Width Distributions and the Upper Critical Dimension of KPZ Interfaces

E. Marinari1, A. Pagnani2, G. Parisi1, and Z. Rácz3

1Dipartimento di Fisica, INFN and INFN, Università di Roma La Sapienza, P. A. Moro 2, 00185 Roma, Italy
2Dipartimento di Fisica and INFN, Università di Roma La Sapienza, P. A. Moro 2, 00185 Roma, Italy
3Institute for Theoretical Physics, Eötvös University, 1117 Budapest, Pázmány sétány 1/a, Hungary
E-mail: Enzo.Marinari@roma1.infn.it, Andrea.Pagnani@roma1.infn.it, Giorgio.Parisi@roma1.infn.it, Racz@pole.elt.hu
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Simulations of restricted solid-on-solid growth models are used to build the width-distributions of \( d = 2 - 5 \) dimensional KPZ interfaces. We find that the universal scaling function associated with the steady-state width-distribution changes smoothly as \( d \) is increased, thus strongly suggesting that \( d = 4 \) is not an upper critical dimension for the KPZ equation. The dimensional trends observed in the scaling functions indicate that the upper critical dimension is at infinity.

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The KPZ equation \([1]\) has been introduced to model growth in terms of a moving interface. The equation is written for the height \( h(\vec{r}, t) \) of the interface above a \( d \)-dimensional substrate

\[
\partial_t h = \nu \nabla^2 h + \lambda (\nabla h)^2 + \eta, \tag{1}
\]

where \( \nu \) and \( \lambda \) are parameters, while \( \eta(\vec{r}, t) \) is a Gaussian white noise. Eq. \([1]\) can also give account of a number of other interesting phenomena (Burgers turbulence, directed polymers in random media, etc.) and, accordingly, a lot of efforts has been spent on finding and understanding the scaling properties of its solutions \([3, 4]\). These intensive studies notwithstanding, a number of unsolved issues remain, the question of upper critical dimension \( (d_u) \) being the most controversial one.

The importance attached to \( d_u \) stems from the hope that, in analogy with equilibrium critical phenomena, a better understanding can be achieved through systematic expansions in terms of \( d_u - d \). The search for \( d_u \) has been on for about a decade \([3, 10]\) and the results range from \( d_u \approx 2.8 \) to \( d_u = \infty \). Analytical estimates originate mainly from mode-coupling theories which yield exact results for \( d = 1 \) [7]. Extending this approach to higher dimensions \([3, 11]\) one obtains values of \( d_u \) which, after refining the self-consistency schemes, appear to settle to \( d_u = 4 \). The result \( d_u = 4 \) also emerges from various phenomenological field-theoretical schemes [12] and some nontrivial consequences of the phenomenological arguments appear to be in agreement with simulations [13].

In contrast to the analytical approaches, numerical solution of the KPZ equation \([13]\), simulations of systems belonging to the the KPZ universality class \([14, 15]\), and the results of real-space renormalization group calculations [14] provide no evidence for a finite \( d_u \). Furthermore, the only numerical study [13] of the mode-coupling equations gives no indication for the existence of a finite \( d_u \) either.

There are, of course, problems with both the analytic approaches and the numerical works. Assumptions about the scaling structure of the solution underlie the field theoretic approaches, and uncontrolled approximations are made when writing down the governing equation in mode-coupling theories. Additional uncertainties come from the use of various selfconsistency schemes in solving the mode-coupling equations. Simulations and numerical works have their own share of difficulties. The systems in higher dimensions cannot be large; the extraction of exponents using fitting procedures which involve unknown correction-to-scaling exponents makes the error estimates suspect, and there may be difficulties with the numerical solution of the mode-coupling equations as well \([14]\).

In view of the above controversy, it is highly desirable to approach the \( d_u \) problem in a way unbiased by approximations and fitting procedures. Such an approach is described below where we study the steady-state width-distributions of \( d = 1 \) to \( d = 5 \) KPZ interfaces.

The width-distributions have been introduced to provide a more detailed characterization of surface growth processes \([13, 22]\), and they have been used to establish universality classes of rather divers phenomena \([23, 24]\). The quantity whose distribution is of interest here is the mean-square fluctuation of the interface defined by

\[
w_2 = \frac{1}{A_L} \sum_{\vec{r}} \left[ h(\vec{r}, t) - \bar{h} \right]^2, \tag{2}
\]

