Journal of Statistical Physics, Vol. 67, Nos. 3/4, 1992

Steady-State Scaling Function of the (1 + 1)-Dimensional Single-Step Model

Lei-Han Tang[1]

Received January 8, 1992

The steady-state height–height correlation function for the $(1+1)$-dimensional single-step model is calculated in a large-scale Monte Carlo simulation. Analysis of the data yields a universal ratio of scaling amplitudes which differs from the value obtained recently from a mode-coupling calculation. An empirical form for a universal scaling function is also presented.

KEY WORDS: Surface roughening; Kardar–Parisi–Zhang theory; driven lattice-gas diffusion; dynamic scaling; universal scaling function.

The Kardar–Parisi–Zhang[1] (KPZ) equation

$$\partial h/\partial t = \nu \nabla^2 h + \tfrac{1}{2}\lambda(\nabla h)^2 + \eta \tag{1}$$

describes the stochastic growth of a rough surface $h(\mathbf{r}, t)$ whose local velocity along a chosen direction on average depends on the local orientation of the surface. Examples of such growth processes include the Eden model, ballistic deposition, and restricted solid-on-solid models (see, e.g., refs. 2 and 13 for recent reviews). The roughness of such a surface exhibits interesting scaling properties both in space and in time. One quantity which characterizes this scaling behavior is the steady-state height–height correlation function

$$C(\mathbf{r}, t) = \lim_{t_0 \to \infty} \langle [\Delta h(\mathbf{r} + \mathbf{r}_0, t + t_0) - \Delta h(\mathbf{r}_0, t_0)]^2 \rangle \tag{2}$$

where $\Delta h(\mathbf{r}, t) = h(\mathbf{r}, t) - \bar{h}(t)$ is the deviation from a mean surface height $\bar{h}(t)$ at time t in a given realization and $\langle \cdots \rangle$ denotes an average over

[1] Institut für Theoretische Physik, Universität zu Köln, D-5000 Köln 41, Germany.

0022-4715/92/0500-0819$06.50/0

different realizations of the stochastic growth process. In the absence of finite-size corrections, the height fluctuation at a given instant has the power-law behavior at large $r = |\mathbf{r}|$,

$$C(\mathbf{r}, 0) \simeq A_r r^{2\zeta} \tag{3a}$$

where ζ is known as the roughness exponent. The auto-height correlation at large t grows as

$$C(0, t) \simeq A_t t^{2\beta} \tag{3b}$$

Equations (3a) and (3b) can be considered as limiting cases of a scaling form

$$C(\mathbf{r}, t) \simeq A_r r^{2\zeta} F(St/r^z) \tag{4}$$

where $z = \zeta/\beta$ and S is a scaling factor related to A_r and A_t.

For the KPZ equation in $(1+1)$ dimensions (one-dimensional surface moving in a two-dimensional space) with an uncorrelated Gaussian noise η, the exponents $\zeta = \frac{1}{2}$ and $\beta = \frac{1}{3}$ are known to be exact.[2,13] Recently, Hwa and Frey[3] showed that, by choosing $S = |\lambda| A_r^{1/2}$, the scaling function $F(\tau)$ in (4) becomes universal. A mode-coupling calculation by Hwa and Frey yielded a numerically determined scaling function $F(\tau)$ which has the limiting behavior $F(\tau) \simeq 0.69\tau^{2/3}$ at large τ. Thus, according to their calculation, there is a universal relationship between the two scaling amplitudes A_r and A_t and the nonlinear parameter λ,

$$A_t = 0.69\, |\lambda|^{2/3} A_r^{4/3} \tag{5}$$

The analysis of Hwa and Frey differs from a number of previous studies,[4] which treat the nonlinear term in (1) perturbatively. The suggestion by Hwa and Frey that the closed set of mode-coupling equations[5] is exact is intriguing from a theoretical point of view. In this paper I present high-precision Monte Carlo data on the single-step model[6] with sublattice updating. The parameters A_r and λ for this lattice model have been calculated exactly.[7] For two different sets of these parameters, the same ratio $R = A_t/(|\lambda|^{2/3} A_r^{4/3}) = 0.725 \pm 0.005$ is obtained. I also present an empirical expression for the scaling function F which fits well with simulation data.

