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Fokker-Planck equation for lattice deposition models

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An asymptotically exact Fokker-Planck equation for the height fluctuations of lattice deposition models is derived from a Van Kampen expansion of the master equation. Using an Edwards-Wilkinson-type model as an example, the solution of the equivalent Langevin equation reproduces the surface roughness and lateral height correlations obtained with kinetic Monte Carlo (KMC) simulations. Our discrete equations of motion thereby provide an exact analytic and computational alternative to KMC simulations of these models.

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The ballistic deposition of particles onto a lattice has broad interest based on the nonequilibrium statistical mechanics of driven systems [1–3], as well as ongoing efforts to use lattice gases to represent macroscopic physical phenomena [4,5]. In deposition models, lattice sites are first chosen randomly at a specified rate. Each deposited particle then relaxes to a nearby site that is determined by some criterion based on the original local configuration. Examples include random deposition, where the deposition site is the initially chosen site, the Edwards-Wilkinson model [6,7], where the deposition site is a local height minimum, the Wolf-Villain model [8,9], where the deposition site is a local coordination maximum, and numerous variations thereon [10–12].

One of the central concerns in the study of lattice models is the expression of the time-development of the system in terms of a stochastic differential equation. For particular cases, the scaling properties of the growth front enable such a relationship to be inferred on the basis of universality classes [2], though this often requires extensive kinetic Monte Carlo (KMC) simulations [13,14]. However, despite several proposals [15–20], there is no rigorous procedure for relating a set of transition rules to a statistically equivalent stochastic equation of motion.

In this Rapid Communication, we use a Van Kampen expansion of the master equation [21] to obtain an asymptotically exact Fokker-Planck equation for the height fluctuations of lattice deposition models. Using an Edwards-Wilkinson-type model [6,7] as an example, the equivalent Langevin equation produces the same surface roughness and lateral height correlations as KMC simulations, but only if the variable transformations in the Van Kampen expansion are used to relate the KMC and Langevin solutions. The Langevin and Fokker-Planck equations therefore embody the statistical properties of the original lattice model and so provide an analytic and computational alternative to KMC simulations.

We consider a one-dimensional lattice on which neither vacancies nor overhangs are permitted. Thus, associated with each site i is a column of height h_i and every surface configuration corresponds to an array $\mathbf{H}=\{h_1,h_2,\ldots\}$. The joint probability of the surface configuration $\mathbf{H}$ at time t is $P(\mathbf{H},t)$. The equation of motion for P from the initial condition $P(\mathbf{H},0)$ is the master equation [21] which, for our purposes, is most conveniently written as

$$\frac{\partial P(\mathbf{H},t)}{\partial t}=\sum_{\mathbf{r}} W(\mathbf{H}-\mathbf{r};\mathbf{r})P(\mathbf{H}-\mathbf{r},t)-\sum_{\mathbf{r}} W(\mathbf{H};\mathbf{r})P(\mathbf{H},t), \tag{1}$$

where $W(\mathbf{H};\mathbf{r})$ is the transition rate from $\mathbf{H}$ to $\mathbf{H}+\mathbf{r}$, and $\mathbf{r}=\{r_1,r_2,\ldots\}$ is the array of jump lengths r_i at each site. The summation over $\mathbf{r}$ is the joint summation over all the r_i.

Master equations provide the same statistical information as KMC simulations and so are amenable to exact solution only in a few cases. Accordingly, we use a Van Kampen expansion [21] to extract the leading fluctuation corrections to the deterministic solution of Eq. (1). The basic assumption of such expansions [21] is that $W(\mathbf{H};\mathbf{r})$ is a sharply peaked function of $\mathbf{r}$ but varies slowly with $\mathbf{H}$, i.e., that there exists a quantity δ such that

$$W(\mathbf{H};\mathbf{r})\approx 0, \quad \text{for } |\mathbf{r}|>\delta; \tag{2}$$

$$W(\mathbf{H}+\Delta\mathbf{H};\mathbf{r})\approx W(\mathbf{H};\mathbf{r}), \quad \text{for } |\Delta\mathbf{H}|<\delta. \tag{3}$$

