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Numerical estimate of the Kardar-Parisi-Zhang universality class in (2+1) dimensions

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We study the restricted solid on solid model for surface growth in spatial dimension $d = 2$ by means of a *multisurface coding* technique that allows one to produce a large number of samples in the stationary regime in a reasonable computational time. Thanks to (i) a careful finite-size scaling analysis of the critical exponents and (ii) the accurate estimate of the first three moments of the height fluctuations, we can quantify the wandering exponent with unprecedented precision: $\chi_{d=2} = 0.3869(4)$. This figure is incompatible with the long-standing conjecture due to Kim and Koesterlitz that hypothesized $\chi_{d=2} = 2/5$.

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The Kardar-Parisi-Zhang (KPZ) equation [1] is one of the simplest and most studied models of out-of-equilibrium surface growth. The equation describes the time evolution of the height $h(\mathbf{r}, t)$ of an interface above a d -dimensional substrate:

$$\partial_t h(\mathbf{r}, t) = \nu \nabla^2 h(\mathbf{r}, t) + \frac{\lambda}{2} |\nabla h(\mathbf{r}, t)|^2 + \eta(\mathbf{r}, t), \quad (1)$$

where ν is the diffusion coefficient, λ is the strength of the nonlinear growth rate, and $\eta(\mathbf{r}, t)$ is a Gaussian white noise of amplitude D :

$$\langle \eta \rangle = 0, \quad \langle \eta(\mathbf{r}, t) \eta(\mathbf{r}', t') \rangle = 2D \delta^d(\mathbf{r} - \mathbf{r}') \delta(t - t'). \quad (2)$$

The universality class induced by Eq. (1) is defined in terms of the scaling properties of the height fluctuations $w_2(L, t) = \langle (h(\mathbf{r}, t) - \langle h(\mathbf{r}, t) \rangle)^2 \rangle$. As a function of the system size L it is believed that $w_2(L, t) \sim L^{2\chi} f(t/L^z)$, where the scaling function is such that $f(x) \rightarrow \text{const}$ for $x \rightarrow \infty$ and $f(x) \sim x^{2\chi/z}$ for $x \rightarrow 0$. The peculiar behavior of f implies that $w_2(L, t) \sim L^{2\chi}$ for $t \gg L^z$ and $w_2(L, t) \sim t^{2\chi/z}$ for $t \ll L^z$. Due to an infinitesimal tilt symmetry of Eq. (1) ($h \rightarrow h + \mathbf{r} \cdot \boldsymbol{\epsilon}$, $\mathbf{r} \rightarrow \mathbf{r} - \lambda t \boldsymbol{\epsilon}$), the two critical exponents are related by the scaling relation $\chi + z = 2$, which is believed to be valid at any dimension d [2].

After decades of intense work in the field, the determination of the two critical exponents χ, z is known rigorously only for $d = 1$ where a fluctuation-dissipation relation leads to the exact result $\chi = 1/2$, $z = 3/2$. At any $d > 1$ the quest for the quantification of the critical exponents is still an open challenge. In particular, in $d = 2$ there is a long-standing conjecture dating back to the seminal paper of Kim and Koesterlitz (KK) [3], which proposes $\chi = 2/5$, $z = 8/5$. Such a conjecture has been supported by a Flory type scaling argument in [4] and later by a field theoretical operator product expansion in [5]. More recently, a nonperturbative renormalization group approximation reported a value of $\chi = 0.33$ [6,7] which, as we will see in the following, is too small compared with our precise measurements. From a numerical point of view the KK conjecture has been put under scrutiny many times in the past [8–15] using different

models belonging to the KPZ universality class and different simulation techniques.

In Table I we resume, to the best of our knowledge, the current state of the art with respect to the numerical check of the KK conjecture: although the statistical uncertainty (when presented in the reference paper) is often too large to exclude the validity of the KK conjecture, yet it is somehow clear that all results fall somehow below the predicted rational guess. Another common feature reported in the previously cited bibliography, is that finite-size scaling corrections to the exponent estimate seem to be particularly relevant, although very few works so far have implemented a systematic procedure to take them into account.

Here, we will investigate the steady state scaling regime $t \gg L^z$ of a restricted solid on solid (RSOS) model for lattice size volumes up to $V = 480^2$ of a very large number of

TABLE I. In this table we display the estimates in different previous work for the exponent χ (with the uncertainty when available), the model used [HSM = hypercubic stacking model, BCSOS = body centered solid-on-solid, KPZ is the direct integration of Eq. (1), BD = ballistic deposition, DLC = dimer lattice gas is a mapping to a discrete model described in detail in [13], DPRM = direct polymer in random medium], and the integration method used (MC = Monte Carlo, FSS = finite-size scaling). The estimate and uncertainty of the last row is obtained by averaging over two results obtained on simple cubic lattices with Gaussian and uniform bond, respectively.