The single-step model in $(1+1)$ dimensions can be described in terms of a surface oriented diagonally on a two-dimensional square lattice.[6] The surface at a given instant can be specified by a set of column heights $\{h_i\}$, $i = 1, \ldots, L$, with the "single-step" constraint $h_{i+1} - h_i = \pm 1$. In a sublattice

updating scheme, one first examines heights of all odd columns. At a local minimum of the surface $h_i = h_{i-1} - 1 = h_{i+1} - 1$, a growth event $h_i \to h_i + 2$ takes place with a probability p^+. At a local maximum, $h_i = h_{i-1} + 1 = h_{i+1} + 1$, an evaporation event $h_i \to h_i - 2$ takes place with a probability p^-. After this is done, the same growth and evaporation rules are applied to all even columns. This completes one time step. The nature of the growth rules allows for simultaneous updating of heights on a given sublattice. Periodic boundary conditions $h_{i+L} = h_i$ are assumed throughout.

It is well known that the single-step model can be mapped to a one-dimensional lattice-gas model with single-particle occupancy and nearest-neighbor hopping.[6] The occupation number of a cell i is simply given by $\sigma_i = (h_i - h_{i-1} + 1)/2$. A growth (evaporation) event corresponds to a particle hopping to the empty cell on its left (right). It has been shown that, for a system of size L with a fixed number of particles N, the steady-state probability distribution of the lattice-gas problem at the completion of each updating cycle has the following factorized form:

$$P(\{\sigma_i\}) = \left[\frac{1-p^+}{1-p^-}\right]^{N_1} \tag{6}$$

where $N_1 = \sum_{i=1}^{L/2} \sigma_{2i-1}$ is the total number of particles in cells with odd indices.[7] In ref. 7 exact expressions for A_r and λ have been obtained from this distribution. In the case $N = L/2$, which corresponds to a surface oriented along the diagonal of the square lattice, we have

$$A_r = \frac{4[(1-p^-)(1-p^+)]^{1/2}}{2-p^+-p^-+2[(1-p^+)(1-p^-)]^{1/2}} \tag{7a}$$

$$\lambda = -(p^+-p^-)/[(1-p^+)(1-p^-)]^{1/2} \tag{7b}$$

Due to the diverging relaxation time $\tau \sim L^z$ with the system size L, it is usually difficult to simulate the steady-state behavior of a large system. In our case, since the steady-state distribution function factorizes, we can circumvent this problem by generating typical steady-state configurations according to (6). Specifically, for a given p^+ and p^-, we compute the average occupancy of odd cells,

$$\frac{2N_1}{L} = \frac{2[(1-p^-)(1-p^+)]^{1/2}}{2-2p^-+2[(1-p^+)(1-p^-)]^{1/2}} \tag{8}$$

For the typical configuration, we assume that exactly N_1 [as determined from (8)] particles are in the odd cells, and the remaining $N_2 = \frac{1}{2}L - N_1$ particles are in the even cells. These N_1 (N_2) particles are then randomly

distributed among the odd (even) cells in the following way. Each time we randomly pick up one of the odd (even) cells. Repeat the process if necessary until an empty cell has been found. Fill the cell with a particle. We then look for the next empty cell and fill it with a particle until all N_1 (N_2) particles are put into the cells. This configuration serves as the initial configuration for our growth simulation.

I have simulated the model at a fixed $p^+ = 1/2$ and three different values of p^-, 0, 1/8, and 1/2. Using a multisite coding algorithm,[8] simulation of a $L = 2^{20} \simeq 10^6$ system can be readily carried out. Although not necessary, I typically equilibrate the system over a period of about 1000 Monte Carlo steps before taking the data. The particle configuration after every 1024 Monte Carlo steps is recorded and then compared with configurations that follow at intervals $t = 1, 2, 4, \ldots, 1024$ to determine $C(r, t)$ as defined by (2) and averaged over r_0. [The choice of exponentially increasing time intervals enables us to examine both the small- and large-time behavior of the correlation function without significantly increasing the computation time needed to take the data. Furthermore, since the dominant contribution to $C(0, t)$ comes from large-wavelength fluctuations whose correlation (or relaxation) time increases algebraically with t, we expect that taking data more frequently will not significantly reduce the effect of statistical errors on the analysis presented below.] The data presented below are obtained from averages over 35 such repeated runs at $p^- = 0$; 24 runs at $p^- = 1/8$; and 20 runs at $p^- = 1/2$. The total amount of CPU time for the $p^- = 0$ simulation is about 200 min on an IBM3090 machine without vector facility. The $p^- = 1/8$ simulation took twice as long to complete due to the more complicated procedure for generating the random bits.

