GROWTH IN SCALE INVARIANCE

Marcel den Nijs
Department of Physics, University of Washington, P.O. Box 351560, Seattle, Washington 98195-1560

What set physics apart from most other disciplines is the drive to discover universal unifying laws of nature. This involves typically digging deeper and deeper into the building blocks of nature. In condensed matter research we often go the opposite way. Instead of cutting up the elements we combine them into stews. Out of this complexity, simplicity can arise as well. One of the most impressive recent examples is the quantum Hall effect. Consider two dimensional (2D) liquid of electrons confined inside a metalic interface layer of a semi-conductor device like GaAs. Make sure it has good electron mobilitiy, but do not care too much about dirt (disorder). Add a perpendicular magnetic field of 10 Tesla, and serve this two dimensional (2D) electron soup at a cool 1 degree Kelvin. Miraculously you can measure $e^2/\hbar$, in terms of the quantum Hall plateaus with an accuracy better than 1 in 10^7. This to the amazement of our atomic physics friends who measure similar fundamental constants of nature by trapping single atoms. (David Thouless referring to a discussion with Hans Dehmelt [1].)

Scale invariant phenomena in strongly fluctuating systems, represent another realization of "simplicity arising out of complexity". The classic examples are critical points in equilibrium statistical mechanics, e.g., those in physisorption on flat substrates. Adsorb one monolayer of He^4 on graphite, one atom for every third puddle in the triangular graphite substrate array. At a few degrees Kelvin, an ordered low temperature structure appears, the so-called $\sqrt{3} \times \sqrt{3}$ phase [2]. The He^4 atoms form a periodic structure with as lattice constant the distance between next nearest neighbour adsorption sites. At the critical point where this order vanishes, the specific heat diverges as $C_v \sim |T - T_c|^\alpha$. The critical exponent α can be measured with an accuracy of a few percent. Its exact value is $\alpha = \frac{1}{3}$ [3,4]. This value is universal, i.e., insensitive of what type of adsorbate orders into the $\sqrt{3} \times \sqrt{3}$ structure (e.g. Kr and N_2 monolayers).

At critical points the correlation length diverges and the large scale fluctuations associated with this are scale invariance. Universality, arises due to insensitivity of those large length scale fluctuations to "most" microscopic details. Only the symmetries of the $\sqrt{3} \times \sqrt{3}$ structure and dimensionality matter. The only danger is to miss spotting some of those symmetries. Not until experimentalists observed incommensurate monolayer structures did it dawn to us theorists that the free energies of the interfaces between the 3 coexisting phases involve chirality [5].

Scaling and universality are well established for 3D equilibrium criticality from very accurate numerical and experimental results, and from the presence of a controllable fixed point (in the sense of renormalization theory) down from an upper-critical dimension. In 2D we are fortunate that in addition to all of the above a free field theory description exists for almost all types of critical phenomena in terms of so-called Coulomb gas representations and conformal field theory [6,5]. 2D critical phenomena are truly exactly solved.

The battle for universality in equilibrium critical phenomena was fought during the 1960's and 1970's at a very detailed level. This was in particular in the context of gas-liquid type critical points. The ultimate acceptance of universality required an accuracy of experimental and theoretical data better than 1%. This attitude has changed dramatically. Students learn about scaling early-on, and take it for granted. Nowadays it is more difficult to convince someone that a phenomenon lacks simple scaling (with only one diverging length scale) than the opposite.

During the last decades, we have been taking scaling and universality on the road. Armed with computers (replacing an unfortunate weakness in experimental input) and with the gospels of scale invariance and universality in hand, we tackle many interesting dynamic stochastic phenomena, like surface growth, surface catalysis, highway traffic, granual materials, and so on. In the following I illustrate some of this in the context of so-called KPZ surface growth [7], which is one of the best known and well studied non-equilibrium stochastic processes [8].