The first condition is always satisfied by deposition models because the difference in successive configurations is one height unit on a single site. However, except for random deposition, the final deposition site is determined by comparing neighboring heights, which is typically accomplished with step functions. Thus, an arbitrarily small change in a height can produce a discontinuous change in W, in clear violation of Eq. (3). This problem can be alleviated by transforming the time as [22]

$$t\to\tau=\Omega^{-1}t, \tag{4}$$

where Ω is a ''largeness'' parameter [21]. Then, in the spirit of the central limit theorem, the h_i are decomposed into a deterministic part ϕ_i and fluctuations ξ_i:

$$h_i(t)=\Omega\phi_i(t)+\Omega^{1/2}\xi_i(t). \tag{5}$$

The incremental change in h_i upon deposition is then

$$h_i-r_i=\Omega\phi_i(t)+\Omega^{1/2}\xi_i(t)-r_i \tag{6}$$

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and $P(\mathbf{H},t)$ transforms as

$$P(\mathbf{H},t)=P(\Omega\mathbf{\Phi}+\Omega^{1/2}\mathbf{\Xi},t)\equiv\Pi(\mathbf{\Xi},t), \tag{7}$$

where $\mathbf{\Phi}=\{\phi_1,\phi_2,\ldots\}$ and $\mathbf{\Xi}=\{\xi_1,\xi_2,\ldots\}$.

The Ω expansion of the master equation can now be carried out in the standard manner [21]. The terms of order $\Omega^{1/2}$ yield equations of motion for the $\phi_i(t)$,

$$\frac{d\phi_i}{d\tau}=K_i^{(1)}(\mathbf{\Phi}), \tag{8}$$

where $K_i^{(1)}$ is the first moment of the transition rate:

$$K_i^{(1)}(\mathbf{\Phi})=\sum_{\mathbf{r}} r_i W(\mathbf{\Phi};\mathbf{r}). \tag{9}$$

The leading correction to this deterministic equation, of order unity, is a Fokker-Planck equation for Π:

$$\frac{\partial\Pi(\Xi,\tau)}{\partial\tau}=-\sum_{ij}\frac{\partial}{\partial\xi_i}\left[\frac{\partial K_i^{(1)}(\mathbf{\Phi})}{\partial\phi_j}\xi_j\Pi(\Xi,\tau)\right]+\frac{a}{2}\sum_i\frac{\partial^2}{\partial\xi_i^2}[K_i^{(1)}(\mathbf{\Phi})\Pi(\Xi,\tau)], \tag{10}$$

where we have used the fact that, for deposition models, all higher moments of the transition rate are diagonal and proportional to the first moment. In particular,

$$K_{ij}^{(2)}(\mathbf{\Phi})=\sum_{\mathbf{r}} r_i r_j W(\mathbf{\Phi};\mathbf{r})=a\,\delta_{ij}K_i^{(1)}(\mathbf{\Phi}). \tag{11}$$

Equations (8) and (10) can be subsumed into a single Fokker-Planck equation for $P(\mathbf{H},t)$:

$$\frac{\partial P(\mathbf{H},t)}{\partial t}=-\sum_i\frac{\partial}{\partial h_i}[K_i^{(1)}(\mathbf{H})P(\mathbf{H},t)]+\frac{a}{2}\sum_i\frac{\partial^2}{\partial h_i^2}[K_i^{(1)}(\mathbf{H})P(\mathbf{H},t)]. \tag{12}$$

In view of Eqs. (4)–(6), this equation is valid to the order $\Omega^{-1/2}$ [23–25].