Table I contains data for $C(0, t)$ from the simulation. Statistical errors generally increase with increasing t, but are less than 0.5% in all cases. The case $p^- = p^+ = 1/2$ is known to be described by (1) with $\lambda = 0$. The exponents for the linear equation[9] are given by $\zeta = 1/2$ and $\beta = 1/4$. There is also an exact relation[10] between the scaling amplitudes in this case, $A_t/A_r = 2(v/\pi)^{1/2}$. The simulation data given in Table I at $p^- = 1/2$ are in excellent agreement with the formula $C(0, t) = 2(vt/\pi)^{1/2}$ using the exact value $v = 1$ obtained by Kandel *et al.*[11] and $A_r = 1$ from (7a).

For $p^- = 0$ the data at $t \geqslant 2$ fit well to the expression

$$C(0, t) = A_t t^{2/3} + C_0 - C_1 t^{-1/3} \tag{9}$$

with $A_t = 0.533$, $C_0 = 0.24$, and $C_1 = 0.2$. Using the values $A_r = 4\sqrt{2}/(3 + 2\sqrt{2}) = 0.97056\ldots$ and $\lambda = -1/\sqrt{2} = -0.7071\ldots$ given by (7), we obtain

$$R = A_t/(|\lambda|^{2/3} A_r^{4/3}) = 0.725 \tag{10}$$

Table I. Data for $C(0, t)$ at $p^+ = 1/2$ and Three Different Values of p^-

t	$p^- = 0$	$p^- = 1/8$	$p^- = 1/2$
0	0	0	0
1	0.568	0.664	1.001
2	0.960	1.060	1.501
4	1.515	1.611	2.187
8	2.358	2.421	3.144
16	3.673	3.642	4.477
32	5.748	5.516	6.358
64	9.042	8.436	9.002
128	14.25	12.99	12.73
256	22.52	20.21	18.04
512	35.62	31.63	25.53
1024	56.40	49.71	36.17

In the case $p^- = 1/8$, data at $t \geqslant 8$ can again be fitted to (9) with another set of parameters $A_t = 0.481$, $C_0 = 0.95$, and $C_1 = 0.9$. The ratio $R = 0.721$ in this case is consistent with (10) in view of the 0.5% statistical errors of the data. Figure 1 shows the data (scaled) in the two cases as compared to (9) using the values for A_t, C_0, and C_1 given above. The linear behavior of each data set with respect to $t^{-2/3}$ at large t indicates that the leading-order correction to scaling is a constant[12] (see also the review by Wolf[13]). A somewhat higher value for A_t would be obtained if no correction to

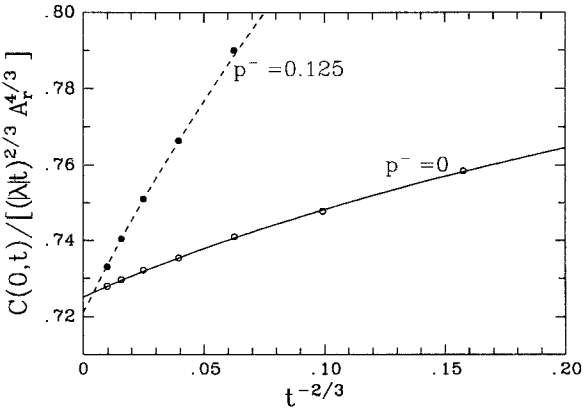

Fig. 1. Scaled data for $C(0, t)$ against $t^{-2/3}$ at $p^- = 0$ (open circles) and $p^- = 1/8$ (solid circles). Solid and dashed lines are calculated according to Eq. (9) using parameter values given in the text.

scaling were taken into account. We thus conclude that the simulation data support a universal value 0.725 ± 0.005 for the ratio $A_t/(|\lambda|^{2/3} A_r^{4/3})$.

