to λ. $\eta(\mathbf{r},t)$ represents the noise. Based on first-order perturbative renormalization-group analysis, Kardar, Parisi, and Zhang [1] found that for the white noise $\eta(\mathbf{r},t)$, the scaling exponents are $\alpha=\frac{1}{2}$ and $\beta=\frac{1}{3}$ for spatial dimension $d=2$. To date, there have been a large number of numerical studies performed on Eq. (3). Amar and Family [8], Chakrabari and Toral [9], Guo, Grossmann, and Grant [10,11] have carried out the numerical solution of Eq. (3) using white noise.

However, the white noise assumption may not always be justified physically. Medina *et al.* [12] have considered a generalization of the nonlinear KPZ equation with the noise term having long-range correlations in space and/or time. The noise spectrum $S(k,w)$ is chosen as

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$$S(k,w) \sim |\mathbf{k}|^{-2\rho} w^{-2\theta} . \tag{4}$$

Using the same first-order renormalization-group method for $d=2$ they predicted that for the noise only spatially correlated ($\theta=0$), for $0<\rho<0.25$ the exponents $\alpha=\frac{1}{2}$ and $\beta=\frac{1}{3}$ remained the same as for white noise, but, for $0.25<\rho<1, \alpha=\frac{1}{3}+2\rho/3$ and $\beta=(1+2\rho)/(5-2\rho)$. Zhang [13] developed some other predictions via replica scaling analysis. His results, based on the equivalent directed polymer problem, were $\beta=\alpha/(2-\alpha)=(1+2\rho)/(3+2\rho)$ for $0<\rho<1/2$. Margolina and Warrier [14] studied the surface growth with the restricted solid-on-solid (RSOS) growth model of Kim and Kosterlitz [15]. They pointed out that their results agreed with Zhang's prediction for $\rho<\frac{1}{4}$. Amar *et al.* [16] also carried out the simulations for both the ballistic deposition and the RSOS model, and Peng *et al.* [17] presented the numerical simulations of ballistic-deposition (BD) and directed-polymer (DP) models. Their results agreed with the prediction of Medina *et al.*

In the present work, the KPZ equation was integrated on a discrete grid using a finite-difference scheme. The largest grid size used was $L=2^{17}=131\,072$. The discrete form of Eq. (3) used is

$$\begin{aligned} h_{\tau+1}(i) = h_\tau(i) + \Delta\tau\{ & \nu[h_\tau(i-1)+h_\tau(i+1)-2h_\tau(i)] \\ & +(\lambda/8)[h_\tau(i+1)-h_\tau(i-1)]^2 \\ & +\eta_\tau(i)\} . \end{aligned} \tag{5}$$

The parameter ν is set equal to unity and calculations were carried out with different values of λ ranging from 1 to 10. It was found that for small λ, the exponent α and β are close to the values associated with the linear equation as expected. When λ gets larger ($\lambda>4$) the resulting values of α and β have little dependence on λ. In the final results, λ was set to 6. The Gaussian white noise in the work of Amar and Family [8] was replaced by the long-range spatially correlated noise, generated by the method introduced originally by Shinozuka [18] and revised over the years [19], and used effectively for some stochastic studies [20,21].

The stochastic one-dimensional noise was simulated by the following series as $N\to\infty$:

$$\eta(x)=\sqrt{2}\sum_{n=0}^{N-1} A_n \cos(k_n x+\Phi_n) , \tag{6}$$

where $A_n=[2S(k_n)\Delta k]^{1/2}, k_n=n\Delta k$, $\Delta k=k_u/N$, and $A_0=0$, or $S(k_0)=0$. k_u represents an upper cutoff wave number beyond which $S(k)$ may be assumed to be zero. The Φ_n appearing in Eq. (6) are independent random phase angles distributed uniformly over the interval $[0,2\pi]$. The period of the stochastic process is $X_0=2\pi/\Delta k$. N is the number of grids used in the noise simulation, while L is the integer measure of the length scale of surface. Because the noise generation is independent and can be applied to other problems, this N should be distinguished from L. However, since we take one period of the simulated noise in order to assure the exact correlation, N and L were set to equal.