KPZ type growth, is named after a 1986 study by Kardar, Parisi, and Zhang [7] of the Langevin equation

$$\frac{dh}{dt} = v_0 + \nu \vec{\nabla}^2 h + \frac{1}{2}\lambda(\vec{\nabla} h)^2 + \eta \tag{1}$$

with uncorrelated Gaussian noise

$$\langle \eta(\vec{r}_1, t_1)\eta(\vec{r}_2, t_2)\rangle = 2\Gamma\delta(\vec{r}_1 - \vec{r}_2)\delta(t_1 - t_2) \tag{2}$$

$h(\vec{r})$ is a height variable defined with respect to an arbitrary reference level. The surface profile is presumed to be single valued. Features like dendritic growth are therefore not addressed. Eq.(1) reads like a Monte Carlo (MC) simulation rule. The local surface height is updated in two stages. First the deterministic part of the growth rate is added, i.e., v_0 modified by the local curvature of the surface (the ν-term), and the local slope (the λ-term). Next, fluctuations are introduced by adding a random number (the η-term). Eq.(1) follows the evolution of one specific sample of the ensemble.

The non-linear λ-term is the soul of the KPZ equation. Without it the equation is linear and trivially soluble. Surface growth in which λ is accidentally tuned-off is known as Edwards-Wilkerson growth. Studies of such linear equations date back to at least the 1950's.

λ is a relevant perturbation. Imagine a renormalization transformation (RT). First all degrees of freedom at length scales $a \leq r < ab$ are removed; a is the lattice cut-off and $b > 1$ is an arbitrary parameter close to unity. This reduction in the resolution does not affect the fluctuations at larger length scales, because at $\lambda = 0$ the theory is linear, and all modes decouple. Next, the cutoff is restored, by rescaling all parameters as $r' = r/b$, $t' = t/b^z$, $h' = h/b^\chi$, and $\lambda' = b^{y_\lambda}\lambda$. We presume that Γ and ν do not rescale ($y_\Gamma = y_\nu = 0$) because we like to compare surfaces with the same noise strength and with the same curvature correction to the growth velocity. Eqs.(1-2) are invariant under this rescaling transformation when the dynamic exponent is equal to $z = 2$ and $\chi = y_\lambda = (2-D)/2$. In $D \leq 2$, $y_\lambda > 0$ is positive, which means that λ appears larger under reduced resolution.

The λ term is generically present in growth proceses, in the sense of Landau theory, and must be included because it is a relevant perturbation. All other higher order terms are generically present as well, but can be neglected because they are irrelevant perturbations, as can be checked easily by the above RT using power counting. They vanish under resolution reduction.

The KPZ equation is equivalent to the Burgers equation for randomly stirred fluids.

$$\frac{d\vec{v}}{dt} + \lambda \vec{v} \cdot \vec{\nabla}\vec{v} = \nu \vec{\nabla}^2 \vec{v} + \vec{f}(\vec{r}, t) \tag{3}$$

This is a vortex free (zero curl) type fluid flow, for which the velocity field obeys the potential form $\vec{v}(r) = -\vec{\nabla}h(r)$. ν now represents viscosity, and $\vec{f} = -\vec{\nabla}\eta$ a random curl-free stirring force. The non-linear term arises here logically as part of the total derivative of the velocity; as conservation of momentum in the absence of viscosity and stirring. The Burgers equation predates the surface growth interpretation by far. The ϵ-expansion type RT (beyond the above zero-loop approximation) was worked out already three decades ago [9].

Unfortunately this RT approach leaves us empty handed. It does not yield a controllable KPZ fixed point. 2D plays the role of critical dimension, but, because the RT equations are third-order in λ, the change in stability of the $\lambda = 0$ fixed point is achieved by spawning-off two new fixed points instead of by a crossing with a single non-trivial one (as in conventional ϕ^4-theory). These 2 new fixed points appear at $D > 2$ and have no bearing on KPZ scaling. They describe the crossover from stable EW growth at small λ to KPZ scaling at large λ. KPZ growth is an intrinsic strong coupling phenomenon. The KPZ fixed point has not been sighted yet (except in 1D, which is very special).

The Burgers equation confirms this intrinsic strong coupling aspect. The stochastic fluid flow must look the same to all moving observers, i.e., obeys Galilean invariance. This implies that λ should not be renormalized. Instead of ν we should choose λ to be invariant under the RT. The relation $z = 2$, implied by the $y_\nu = 0$ choice, is replaced by $\chi + z = 2$ in this new $y_\lambda = 0$ gauge. This exponent relation is well established numerically, and is one of the few firm results for KPZ scaling [8].

