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Scaling of ballistic deposition from a Langevin equation

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An exact lattice Langevin equation is derived for the ballistic deposition model of surface growth. The continuum limit of this equation is dominated by the Kardar-Parisi-Zhang (KPZ) equation at all length and time scales. For a one-dimensional substrate the solution of the exact lattice Langevin equation yields the KPZ scaling exponents without any extrapolation. For a two-dimensional substrate the scaling exponents are different from those found from computer simulations. This discrepancy is discussed in relation to analytic approaches to the KPZ equation in higher dimensions.

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Surface growth is often described by idealized lattice models [1,2] in which the complex interactions between individual atoms or molecules are replaced by simple rules for the occupancies of lattice sites. If these rules generate heights whose sum (or integral) is not equal to the material deposited (e.g., because of evaporation or defect formation), one speaks of *nonconserved* surface growth. Such models are used to account for a great variety of phenomena, ranging from sputter deposition to the growth of bacterial colonies [1,2]. Arguably the most studied continuum theory for nonconserved surface growth is the Kardar–Parisi–Zhang (KPZ) equation [3],

$$\frac{\partial u}{\partial \tau} = \nu \nabla^2 u + \lambda (\nabla u)^2 + \xi, \tag{1}$$

where $u(\mathbf{x},\tau)$ is the deviation from the mean height at time τ and position $\mathbf{x}$ on a d-dimensional substrate, and $\xi(\mathbf{x},\tau)$ is a Gaussian noise with zero mean and covariance

$$\langle \xi(\mathbf{x},\tau)\xi(\mathbf{x}',\tau')\rangle = 2D\delta(\mathbf{x}-\mathbf{x}')\delta(\tau-\tau'). \tag{2}$$

Despite an extensive body of work, even basic properties of the KPZ equation, such as the scaling exponents for $d>1$ and the existence of an upper critical dimension, remain controversial [4–16].

In the absence of a generally accepted analysis of the KPZ equation for $d>1$, the theoretical investigation of nonconserved surface growth has relied largely on kinetic Monte Carlo (KMC) simulations of lattice models. A prototype model for nonconserved surface growth is ballistic deposition (BD). Originally introduced as a model for vapor deposition [17,18], BD was among the first surface growth models to be studied with KMC simulations [19]. However, the relation between BD and the KPZ equation is still not completely understood. KMC simulations for $d=1$ reveal a systematic discrepancy between the scaling properties of the KPZ equation and those of BD [20,21] that is alleviated only if the results of computer simulations are extrapolated to infinitely large system sizes [22]. Similar problems have been reported for other lattice models of nonconserved surface growth [15,16]. As a result, the universality of results obtained from KMC simulations for $d>1$ has been called into question [10,12,14,15]. The absence of a direct relation between lattice models and the KPZ equation has proven to be a major obstacle to further progress, not least because the scaling behavior inferred from KMC simulations can be masked by crossover.

In this Rapid Communication, we examine the relation between BD and the KPZ equation from a somewhat different perspective. Our discussion is based on the lattice Langevin equation [23,24] for BD. This formulation is statistically equivalent to KMC simulations and constitutes a computational alternative to such simulations [24,25]. The regularized expression of the lattice Langevin equation provides initial conditions for renormalization-group transformations, which allows a hierarchy of continuum equations to be obtained across all length and time scales. For BD, however, we find that even the microscopic equation of motion is very close to the KPZ fixed point. The direct solution of the lattice Langevin equation for BD is therefore a convenient method to investigate the scaling properties of the KPZ equation. This is demonstrated for one- and two-dimensional substrates.

