

Mapping of (2+1)-dimensional Kardar-Parisi-Zhang growth onto a driven lattice gas model of dimers

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We show that a (2+1)-dimensional discrete surface growth model exhibiting Kardar-Parisi-Zhang (KPZ) class scaling can be mapped onto a two-dimensional conserved lattice gas model of directed dimers. The KPZ height anisotropy in the surface model corresponds to a driven diffusive motion of the lattice gas dimers. We confirm by numerical simulations that the scaling exponents of the dimer model are in agreement with those of the (2+1)-dimensional KPZ class. This opens up the possibility of analyzing growth models via reaction-diffusion models, which allow much more efficient computer simulations.

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I. INTRODUCTION

The Kardar-Parisi-Zhang (KPZ) equation [1] motivated by experimentally observed kinetic roughening has been the subject of a large number of theoretical studies [2,3]. Later it was found to model other important physical phenomena such as randomly stirred fluids [4], dissipative transport [5,6], directed polymers [7], and the magnetic flux lines in superconductors [8]. It is a nonlinear stochastic differential equation, which describes the dynamics of growth processes in the thermodynamic limit specified by the height function $h(\mathbf{x}, t)$,

$$\partial_t h(\mathbf{x}, t) = v + \sigma \nabla^2 h(\mathbf{x}, t) + \lambda [\nabla h(\mathbf{x}, t)]^2 + \eta(\mathbf{x}, t). \quad (1)$$

Here v and λ are the amplitudes of the mean and local growth velocity, σ is a smoothing surface tension coefficient, and η roughens the surface by a zero-average Gaussian noise field exhibiting the variance

$$\langle \eta(\mathbf{x}, t) \eta(\mathbf{x}', t') \rangle = 2D \delta^d(\mathbf{x} - \mathbf{x}') (t - t'). \quad (2)$$

Here d is used for the dimension of the surface, D for the noise amplitude, and $\langle \rangle$ denotes the average over the noise distribution. In 1+1 dimensions the equation is exactly solvable [7], but in higher dimensions only approximations are available (see [9]). In $d > 1$ spatial dimensions, due to the competition of roughening and smoothing terms, models described by the KPZ equation exhibit a roughening phase transition between a weak-coupling regime ($\lambda < \lambda_c$), governed by the $\lambda = 0$ Edwards-Wilkinson fixed point [10], and a strong-coupling phase. The strong-coupling fixed point is inaccessible by the perturbative renormalization method. Therefore the KPZ phase space has been the subject of controversies, and the value of the upper critical dimension has been debated for a long time. Very recently, nonperturbative renormalization and mode coupling theory has revealed a rich phase diagram, with more than one line of fixed point solutions in the d - λ space [11]. This suggests an upper critical dimension $d_c = 4$ for the KPZ model, but earlier numerical work [12] does not support this claim.

In one dimension (1D) a discrete, restricted solid-on-solid realization of KPZ growth is equivalent to the asymmetric

simple exclusion process (ASEP) of particles [13,14] (see Fig. 1). In this discrete so-called “roof-top” model the heights are quantized and the local derivatives can take the values $\Delta h = \pm 1$. By considering the up derivatives ($\Delta h = 1$) as particles and the down ones as holes, the roughening dynamics can be mapped onto a driven diffusive system of particles with single site occupancy. The ASEP model, on the other hand, is well known and its scaling properties have been explored (for a recent review see [15]).

The extension of this kind of lattice gas analogy to higher dimensions has not been considered to our knowledge. Instead, hypercube stacking models were constructed [14,16,17] and surface configurations were mapped onto the d -state Potts spins defined on the substrate lattice itself. In particular, (2+1)-dimensional surfaces were shown to be related to the six-vertex model with equal vertex energies [18] and to the ground-state configurations of the anisotropic Ising model defined on the triangular lattice [19]. As a consequence the height-height correlation functions can be related to four-spin-correlation functions of the spin system. Very recently the conformal invariance of the isoheight lines has also been pointed out [20].

Here we show that a (2+1)-dimensional growth model exhibiting KPZ scaling can also be mapped onto a driven lattice gas. This is important from a theoretical point of view, because the scaling behavior of driven diffusive systems (DDSs) has been studied intensively for a long time (for a review, see Ref. [21]); thus results for DDSs may be exploited to understand the KPZ model better, and vice versa [22]. Furthermore, this conserved lattice gas and its generali-

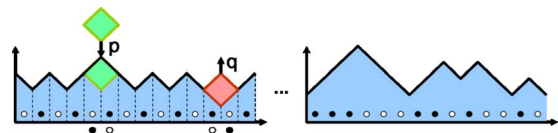


FIG. 1. (Color online) Mapping of the (1+1)-dimensional surface growth onto the 1D ASEP model. Surface attachment (with probability p) and detachment (with probability q) correspond to anisotropic diffusion of particles (bullets) along the 1D base space.