The solution of Eq. (12) will be obtained from the equivalent Langevin equation [23]:

$$\frac{dh_i}{dt}=K_i^{(1)}(\mathbf{H})+\eta_i, \tag{13}$$

where the η_i are Gaussian noises that have zero mean, $\langle\eta_i(t')\rangle=0$, and covariances

$$\langle\eta_i(t)\,\eta_j(t')\rangle=aK_i^{(1)}(\mathbf{H})\,\delta_{ij}\delta(t-t'). \tag{14}$$

The numerical integration of this equation is carried out with the following time-explicit scheme:

$$h_i(t+\Delta t)=h_i(t)+[K_i^{(1)}(\mathbf{H})+\eta_i(t)]\Delta t, \tag{15}$$

where $\mathbf{H}$ is the height array at time t. Periodic boundary conditions are imposed on a lattice with L sites and the initial conditions are $h_i(0)=0$, for $i=1,2,\ldots,L$. Then, with $t_n=n\Delta t$, Eqs. (4) and (5) relate the solution $h_i(t_n)$ of Eq. (15) to the height in the original time variable by

$$h_i(t_n)\rightarrow\Omega h_i(\Omega t_n). \tag{16}$$

This transformation is the basis for the statistical equivalence of the Langevin equation (13), or the Fokker-Planck equation (12), and the original lattice model.

In one-dimensional models for which deposition is onto the original site or a nearest-neighbor site, the transition rates are of the general form

$$W(\mathbf{H};\mathbf{r})=\frac{1}{\tau_0}\sum_k\left[w_k^{(1)}\delta(r_k-a)\prod_{j\neq k}\delta(r_j)+w_k^{(2)}\delta(r_{k-1}-a)\prod_{j\neq k-1}\delta(r_j)+w_k^{(3)}\delta(r_{k+1}-a)\prod_{j\neq k+1}\delta(r_j)\right], \tag{17}$$

where τ_0 is the deposition rate, a is the height unit, and the $w_k^{(i)}$ determine whether deposition is onto the original site ($i=1$) or a nearest-neighbor site ($i=2,3$). For all such models [17]

$$K_i^{(1)}=\frac{a}{\tau_0}[w_i^{(1)}+w_{i+1}^{(2)}+w_{i-1}^{(3)}]. \tag{18}$$

We consider a model [17] where a particle remains on the incident site only if its height is less than or equal to both nearest-neighbor heights. If only one nearest-neighbor height is lower than that of the original site, deposition is onto that site. But, if both nearest-neighbor heights are lower than that of the original site, the deposition site is chosen randomly between the two. Thus,

$$w_k^{(1)}=\theta_k^+\theta_k^-,$$

$$w_k^{(2)}=\theta_k^+(1-\theta_k^-)+\tfrac{1}{2}(1-\theta_k^+)(1-\theta_k^-), \tag{19}$$

$$w_k^{(3)}=\theta_k^-(1-\theta_k^+)+\tfrac{1}{2}(1-\theta_k^+)(1-\theta_k^-),$$

where $\theta_k^{\pm}=\theta(h_{k\pm1}-h_k)$ and $\theta(x)$ is defined by

$$\theta(x)=\begin{cases}1, & \text{if } x\geq 0;\\ 0, & \text{if } x<0.\end{cases} \tag{20}$$

Our comparison between KMC simulations and the solution of Eq. (15) is based on the surface roughness and the lateral height correlations. The surface roughness is