In the classic BD model [17–19], a particle impinges onto a randomly chosen lattice site and irreversibly attaches to the first vertical or lateral nearest-neighbor encountered. For simplicity all calculations are illustrated for a one-dimensional substrate, but this is not an inherent limitation of our method. The updating algorithm for site i with integer height H_i at time step $t+1$ can be expressed as

$$H_i(t+1) = \max(H_{i-1}(t), H_i(t)+1, H_{i+1}(t)), \tag{3}$$

for $i=1,2,\ldots,L$, where t is defined as the number of particles deposited, $\max(x,y,z)$ yields the maximum of the three arguments, and the deposition unit has been set equal to unity. The statistical properties of the BD model are embodied by the Chapman–Kolmogorov equation [26] for the transition probability $T_{t+t'}(\mathbf{H}_3|\mathbf{H}_1)$ from height configuration $\mathbf{H}_1$ to configuration $\mathbf{H}_3$ in the time interval $t+t'$,

$$T_{t+t'}(\mathbf{H}_3|\mathbf{H}_1) = \sum_{\mathbf{H}_2} T_{t'}(\mathbf{H}_3|\mathbf{H}_2) T_t(\mathbf{H}_2|\mathbf{H}_1), \tag{4}$$

where $t=t_2-t_1$ and $t'=t_3-t_2$. Equation (4) is satisfied by all Markovian lattice models and has the master equation as a familiar limiting case [26].

The Chapman–Kolmogorov equation can be rendered more analytically tractable by carrying out a Kramers–Moyal–van Kampen expansion [23,24,26]. We identify the largeness parameter Ω governing intrinsic fluctuations [26] as the reciprocal of the deposition unit [24]. By transforming to the continuous time and height variables $\tau=\Omega^{-1}t$ and $h_i=\Omega^{-1}H_i$, we obtain, for $\Omega\to\infty$, the lattice Langevin equation [24]

$$\frac{dh_i}{d\tau} = K_i^{(1)} + \eta_i, \tag{5}$$

for $i=1,2,\ldots,L$, where $K_i^{(1)}$ is the first moment of the transition rate and the η_i are Gaussian noises that have zero mean and covariances

$$\langle \eta_i(\tau)\eta_j(\tau')\rangle = K_{ij}^{(2)}\delta(\tau-\tau), \tag{6}$$

in which $K_{ij}^{(2)}$ is the second moment of the transition rate. The transition moments are defined by

$$K_i^{(1)}(\mathbf{h}) = \int d\mathbf{r} r_i W(\mathbf{h};\mathbf{r}), \tag{7}$$

$$K_{ij}^{(2)}(\mathbf{h}) = \int d\mathbf{r} r_i r_j W(\mathbf{h};\mathbf{r}), \tag{8}$$

where $W(\mathbf{h};\mathbf{r})$ is the transition rate from $\mathbf{h}$ to $\mathbf{h}+\mathbf{r}$, and $\mathbf{r}$ is the array of jump lengths.

A limit theorem due to Kurtz [27–29] mandates that the Langevin equation (5) is statistically equivalent to the Chapman–Kolmogorov equation (4) in that the two formulations produce identical results for quantities that characterize surface morphologies. Solutions of Eq. (5) are related to the results of KMC simulations through [24]

$$\langle F(\{H_i(t)\})\rangle = \left\{ F\left[\left(H_i(0) + \int_0^t [K_i^{(1)}(\mathbf{h}(\tau)) + \eta_i(\tau)]d\tau \right) \right] \right\}, \tag{9}$$

where F is a function of the surface profile, such as the variance or the lateral height correlation. Equation (9) has been verified for several standard lattice growth models [24,25].

For the BD model, Eqs. (7) and (8) yield

$$K_i^{(1)} = w_i^{(1)} + (h_{i-1}-h_i)w_i^{(2)} + (h_{i+1}-h_i)w_i^{(3)},$$

$$K_{ij}^{(2)} = \delta_{i,j}[w_i^{(1)} + (h_{i-1}-h_i)^2 w_i^{(2)} + (h_{i+1}-h_i)^2 w_i^{(3)}], \tag{10}$$

where $\delta_{i,j}$ is the Kronecker delta, $w_i^{(1)}$ is the local transition rate for increasing h_i by one unit, and $w_i^{(2,3)}$ are the transition rates for increasing h_i to $h_{i\mp1}$:

$$w_i^{(1)} = \theta_{i,i-1}\theta_{i,i+1}, \tag{11}$$

$$w_i^{(2)} = \Theta_{i,i-1}\theta_{i,i+1} + \Theta_{i,i-1}\Theta_{i,i+1}\Theta_{i+1,i-1} + \tfrac{1}{2}\Theta_{i,i-1}\Theta_{i,i+1}\delta_{i+1,i-1}, \tag{12}$$

with $w_i^{(3)}$ obtained from $w_i^{(2)}$ by making the replacements $i\pm1\to i\mp1$. In these expressions, we use the notation $\Theta_{x,y}=1-\theta_{x,y}$, $\delta_{x,y}=\theta_{x,y}+\theta_{y,x}-1$, $\theta_{x,y}=\theta(h_x-h_y)$, and the "discrete step function" $\theta(n)$ for integer n is

$$\theta(n) = \begin{cases} 1 & \text{if } n \geqslant 0; \\ 0 & \text{if } n \leqslant -1. \end{cases} \tag{13}$$

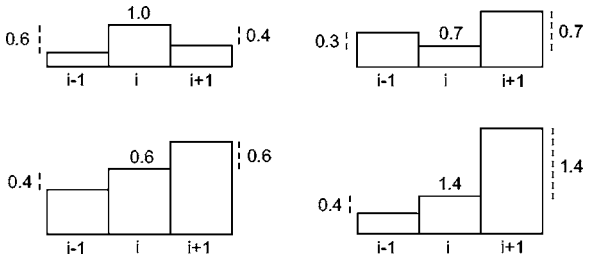

FIG. 1. Local growth rates at a randomly chosen site i for several representative configurations of the BD model using $a=0.1$ in Eq. (14). Height differences between this site and nearest-neighbor sites are shown at the sides of each configuration.

The continuation of $\theta(\Delta h)$ to the range $-1<\Delta h<0$ must be carried out such that the rules of the lattice model are faithfully generalized from discrete to continuous height variables [24]. A representation for $\theta(\Delta h)$ consistent with this criterion is [24,30]

$$\theta(\Delta h) = \frac{1}{a}[\max(\Delta h + a, 0) - \max(\Delta h, 0)], \tag{14}$$

where $a>0$. As illustrated in Fig. 1, the rules of BD are satisfied for continuous deposition events if a is infinitesimal. Operationally, we can either choose a value of a small enough to satisfy Eq. (9) to some prescribed tolerance, or take $a\to0$ after having performed the Kramers–Moyal–van Kampen expansion.

Equations (10)–(12) and (14) completely define the lattice Langevin equation (5) for BD. They can be used to derive appropriate continuum equations for any length and time scales. Our first step is to introduce the continuous space variable x and the interpolating height function $u(x,\tau)$ such that

$$h(i\pm n,\tau) = \sum_{k=0}^{\infty} \left(\frac{\partial^k u}{\partial x^k} \right) \Bigg|_{x=i} \frac{(\pm a_{\|} n)^k}{k!}, \tag{15}$$

where $a_{\|}$ is the lateral lattice constant. The discrete step function $\theta(\Delta h)$ is regularized through

$$\theta(\Delta h;\delta) = \frac{1}{2a}\int_{-\infty}^{\Delta h} \{\mathrm{erf}[(s+a)\delta] - \mathrm{erf}(s\delta)\} ds, \tag{16}$$

where $\delta>0$ and $\mathrm{erf}(x)$ is the error function. We have that $\lim_{\delta\to\infty}\theta(\Delta h;\delta)=\theta(\Delta h)$ for all real values of Δh.

The substitution of the Taylor expansions of u and θ into Eqs. (5)–(8) yields the continuum equation for the BD model. For $\delta\to\infty$, the resulting large-order differential equation retains the atomistic information of the lattice Langevin equation. Decreasing δ suppresses the coefficients of higher-order derivatives and leads to an effective lower-order differential equation. For $0<\delta\lesssim0.1$, we find for one- and two-

dimensional substrates that all terms apart from $\nabla^2 u$ and $(\nabla u)^2$ have coefficients that render them negligible. In $d=1$, the microscopic continuum equation is therefore within the domain of attraction of the KPZ fixed point, since the higher order corrections do not modify the universal scaling behavior [3]. A renormalization-group analysis for the KPZ equation is not available in $d=2$, but the fact that our regularized equation is close to this equation provides confidence that ballistic deposition follows KPZ behavior.