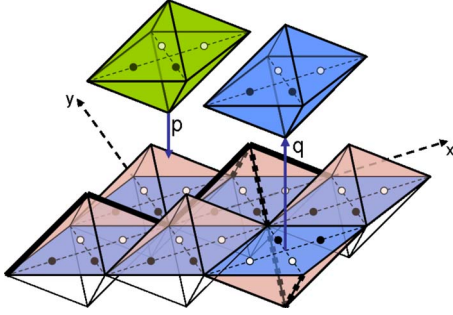


FIG. 2. (Color online) Mapping of the (2+1)-dimensional surface growth onto the 2D particle model (bullets). Surface attachment (with probability p) and detachment (with probability q) correspond to Kawasaki exchanges of particles, or to anisotropic diffusion of dimers in the bisectrix direction of the x and y axes. The crossing points of dashed lines show the base sublattice to be updated. Thick solid (dashed) lines on the surface show the x (y) cross sections, corresponding to the 1D model (Fig. 1).

zations with anisotropies, disorder, or higher-order terms can be studied effectively by bit-coded algorithms, for example.

II. MAPPING ONTO LATTICE GAS IN TWO DIMENSIONS

As a generalization of the (1+1)-dimensional roof-top model, where the building blocks are squares, let us put octahedra on the square lattice, such that we get back the (1+1)-dimensional model in the x or y direction as shown in Fig. 2. Surface adsorption or desorption events correspond to attachment or detachment of octahedra, respectively. The surface built up from the octahedra can be described by the edges meeting at the up (down) middle vertices. The up edges in the x or y directions are represented by $+1$'s, and the down ones by -1 's in the model. In this way a single site deposition flips the four edges and means two $+1 \leftrightarrow -1$ (Kawasaki) exchanges: one in the x and one in the y direction. This can also be understood as a special 2D cellular automaton [23] with the generalized Kawasaki updating rules

$$\begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} \rightleftharpoons \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \quad (3)$$

with probability p for attachment and probability q for detachment. We can also call the $+1$'s particles and the -1 's holes of the base square lattice. In this way an attachment (detachment) update can be mapped onto a single step motion of an oriented dimer in the bisectrix direction of the x and y axes. To make a one-to-one mapping, we update the neighborhood of sublattice points, which are denoted by the crossing points of the dashed lines only.

Since the three-dimensional space cannot be filled fully by octahedra, holes can occur among them, below the surface. Therefore this approximation of a surface growth may not sound faithful and the validity of KPZ growth rules requires confirmation. Note, however, that in reality atoms are not cubes either and do not tile the three-dimensional space completely. Furthermore, very recently in bidisperse ballistic deposition models [24,25], in which under-surface vacancies

may occur, KPZ scaling has been reported as well.

The deterministic part of the KPZ equation (1), which can be obtained by averaging over the noise, can be derived from the surface-dimer model similarly as was done in the 1+1 dimension [13]. If we apply the transformation

$$\mathbf{v}(\mathbf{x}, t) = \nabla h(\mathbf{x}, t), \quad (4)$$

we get the Burgers' equation for the height profile

$$\partial_t \mathbf{v}(\mathbf{x}, t) = \sigma \nabla^2 \mathbf{v}(\mathbf{x}, t) + \lambda \mathbf{v}(\mathbf{x}, t) \nabla \mathbf{v}(\mathbf{x}, t). \quad (5)$$

Our system is represented by two matrices Δ_x and Δ_y of sizes $L \times L$, which contain discrete derivatives $+1$ or -1 in the x and y directions, respectively [see Eqs. (10) and (11)]. In two dimensions we introduce the vector variable $\bar{\sigma}_{i,j} = (\Delta_x(i-1, j), \Delta_y(i, j-1))$. This has the value $(1, 1)$ in the case of a dimer and $(-1, -1)$ for a pair of holes. By setting up the master equation

$$\partial_t P(\{\bar{\sigma}\}, t) = \sum_{i,j} w'_{i,j}(\{\bar{\sigma}\}) P(\{\bar{\sigma}\}, t) - \sum_{i,j} w_{i,j}(\{\bar{\sigma}\}) P(\{\bar{\sigma}\}, t) \quad (6)$$

