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Physica A 267 (1999) 406–413

PHYSICA A

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The Edwards–Wilkinson model revisited: large-scale simulations of dynamic scaling in 2+1 dimensions

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Received 28 October 1998

Abstract

Using extensive simulations of surface growth in the 2+1 dimensional atomistic model of Edwards and Wilkinson (EW), we have calculated both interfacial width and the structure factor, to extract the dynamic exponent z. In contrast to theoretical expectations, finite-size scaling of the data for both surface properties is achieved using $z \sim 1.63$, instead of the predicted value of 2.0. A restricted variant of the EW model gives $z \sim 2.0$. Clarifying these non-trivial differences in dynamical correlations, now represents an intriguing theoretical challenge.

PACS: 05.70.Ln; 64.60.Ht; 82.65.Dp; 02.50.Ng

Keywords: Large-scale simulations; Surface growth model; Dynamic scaling; Edwards–Wilkinson model

The general study of surface phenomena and surface characterization has been an exciting field of research over several decades. Efforts to understand microscopic, non-equilibrium behavior at growing surfaces are, however, more recent and are attributable to rapid technological advances. In recent years there has been tremendous activity in the study of surface growth models, as part of an attempt to produce a theoretically complete and robust description of non-equilibrium growth behavior [1,2]. One motivation for such studies is the desire to determine what factors affect the essential properties of surface fluctuations which, in turn, decide the dynamic universality classes. In this regard, atomistic models, which include deposition and some form of accompanying diffusion, have been used with some degree of success. Apart

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0378-4371/99/$ – see front matter
PII: S0378-4371(98)00641-4

from the use of such models, which can be most effectively solved using computer simulations, an alternative approach that has been pursued is the construction of differential equations for surface fluctuations, as growth proceeds in the continuum limit. Although most studies are in general helpful in understanding the dynamical behavior of a growing surface, our knowledge of the nature (or mechanism) behind such observed dynamical behavior is incomplete.

We have studied two forms of the Edwards–Wilkinson surface growth model, using slightly different hopping (diffusion) rules, which produce markedly different behavior of the long-time and large-scale properties. By exploiting the differences between these two models, we show how the interplay of the external flux, and local hopping rules can, in some cases, induce non-trivial dynamical correlations at a growing surface. The Edwards–Wilkinson (EW) model plays an important role in the study of non-equilibrium surface growth due to the simplicity of its growth process. In a seminal paper [3] the lattice model was introduced for the study of fluctuations in a surface, growing by random deposition of particles with immediate relaxation to nearest-neighbor sites. Based on the lattice model, Edwards and Wilkinson derived an equation which is purported to describe the surface fluctuations during growth. The EW equation is written as

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \phi \,, \tag{1}$$

where $h(\mathbf{r},t)$ is the height of the surface at position $\mathbf{r}$ and time t, ν is the surface tension, and ϕ is the stochastic contribution to the surface fluctuations. Note that in the original EW formulation $\nu = Fa^2$, F is the flux, and a is the lattice constant. The noise ϕ has zero mean i.e. $\langle \phi(\mathbf{r},t)\rangle = 0$, and correlations are defined as $\langle \phi_{\mathbf{k},\omega}\phi_{\mathbf{k}',\omega'}\rangle = FL^2\tau v^2 \exp(-k^2a^2)\delta(k+k')\delta(\omega+\omega')$, where τ is the maximum time up to which particles are deposited, v is the volume of each particle, L is the lateral extent of the system, and $\mathbf{k}$ is the surface wave vector. It is unclear if this form of the noise–noise correlations correctly describes the development of dynamical correlations arising due to deposition and relaxation of incident particles as envisaged by EW; however, it is interesting that such an approach was used to incorporate the effects of flux and relaxation, i.e. to describe the system in a non-equilibrium state. The irreversibility in surface fluctuations during growth is essentially reflected through the correlated noise. (To see how correlations can build up during deposition, see some recent experiments on sedimentation [4].)

The EW model was the first manifestly non-equilibrium model used to attempt to understand surface fluctuations in a non-equilibrium system, although it was inappropriately characterized as a model that represents the equilibrium scenario [5–7]. (This conclusion was based on the simulation results of a 1+1 dimensional EW model, and the comparison with a continuum equation that represents equilibrium surface fluctuations.)