The moments of the height distribution

$$W_n(L,t) = L^{-1} \sum_{\vec{r}} \langle (h_{\vec{r}} - h_{av})^n \rangle \tag{4}$$

scale as

$$W_n(L,t) = b^{\alpha_n} W_n(b^{-1}L, b^{-z}t) \tag{5}$$

with L the lattice size. Unlike models for turbulence, multi-scaling is believed to be absent, such that the exponents obey the relations $\alpha_n = n\chi$. Eq.(5) is a finite size scaling relation. Under a rescaling of all lengths, as $r' = r/b$, the interface is invariant if time is rescaled, as $t' = b^{-z}t$, and height as $h' = b^{-\chi}h$.

The non-linear λ term is absent in equilibrium dynamics because of detailed balance. Equilibrium surface roughness is therefore universal with exponent $\chi = (2-D)/2$. In particular, 2D equilibrium interface widths scale as $W \sim \log(L)$. During KPZ type growth the surface is much rougher.

The Kim-Kosterlitz (KK) model in one of many KPZ type lattice growth models. Such models provide direct tests of universality; as equilibrium Ising type models do with respect to ϕ^4-theory. In the KK model the atom stacking is simple cubic, with as constraint that nearest neighbour columns can differ by at best one, $S^z(\vec{r}, \vec{r}') = h_{\vec{r}} - h_{\vec{r}'} = 0, \pm 1$. These spin type bond variables represent a discretized lattice version of the Burger equation velocity field. The MC update rule is as follows. After choosing a column at random, a particle can deposit with probability p or disorb with probability q, irrespective of the local surface configuration except for the $S^z = 0, \pm 1$ constraints.

A second important lattice version of KPZ growth is the body-centered solid-on-solid (BCSOS) model. Here the atoms can be viewed as rectangular bricks, with an alternating stacking. The surface heights at the black checkerboard fields are even integers and those at the white fields are odd. The velocity field spin variables can take only two values, $S^z(\vec{r}, \vec{r}') = \pm 1$. The BCSOS model is exactly soluble in 1D by the Bethe Ansatz [11]; the master equation represents a special line in the famous 6-vertex model. The critical exponents are $\alpha = \frac{1}{2}$ and $z = 2 - \alpha = \frac{3}{2}$. The S^z velocity field is completely random in the stationary growing state.

As models for surface growth the above processes are rather naive. One could try to duck the issue by arguing that this is what universality is all about, and draw on the analogy with the Ising model. That is a rather crude model for a gas-liquid transition, but the large scale fluctuations do not depend on "those" details. However, in equilibrium critical phenomena we learned to be careful as well, to be certain we identified all symmetries and conservation laws that might influence the universality class of the transition. Likewise, in surface growth there are a number of details can change the scaling properties. Examples are: extra degrees of freedom (like heat flux to carry away latent heat), surface diffusion, and particle conservation. In epitaxial growth the rejection of a deposition attempt is unphysical, because a particle aimed at an unfavorable site does not vanish in thin air.

Nevertheless, there are a few experimentally confirmed KPZ processes. Fig.1 shows the time evolution of a front in slow paper combustion from the experiments by the Finish Jyvaskyla group [13]. After letting many sheets of copier and lens type paper go up in smoke and ash (it is slow flameless type combustion) they obtained statistical accurate data for the surface width exponents. At length scales larger than about $r_c \simeq 0.5$ cm the exponents agree with 1D KPZ scaling; $\beta = z/\alpha \simeq 0.35(1)$ and, as shown in Fig.2, $\alpha \simeq 0.49(2)$. Below r_c the front is rougher (visible as local bumps in Fig.1). The current discussion centers on whether this crossover is due to directed percolation type depinning or not [13].

The properties of KPZ scaling in $D \geq 2$ remain intriguing. Recent analytical progress forces us to push towards more accurate numerical simulations. Lässig [12] derived a quantization condition for the stationary state roughness exponents, $\chi = 2/k$ with $k > 3$ an odd integer, under the assumption that an operator product expansion exists and also that the spectrum lacks multiscaling. The dimension is not specified, but the first two values, $\alpha = 2/5$ and $\alpha = 2/7$, are close to the numerical 2D and 3D results. The challenge is to show numerically whether this theory is correct, and if so to build on it, to gain analytic insight into more detailed aspects of the stationary state distribution such as amplitude ratios of its moments.