for the probability distribution $P(\{\bar{\sigma}\}, t)$, where the prime denotes a state resulting from a generalized Kawasaki flip (3), the transition probability is given by

$$w_{i,j}(\{\bar{\sigma}\}) = \frac{1}{8} \left(2 - \bar{\sigma}_{i+1,j+1} \bar{\sigma}_{i,j} + \lambda (\bar{\sigma}_{i+1,j+1} - \bar{\sigma}_{i,j}) - \frac{(1-\lambda)}{2} (\bar{\sigma}_{i+1,j+1} \times \bar{\sigma}_{i,j})^2 \right), \quad (7)$$

with $\lambda = 2p/(p+q) - 1$ parametrization. This formally looks like the one-dimensional Kawasaki exchange probability (shown in [13]), except for the cross-product term, which is necessary to avoid surface discontinuity creation. The cross product as a determinant cancels updates between configurations such as $(1, 1) \rightarrow (1, -1)$. The nonlinear term vanishes for $p=q$ ($\lambda=0$). The sign of the coefficient λ of the nonlinear term can be interpreted as follows. For $p > q$ positive nonlinearity (positive excess velocity) it is a consequence of growth with voids.

To obtain Eq. (5) first one averages over the slope vectors

$$\langle \bar{\sigma}_{i,j} \rangle = \sum_{\{\bar{\sigma}\}} \bar{\sigma}_{i,j} P(\{\bar{\sigma}\}, t). \quad (8)$$

Then, by calculating its time derivative using the master equation, the cross-product term drops out and one obtains

$$2\partial_t \langle \bar{\sigma}_{i,j} \rangle = \langle \bar{\sigma}_{i-1,j-1} \rangle - 2\langle \bar{\sigma}_{i,j} \rangle + \langle \bar{\sigma}_{i+1,j+1} \rangle + \lambda \langle \bar{\sigma}_{i,j} (\bar{\sigma}_{i+1,j+1} - \bar{\sigma}_{i-1,j-1}) \rangle. \quad (9)$$

Here one can see the discrete second and first differentials of $\bar{\sigma}_{i,j}$ corresponding to the operators of (5). These differentials are one dimensional because the dimer dynamics is also one dimensional. Making a continuum limit in both directions and taking into account the relation of height and slope variables (4), we can arrive at the deterministic part of the KPZ equation (1).

This agreement does not prove the equivalence of the KPZ and the dimer models, since they are just the first equa-

tions in the hierarchy of equations for correlation functions. On the other hand, from the universal scaling point of view they show the equivalence of the leading order terms. We will show by numerical simulation that our mapping is faithful and reproduces the KPZ class surface growth behavior.

III. THE SIMULATION ALGORITHM

In the algorithm we extend the sequence of discrete slopes of the 1D ASEP model (Fig. 1) to local derivatives at (i,j) sites in x and y directions of the surface (see Fig. 2). The initially flat surface is presented as a regular sequence of +1's and -1's within both matrices. Periodic boundary conditions are applied to the x and y directions. The system's evolution is simulated as follows.

A site (i,j) on the substrate plane is selected randomly. Then, we choose an attachment or detachment attempt according to their probabilities p and q . Generalized Kawasaki exchanges (3) of attachment or detachment are realized if

$$\begin{pmatrix} \Delta_x(i-1,j) & \Delta_x(i,j) \\ \Delta_y(i,j-1) & \Delta_y(i,j) \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ -1 & 1 \end{pmatrix} \quad (10)$$

or

$$\begin{pmatrix} \Delta_x(i-1,j) & \Delta_x(i,j) \\ \Delta_y(i,j-1) & \Delta_y(i,j) \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix}, \quad (11)$$

respectively. Throughout this paper the time is measured by Monte Carlo steps (MCSs), i.e., $L \times L$ jump attempts correspond to one MCS. After certain time intervals data evaluation requires the reconstruction of the surface heights $h_{x,y}(t)$ by summing up the sequence of local slopes Δ_x, Δ_y .