In this paper, we report large-scale Monte Carlo simulations, which are used to study the dynamic finite-size scaling relation of the physical model of EW in 2+1 dimensions. Our primary aim is to characterize its non-equilibrium behavior through

the determination of the dynamic exponent z, and to classify it in an appropriate non-equilibrium universality class. In addition, we study a restricted variant of the EW model (REW), with slightly modified local dynamics, which we believe sheds some light on the origin of noise correlations. The surface properties are characterized by measuring the structure factor, and the root mean square of surface fluctuations, (commonly defined as the interfacial width.) For sufficiently long times t, and large substrate sizes L, the interfacial width $W(L,t)$ is expected to satisfy the dynamic scaling relation [8]

$$W^2(L,t) = A \ln\left[Lf\left(\frac{t}{L^z}\right)\right], \tag{2}$$

where $f(x)$ is the scaling function, and z is the dynamic exponent. The scaling function has the property $f(x) \sim x^{\beta}$, for $x \ll 1$ and $f(x) \to constant$, for $x \gg 1$. The exponents z and β satisfy the relation $z\beta = 1$. This identity, along with the particular form of the scaling function ensures that for small times the interfacial width behaves as $W^2 \sim A\beta \ln t$, and at very long times the saturated value of the interfacial width (W_∞) satisfies the relationship $W_\infty^2 - A \ln L \sim constant$.

The structure factor $S(L,kL,t)$ can be obtained by measuring the Fourier transform of the spatial correlation function, and should satisfy the dynamic scaling law [9],

$$S(L,kL,t) = L^{(2-\eta)} g(t/L^z, kL)\ , \tag{3}$$

where $kL = 2n\pi$, n being an integer, and z is the dynamic exponent. The long-wavelength behavior of the surface can be probed by using a small value of k. In this limit, and for large lattice sizes, the structure factor obeys the scaling function $g(x,kL) \sim x^{\gamma}$, for $x \ll 1$ and $g(x,kL) \to constant$, for $x \gg 1$. Note that kL is kept fixed during the simulation, and only L is varied. The exponent γ is related to the dynamic exponent by $\gamma = (2-\eta)/z$.

To simulate the physical model of EW, particles are randomly deposited on an initially flat substrate of size $L \times L$ with periodic boundary conditions. A deposited particle is allowed to move only once to the nearest-neighbor column with minimum height, indicating a relaxation similar to that in the presence of a gravitational field. Each particle can move to a nearest-neighbor column after hitting the surface, only if the nearest-neighbor columns are at a lower height. In case there are two or more sites of equal height to which a particle can hop, the final site is chosen randomly. The REW model can be made by modifying the EW model, such that an adatom has the only choice to move into a single nearest-neighbor column of largest depth that is uniquely defined, i.e. if two or more sites are in competition, then the move is rejected. If a unique site is not available, the adatom loses its chance to move and remains at its initially deposited site. We measure the interfacial width and the structure factor along the (1,0) direction for the EW model to characterize the roughness of the growing surface. For the REW model we report only the results for the structure factor. The interfacial width is defined as $W(L,t) = [\langle h^2(\mathbf{r},t)\rangle - \langle h(\mathbf{r},t)\rangle^2]^{1/2}$, where $\langle h(\mathbf{r},t)\rangle = L^{-2}\sum_r h(\mathbf{r},t)$, while the structure factor can be written as $S(k,t) = \langle h_k(t) h_{-k}(t)\rangle$, where $h_k(t) = L^{-1}\sum_r (h(\mathbf{r},t) - \langle h(\mathbf{r},t)\rangle)\exp(i\mathbf{k}.\mathbf{r})$. Lattice sizes ranging from $L = 20$ to 1280