Until recently, the 2D numerical values were surprisingly inaccurate. For the BCSOS model, they were in the $\alpha \simeq 0.38$ range, while for the Kim-Kosterlitz model, $\alpha \simeq 0.40$. This spread serves as an example of how much univerality is taken for granted nowadays. Nobody seems to doubt the universality of KPZ type scaling, but those data did not support it. The quoted error bars are often smaller than the spread in these numbers.

In a typical MC simulation, the width W_2, is monitored as function of time for a set of system sizes L. After an initial short time interval, where the initial condition dominates, the powerlaw $W_2 \sim t^\beta$, with $\beta = \alpha/z$ sets-in, until the width saturates at the system width. The analogy with self diffusion in a finite box might be helpful. An arbitrary shaped particle cloud (the initial state) first develops into a Gaussian wavepacket. Next, it keeps broadening and does so in a universal shape invariant manner. Finally it hits the box boundaries and reaches the uniform distributed stationary state.

A typical analysis of the data involves plotting $\log(W_2)$ versus L and looking for a straight line as shown in Fig.3 for the 2D BCSOS model. The drawn line with slope $\alpha_2 = 2\chi = 4/5$ is shown for comparision. By eye it looks as if α_2 converges to a smaller value. However, corrections to scaling powerlaws are deceptive. A proper finite size scaling analysis proceeds by creating estimates for α from sets of nearby L's (by solving $W \sim AL^\alpha$ as a set of 2 equations with 2 unknowns). Fig.4 shows such estimates as function of L for the 2D BCSOS model [14]. The data are noisy at large L, but that is to expected for MC data, and without analysing the data upto the edge of the noise we would be under utilizing their accuracy. The curve inside the data points represents averages over local ranges of L. Again, the curve seems to converge to a value $\alpha_2 < 4/5$. The definite slope indicates strong corrections to scaling of the form $W_2 = AL^{\alpha_2}(1+BL^{y_{ir}}\cdots)$. The slope is proportional to B and is not a universal property. It is a measure of the distance to the RT fixed point. Kim and Kosterlitz proposed that $\chi = 2/5$. They were lucky, in their model the slope is almost absent (virtually drowned out by MC noise), see Fig.5 [14]. The KK model must be very near the fixed point and the BCSOS model rather far away.

Assuming that $\chi = 2/5$ we can estimate the values of the leading correction to scaling exponents from the BCSOS data. We find $y_{ir} \simeq -0.6(2)$ for the even moments and $y_{ir} \simeq -1.7$ (3) for the odd ones [14]. This powerlaw fit is satisfactory stable. Still, it remains a strain to the eye. While looking at Fig(4), we tend to perform a least square fit in our head, which points to $\alpha_2 \simeq 0.38(1)$ and leaves $\alpha_2 = 4/5$ beyond the error bar. The pitfall is that corrections to scaling with exponents $y_{ir} > -1$ converge very slowly. This serves as example of how easily it is to underestimate error bars in scale invariant phenomena.

The above finite-size scaling analysis does not prove that KPZ universality exists, nor that the Kim-Kosterlitz-Lässig conjecture is correct. It merely shows that both assumptions are consistent with the current data. We need to push the numerical accuracy by at least one more order of magnitude before we can put these issues to rest.

The most intriguing aspect of KPZ type growth is the nature of universal stationary state. In 1D it is still a simple Gaussian, and skewness appears only in the form of finite size corrections to scaling [15]. In higher dimensions the stationary state is intrinsically skewed. The odd moments of the distribution are non-zero. The physical visualization of skewness, is of a landscape where on average hill tops are wider (flatter, less sharp) than valley bottoms. Such a statement is meaningless without the specification of a cut-off. The definition of what constitutes a mountain and what represents a local hump depends on the length scale at which the surface configuration is being viewed. (Humans do not interpret grains of sand as hills.) Skewness is a scale dependent property. The asymptotic scaling of the moments tells us how asymmetric the hills and valleys are in the large length scale limit.

The amplitude ratios $R_n = W_n/(W_2)^{\frac{n}{2}}$ characterize such aspects of the universal stationary state distribution. We find numerically, $R_3 = -0.27(1)$ and $R_4 = +3.15(2)$ [14]. Their BCSOS and KK model values agree much better than the large spread in the absolute values for the α_n would suggest. Universal amplitude ratio's like this can only be the beginning. More details of the universal stationary state need to follow, in particular within the context of Lässig's theory.