IV. RESULTS

Starting from a periodic, vertically striped particle distribution, which corresponds to a flat initial surface, we update the particle model by the rules defined in the previous section. At certain time steps we calculate the $h_{x,y}(t)$ heights from the height differences $\Delta_{x,y}$. The morphology of a growing surface is usually characterized by its width,

$$W(L,t) = \left[\frac{1}{L^2} \sum_{x,y} h_{x,y}^2(t) - \left(\frac{1}{L^2} \sum_{x,y} h_{x,y}(t) \right)^2 \right]^{1/2}. \quad (12)$$

In the absence of any characteristic length, growth processes are expected to show power-law behavior of the correlation functions in space and height, and the surface is described by the Family-Vicsek scaling [26]

$$W(L,t) \propto \begin{cases} t^\beta & \text{for } t_0 \ll t \ll t_s, \\ L^\alpha & \text{for } t \gg t_s. \end{cases} \quad (13)$$

Here α is the roughness exponent and characterizes the deviation from a flat surface in the stationary regime ($t \gg t_s$) in which the correlation length has exceeded the linear system size L and β is the surface growth exponent, which describes the time evolution for earlier (nonmicroscopic $t \gg t_0$) times. The dynamical exponent z can be expressed by the ratio

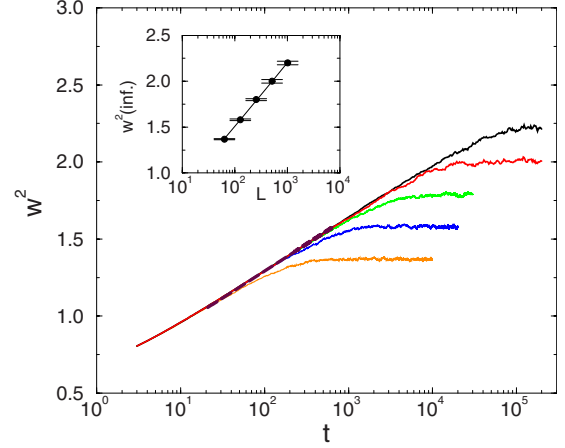


FIG. 3. (Color online) Logarithmic surface growth in the case of up-down symmetry for different sizes $L=64, 128, 256, 512, 1024$ (bottom to top). The dashed line shows the fitting with the form (16). Inset: width saturation values for different system sizes L in the long-time limit.

$$z = \alpha/\beta. \quad (15)$$

In the case of up-down symmetry ($p=1, q=1$) the nonlinear term is dropped, and the KPZ equation (1) simplifies to the Edwards-Wilkinson (EW) equation [10]. Since the upper critical dimension of this equation is $d_c=2$, mean-field behavior, characterized by $\alpha=\beta=0$ and logarithmic scaling, is expected by field theory. Indeed, the width of the surface grows as

$$W^2(t) = a \ln(t) + b, \quad (16)$$

as shown in Fig. 3. The prefactor a obtained by fitting the $L=1024$ curve in the $20 < t < 1000$ region with the form (16) is $a=0.152(8)$. This is in agreement with the theoretical estimate for the EW equation $D/(4\pi\sigma)$ [27] if we take into account the exact value for the stiffness constant (or surface tension) $\bar{\sigma}/D=\pi/9$. This constant was identified in [19] through the correspondence between the exact calculation of the four-spin correlation function of the zero-temperature triangular Ising antiferromagnet [28] and the discrete height-height correlation function in real space in the interface model. The factor $\bar{\sigma}=2/3\sigma$ is coming from the $2/\sqrt{3}$ triangular lattice site per surface element and the $1/\sqrt{3}$ of the octahedron vs cube surface fraction; thus the theoretical estimate is $a \approx 0.151981$.

The saturation values are expected to exhibit logarithmic growth,

$$W^2(\text{inf}) = \lim_{t \rightarrow \infty} W^2(t) = c \ln(L) + d, \quad (17)$$

with the system size [27]. As can be seen in the inset of Fig. 3 this really happens with the prefactor $c=0.30(1)$, which agrees with the theoretical value $c=2a \approx 0.304$ again.

For pure deposition $p=1, q=0$, or in the case of other general up-down asymmetric cases, we saw power-law increase of the surface width, in agreement with the scaling hypothesis (13) (see Fig. 4). For the largest system that we have investigated ($L=1024$), we fitted $W(t)$ in the $100 < t$

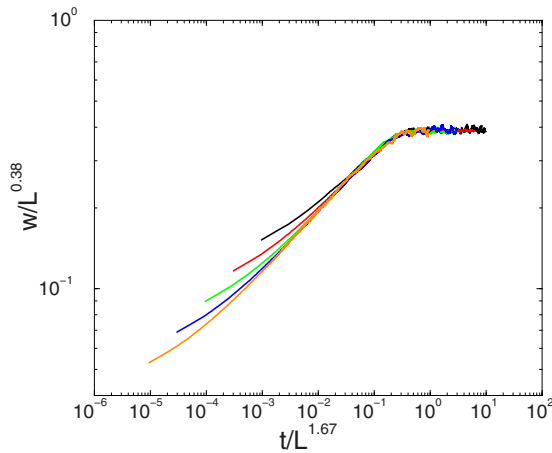


FIG. 4. (Color online) Scaling collapse for $p=1, q=0$ with $(2+1)$ -dimensional KPZ class exponents for different sizes $L = 64, 128, 256, 512, 1024$ (bottom to top).