Finally, I present the simulation data for $C(r, t)$ at $r = 2, 4, 8, ..., 512$ and $p^- = 0$ and 1/8. For $t = 0$ the data in both cases are in very good agreement with the exact expression $C(r, 0) = A_r r$ obtained from (6) for an even integer r. Figures 2a and 2b are scaling plots of the data according to the scaling form (4) without taking corrections to scaling into account. The

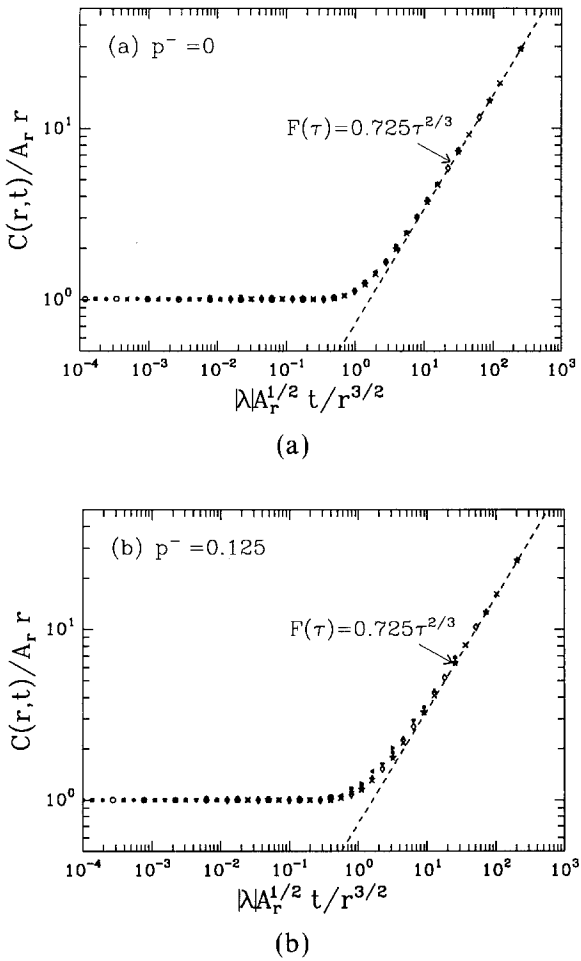

Fig. 2. Scaling plot of the steady-state height–height correlation function $C(r, t)$ using exact values for A_r and λ. (a) $p^- = 0$; (b) $p^- = 1/8$. The same plotting symbol is used for data at a given t.

same plotting symbol is used for data at a given t but different r. The two data-collapsing curves agree well with each other, and agree with the limiting form $F(\tau)=0.725\tau^{2/3}$ at large τ as determined above. In the case $p^-=1/8$, there are noticeable deviations from the universal curve for data at small r, which can be attributed to the correction-to-scaling terms as in Eq. (9).

To obtain an analytical representation of the scaling function, I have analyzed the scaling curve for $p^-=0$ in two limiting cases. At large τ, the correction to $F(\tau)=0.725\tau^{2/3}$ is of the form $\tau^{-2/3}$. For small τ, $F(\tau)-1$ approaches 0 as an exponential function of $\tau^{-2/3}$. A good empirical form for $F(\tau)$ which fits the data is given by

$$F(\tau)=\begin{cases}1+3e^{-3.15\tau^{-2/3}} & \text{for} \quad \tau<\tau_0 \\ 0.725\tau^{2/3}+0.4\tau^{-2/3} & \text{for} \quad \tau\geqslant\tau_0\end{cases} \tag{11}$$

Figure 3 shows the scaled data for $p^-=0$ as compared to (11) in the region around $\tau_0\simeq 2.3$. The agreement is satisfactory.

