

Nonequilibrium critical dynamics: upturns from surface kinetic roughening

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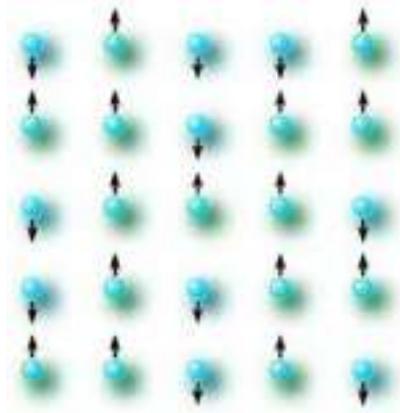


<https://sites.google.com/view/rodolfo-cuerno-rejado/home>

Outline of the talk

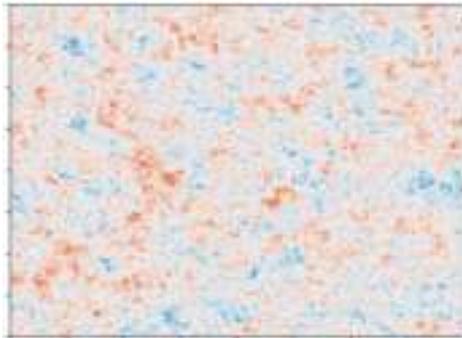
- Introduction: (non-)equilibrium critical dynamics (Ising)
- Surface kinetic roughening
- KPZ equation
- What defines a universality class?
- KPZ nonlinearity vs: Scaling exponents
 Field statistics
 Dynamic scaling ansatz
- Upturns from surface kinetic roughening (Ising)
- Conclusions

Ising model



$$\mathcal{H}_{\text{Ising}} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i, \quad s_i = \pm 1$$

$$Z = \sum_{\{s_i\}} e^{-\mathcal{H}_{\text{Ising}}/k_B T}$$



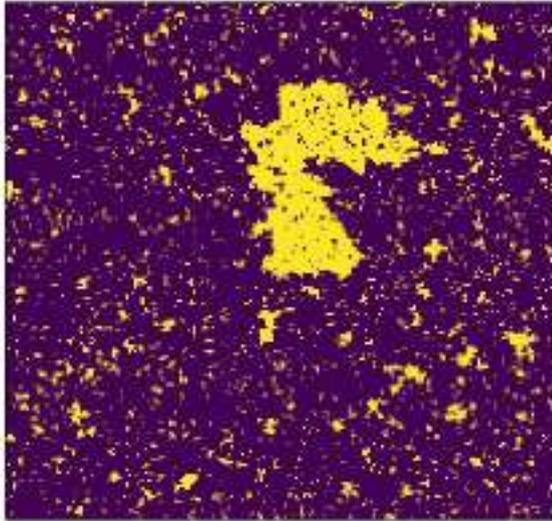
$$\text{Local magnetization } \phi(\mathbf{r}) = \frac{1}{N(\mathbf{r})} \sum_{i \in \mathbf{r}} s_i$$

$$\mathcal{L}[\phi] = \int d\mathbf{r} \left\{ \frac{r}{2} \phi^2 + \frac{u}{4} \phi^4 + \frac{\nu}{2} (\nabla \phi)^2 \right\}$$

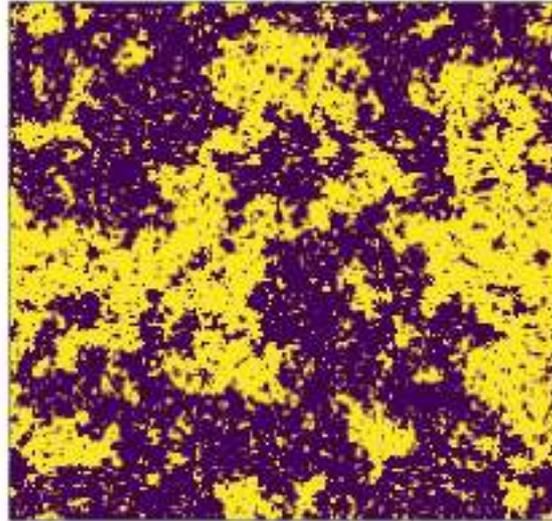
$$Z = \int \mathcal{D}\phi e^{-\mathcal{L}/k_B T}$$

Equilibrium 2nd. order (continuous) transition

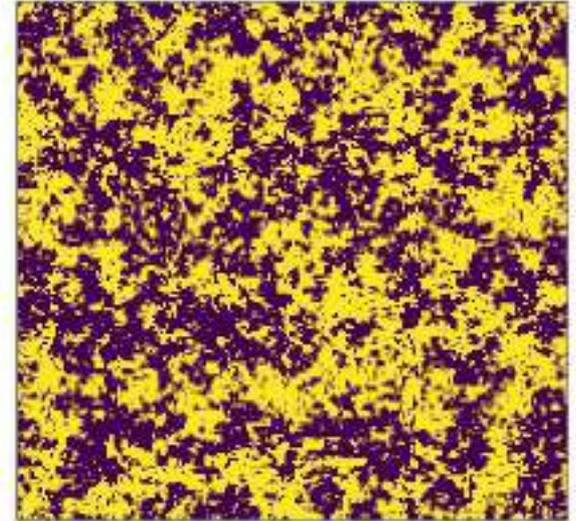
$T < T_c$



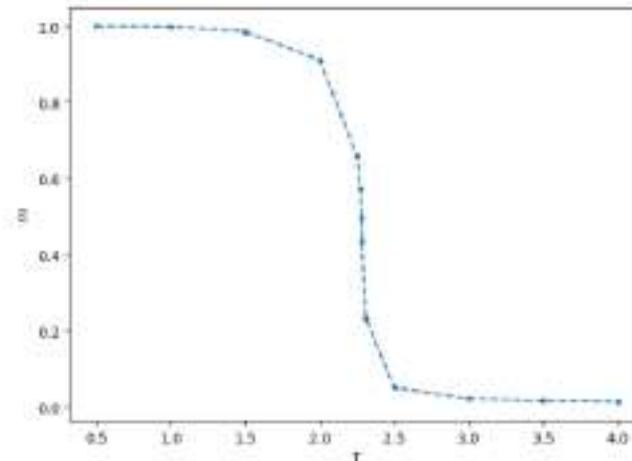
$T \approx T_c$



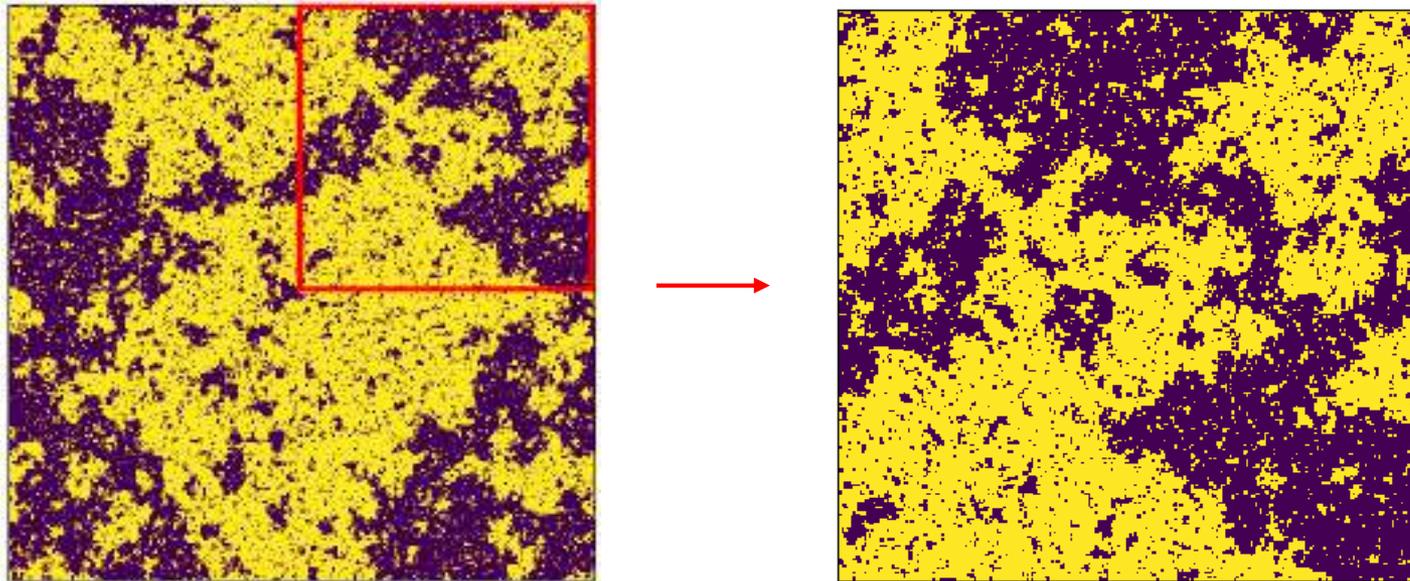
$T > T_c$



$$\langle m \rangle = \frac{1}{N} \langle \sum_i s_i \rangle$$

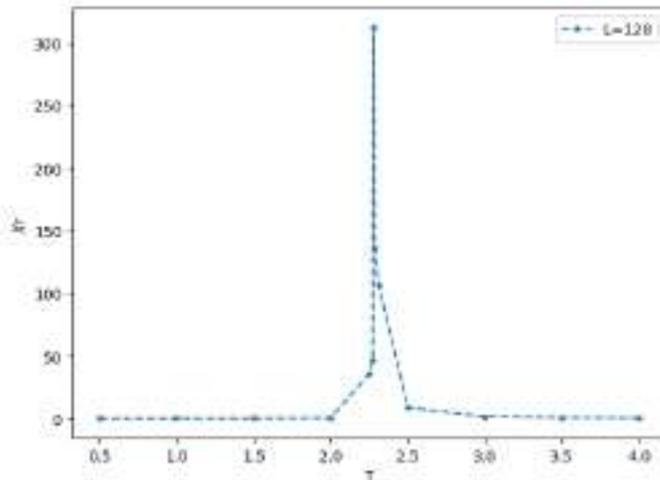


Scale invariance at $T=T_c$

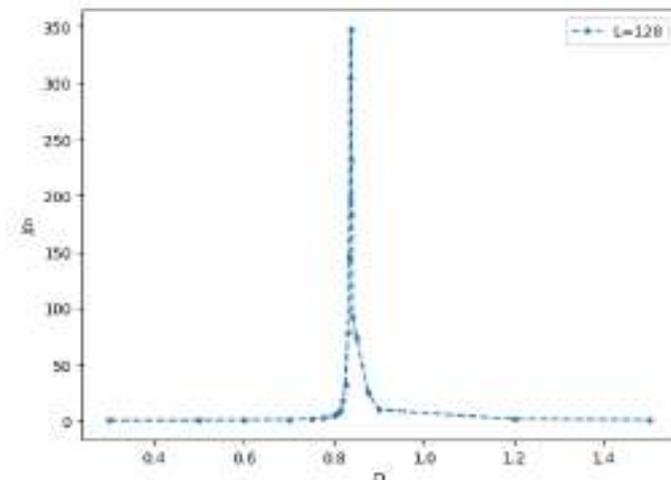


Criticality

$$\chi = \frac{\partial m}{\partial H} \propto \langle m^2 \rangle - \langle m \rangle^2$$