In this study, the stochastic field is spatially correlated and temporally uncorrelated. The power spectrum density $S(k,w)$ is

$$S(k,w)=S(k)=k^{-2\rho} . \tag{7}$$

The noise-noise correlation function $R(r)$ for the generated noise was computed for $\rho=0.0$–0.5, and the log-log plot of $R(r)$ vs r shows that when $\rho\leq 0.3$ the correlation function $R(r)$ follows the expected $r^{2\rho-1}$. But for large ρ, the simulated noise has smaller value, and at the extreme end for $\rho=0.5$, the simulated noise decays with $\rho'\sim 0.44$, where ρ' is the value of ρ obtained from simulated noise and will be referred to as "effective" ρ. Figure 1 shows the log-log plot of the noise-noise correlation function $R(r)$ vs r with (a) $\rho=0.3$ and (b) $\rho=0.5$. In Fig. 1(b) it can be seen that the curve is not linear as r increases. This is due to the fact that the noise correlation itself has singularity at $r=0$. When ρ is larger, the power

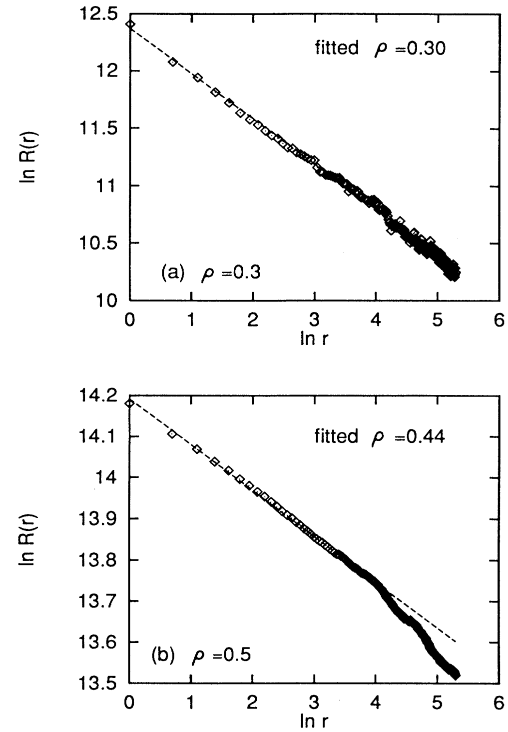

FIG. 1. Log-log plot of noise-noise correlation $R(r)$ vs r. (a) $\rho=0.3$ when the fitted line with 200 sites shows the effective $\rho'=0.3$; (b) $\rho=0.5$ when the effective $\rho'\sim 0.44$ fitted with 55 sites.

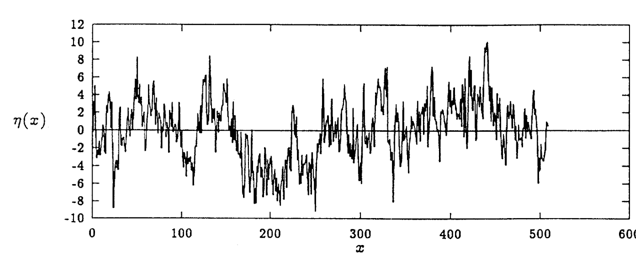

FIG. 2. Simulated one-dimensional noise $\eta(x)$ ($\rho=0.5$).

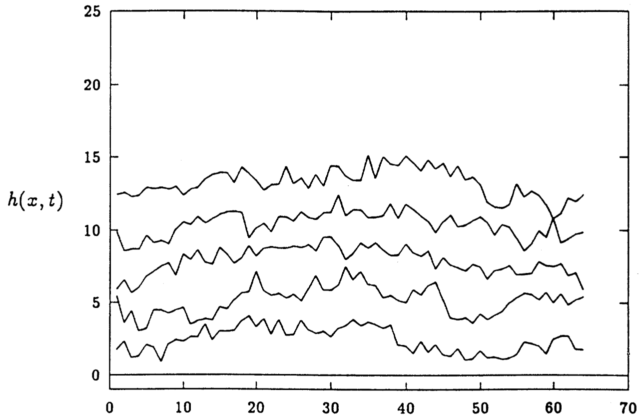

FIG. 3. Simulated done-dimensional surface growth according to the KPZ equation with a long-range spatially correlated noise ($\rho=0.5$). Each drawn surface was 50 time steps apart, with the time step $\Delta t=0.05$.

spectrum density $S(k)$ decays more sharply near zero, which involves larger error when we set $S(0)=0$ for the use of fast Fourier transform (FFT). The effective ρ' was found to scale over a range of 200 sites except for $\rho=0.5$, in which case the range was 55 sites. In the results presented below, the effective ρ' was used.