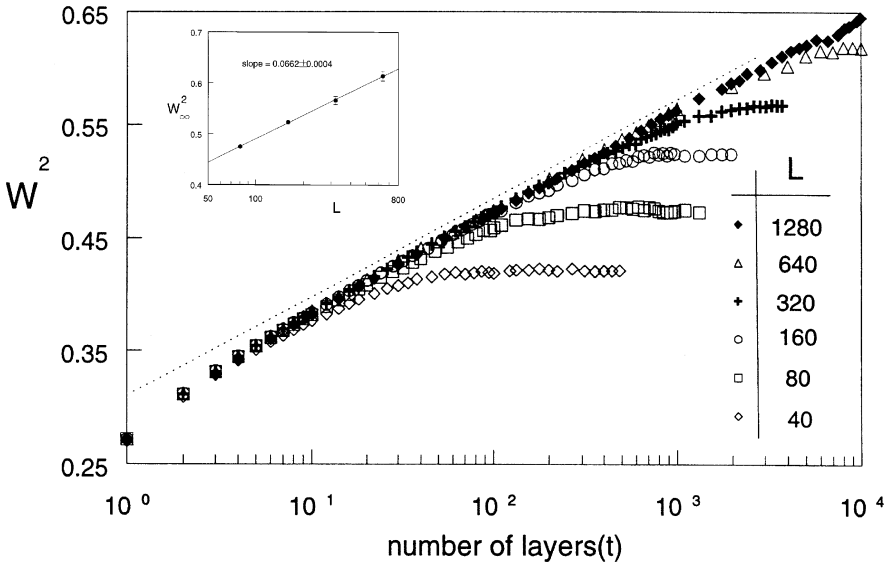

Fig. 1. The square of the interfacial width for the EW model vs. the number of deposited layers for several lattice sizes $40 \leqslant L \leqslant 1280$, on a semi-logarithmic scale. (Error bars are roughly the size of the points.) A linear fit through the data has a slope $A\beta = 0.040 \pm 0.001$ (shown as a dotted line). The inset shows the saturated interfacial width (W_∞) for various lattice sizes in a semi-logarithmic scale. A fit through the data points has a slope $A = 0.0662 \pm 0.0004$. Note that the x-axis needs to be converted to natural logarithm, to obtain the slopes reported here.

were used for the simulations, and data were averaged over multiple runs (starting with different random number seeds.) The number of runs varied from 50 for $L = 1280$ to 2000 for $L = 40$ lattices. Because of the need for both large lattices and large numbers of runs, each of which required growth to a large number of layers, this study was computationally demanding: The computer time invested in this accurate study of both the EW and the REW model totaled about 30,000 Workstation CPU hours.

The evolution of the interfacial width for the EW model is shown in Fig. 1 on a semi-logarithmic scale. For the largest lattice size, the data can be well fitted by a straight line starting from ≈ 20 layers up to 10^4 layers. A similar plot on a log–log scale did not produce linear behavior over substantial time scales. Thus the square of the interface width evolves logarithmically with time (t), i.e. $W^2 \sim A\beta \ln(t)$ where t is proportional to the number of deposited layers. By fitting a straight line through the linear portion of the graph, the slope is estimated to be $A\beta = 0.040 \pm 0.001$. The square of the saturated interface width, i.e. ($W^2(L, t \to \infty) \equiv W^2_\infty$), is also found to depend logarithmically on substrate sizes L, (shown as an inset). A linear fit through the data points yields an estimated slope of $A = 0.0662 \pm 0.0004$. Hence using the identity $z\beta = 1$, we determine the dynamic exponent to be $z = 1.65 \pm 0.05$. This dynamic exponent can be verified self-consistently by attempting full finite-size scaling of the data points according to Eq. (2). Excellent scaling of data (shown in Fig. 2) is obtained by using

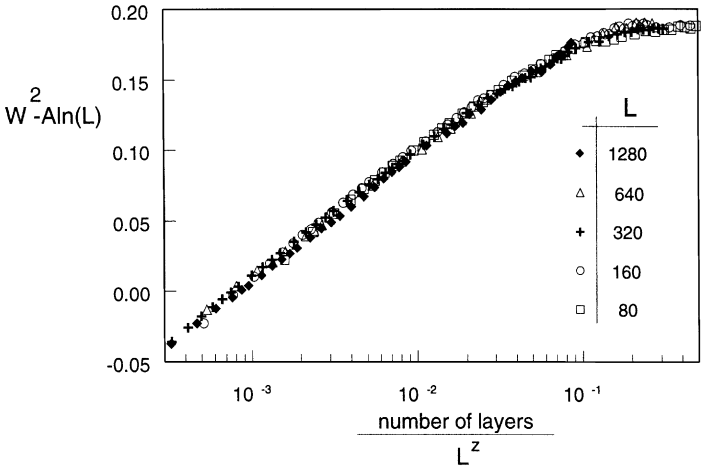

Fig. 2. Dynamic scaling plot of the interfacial width for $z = 1.63$ is shown in a semi-logarithmic scale for the EW model. A is chosen as 0.066. The data show good scaling, which self-consistently agrees with the scaling equation.