$$T_c = 2.277$$



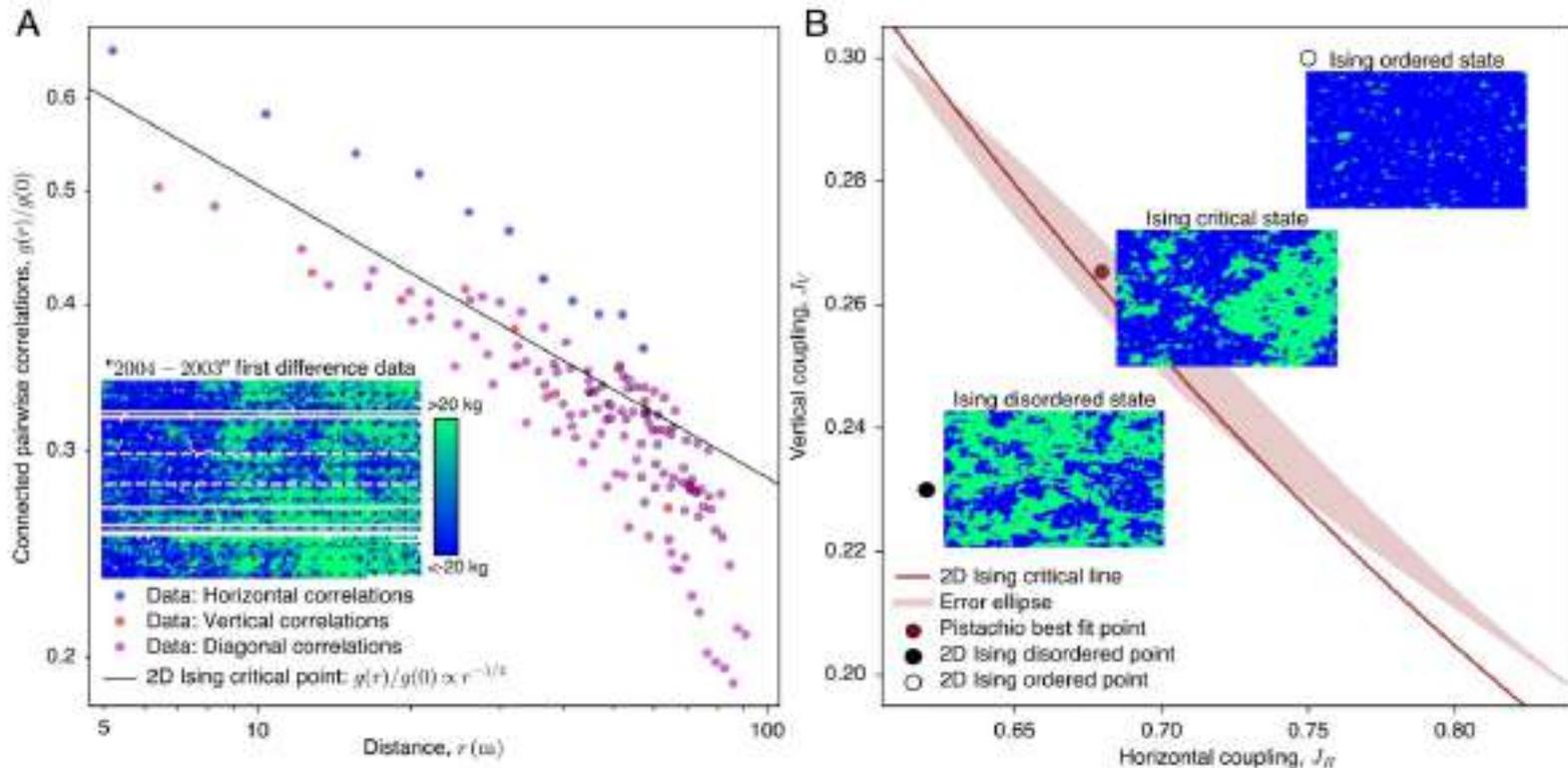
$$D_c = 0.835$$

$$\chi \propto \sum_r G_r \quad G_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$$

$$G(r) = \langle \phi(\mathbf{r}) \phi(\mathbf{0}) \rangle = \int d\mathbf{k} e^{i\mathbf{k}\mathbf{r}} \langle |\phi(\mathbf{k})|^2 \rangle \approx \int d\mathbf{k} e^{i\mathbf{k}\mathbf{r}} \frac{1}{\xi^{-2} + k^2}$$

$$T = T_c \Rightarrow \xi \rightarrow \infty \Rightarrow G(r) \sim \frac{1}{r^{d-2+\eta}} \Rightarrow \chi \rightarrow \infty$$

Oscillating populations: Pistachio production



$$\phi_{i,j} \equiv X_{i,j,2004} - X_{i,j,2003} - (X_{2004} - X_{2003})$$

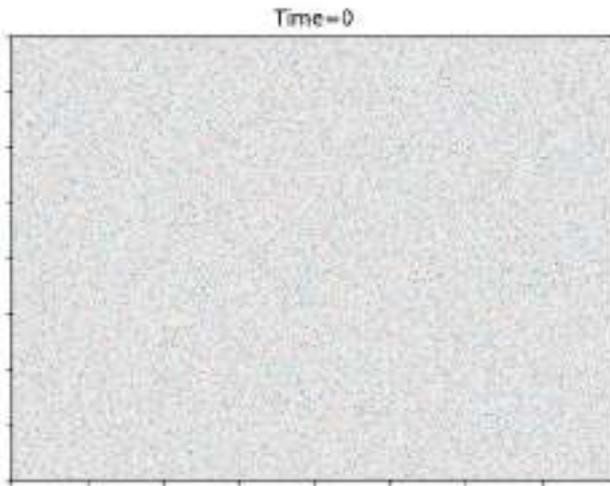
$$g_D(\Delta i, \Delta j) = \frac{1}{2N_{\Delta i, \Delta j}} \sum_i \sum_j \bar{\phi}_{i,j} \bar{\phi}_{i+\Delta i, j+\Delta j}$$

(Critical) dynamics

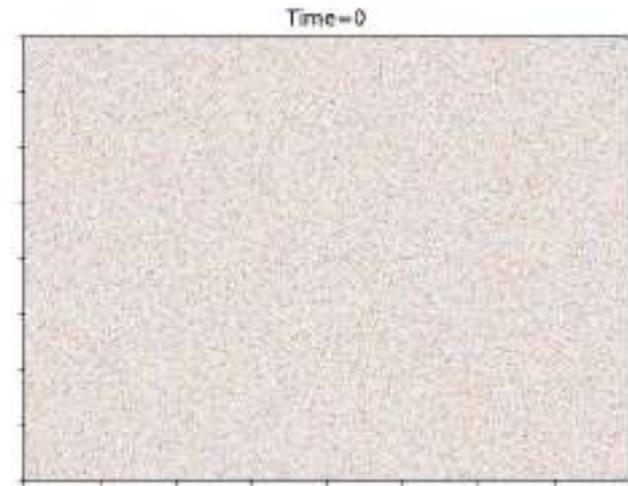
Stochastic time-dependent
Ginzburg-Landau equation (STDGL)

$$\frac{\partial \phi(\mathbf{r}, t)}{\partial t} = -r\phi(\mathbf{r}, t) - \zeta(\mathbf{r}, t) + \nu \nabla^2 \phi(\mathbf{r}, t) + \zeta(\mathbf{r}, t)$$

Subcritical ($T=0$)

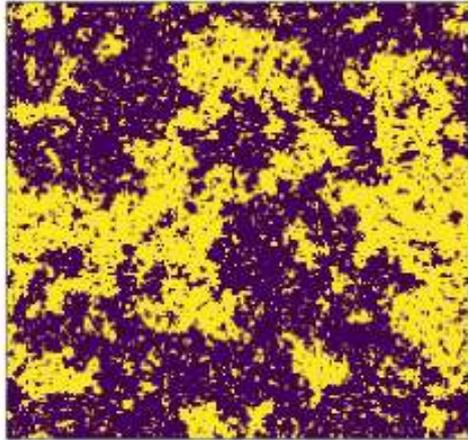


Critical ($T=T_c$)



Critical dynamics

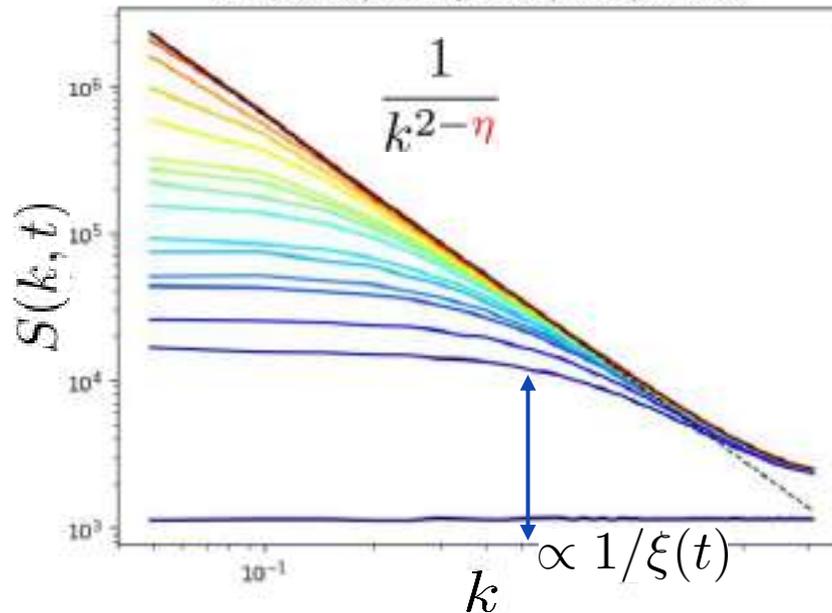
$T=T_c$



$$S(k, t) = \langle |\phi(\mathbf{k}, t)|^2 \rangle$$

$$G(r, t) = \int d\mathbf{k} e^{i\mathbf{k}\mathbf{r}} S(k, t) \xrightarrow{t \rightarrow \infty} \frac{1}{r^{d-2+\eta}}$$