where \( A_L \) is the area of the substrate of characteristic linear dimension \( L \), and \( \bar{h} = \sum_{\vec{r}} h(\vec{r}, t)/A_L \) is the average height of the surface. Sampling \( w_2 \) in the steady state, one can build the so called width distribution \( P_L(w_2) \) for \( w_2 \) defined as the probability that \( w_2 \) is in the interval \([w_2, w_2 + dw_2]\). If the quantities \( h(\vec{r}, t) - \bar{h} \) were uncorrelated at large distances the probability distribution of \( w_2 \) would be approaching \( \delta(w_2 - \langle w_2 \rangle_L) \) for \( L \to \infty \). On the contrary, the fact that the distribution is non trivial implies that these quantities are strongly correlated at large distance.
The usefulness of this distribution lies in the follow- ing observation supported by all the examples studied so far (including \(d = 1\) and 2-dimensional KPZ surfaces [19, 21, 27]). Namely, in systems where the steady-state roughness diverges \(\langle w_2 \rangle_L \rightarrow \infty\) in the \(L \rightarrow \infty\) limit, \(P_L(w_2)\) assumes a scaling form
\[
P_L(w_2) \approx \frac{1}{\langle w_2 \rangle_L} \Phi_d \left( \frac{w_2}{\langle w_2 \rangle_L} \right),
\]
where \(\Phi_d(x)\) is an universal scaling function characteristic of the universality class of a given nonequilibrium dynamics in dimension \(d\). This universality is understandable, it is a consequence of the facts that (i) a steady state can be considered as a critical state if the fluctuations diverge, and (ii) in critical systems, the distribution functions of macroscopic quantities (such as \(\langle w_2 \rangle\)) are characterized by scaling functions which are universal.

The universality of \(\Phi_d(x)\) allows the investigation of the problem of \(d_u\), once it is noted that the scaling functions depend on dimensionality up to \(d = d_u\) and they are expected to take on a fixed shape for \(d \geq d_u\). Thus if one finds that scaling functions vary smoothly in dimensions \(1 \leq d \leq d_u\), one can conclude that \(d - 1 < d_u\). This is the line of argument we employ below for KPZ systems. We shall compare the scaling functions \([3]\) for \(1 \leq d \leq 5\) using the exact results for the \(d = 1\) steady state [19], previously obtained simulation data for \(2 \leq d \leq 4\) restricted solid-on-solid (RSOS) growth models [13], and by generating new data for the \(d = 5\) RSOS model. Our main finding is that the \(\Phi_d(x)\)'s change smoothly as \(d\) is varied thus suggesting that \(d_u > 4\).

It is important to recognize that there are no fitting procedures in the above approach. The width- distributions are just histograms calculated from Monte- Carlo (MC) simulations. Both quantities \(w_2\) and \(\langle w_2 \rangle_L\) entering \([3]\) are measured and no scaling properties of \(\langle w_2 \rangle_L\) are used or assumed. The only approximation is the finite size of the systems investigated. It should be noted, however, that our approach relies only on the shape of the scaling functions. Since the important size- dependences reside in the argument of these functions the functional forms converge at small sizes. A further and rather important observation that helps to reach our conclusion is that, as we shall show below, the scaling functions converge to well distinguished forms for \(1 \leq d \leq 5\).

Let us now present and discuss the evidence for our conclusion of \(d_u > 4\). The scaling functions \([3]\) for dimensions \(d = 1 - 5\) are displayed in Figs. 1 and 2. The \(d = 1\) curve is an exact result [19]. The rest is obtained from simulations of the RSOS model that is believed to belong to the universality class of the KPZ equation [23]. The RSOS model and its simulations are described in [15] where hypercubes of volume \(L^d\) with periodic boundary conditions were simulated and a multi-surface coding technique allowed to obtain excellent steady-state statistics for systems up \(d = 4\). We take the results from this work to build \(\Phi_d(x)\) for \(d = 2 - 4\) and, in this paper, we extend these simulations to find \(\Phi_d(x)\) for \(d = 5\) as well.

As one can see on Figs. 1 and 2, the scaling functions change smoothly as \(d\) increases. The \(\Phi_d(x)\)'s get narrower and more centered on \(x = 1\), and there does not seem to be any break in this behavior at \(d = 4\). The equality of the \(d = 4\) and 5 scaling functions appears to be excluded. Since our conclusion about \(d_u > 4\) rests on the above observations we must now discuss some details in order to make it more than a visual observation.

The basic problems that may arise in measuring steady state properties are the problems of statistics, relaxation, and finite-size. Since the multi-surface coding allowed the simulations of 32 or 64 systems in one run, we had
no problem gathering data with good statistics. The relaxation time problems were taken care by having very long runs and being in the asymptotic plateau region of \( w_2 \) for at least an order of magnitude longer period than the time of reaching the plateau (for details see discussion and Figs. 3, 5, and 7 in [13]).

The solution to the problem of finite size is less obvious. In general, one can observe that the \( \Phi_d \)'s converge to their limiting shape when the number of sites \( (N = L^d) \) becomes about a factor 2 larger than the number of sites on the surface \( (N_s) \). Fig. 3 demonstrates this observation for the \( d = 2 \) and 4 systems. Results for linear sizes of \( L = 7 \) \( (N = 2N_s) \) and \( L = 157 \) \( (N = 40N_s) \) are compared for \( d = 2 \) and one can see that they have the same \( \Phi \)'s within the the statistical errors of the simulations [30]. Similar conclusion can be drawn by comparing the \( L = 13 \) \( (N = 2N_s) \) and \( L = 25 \) \( (N = 3.5N_s) \) systems in \( d = 4 \) (analogous results for \( d = 3 \) are not displayed on Fig. 3 in order to keep clarity in presentation).