The noise distribution $\eta(x)$ with spatial correlation was generated independently at each time step (thus yielding a noise δ correlated in time). Smaller time steps were used to ensure convergence and it was indeed verified that the obtained results were numerically stable. Figure 2 shows the simulated one-dimensional noise $\eta(x)$. Figure 3 shows the simulated surface growth at different times.

The exponents α and β which characterize the scaling

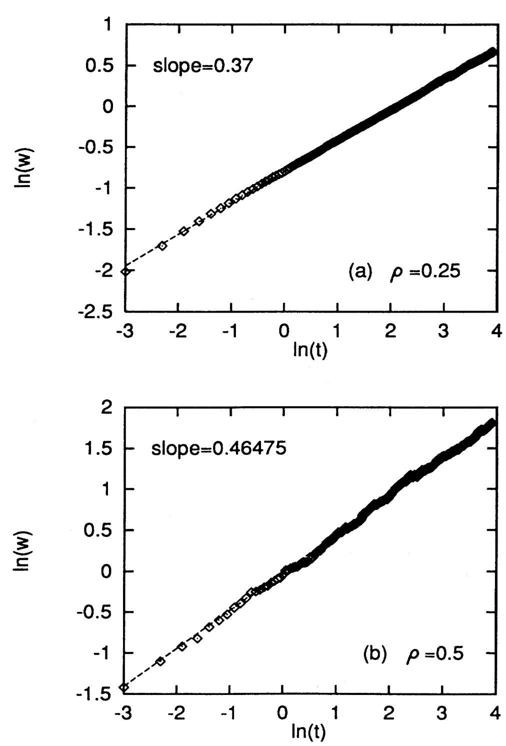

FIG. 4. Log-log plot of w vs t for $L=131\,072$, time step, $\Delta t=0.05$ and $\lambda=6$. (a) $\rho=0.25$; (b) $\rho=0.5$.

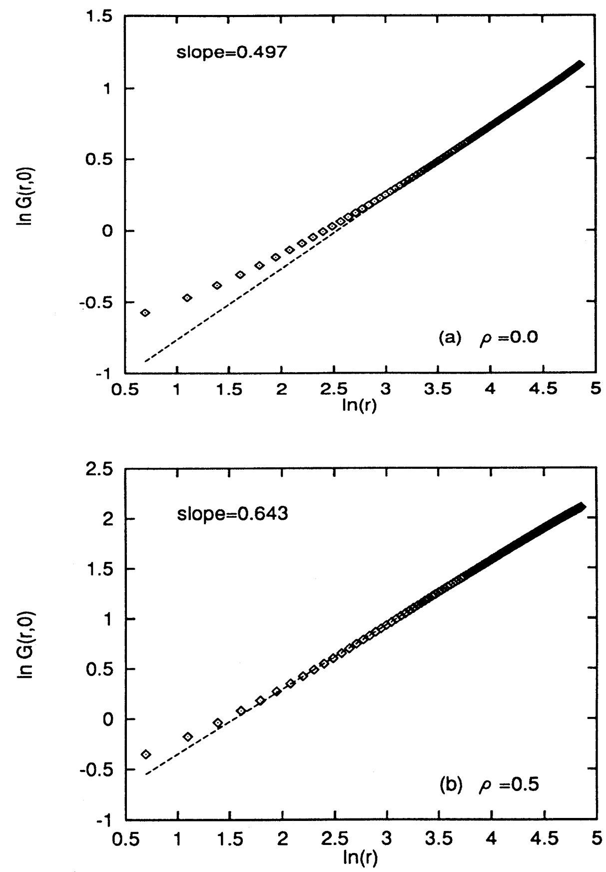

FIG. 5. Log-log plot of $G(r,0)$ vs r for $L=131\,072$, time step $\Delta t=0.05$, 10^5 time steps and $\lambda=6$. (a) $\rho=0.0$; (b) $\rho=0.5$.