GL 128x128, dim: 2, Δt: 0.1, r: 0.5, D: 0.835



$$\xi^{-1}(t) \sim \frac{1}{t^{1/z}}$$

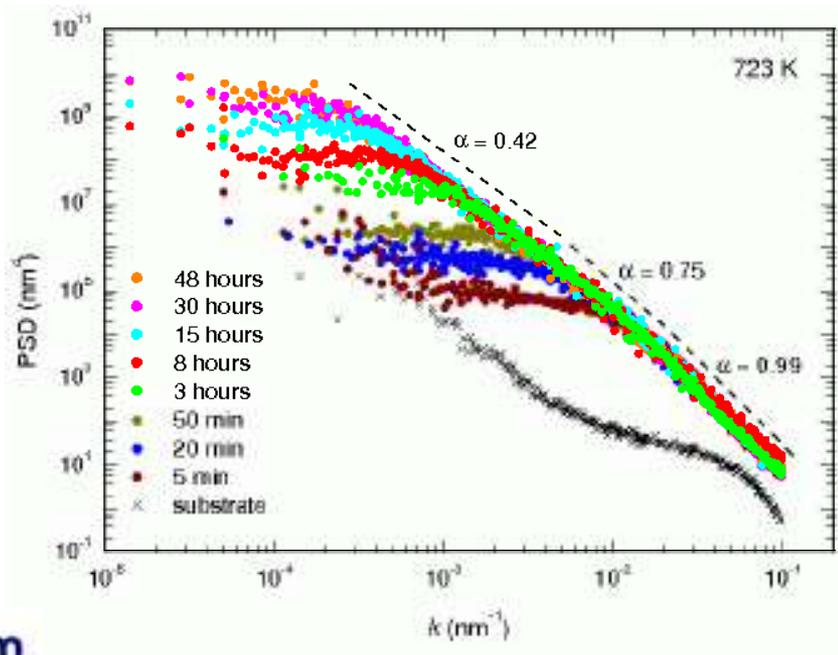
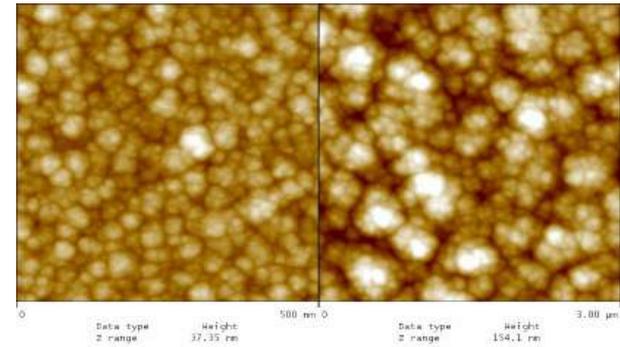
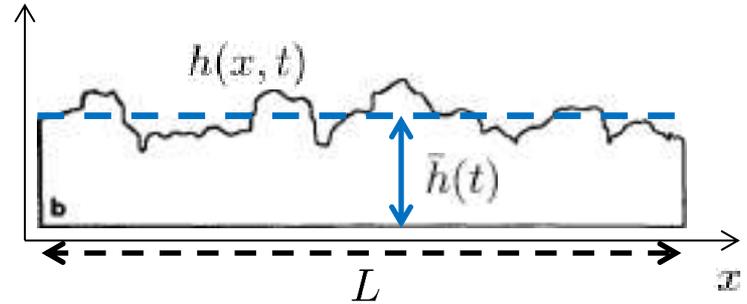
$$\phi(\mathbf{r}, t = 0) = 1$$

Surface analysis

Height power spectral density:

$$h(k, t) = \mathcal{F}(h(x, t) - \bar{h}(t))$$

$$S(k, t) = \langle |h(k, t)|^2 \rangle \rightarrow \frac{1}{k^{2\alpha+2}}$$



$$\xi^{-1}(t) \sim \frac{1}{t^{1/z}}$$



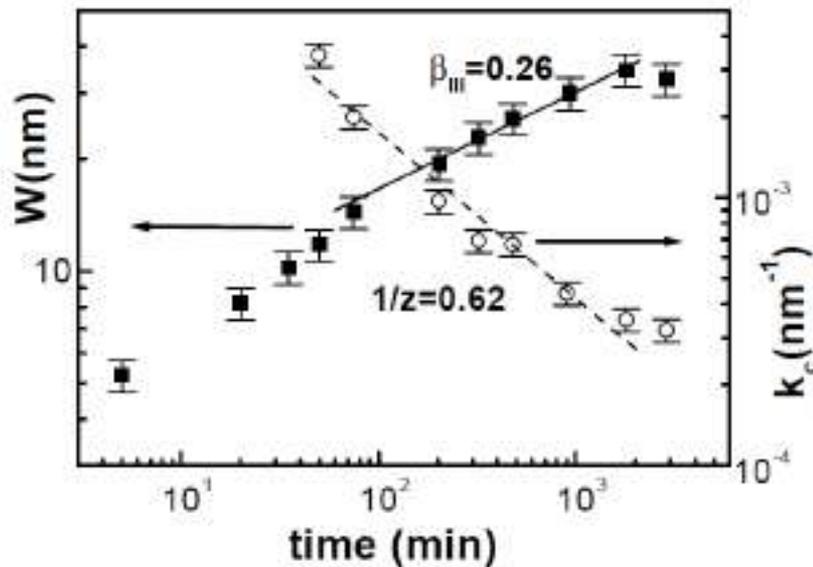
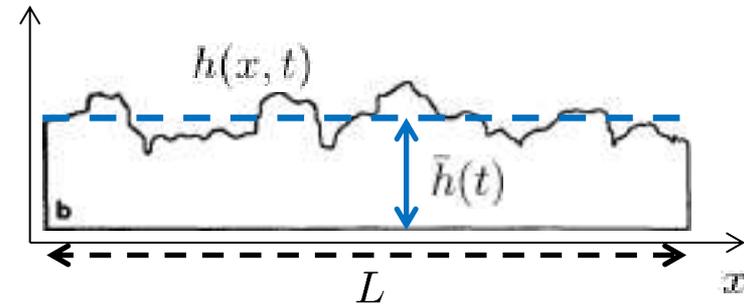
like dynamics of Ising model at $T=T_c$!

Surface analysis

Surface roughness:

$$W^2(L) = \frac{1}{L^2} \sum_x [h(x, t) - \bar{h}(t)]^2$$

$$= \sum_{k \neq 0} S(k, t)$$



$$W(t) \sim t^\beta$$

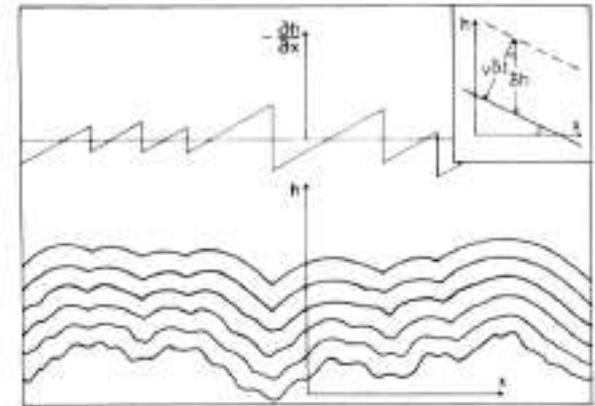
$$\beta = \frac{\alpha}{z}$$

Kardar-Parisi-Zhang equation

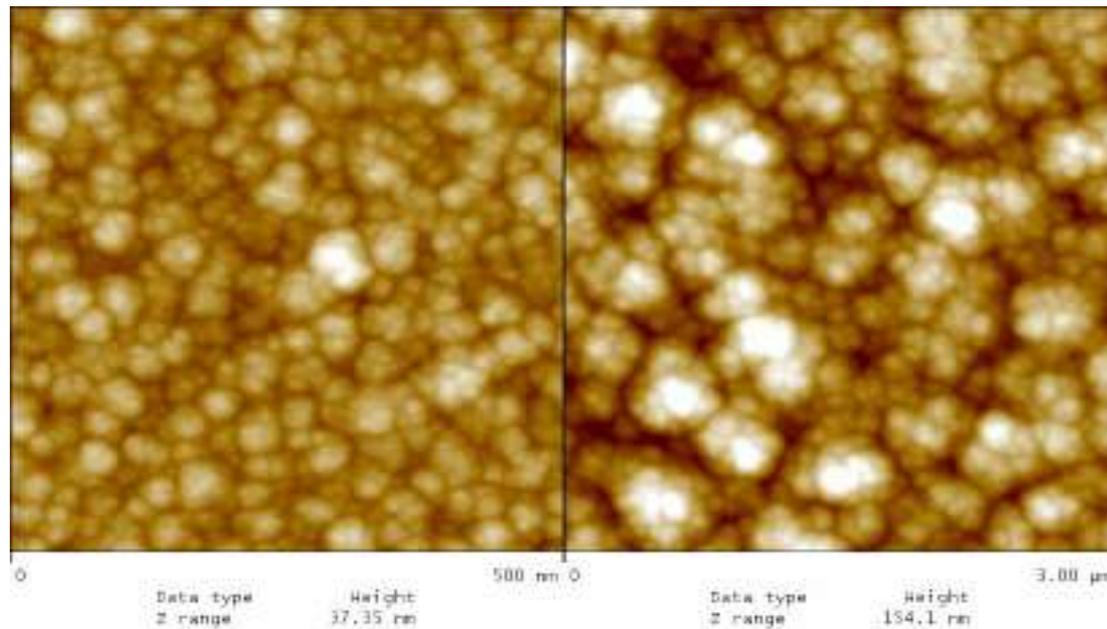
$$\partial_t h = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta$$

$$\langle \eta(\mathbf{r}, t) \eta(\mathbf{r}', t') \rangle = D \delta(\mathbf{r} - \mathbf{r}') \delta(t - t')$$

M. Kardar, G. Parisi & Y.-C. Zhang Phys. Rev. Lett. **56**, 889 (1986)

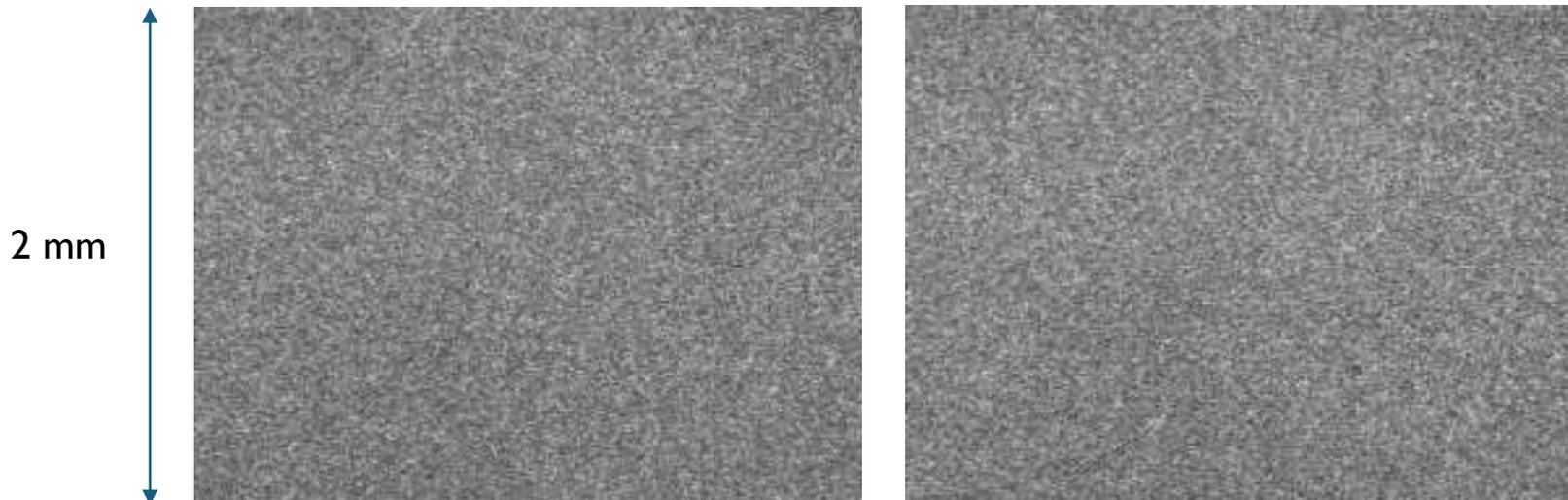
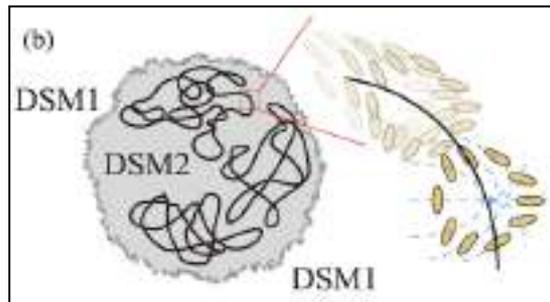