$z = 1.63$, which is well within the estimates from the previous analysis. Note that with the increase in lattice size, the region over which the data scale, becomes larger, and $L = 1280$ obeys asymptotic scaling from ≈ 50 layers to more than 10^4 layers. When we use $z = 2.0$, scaling fails.

We now consider the behavior of the structure factor. Note that the exact solution of the linear EW equation [7] gives the following expression for the structure factor: $n^2 S(L, kL, t) = L^2(D/v)(1 - \exp(-8n^2\pi^2 v L^{-2} t))$, where D and v are constants. For $L \to \infty$, and short times $S(L, kL, t) \sim t$ while at large times $S(L, kL, t \to \infty) \to L^2$. We have calculated the structure factor for both the EW and the REW model for several lattice sizes. As time increases, large-scale structures develop and finally the structure factor saturates due to finite-size effects. We find that for the EW model $S(L, kL, t) \sim t^{\gamma}$ where $\gamma = 1.23 \pm 0.01$, while for the REW model $\gamma = 1.01 \pm 0.02$. For both the models, the saturated structure factor scale as L^{δ}, with $\delta = 2.02 \pm 0.03$, and $\delta = 2.03 \pm 0.04$ for the EW and REW models, respectively.

Based on our observations we propose the following dynamic scaling equation for the structure factor, $S(L, kL, t) = L^2 f(t/L^z, kL)$, where z is the dynamic exponent. The scaling function $f \to constant$, for $t \to \infty$, and in the limit of small times and large lattice sizes, the scaling function approaches the general form (as shown in Eq. (3)). This can be written as $f \sim (L^{-z}t)^{\gamma}$, where $z\gamma = 2$ and $\eta = 0$. This gives, $z = 1.64 \pm 0.04$ for the EW model, and $z = 2.01 \pm 0.08$ for the REW model. The results for the EW model are in good agreement with our earlier observation, and also agrees well with the scaled structure factor data as shown in Fig. 3. Fig. 4 shows scaling of the structure factor data for the REW model with $z = 2.0$, a value which agrees quite well with the solution of the linear EW equation.

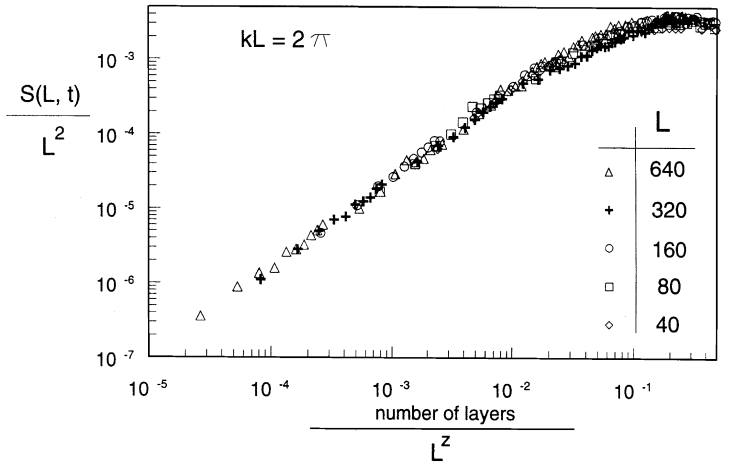

Fig. 3. Dynamic scaling plot of the structure factor for the EW model. The lattice sizes range from 40 to 640, and the data points represent averages ranging from 2000 to 250 runs, respectively. Excellent scaling is obtained over several decades with a log–log plot using $z = 1.63$.