![Fig. 3. Finite-size effects on the scaling function [eq.(3)] in dimensions \( d = 2, 4 \) and 5. \( L \) denotes the linear size of the hypercubes investigated.](image)

We need the \( N \approx 2N_s \) convergence rule because the largest \( d = 5 \) system we can investigate has \( L = 15 \), corresponding to \( N \approx 2N_s \). The results for \( \Phi_5 \) displayed in Fig. 3 indicate that the \( N \approx 2N_s \) rule applies to \( d = 5 \) as well. Indeed, systematic deviations between the \( L = 11 \) and \( L = 15 \) curves can be detected only at small values of \( \Phi_5 \) in the region of \( x \leq 0.85 \). An important feature of the size-dependence of \( \Phi_5 \) that can be seen in Fig. 3 is that the maximum of \( \Phi_5 \) slightly increases with size. This means that, near the maximum, \( \Phi_5 - \Phi_4 \) becomes larger with increasing \( L \), thus excluding the possibility of the two functions \( \Phi_5 \) and \( \Phi_4 \) becoming equal. The different functional forms for the scaling functions in \( d = 4 \) and 5 then indicate that \( d = 4 \) is not the upper critical dimension for the KPZ systems.

The concept of smooth changes across \( d = 4 \) can be put on a more quantitative basis by examining the dimensional trend in the spread of the scaling function around its average \( x = 1 \)

\[
\sigma_d^2 = \int_0^\infty dx \frac{(x-1)^2}{\langle (w_2)^2 \rangle - 1}, \tag{4}
\]

that is related to relative mean-square fluctuations of \( w_2 \). Apart from the case of \( d = 1 \), the \( L \) dependence of \( \sigma_d \) is very weak and plotting \( \sigma_d(L) \) against \( 1/L \) one can get accurate estimates of \( \sigma_d(\infty) \). The values of \( \sigma_d(\infty) \) as a function of \( 1/d \) are displayed on Fig. 4. As one can see, apart from the \( d = 1 \) result, the straight line \( \sigma_d \approx 0.71/d \) gives an excellent description of the dimensional dependence of \( \sigma_d \).

![Fig. 4. Dimensional dependence of the relative fluctuations of \( w_2 \). The extrapolated values \( \sigma_d(L \to \infty) = \sigma_d(\infty) \) [see eq.(4)] are plotted against \( 1/d \) with the solid line given by \( \sigma_d = 0.71/d \).](image)

The result \( \sigma_d \approx 0.71/d \) indicates that \( \sigma_d \to 0 \) for \( d \to \infty \) i.e. the scaling function converges to a delta-function, \( \delta(x) \), at \( d = \infty \). Remarkably, the convergence \( \Phi_d(x) \to \delta(x) \) also takes place in a related surface-growth model, in the Edwards-Wilkinson model if \( d = 2 \) [20]. Since \( d = 2 \) happens to be the upper critical dimension of this model (the interface becomes flat for \( d > d_u = 2 \) one may speculate that the results displayed on Fig. 4 actually give support to the suggestion that failure of numerical attempts at locating a finite \( d_u \) means that \( d_u = \infty \) for KPZ systems [31].

In summary, we believe that the main results of this paper (Fig. 4 and 2) provides strong evidence that \( d_u \geq 5 \) and, furthermore, Fig. 4 suggests that \( d_u = \infty \). As a final remark, let us note that the results displayed on Fig. 4 and 2 can be appreciated from another point of view. Namely, we have constructed the scaling functions of width distributions for the KPZ universality class. Thus we have expanded the picture gallery of scaling functions that may be used for identifying the universality classes of nonequilibrium steady states.
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[30] A non-negligible contribution to the statistical error comes from the fact that the number of possible $w_2$ values is small for small systems. This causes problems with the choice of binsize, $dw_2$, when building $P(w_2)$. Namely, $dw_2$ must be significantly larger than the difference between neighboring $w_2$ values, otherwise small changes in $dw_2$ yield large fluctuations in $P(w_2)$. On the other hand, $dw_2$ must be smaller than the scale on which relevant changes occur in $P(w_2)$. Finding appropriate values of $dw_2$ does not pose a problem for the system sizes we studied, in general. The $d = 2$, $L = 7$ system, however, is an exception where the fluctuations coming from binsize choice are clearly visible.
[31] In addition to obtaining $\sigma_2$, the simulations of the $d = 5$ KPZ system can also be used to determine the critical exponents in the finite-size scaling of the width, $w_2 \approx A_2 L^{2\chi} (1 + B_2 L^{-\omega})$. One finds that $\chi = 0.205 \pm 0.015$ and $\omega = 1.07 \pm 0.14$. Although these results are obtained by fitting and thus are not used in the main line of argument of the paper, it should be noted that, taken together with the results of the $d = 2 \rightarrow 4$ simulations, they give additional support to the notion of smoothly changing criticality across $d = 4$. We also note that the $d = 5$ simulations did not show any evidence of a glassy phase that has been discussed as a possibility for $d > 4$ KPZ systems.
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