Reference	χ	Model	Annotation
[16]	0.385(5)	HSM	MC
[8]	0.38(1)	BCSOS	FSS
[9]	0.38(8)	RSOS	Nonlinear measures
[10]	0.393(3)	RSOS	Multispin coding and FSS
[11]	0.366, 0.363	BD	MC and FSS
[12]	$0.38 \leq \chi \leq 0.40$	KPZ	Direct integration
[13]	0.377(15)	DLC	MC and FSS
[14]	0.393(4)	DLC	Bit-coded MC on GPUs and FSS
[15]	0.388	KPZ	Eulerian integration
[15]	0.385(4)	DPRM	Transfer matrix method

TABLE II. In this table we display the lattice linear size L , the base 2 logarithm of the number of Monte Carlo sweeps (full lattice updates), and the number of samples produced in our simulations.

L	\log_2 (No. sweeps)	No. samples
26	24	96
30	24	1140
40	27	30
60	26	280
80	27	60
120	27	312
160	27	156
240	27	305
320	27	492
480	25	687

surface samples to reduce as much as possible the statistical error in the estimate of the critical exponent. The RSOS model can be simulated in the following way: at any time t we randomly select a site i on the d -dimensional lattice and we let the surface height h_i at that point grow of a unit $h_i(t+1) = h_i(t) + 1$ only if $\max_{j \in \partial_i} |h_i(t) - h_j(t)| \leq 1$, where with ∂_i is the set of four nearest neighbors of i in $d = 2$ assuming periodic boundary conditions. We used an improved multispin coding algorithm which has already been described in detail elsewhere [17]. We simulated two-dimensional lattices of volume $V = L^2$ for lattices of linear size $L = 26, 30, 40, 60, 80, 120, 160, 240, 320, 480$. A summary of our simulations is provided in Table II.

The numerical strategy adopted here is to achieve a fair statistical sampling of the asymptotic regime $t > L^z$. At any time t and for each sample we measure the first three connected moments $w_n(L, t) = \sum_{i=1}^V (h_i(t) - \langle h(t) \rangle)^n / V$, where $\langle h(t) \rangle = \sum_{i=1}^V h_i(t) / V$, and $n = 2, 3, 4$. Eventually, we define our asymptotic (in time) estimate as

$$w_n(L) = \frac{1}{T_0 - T_1 + 1} \sum_{t=T_1}^{T_0} w_n(L, t). \quad (3)$$

In this way in practice we just consider the second half of the simulation being able at the same time to judge how deep in the

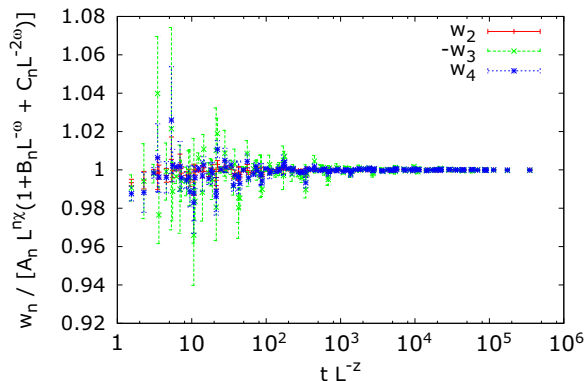


FIG. 1. (Color online) Scaling plot of the rescaled second moment $w_2 / [A_2 L^{2\chi} (1 + B_2 L^{-\omega})]$ vs the rescaled time t / L^z .

TABLE III. In this table we display the lattice linear size, the minimal lattice size from which we start fitting the data; the best-fit estimates of the exponents χ and ω ; the variance of the reduced χ square per degree of freedom ($\sqrt{\text{WSSR}/\text{NDF}}$), and the number of degrees of freedom.

FIT I Eq. (4)				
Starting L	χ	ω	$\sqrt{\text{WSSR}/\text{NDF}}$	NDF
26	0.3904(4)	0.9(1)	8.53	22
30	0.3903(4)	0.9(1)	8.41	19
40	0.3898(5)	0.9(1)	5.36	16
60	0.3893(6)	0.9(2)	3.22	13
80	0.3892(7)	0.9(3)	2.40	10
FIT II Eq. (5)				
26	0.3869(4)	0.57(5)	1.2085	19
30	0.3866(6)	0.53(6)	1.27627	16
40	0.3868(7)	0.5(1)	1.22814	13
60	0.383(4)	0.3(2)	1.09807	10