SiO₂ on Si
AFM top view



I+I KPZ universality: experiments + equation

Driven liquid crystals: laser-induced nucleation of favorable turbulent phase



I+I KPZ universality: experiments + equation

$$\frac{\partial h}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta$$

T. Sasamoto & H. Spohn PRL **104**, 230602 (2010)

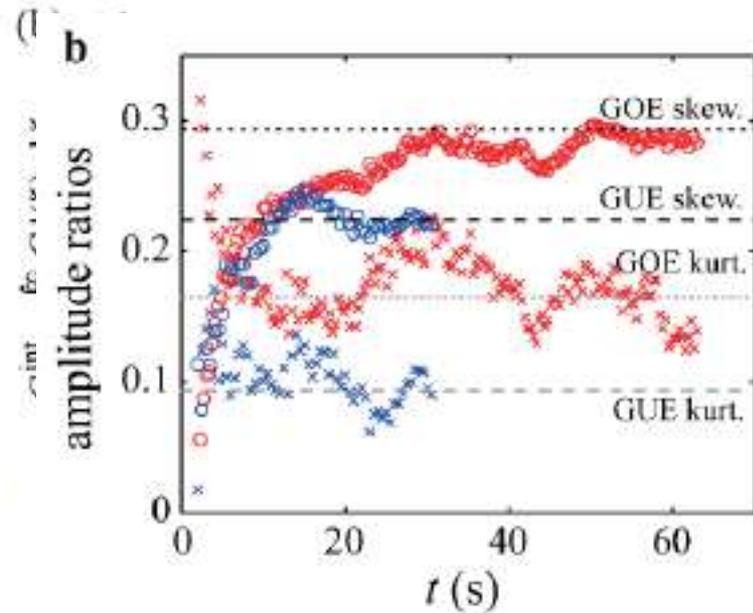
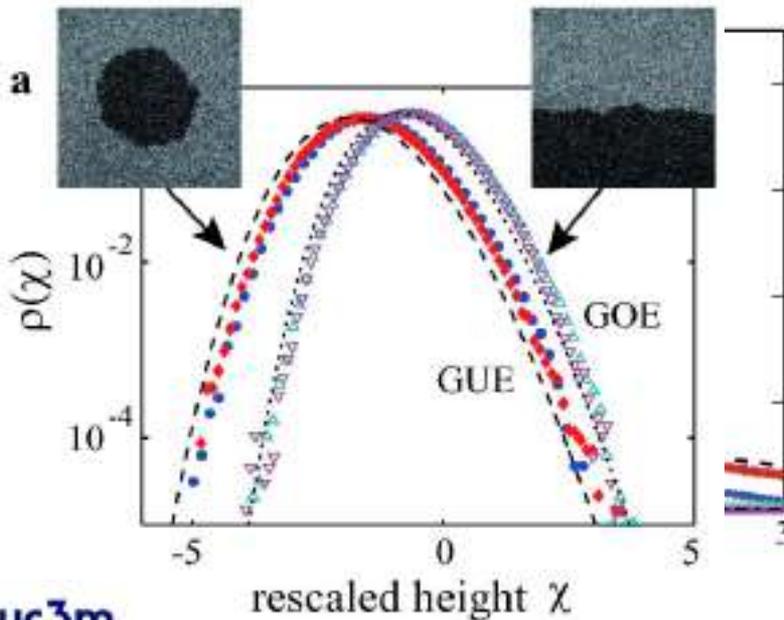
P. Calabrese, P. Le Doussal, & A. Rosso EPL **90**, 20002 (2010)

G. Amir, G. I. Corwin & J. Quastel Comm. Pure Appl. Math. **64**, 0466 (2011)

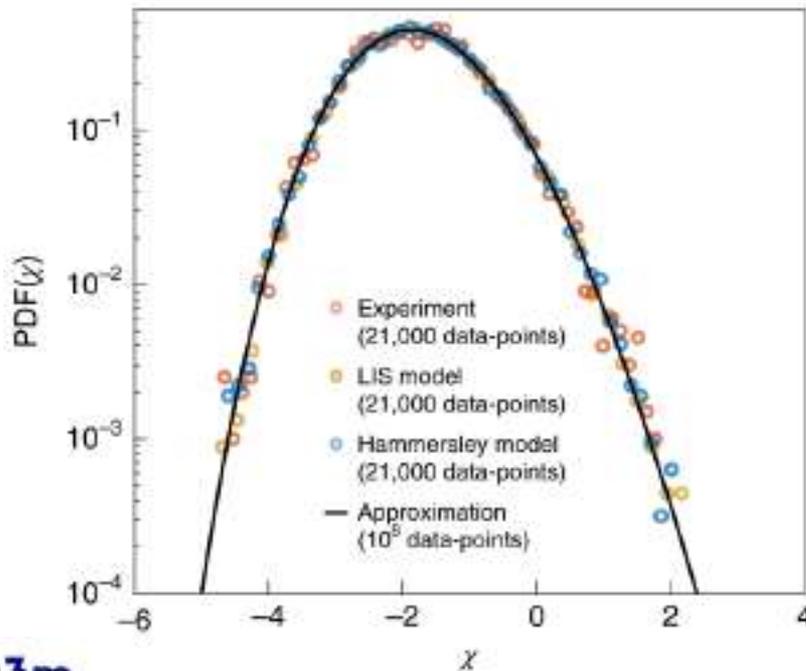
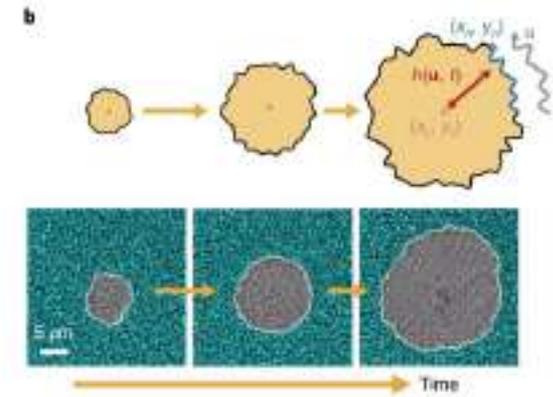
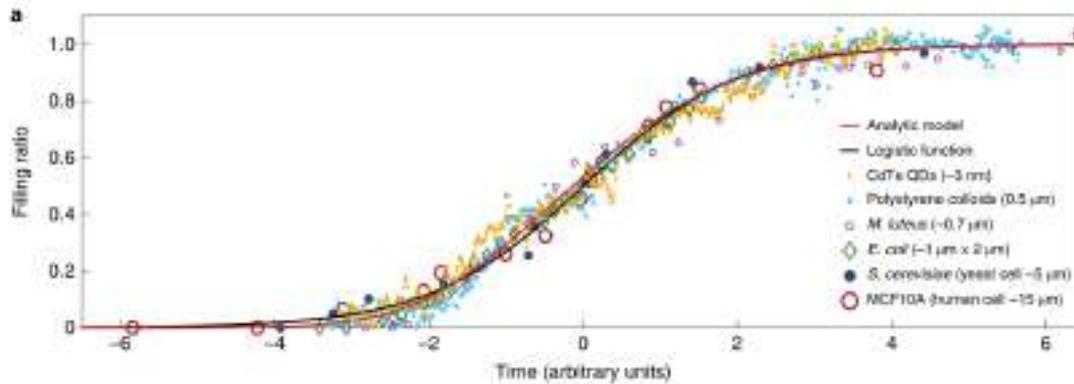
P. Calabrese & P. Le Doussal PRL **106**, 250603 (2011)

$$h \approx \frac{C_s(l, t)}{v_\infty t} + \frac{\overline{(\Gamma t)^\beta} \langle h(x+l, t) h(x, t) \rangle - \langle h(x+l, t) \rangle \langle h(x, t) \rangle}{v_\infty t}$$

Universal amplitude ratios



Universal fluctuations

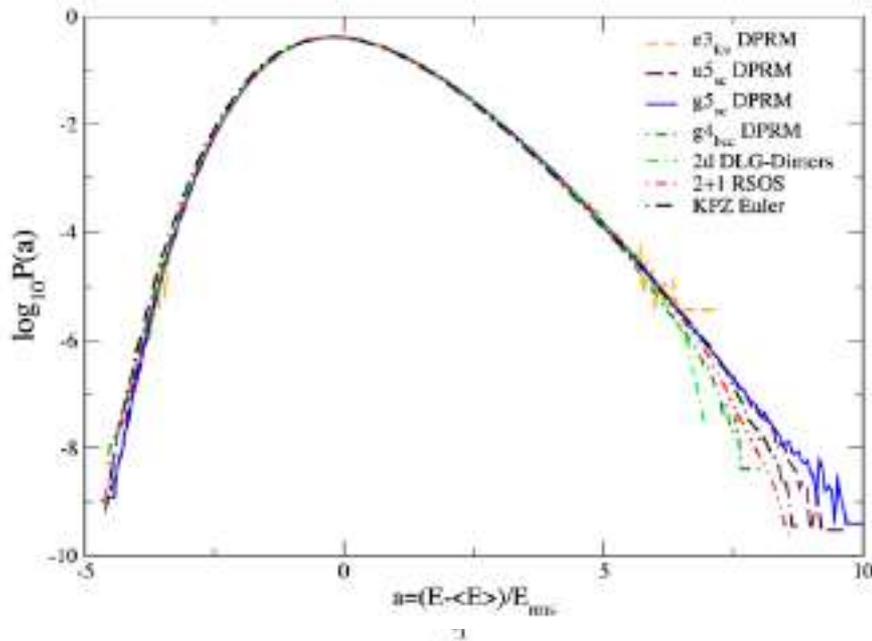


$$\chi = \frac{\Delta h(\Delta t) - \overline{\Delta h(\Delta t)}}{W(\Delta t)}$$

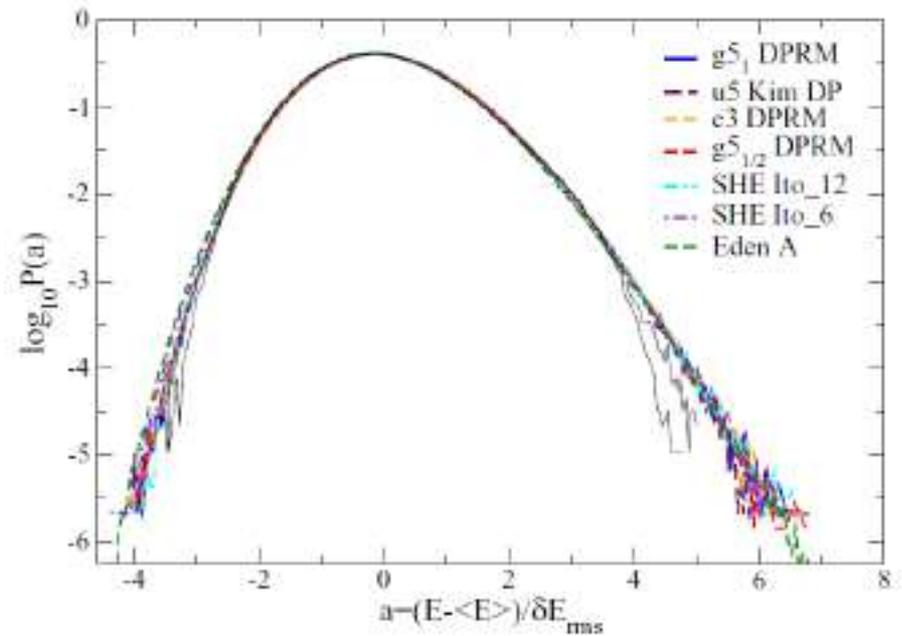
$$\Delta h(\Delta t) = h(t_0 + \Delta t) - h(t_0)$$

2+1 KPZ universality: equation+models

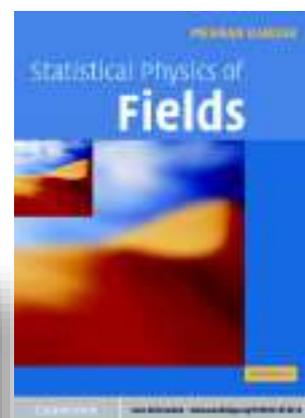
Flat initial condition



Enlarging substrate



T. Halpin-Healy PRL **109**, 170602 (2012). Alves & S.C. Ferreira PRE **87**, 041021 (2013).
 T. Halpin-Healy PRL **87**, 041021 (2001). T. Halpin-Healy PRL **88**, 042118 (2013).