The identification of other surface growth universality classes, besides KPZ growth, is well on its way. This can be addressed by ad-hoc modifications of the KPZ equation, e.g., by addding extra degrees of freedom, or by changing the white (Markovian) noise into correlated noise [8]. The mapping-out of global phase diagrams is another route to research such issues.

The KK model is a special point in the so-called Restricted solid-on-solid (RSOS) model, in which the transition probabilities vary by means of temperature via the step energy,

$$E = \sum_{\vec{r},\vec{r}'} K(h_{\vec{r}} - h_{\vec{r}'})^2 \tag{6}$$

The summation runs over nearest neighbour collumns only and E and K are in units of $k_B T$. Equilibrium simulations mostly apply the Metropolis update rule (go with probability $P = 1$ when the energy is lowered, go with $P = \exp(-\Delta E)$ if it raised). A deposition bias can be introduced by multiplying the transition probabilities with deposition and desorption factors, p and q. The KK model is the infinite temperature limit ($K = 0$).

In equilibrium, a roughening transition takes place at a specific positive value of K. In driven non-equilibrium surfaces this transition does not occur. The growing surface is always rough. Near equilibrium, below the equilibrium roughening temperature, the surface grows by so-called layer-by-layer growth but at large enough length scales (which might be academically large) the growing surface is still KPZ rough.

At the $K < 0$ side of the phase diagram an Ising type equilibrium phase transition takes place. The $S^z = 0$ (no-step) degrees of freedom become frozen out at $K << 0$, and the model reduces to the BCSOS model with $S^z = \pm 1$. Which checkerboard sublattice ends up with the even or the odd heights is arbitrary. This is an Ising type spontaneous broken symmetry. In the context of surface reconstructions it represents a so-called rough reconstructed phase [16]. In our simulations for the growing surface [17] we find a peak in the susceptibility of the Ising order parameter as well, but it keeps moving with lattice size. $S^z = 0$ excitations form closed loops. Such loops are nucleated in the valley bottoms. They run up hill very fast, but then get stuck on top of a ridgeline of the fluctuating growing surface, as illustrated in Fig.6. There they stay trapped, slaved to the growth of the surface, until those KPZ fluctuations shrink the enclosed valley to zero, or until a new loop nucleates out of the valley. There is no phase transition in a pure mathematical sense. The susceptibility peak signals the crossover length scale below which the life time of trapped loops is dominated by KPZ fluctuations, and the surface looks as if reconstructed. Moreover, the KPZ fluctuations are critical and induce critical fluctuatons in this quasi-reconstruction order.

KPZ type scaling and this last example of ridgeline loop trapping are illustrations of the richness of phenomena that are being found in driven stochastic processes and other complex systems. Scale invariance and universality are generically occuring phenomena. Moreover, for some cases, like KPZ growth, analytic insight has grown to the point that the numerical accuracy required to settle the details begins to rival that of equilibrium critical phenomena several decades ago.

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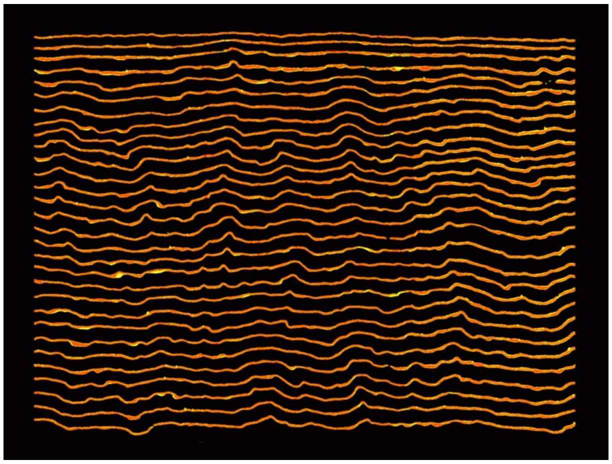

FIG. 1. Time evolution of fronts in slow paper combustion. The time steps between succesive fronts is 10 seconds. The fronts are approximately 30 cm wide.