asymptotic regime ($t \gg L^z$) our simulations are: Fig. 1 shows clearly that our data for all lattice size produce a fair sampling of the steady state regime. We already mentioned how relevant finite-size scaling correction to the critical exponent is in two-dimensional KPZ. To keep the size dependence of the scaling under control in a reliable way we opted to fit simultaneously the first three moments $w_{2,3,4}$, which at the leading order, scale as $L^{n\chi}$ with $n = 1, 2, 3$. The first order corrections to the scaling are encoded in the exponent ω in the following way [10,17]:

$$\begin{aligned} w_2 &= A_2 L^{2\chi} (1 + B_2 L^{-\omega}), \\ w_3 &= S A_2^{3/2} L^{3\chi} (1 + B_3 L^{-\omega}), \\ w_4 &= K A_2^2 L^{4\chi} (1 + B_4 L^{-\omega}). \end{aligned} \quad (4)$$

As we will see in the following, finite-size scaling corrections turn out to be particularly severe, so we analyzed our data

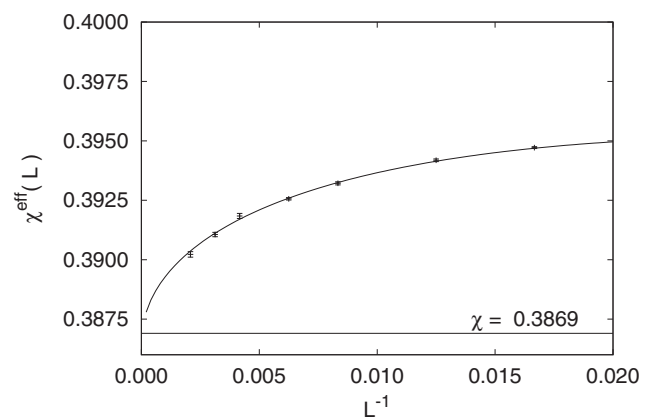


FIG. 2. Local slope of w_2 is displayed as a function of L^{-1} . Dots with error bars are values obtained by simulations, while the line is the 11-parameters best fit reported in Table IV. The solid horizontal line is at $\chi = 0.3869$, i.e. the best-fit prediction for the wandering exponent. The highest tick on the y axis is 0.4, which is the KK conjecture.

TABLE IV. In this table we display the best-fit values together with their statistical error of the parameters defined in Eqs. (4) and (5).

	χ	ω	A_2	B_2	C_2	S	B_3	C_3	K	B_4	C_4
FIT I	0.3893(6)	0.8(2)	0.118(1)	-0.4(2)	NA	-0.2669(4)	-1.1(6)	NA	3.146(2)	-0.9(5)	NA
FIT II	0.3869(4)	0.57(5)	0.1226(1)	-0.37(2)	0.6(2)	-0.2657(4)	-0.46(7)	-1.0(1)	3.145(1)	-0.73(6)	1.0(3)

using the following second order fitting scheme:

$$\begin{aligned}
 w_2 &= A_2 L^{2\chi} (1 + B_2 L^{-\omega} + C_2 L^{-2\omega}), \\
 w_3 &= S A_2^{3/2} L^{3\chi} (1 + B_3 L^{-\omega} + C_3 L^{-2\omega}), \\
 w_4 &= K A_2^2 L^{4\chi} (1 + B_4 L^{-\omega} + C_4 L^{-2\omega}).
 \end{aligned} \quad (5)$$

The relevance of the finite-size scaling corrections is best appreciated from Table III, where we display, as a function of the minimal linear lattice size, the outcome of the fit. As far as the scheme proposed in Eq. (4) is concerned, we see clearly how the larger the lattice size, the lower the best-fit value for χ . The variance of the reduced χ square, although decreasing sensibly in the size interval considered, due to the extreme precision in our estimation of the moments, remains too large. The scenario becomes even more satisfactory with the second fitting scheme defined in Eq. (5) where, upon increasing the minimal lattice size, the resulting best-fit values remain remarkably stable with a reduced χ square around 1. For these reasons we choose Eq. (5) as best fitting scheme using as minimal linear size $L = 26$. Our final estimate yields $\chi = 0.3869(4)$ and $\omega = 0.56(5)$, and the best-fit values for the two fitting schemes are reported in Table IV. The values $\chi = 0.33$, $\omega = 0.7$ reported in [6,7] are still far from our numerical estimate.