$< 10\,000$ time window with a power law and obtained $\beta = 0.23(1)$. This value agrees quite well with the numerical estimate for the $(2+1)$ -dimensional KPZ class ($\beta=0.24$) provided in Ref. [9]. Note, however, that for smaller system sizes the exponent estimate is somewhat smaller, due to corrections to scaling, but one can clearly see a convergence toward higher values and a better collapse as $L \rightarrow \infty$. Large-scale simulations with an effective, bit-coded version of our algorithm could result in very precise estimates. The systematic tendency toward an asymptotic behavior has been found in Fig. 4.

The saturation values $W(\text{inf})$ for different system sizes also scale well with (14) and with the exponent $\alpha=0.38(1)$ of the $(2+1)$ -dimensional KPZ class [9,29]. Assuming corrections to scaling of the form $W \approx A_2 L^\alpha (1 + B_2 L^{-\omega})$, the fitting to our data resulted in a very small effect, $\alpha=0.377(15)$, which marginally overlaps with the value of [29] but does not support the proposal $\alpha=2/5$ of [30]. Using these surface exponents and the scaling law (15) we estimated the dynamical exponent to be $z=1.64(1)$, which is somewhat greater than what was found for the $(2+1)$ -dimensional KPZ class in [9] ($z=1.58$). We think that this is due to the correction to scaling observed in the time dependence discussed above. If we scale the time with the dynamical exponent $z=1.64$, we obtain a good scaling collapse of the growth data for different sizes (Fig. 4) in agreement with the (13), (14) law again. Our exponent estimates also satisfy the $\alpha+z=2$ scaling relation within the error margin. This implies that Galilean invariance holds and the lattice model indeed lies in the $(2+1)$ -dimensional KPZ universality class.

V. CONCLUSIONS AND OUTLOOK

We have pointed out the possibility of mapping a discrete surface growth process onto a conserved, driven lattice gas

model of oriented dimers, which move perpendicularly in two dimensions. The straight line motion of dimers in the two-dimensional space is very similar to the motion of particles of the ASEP process. The difference is that, since the dimers are extended objects, their motion is slowed down by dimer particle exclusion and the sublattice update as compared to the single particles of the ASEP. As a consequence their motion is described by a somewhat larger dynamical exponent ($z \approx 1.64$) than that of the ASEP ($z=3/2$), so the change of $z(d)$ seems to be a purely topological phenomenon in KPZ. This provides a better understanding of the relation of universality classes of surface classes to those of the reaction-diffusion models [31–33]. Interestingly the x - y symmetric surface dynamics maps onto a strongly anisotropic reaction-diffusion model.

We have found KPZ or EW scaling by numerical simulations; hence we showed that lattice anisotropy and under-surface vacancies are irrelevant. Our simulation results for the $(2+1)$ -dimensional EW case reproduced the theoretically expected logarithmic scaling, with the correct leading order coefficients. For the KPZ scaling, our roughness exponent result is in the middle of the range obtained by various numerical exponent estimates: i.e., between $\alpha=0.36$ [34,35] and the field theoretical value $\alpha=0.4$ [30]. Our $\alpha=0.377(15)$ coincides with that of the numerical study [36] and agrees with the renormalization result $\alpha=0.38$ [37]. It overlaps marginally with the simulation result $\alpha=0.393(3)$ [29] as well. Our growth exponent estimate $\beta=0.23(1)$ matches the results of [34] [$\beta=0.221(2)$] and [36] [$\beta=0.229(5)$], obtained by independent numerical fitting procedures. The dynamical exponent of this study is also in the range provided in [36].

Our model provides an efficient way of simulation and opens the possibility of studying more complex growth models relevant for the recent interest in self-organizing surface nanosystems [38]. An optimized, bit-coded version of our code, which manipulates the two-dimensional bit field by logical operations, runs roughly ten times faster than the current version and will be presented elsewhere. For example, the Bradley-Harper [39] and the debated Kuramoto-Sivashinsky [40] models with their modifications can be investigated numerically and are the subject of forthcoming presentations.

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