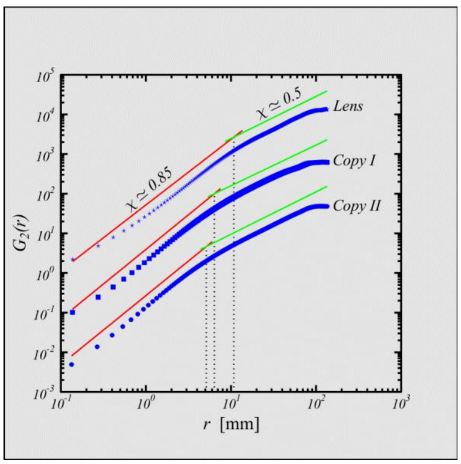

FIG. 2. Stationary state scaling of the height-height correlation function, $G(r) \sim r^{2\chi}$, in slow paper combustion experiments.

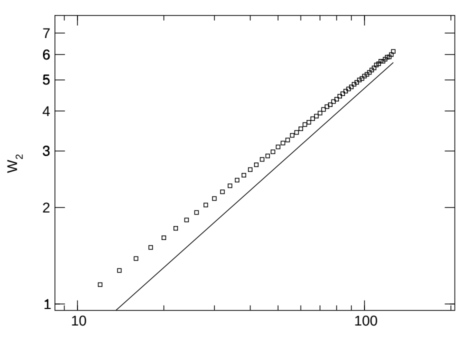

FIG. 3. Log-log plot of the surface width W_2 versus lattice size L in the 2D BCSOS model. The reference line has a slope $\chi = 2/5$.

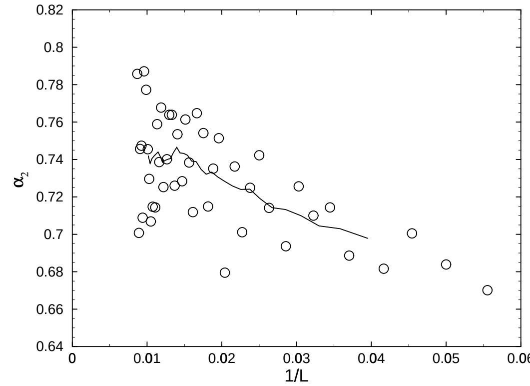

FIG. 4. Finite size scaling analysis of the surface width exponent $\alpha_2 = 2\chi$ in the 2D BCSOS model.

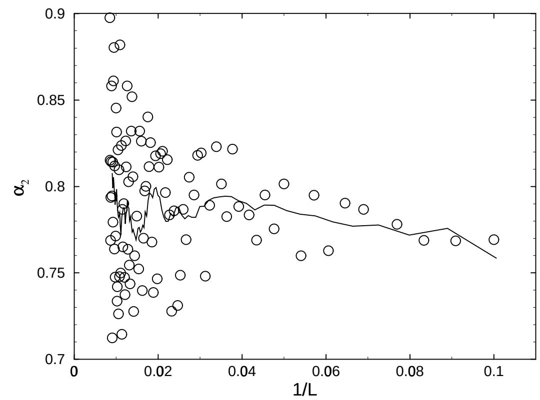

FIG. 5. Finite size scaling analysis of the surface width exponent $\alpha_2 = 2\chi$ in the 2D Kim-Kosterlitz model.

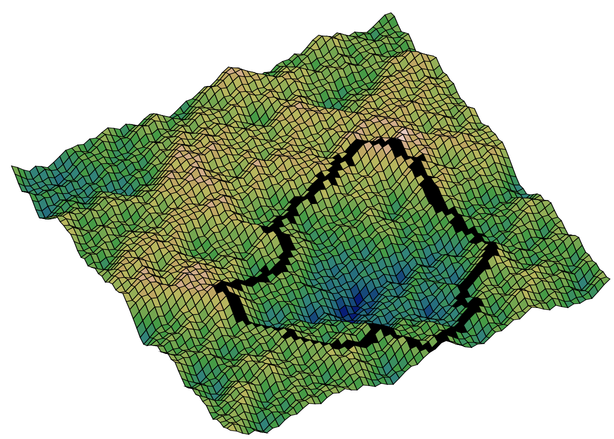

FIG. 6. Surface configuration in the RSOS model for $K << 0$ with a loop of $S^z = 0$ states trapped on surface ridgelines.