The foregoing considerations demonstrate that, even for small lattice sizes, the universal behavior of BD is close to that of the KPZ equation. Hence, the lattice Langevin equation (5) can be used to investigate the scaling properties of the KPZ equation without having to make any extrapolation. For the BD model, the numerical integration of Eq. (5) is achieved through the algorithm [24]

$$h_i(\tau+\Delta\tau) = h_i(\tau) + K_i^{(1)}(\mathbf{h})\Delta\tau + K_i^{(1)}(\mathbf{h})\Delta W_i(\tau), \quad (17)$$

with $\Delta W_i(\tau) = W_i(\tau+\Delta\tau) - W_i(\tau)$, where $\langle \Delta W_i(\tau)\rangle = 0$, $\langle [\Delta w_i(\tau)]^2\rangle = \Delta\tau$, and $K_i^{(1)}$ is defined in Eq. (10). We have used $\Delta\tau = 1/10$ for $d=1$ and $\Delta\tau = 1/20$ for $d=2$. Such relatively small increments [24] ensure the stability of the above algorithm for our model, but the numerical integration in Eq. (17) takes considerably longer than the corresponding KMC simulations. In some cases, if only the scaling behavior in the unsaturated regime is of interest, much larger values of $\Delta\tau$ can be used [24].

Surface morphologies obtained from Eq. (17) can be characterized by the standard deviation $w(L,\tau)$ of the height profile. For many models of surface growth, including Eq. (1), $w(L,\tau)$ exhibits dynamic scaling [1,2],

$$w(L,\tau) \equiv [\langle h^2(\tau) - \langle h(\tau)\rangle^2\rangle]^{1/2} \sim L^{\alpha} f\left(\frac{\tau}{L^z}\right), \quad (18)$$

where $\langle h^n(\tau)\rangle \equiv L^{-1}\Sigma_i h_i^n(\tau)$ for $n=1,2$, the scaling function $f(x) \sim x^{\beta}$ for $x \ll 1$ and $f(x) \to$ const. for $x \gg 1$, α is the roughness exponent, z is the dynamic exponent, and $\beta = \alpha/z$ is the growth exponent. As in Ref. [16], we use measurements of the saturated interface width w_{sat} for various system sizes to estimate α, from which z can be calculated by $z = 2-\alpha$ [3].

Figure 2(a) shows values for w_{sat} obtained with Eq. (17) for $d=1$. We find $\alpha = 0.495 \pm 0.008$, in excellent agreement with the generally accepted value $\alpha = 1/2$ of the KPZ universality class [3]. This validates our previous suggestion [25] that, even for small system sizes, the universal behavior of BD is very well described by the KPZ equation. KMC simulations of BD, on the other hand, generally find smaller values of α before extrapolation (see Table I). This apparent disagreement between the lattice Langevin equation and KMC simulations comes as a surprise: On basis of Kurtz's theorems [27–29] and results for other conserved [24] and nonconserved [25] lattice models the two formulations are expected to yield statistically equivalent surface morphologies in the sense of Eq. (9). A possible explanation for the discrepancy is the previous demonstration [20,21] that KMC simulations of BD couple strongly to correlations in pseudorandom number generators. For the lattice Langevin equation, Eq. (10) indicates that the noise can vary at each lattice site, so this representation does not suffer from such problems by allowing a greater exploration of configuration space.