$$W(L,t)=[\langle h^2(t)\rangle-\langle h(t)\rangle^2]^{1/2}, \tag{21}$$

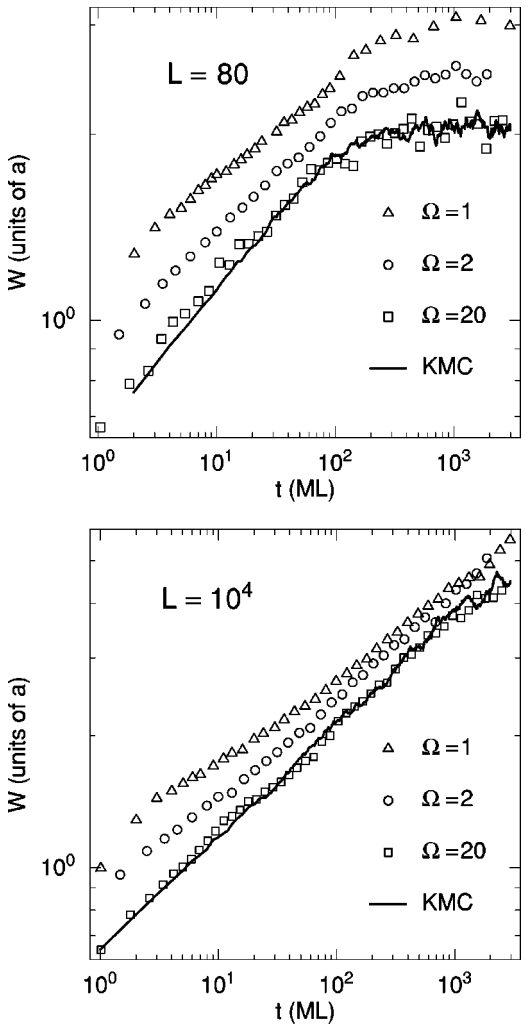

FIG. 1. Surface roughness obtained from the Langevin equation (15) and KMC simulations for systems of size $L=80$ and $L=10^4$ for $\Omega=1,2,20$. Data sets for $L=80$ were averaged over 200 independent realizations. Those for $L=10^4$ were obtained from a single realization. The time is measured in units of monolayers (ML) deposited.

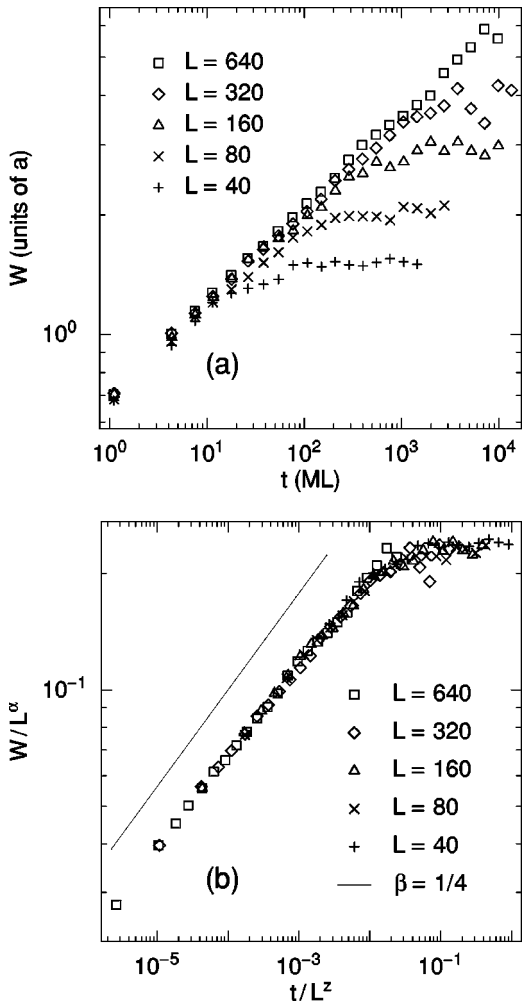

FIG. 2. (a) Surface roughness obtained from the Langevin equation (15) for $\Omega=10$ and the indicated system sizes. Each data set was averaged over 200 independent realizations. (b) Data collapse for all system sizes in (a) obtained by plotting $WL^{-\alpha}$ vs tL^{-z} for $\alpha=\frac{1}{2}$ and $z=2$. The slope $\beta=\frac{1}{4}$ is shown for comparison.

where $\langle h^n(t)\rangle = L^{-1}\Sigma_i h_i^n(t)$, for $n=1,2$. For sufficiently long times and large substrate sizes, W conforms to the dynamical scaling hypothesis [2],

$$W(L,t)\sim L^{\alpha} f(t/L^{z}), \tag{22}$$

where $f(x)\sim x^{\beta}$ for $x\ll 1$, $f(x)\rightarrow$constant for $x\gg 1$, and $z=\alpha/\beta$. The lateral height correlation function is