A widely encompassing universality class

- (1) As long as the rearrangements of particles on the surface can result in holes and vacancies, there is no conservation law.
- (2) There is a *translation symmetry*, $v[h(\mathbf{x}) + c] = v[h(\mathbf{x})]$, implying that v depends only on gradients of $h(\mathbf{x})$.
- (3) For simplicity, we shall focus on *isotropic* surfaces, in which all directions in \mathbf{x} are equivalent [See, however, D. Wolf, Phys. Rev. Lett. **67**, 1783 (1991)].
- (4) There is no up–down symmetry, i.e. $v[h(\mathbf{x})] \neq -v[-h(\mathbf{x})]$. The absence of such symmetry allows addition of terms of both parities.

With these conditions, the lowest order terms in the equation of motion give [M. Kardar, G. Parisi, and Y.-C. Zhang, Phys. Rev. Lett. **56**, 889 (1986); E. Medina, T. Hwa, M. Kardar, and Y.-C. Zhang, Phys. Rev. A **39**, 3053 (1989)],

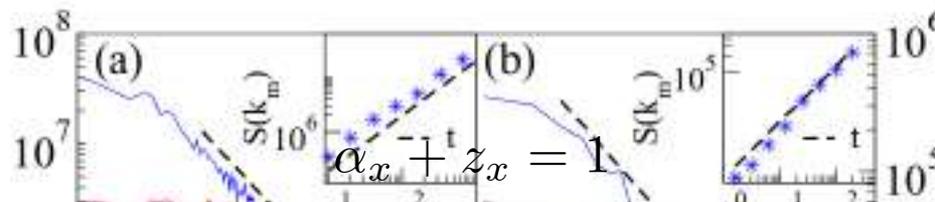
$$\frac{\partial h(\mathbf{x}, t)}{\partial t} = u + v \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \dots + \eta(\mathbf{x}, t), \quad (9.81)$$

with the non-conservative noise satisfying the correlations in Eq. (9.74).

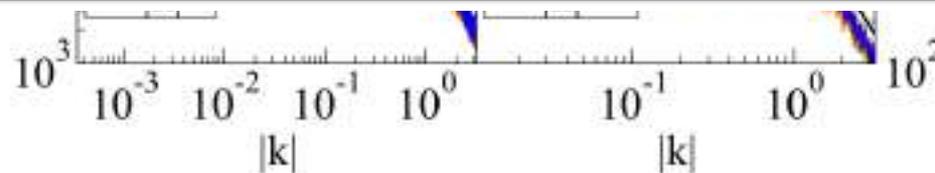
Lack of up-down symmetry \Rightarrow TW statistics: Burgers equation with non-conserved noise

J. Krug Adv. Phys **46**, 139 (1997)

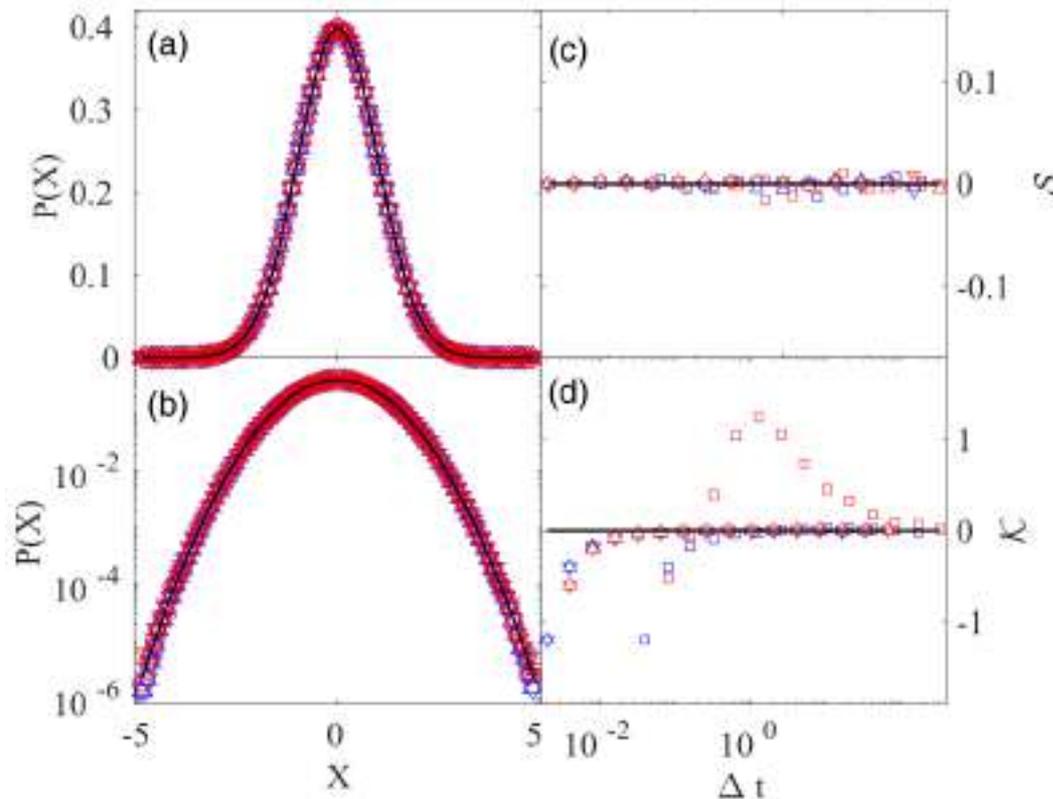
The skewness is a measure of the distribution, to be expected because the growth direction breaks the z -symmetry while \mathcal{L} gauges the weight \mathcal{L} is Gaussian: for a



Equation	α_x	α_y	z_x	z_y
1D Burgers	0	not defined	1	not defined
Hwa-Kardar	$-1/5$	$-1/3$	$6/5$	2
Generalized Hwa-Kardar	$-1/3$	$-1/3$	$4/3$	$4/3$



Lack of up-down symmetry \Rightarrow TW statistics: Burgers equation with non-conserved noise



$$X(x, \Delta t, t_0) = \frac{\Delta\phi - \overline{\Delta\phi}}{(\Gamma\Delta t)^\beta}$$

$$\Delta\phi(x, \Delta t, t_0) = \phi(x, t_0 + \Delta t) - \phi(x, t_0)$$

- Burgers
- △ HK
- ▽ gHK

Growth regime: $t_0=0, \Delta t < t_{\text{sat}}$

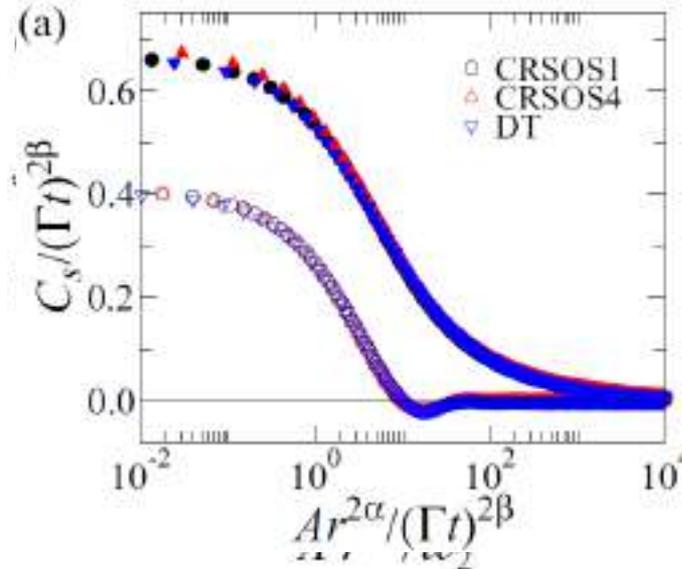
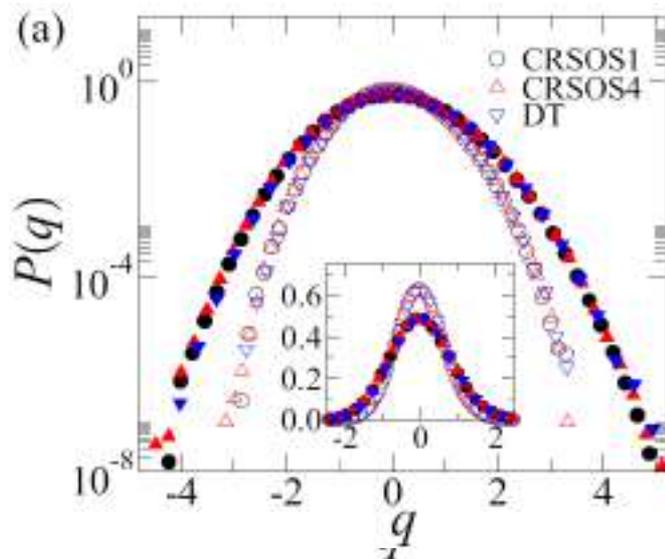
Saturation: $t_0 > t_{\text{sat}}$

Analogous universal traits: Non-linear MBE class

$$\partial_t h = F - \nu_4 \nabla^4 h + \lambda_4 \nabla^2 (\nabla h)^2 + \eta$$

$$h = Ft + (\Gamma t)^\beta \chi \quad \text{Prähofer-Spohn ansatz}$$

2+1 growth

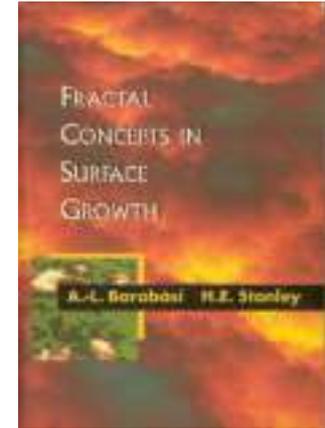


Open symbols:
Flat init. cond.

Closed symbols:
Enlarging substr.

Universality class = exponent values?