To summarize, the steady-state height–height correlation function for the single-step model is obtained via Monte Carlo simulation of a large system. Analysis of the data at two different values of the evaporation rate p^- yields a universal amplitude ratio $A_t/(|\lambda|^{2/3}A_r^{4/3})=0.725\pm 0.005$. This number is close to the value 0.58 obtained by Hwa and Frey via numerical solution of exact mode-coupling equations. An empirical form for the scaling function is also given.

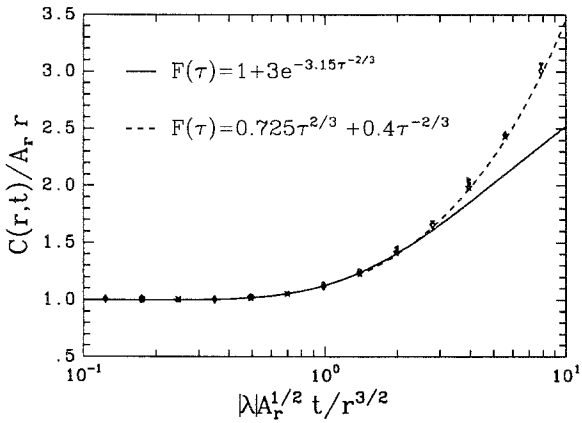

Fig. 3. Scaled data for $p^-=0$ as compared to the analytic expression (11).

ACKNOWLEDGMENTS

I am indebted to Bruce Forrest and Dietrich Wolf for teaching me the multisite coding technique, Erwin Frey for an informative discussion, and Dietrich Stauffer for many helpful suggestions on presentation. I would also like to thank the Institut für Festkörperforschung des Forschungszentrums Jülich for hospitality, where part of the work was carried out. Upon completion of this work I received a preprint by J. G. Amar and F. Family where a value 0.71 for the amplitude ratio was reported.

REFERENCES

1. M. Kardar, G. Parisi, and Y.-C. Zhang, *Phys. Rev. Lett.* **56**:889 (1986).
2. J. Krug and H. Spohn, in *Solids far from Equilibrium: Growth, Morphology and Defects*, C. Godrèche, ed. (Cambridge University Press, Cambridge, 1991); see also F. Family and T. Vicsek, eds., *Dynamics of Fractal Surfaces* (World Scientific, Singapore, 1991).
3. T. Hwa and E. Frey, *Phys. Rev. A* **44**:R7873 (1991).
4. D. Forster, D. R. Nelson, and M. J. Stephen, *Phys. Rev. A* **16**:732 (1977); M. Kardar and Y.-C. Zhang, *Phys. Rev. Lett.* **58**:2087 (1987); E. Medina, T. Hwa, M. Kardar, and Y.-C. Zhang, *Phys. Rev. A* **39**:3053 (1989); L.-H. Tang, T. Nattermann, and B. M. Forrest, *Phys. Rev. Lett.* **65**:2422 (1990).
5. H. van Beijeren, R. Kutner, and H. Spohn, *Phys. Rev. Lett.* **54**:2026 (1985); H. K. Janssen, and B. Schmittmann, *Z. Phys. B* **63**:517 (1986).
6. P. Meakin, P. Ramanlal, L. M. Sander, and R. C. Ball, *Phys. Rev. A* **34**:5091 (1986); M. Plischke, Z. Rácz, and D. Liu, *Phys. Rev. B* **35**:3485 (1987).
7. L.-H. Tang, B. M. Forrest, and D. E. Wolf, *Phys. Rev. A*, in press.
8. B. M. Forrest and L.-H. Tang, *J. Stat. Phys.* **60**:181 (1990).
9. P. G. de Gennes, *Faraday Symp.* **1971**(5):61.
10. T. Nattermann and L.-H. Tang, *Phys. Rev. A*, in press.
11. D. Kandel, E. Domany, and B. Nienhuis, *J. Phys. A* **23**:L755 (1990).
12. D. E. Wolf and J. Kertész, *Europhys. Lett.* **4**:561 (1987).
13. D. E. Wolf, in *Kinetics of Ordering and Growth at Surfaces*, M. Lagally, ed. (Plenum Press, New York, 1990).