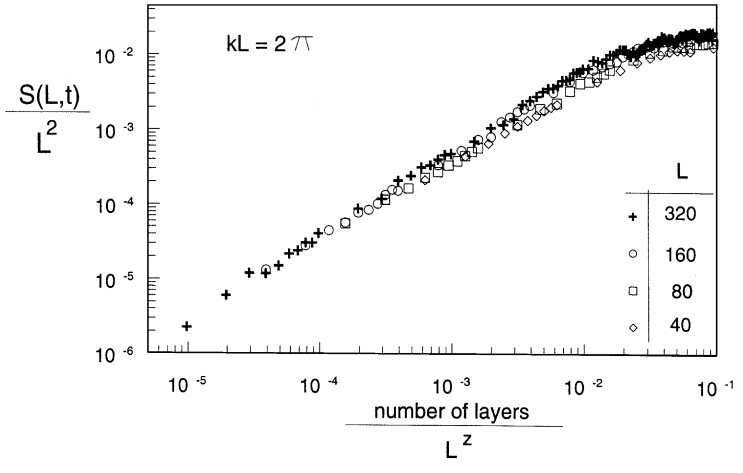

Fig. 4. Dynamic scaling plot of the structure factor is shown for the REW model in a log–log scale, using $z = 2.0$. As the lattice size is increased, the quality of collapse in the scaled data improves substantially, with $L = 160$, and 320 showing very nice scaling. This indicates that asymptotic scaling is obeyed for the REW model using $z = 2.0$.

The fact that data for both the EW and REW model show good scaling but with *different* dynamic exponents is intriguing. Certainly the REW model can be described by the linear Langevin equation, with uncorrelated noise. One might intuitively expect that the addition of apparently uncorrelated randomness (in the diffusion) to the REW model would not introduce any new correlation effects and thus should not effect the dynamic behavior. The subtle change in the local dynamics has resulted in completely

different scaling behavior. We do not presently understand why this is the case and view the need for a clear, convincing explanation to be an important theoretical challenge!

One speculative argument for the origin of this apparent violation of dynamic universality is the following. A standard approach in critical phenomena to study the long-time, large length-scale properties of a dynamical system is to begin with a semi-phenomenological equation of motion in a small set of semi-macroscopic variables ξ_i, $i=1,2,\ldots,N$, whose dynamical evolution is slow compared to the remaining microscopic degrees of freedom. In these equations the remaining "fast" variables enter only in the form of random forces (usually called the noise ϕ_i) as shown:

$$\frac{\partial \xi_i}{\partial t} = -\sum M_{ij} \frac{\delta \mathscr{F}}{\delta \xi_j} + \phi_i \,, \tag{4}$$

where $\mathscr{F}$ is the Ginzburg–Landau coarse-grained free energy functional, and M is the matrix of generalized Onsager coefficients. The EW equation is a simple example of this approach in which the noise is delta correlated in time. It may be that in the atomistic EW model, noise in the flux is somehow coupled to the local dynamics to produce non-trivial, temporal noise correlations in the dynamical equation. These are missing, of course, from the REW model.

In previous studies, the non-trivial dynamical correlations have been accounted for by assuming the presence of a non-linear term in the linear Langevin equation [10]. This equation is then solved perturbatively using the dynamic renormalization group methods. The anomaly in such a procedure is that the surface shape resulting from such a growth equation still remains invariant in time [11], although it is well known that non-equilibrium systems are generally irreversible, and consequently do not remain invariant under time translation. The irreversiblity in the evolution of dynamic properties can be taken into account by assuming that the stochastic noise has correlations in time. By introducing such a construct, the apparently-linear hydrodynamic equation can exhibit non-linearities through the noise correlations, thus altering the value of the dynamic exponent z from the linearized hydrodynamic value of 2.0.

In conclusion, we have performed large-scale simulations of the atomistic model of EW to extract the dynamic exponent z from calculations of both the interfacial width and the structure factor. Contrary to the expected theoretical value of 2.0, we obtained $z \approx 1.63$ from the simulations. We show that when all randomness in the diffusion is removed, the dynamic exponent convincingly changes to $z \sim 2.0$. The study provides a tantalizing hint of the effect of dynamical correlations, and suggests that more complex correlations are needed in the linear Langevin (EW) equation if it is to accurately describe surface fluctuations under the combined influence of external flux and diffusion.

This research was supported in part by NSF Grant No. DMR-9405018. We wish to thank F. Abraham, J. Banavar, K. Binder and D. Wolf for enlightening discussions, and J. Lees for help with computation. S.P. acknowledges funding in PSU from NASA and the Petroleum fund administered by the American Chemical Society.

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