There are a number of questions that we must answer if we wish to classify the growth equations in terms of universality classes. For example, what exactly is a universality class? We shall use here the standard working definition, that two systems belong to the same universality class if they share the same set of scaling exponents. This



E.g. 1+1 dimensional nonlinear MBE equation [H.K. Janssen PRL 78, 1082 \(1997\)](#)

$$\partial_t h = -\nu_4 \partial_x^4 h + \lambda_4 \partial_x^2 (\partial_x h)^2 + \eta$$

$$\alpha_\delta = 1 - \delta$$

$$z_\delta = 3 - 2\delta$$

$$\delta \simeq 0.03$$

Non-Gaussian PDF

$$2\alpha_\delta + 1 = z_\delta$$

Same exponents as

Non-renormalization of noise

$$\partial_t h_k = -\nu_4 |k|^{z_\delta} h_k + \eta_k$$

$$2\alpha_\delta + 1 = z_\delta$$

Linear equation

But Gaussian PDF!

A family of non-local equations

Competition between (nonlocal) instabilities and KPZ nonlinearity

$$\partial_t h_{\mathbf{k}} = (\nu |k|^\mu - \mathcal{K} k^m) h_{\mathbf{k}} + \frac{\lambda}{2} \mathcal{F}[(\nabla h)^2] + \eta_{\mathbf{k}}$$

$$0 < \mu < 2, m \geq 2$$

Many celebrated particular cases (μ, m) :

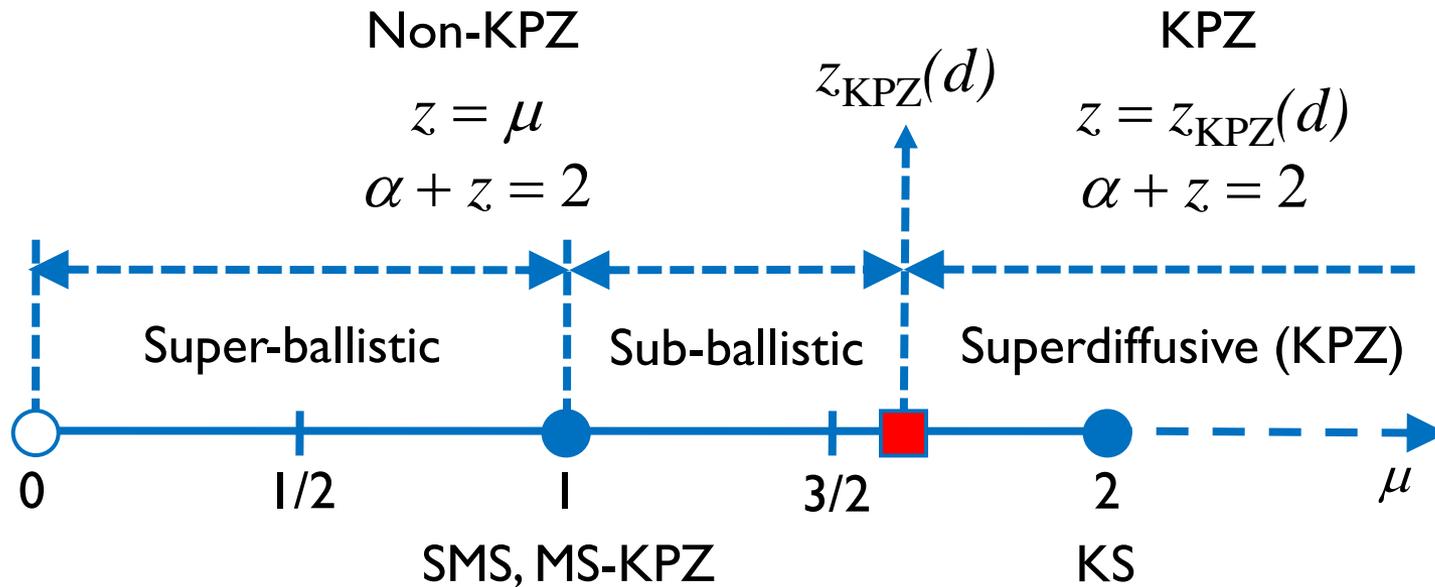
Saffman-Taylor = Mullins-Sekerka = (1,3)

Michelson-Sivashinsky = (1,2)

Kuramoto-Sivashinsky = (2,4)

...

DRG and numerics



Examples:

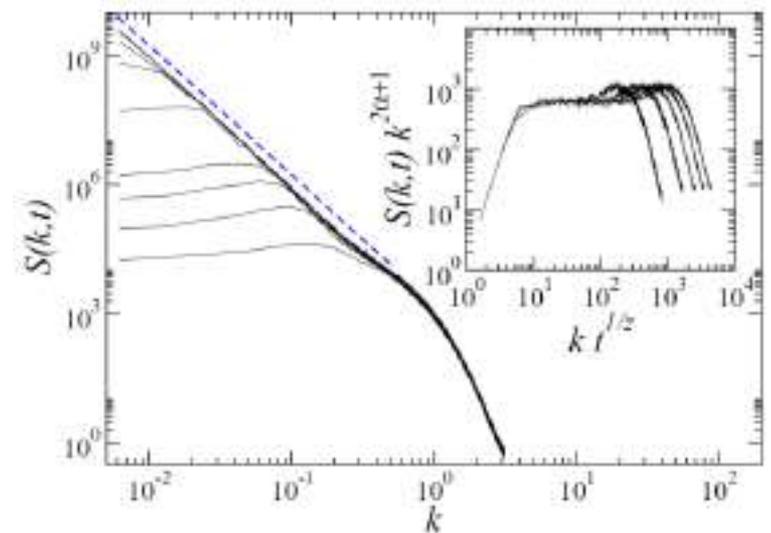
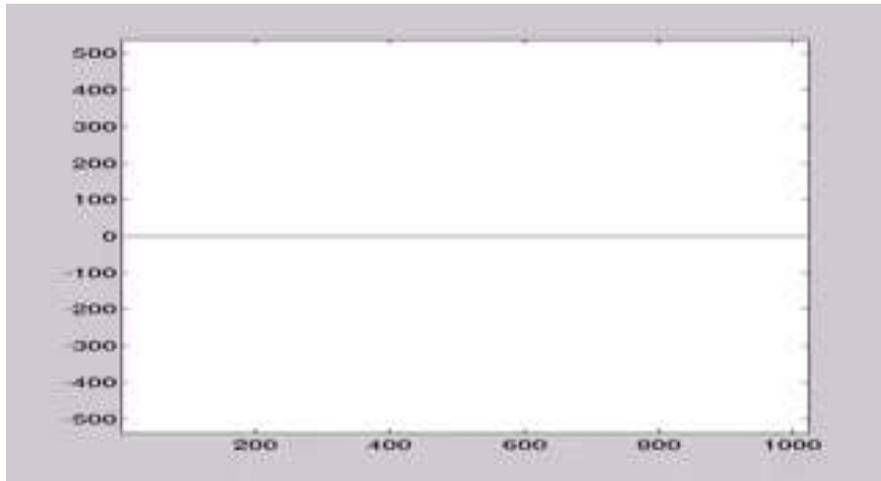
μ	$d=1$ $z_{\text{KPZ}}=3/2$	$d=2$ $z_{\text{KPZ}}=1.61$
1	NON-KPZ	NON-KPZ
3/2	KPZ	NON-KPZ
7/4	KPZ	KPZ

Diffusion-limited growth (I+I growth)

Highly efficient growth events \rightarrow non-local instability

$$\frac{\partial h_k}{\partial t} = [a_1 |k| - a_3 |k|^3] h_k + \frac{v}{2} \mathcal{F} [(\partial_x h)^2] + \eta_k$$

Mullins-Sekerka
Cusp dynamics
Disordered asymptotics



NON-KPZ universality class:

$$\alpha = z = 1, \quad \alpha + z = 2$$

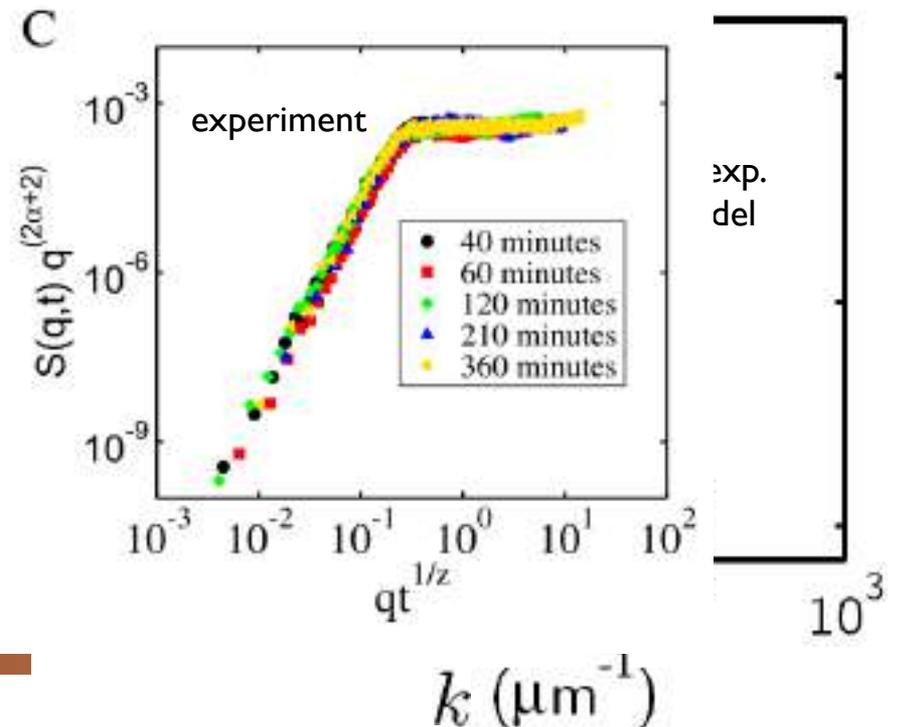
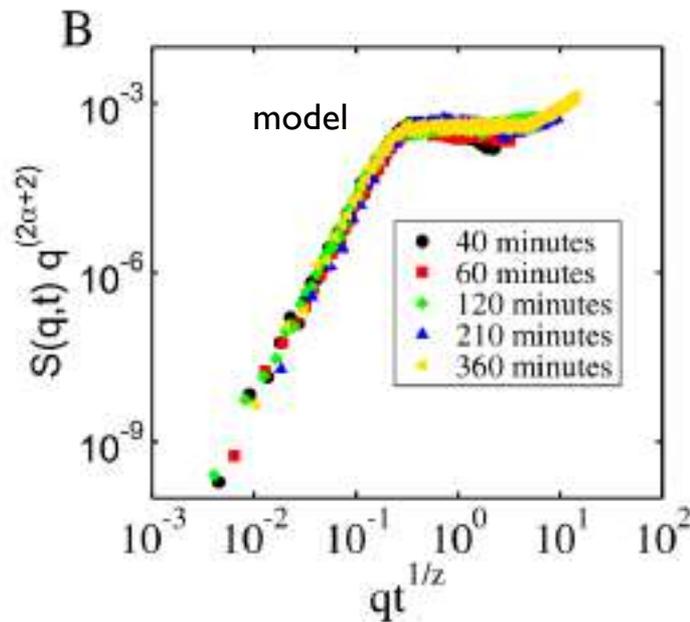
CVD growth with fast interface kinetics (2+1 growth)