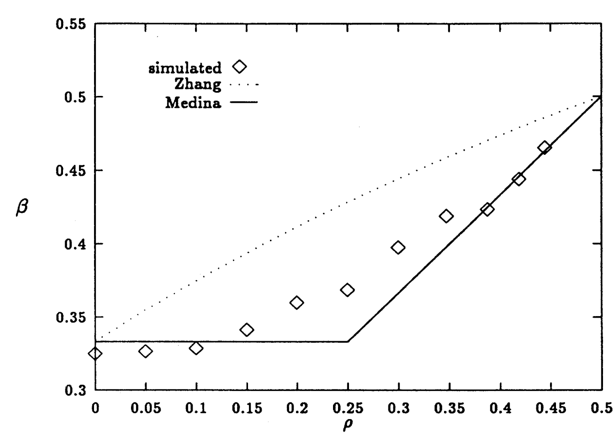

FIG. 6. Growth exponent β as a function of the correlation exponent ρ. Dashed curve is the prediction by Zhang. Solid curve is the prediction by Medina *et al.*

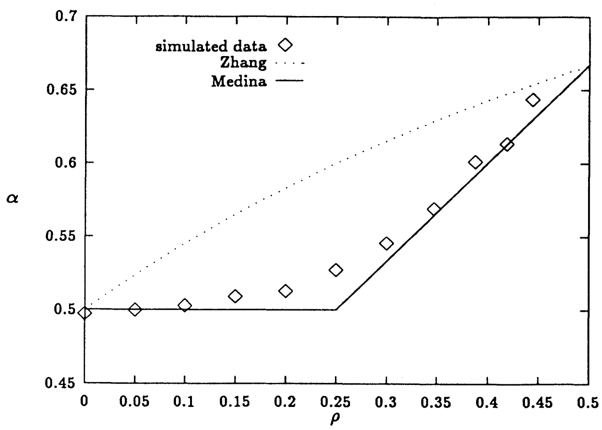

FIG. 7. Roughness exponent α as a function of the correlation exponent ρ. Dashed curve is the prediction by Zhang. Solid curve is the prediction by Medina *et al.*

behavior $w(L,t) \sim L^{\alpha} f(t/L^{\alpha/\beta})$ are important parameters in this study. They were obtained in the following manner: For each value of ρ, the exponent β was determined from the slope of the log-log plots of the surface width w vs time, which were obtained from runs of the order of 10^3 time steps, with averages taken over five runs. Figure 4 shows the log-log plot of w vs t; the surface roughness exponent α was determined from the slope of the log-log plots of the correlation function $G(r,t)$ vs distance r at later times ($t \sim 10^5$ time steps). The range of scaling is 128 sites. Due to the nature of this specific noise correlation, the error at small r is expected, and only a few points (≤ 10 out of 128) for small r is somewhat off the fitted line. Figure 5 shows the log-log plot of the height-height correlation function $G(r,t)$ vs r after 10^5 time steps. Figures 6 and 7 show the results of the growth exponent β and roughness α, respectively, as functions of ρ, from the numerical solution of the KPZ equation with a long-range spatially correlated noise. The obtained results are also compared with different predictions by Medina *et al.* [12] and Zhang [13] in these figures.

III. CONCLUSION

Extensive numerical simulations of the KPZ equation subjected to a long-range spatially correlated noise were carried out using a methodology involving uniform random variates and FFT. The results are in good agreement with the prediction by Medina *et al.* [12] and the simulation results by Amar *et al.* [16] via RSOS and ballistic models and Peng *et al.* [17] via BD and DP models. This study shows that the critical point ρ_c, where α and β start to vary from the values corresponding to the white noise, is smaller than the predicted value $\rho=0.25$ by Medina *et al.* The general agreement of the present results with the theoretical prediction of Medina *et al.* also shows that the unique method of colored noise simulation is effective. This method of simulation can be easily extended to simulate a three-dimensional noise $\eta(x,y,t)$, and is thus applicable to the case where a spatially two-dimensional surface grows according to the KPZ equation. A work in this direction is in progress.

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