To appreciate more clearly the finite-size effects on χ , we evaluate the effective exponent χ_2^{eff} as the discrete logarithmic derivative of Eqs. (5), which in our case reads

$$\chi_2^{\text{eff}}(L) = \frac{\log\left(\frac{w_2(L)}{w_2(L')}\right)}{2 \log\left(\frac{L}{L'}\right)}, \quad (6)$$

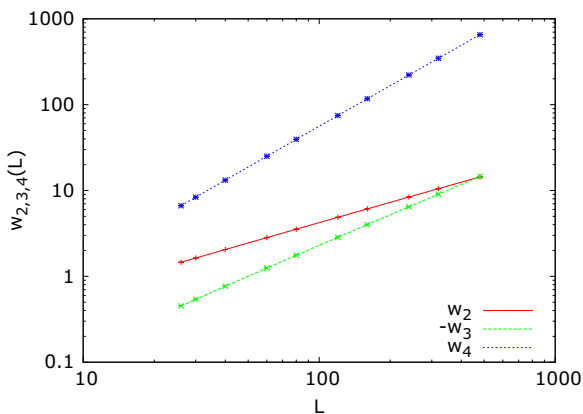


FIG. 3. (Color online) The quantities $w_2, -w_3, w_4$ obtained by the best-fit value of Eq. (5) are displayed as a function of L (lines) on double logarithmic scale. Dots with error bars are values obtained by simulations. Note that all w_2 values are larger than one even for the smaller lattice sizes.

where $L/L' = 2$. In Fig. 2 we display χ_2^{eff} as a function of L^{-1} and we superpose to the data points the best-fit estimate for χ . Note also how the effective exponent, upon increasing the lattice size, departs substantially from the KK conjecture value $\chi_{\text{KK}} = 2/5 = 0.4$, which in Fig. 2 coincides with the upper extremal y -axis tick.

A matter of concern, when studying numerically scaling related properties of system at criticality, is the ability to define how deeply inside the critical phase the system under study is. For a discrete model such as RSOS, a practical way to check this property is to compare to the typical size of the fluctuations (given by w_2) with the lattice spacing, which in our model is equal to 1 [18]. In Fig. 3 we display the values of $w_{2,3,4}$ measured in our simulations as a function of the linear size of the systems. We can easily convince ourselves that all our simulations are characterized by typical fluctuations which are larger than the lattice spacing. At odds with what happens in $d = 1$, where in the asymptotic regime the fluctuations of the surface are known to be Gaussian, the moments of the distribution show a strong departure from the $d = 1$ case. This is best appreciated in terms of the ratio of the cumulants $R_4 = w_4/w_3^2$ vs $R_3 = w_3/w_2^{3/2}$ as shown in Fig. 4, where a scatter plot of R_4 vs R_3 is shown (note that increasing lattice sizes are from right to left). The linear scaling behavior of the plot was already observed in [8,10], and here again is clearly indicating a strong departure from a normal distributed fluctuation of the surface, as $R_4^{\text{Gauss}} = 3$.

The numerical technique we developed [17], allowed us to run very accurate numerical simulations of the RSOS model in $d = 2$. We have been able to estimate with an unprecedented accuracy the critical exponent $\chi = 0.3869(4)$ in a reasonable amount of computational time. The typical fluctuations length

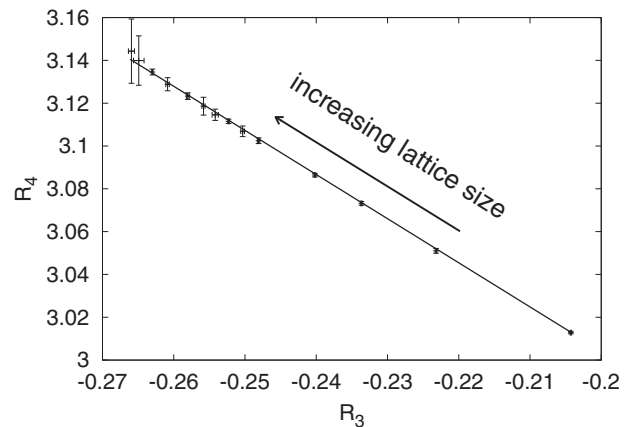


FIG. 4. Scatter plot of the ratio of the cumulant $R_4 = w_4/w_3^2$ vs $R_3 = w_3/w_2^{3/2}$. The continuous line is the linear fit to the data. Note that the lowest tick in the y axis should represent the value of the R_4 ratio for a normal distribution.

scale of our simulations and our careful finite-size scaling analysis clearly indicate that (i) the system reached a controlled scaling regime, (ii) the measured scaling exponents are reliable and not affected by a preasymptotic crossover regime, and (iii) the distribution of the fluctuations is non-Gaussian. A shrewd use of the simultaneous fit of the three cumulants as a function of the lattice size, we are finally able to disprove the KK conjecture that the value of the exponent $\chi = 2/5$, a figure

that, given the small statistical uncertainty of our estimate, lays at more than 32 standard deviations away from our prediction.

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