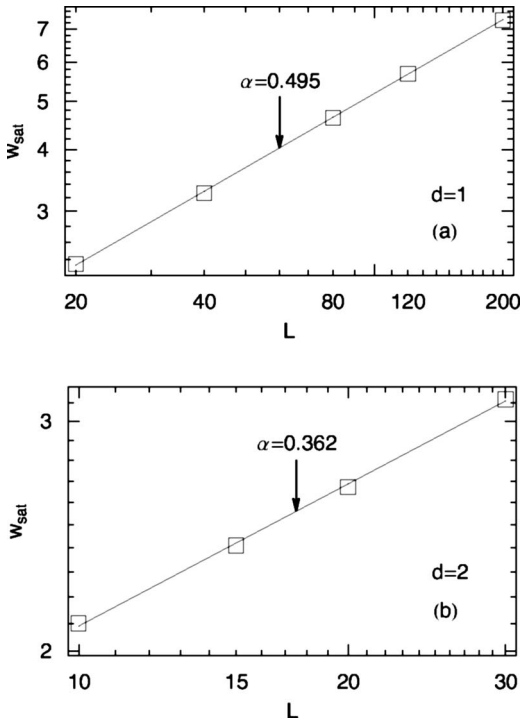

FIG. 2. The saturated interface width w_{sat} obtained from Eq. (17) for BD versus the linear system size L for (a) $d=1$ and (b) $d=2$. The error bars associated with the data points are smaller than the symbol size. The lines with slope $\alpha=0.495$ in (a) and $\alpha=0.362$ in (b) are optimal fits.

Figure 2(b) shows our results for BD onto two-dimensional substrates. As for $d=1$ the continuum limit of the lattice Langevin equation for $d=2$ is the KPZ equation (1) even before any renormalization-group transformations are carried out. Hence, our results for $d=2$ directly reflect the properties of the KPZ equation without any substantial corrections to scaling due to higher-order terms. From the data displayed in Fig. 2(b), we obtain the value $\alpha = 0.362 \pm 0.015$. As summarized in Table I extensive KMC simulations carried out recently [15,16] have yielded larger values. However, simulations [35] that only consider data for which the probability distribution of local height differences is stationary find a value of α close to our result.

Recently there have been some promising analytic attempts [10–14] at characterizing the behavior of the KPZ equation for $d>1$. Field-theoretic methods [12] have been used to calculate the value $\alpha = 2/5$ for $d=2$. On the other hand, the mode-coupling approximation [7,14] suggests the value $\alpha \simeq 0.38$ [14]. The aforementioned KMC simulations have either rejected both these predictions [16] or only the value $\alpha = \frac{2}{5}$ [15]. However, the values for α obtained from KMC simulations rely on an extrapolation to infinitely large system sizes [15,16] and, hence, can only be accurate if the assumptions made about the corrections to scaling are valid [15]. Our results confirm the trend observed in recent KMC simulations [15,16,35] that the predictions of available ana-

TABLE I. Values of the roughness exponent α obtained through computer simulations in the indicated articles and Eq. (17) for BD in the present study. The simulations use the BD model for $d=1$, and various nonconserved lattice models for $d=2$.

$d=1$	0.42 ± 0.03[a]	0.42 ± 0.02[c]	0.45[e]	0.47[g]	0.45[h]	0.495 ± 0.008 [This study]
$d=2$	0.383 ± 0.008[b]	0.393 ± 0.003[d]	0.385 ± 0.005[f]	$0.33-0.36$[g]	0.36[i]	0.362 ± 0.015 [This study]

[a]Ref. [19].
[b]Ref. [15].
[c]Ref. [20].
[d]Ref. [16].
[e]Ref. [31].
[f]Ref. [34].
[g]Ref. [32].
[h]Ref. [33].
[i]Ref. [35].

lytic approaches [12,14] do not yield good agreement with results obtained from discrete lattice models.

In summary, we have described a multiscale approach to the analysis of ballistic deposition. Our methodology provides an analytic augmentation of KMC simulations, but also allows the direct derivation of essentially exact continuum equations. Hence, we showed that, even before any coarse-graining, the scaling properties of the BD model are described by the KPZ equation to a very good approximation for $d=1$ and $d=2$. This was confirmed by the demonstration that for $d=1$ the lattice Langevin equation for BD yields the KPZ scaling exponents for small lattice sizes. For $d=2$ our approach leads to scaling exponents which are different from those obtained from recent KMC simulations [15,16] and analytic arguments [12,14]. The wider significance of our work stems from the lattice Langevin equation providing a starting point for a systematic multiscale analysis of lattice models previously studied only through KMC simulations.

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