$$C(r,t)=\langle [h_i(t)-h_j(t)]^2\rangle^{1/2}, \tag{23}$$

where $r=|i-j|$. For r much smaller than the lateral correlation length [2],

$$C(r,t)\sim r^{\alpha}. \tag{24}$$

The comparison of $W(L,t)$ obtained from KMC simulations and from Eq. (15) is shown in Fig. 1 for $L=80$ and $L=10^4$, each for $\Omega=1,2,20$. With increasing Ω, the roughness obtained for both lattice sizes approaches that of the KMC simulation at all times. The convergence with Ω is quite rapid, but there are appreciable discrepancies for small Ω. For $L=80$ and $\Omega=1$, the growth front is much rougher, the saturation time is delayed, and the presaturation slope is smaller than in the KMC simulation. There are remnants of these discrepancies for $L=10^4$, though the slope appears to cross over to that of the simulation at long times even for $\Omega=1$.

Figure 2(a) shows the surface roughness obtained from Eq. (15) for lattices of sizes $L=40,80,160,320,640$ with $\Omega=10$. According to Eq. (22), a plot of $WL^{-\alpha}$ versus tL^{-z} should, with appropriately chosen values of α and z, yield a collapse of the data onto the scaling function f. This is shown in Fig. 2(b) for $\alpha=\frac{1}{2}$ and $z=2$. The quality of the data collapse indicates not only that these are the correct exponents, but that the solution of Eq. (15) with $\Omega=10$ is capable of reproducing such scaling behavior.

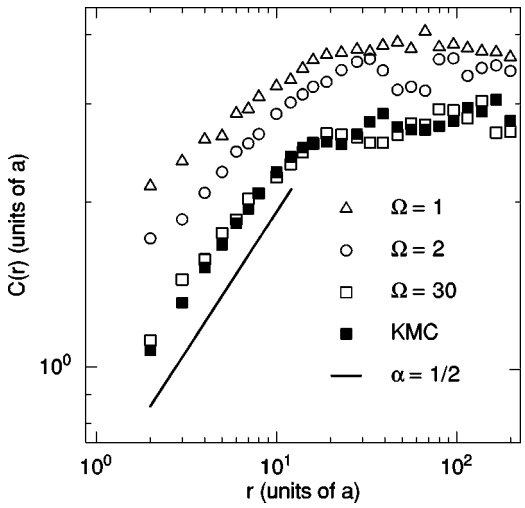

FIG. 3. The lateral height correlation function obtained from the Langevin equation (15) and KMC simulations after the deposition of 100 ML on a system of size $L=1000$ for $\Omega=1,2,30$. The slope $\alpha=\frac{1}{2}$ is shown for comparison.

The fact that calculations with finite Ω produce a rougher surface than KMC simulations can be understood as follows. In the Langevin equation, the relaxation at *every* site at a given time step is determined from the local configuration at the *preceding* time step. In the simulations, however, the surface configuration is updated with each deposition event. Given that $0\leqslant K_i^{(1)}\leqslant 3a/\tau_0$, with the lower bound produced by ''peaks'' in the height profile and the upper bound by ''troughs,'' deposition (including the noise) is strongly biased toward sites at deep local minima. Thus, for $\Omega=1$, the surface is rougher than in the KMC simulations, but, for $\Omega>1$, this effect is counterbalanced by Eq. (16), which transforms the Langevin time t to a *later* KMC time Ωt, with a corresponding rescaling of the height.

Figure 3 compares $C(r,t)$ determined from KMC simulations with that obtained from solutions of Eq. (15) for $L=1000$ with $\Omega=1,2,30$. The convergence with Ω is again evident, especially for the lateral correlation length and the scaling behavior in Eq. (24). Neither is reproduced by correlation functions obtained with $\Omega=1$ and $\Omega=2$. This comparison provides a somewhat more stringent test of our method than that based solely on the roughness because it shows that the statistics of the spatial arrangements of heights are correctly described.

Finally, we note that our method can be applied to models other than those involving only deposition. In particular, site-to-site hopping is amenable to the approach taken here [17], but because the noise covariances are not site-diagonal in this case, there is no apparent computational advantage over KMC simulations. Nevertheless, our method does establish a direct connection between lattice transition rules and statistically equivalent discrete stochastic differential equations.

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