MS+KPZ

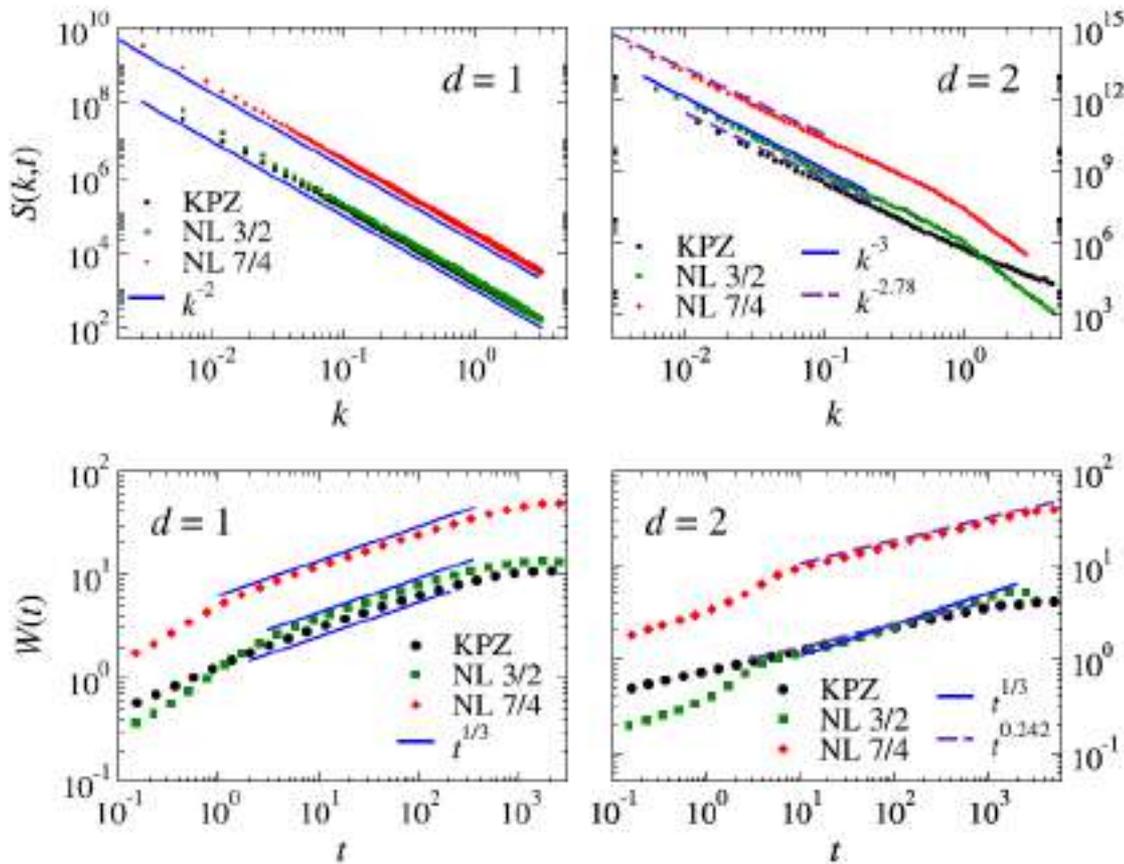
AFM $1 \mu\text{m}^2$

NON-KPZ universality class
(dimension-independent exponents):

$$\alpha = z = 1, \quad \alpha + z = 2$$



Departure from KPZ scaling in 2+1 dimensions



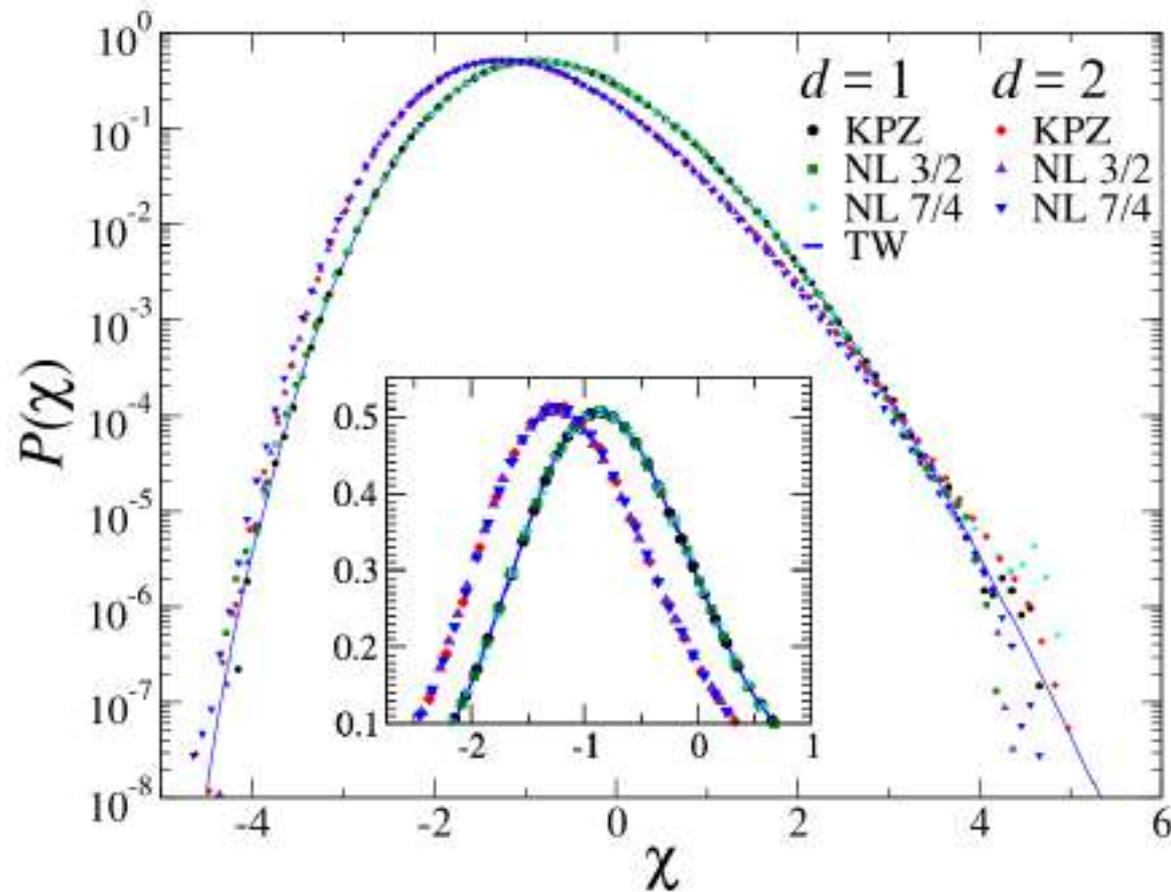
μ	d=1 $z_{\text{KPZ}}=3/2$	d=2 $z_{\text{KPZ}}=1.61$
3/2	KPZ	NON-KPZ
7/4	KPZ	KPZ

The $\mu=3/2$ system changes universality class with dimension

S. Das Sarma, P. Punyindu & Z. Toroczkai PRE **65**, 036144 (2002) for MBE SOS models

Departure from KPZ scaling in 2+1 dimensions

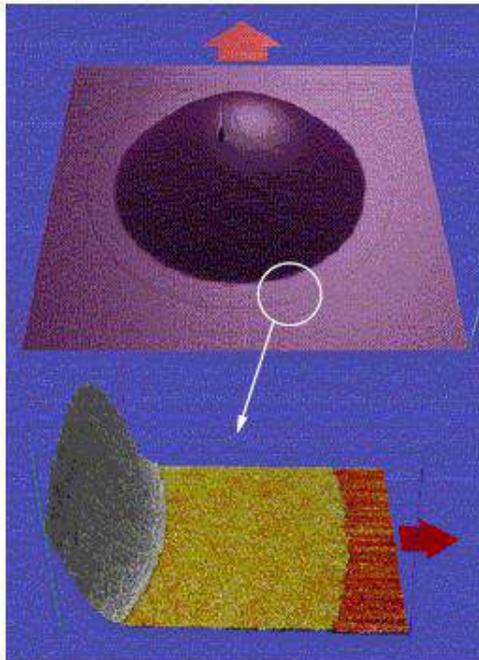
Consistent KPZ PDF behavior in $d=1$ and 2 with non-KPZ exponents ($d=2$)



TW with “very” non-KPZ exponents: precursor spreading

Precursor film dynamics:

Under complete wetting conditions, a layer of molecular thickness forms that precedes the macroscopic wetting front and grows as $t^{1/2}$ (cf. Tanner’s laws $t^{1/10}$ or $t^{1/7}$)



AFM

Polystyrene on Si

Droplet height: 80 nm

Droplet diameter: 12 μm

Height precursor film: 0.7 nm

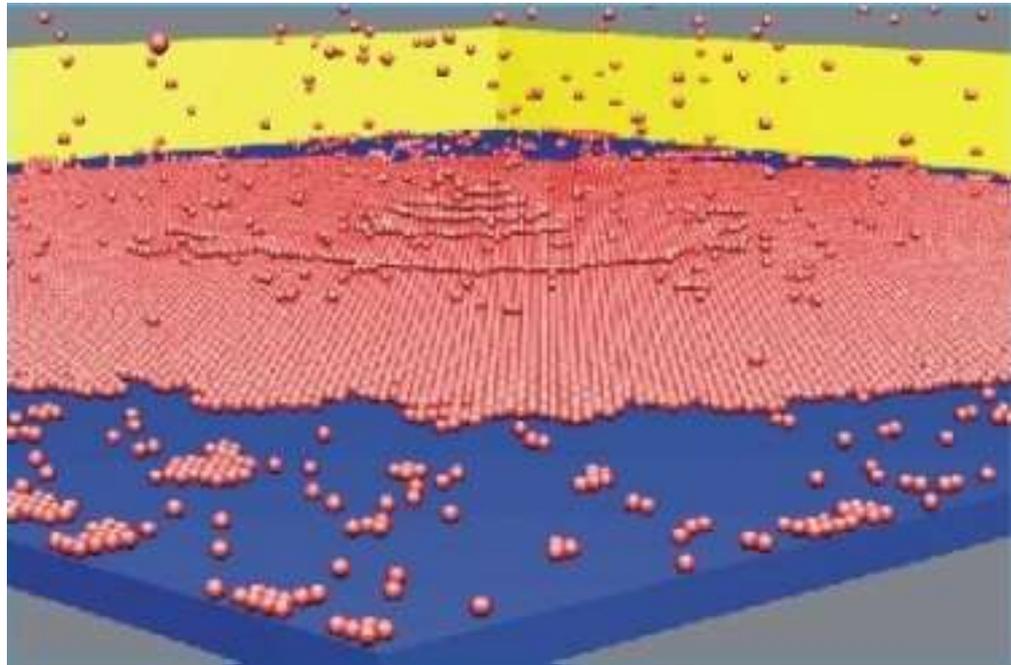
NanoScience Group

University North Carolina

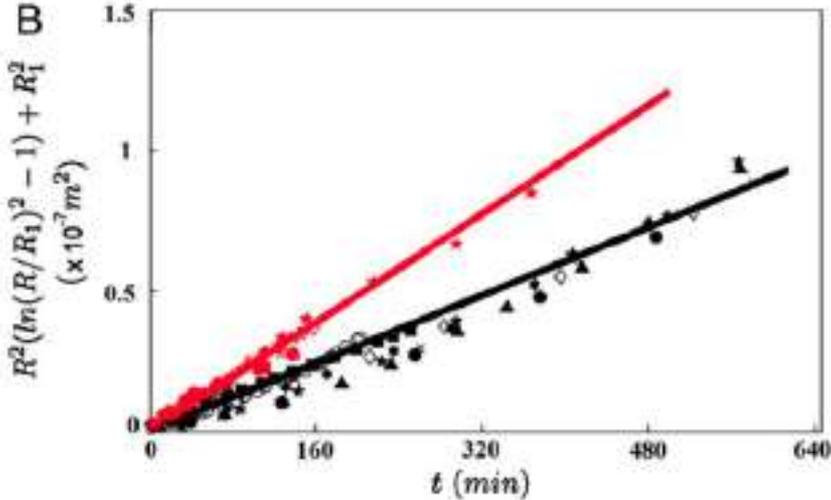
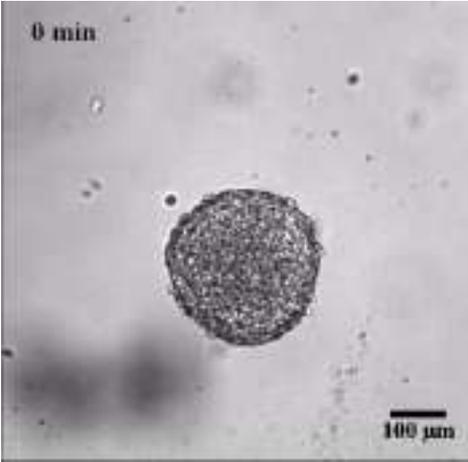
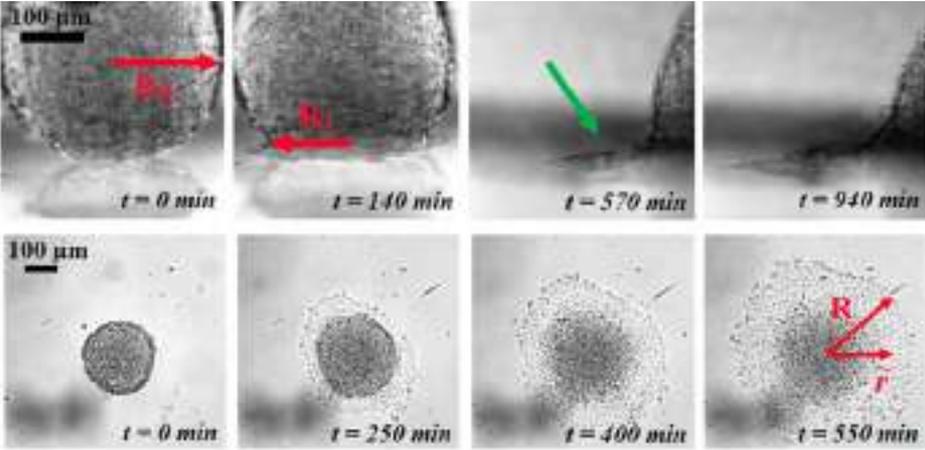
TW with “very” non-KPZ exponents: precursor spreading

Precursor film dynamics:

Under complete wetting conditions, a layer of molecular thickness forms that precedes the macroscopic wetting front and grows as $t^{1/2}$ (cf. Tanner’s laws $t^{1/10}$ or $t^{1/7}$)



Precursor spreading

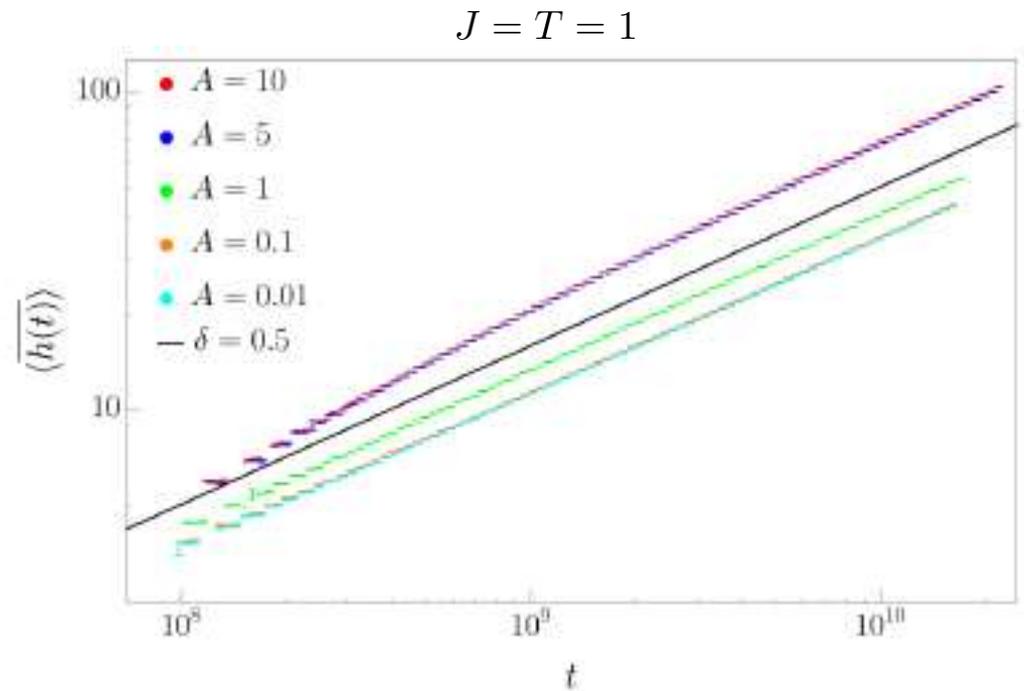
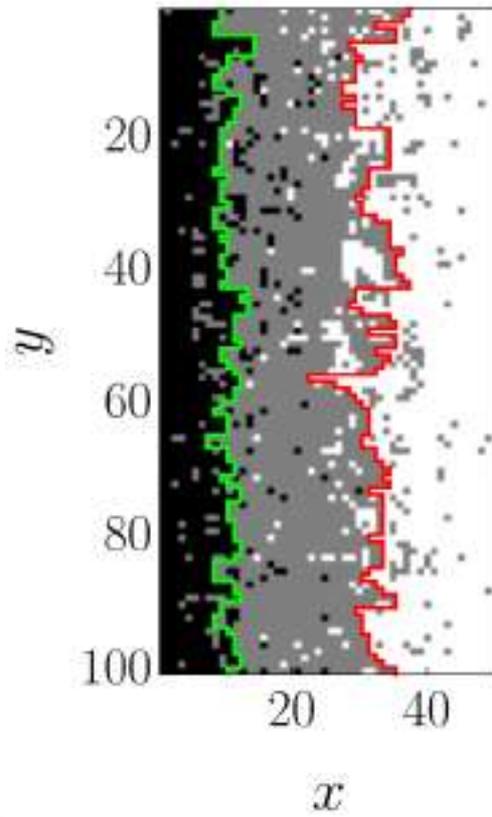


$$R(t) \sim t^{1/2}$$

Precursor spreading: kMC model

A. Lukkarinen, K. Kaski & D. B. Abraham PRE 51, 2199 (1995)

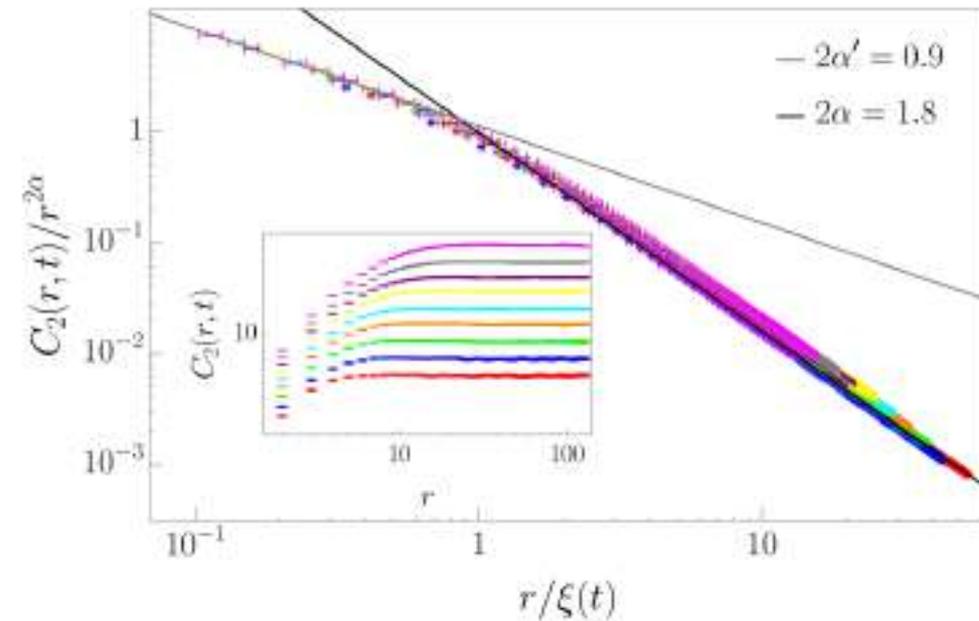
$$\mathcal{H} = -J \sum_{\langle r,s \rangle} n(\mathbf{r}, t)n(s, t) - A \sum_r \frac{n(\mathbf{r}, t)}{Z^3}$$



Precursor spreading: intrinsic anomalous scaling

$$C_2(r, t) = \frac{1}{L_y} \sum_y \langle [h(y+r, t) - h(y, t)]^2 \rangle$$

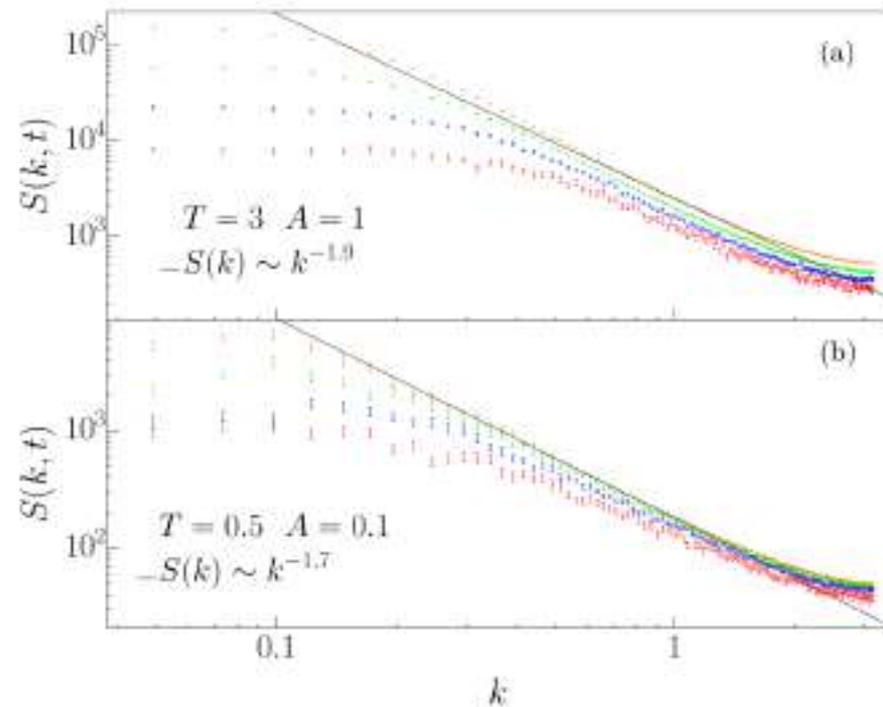
$$J = T = A = 1$$



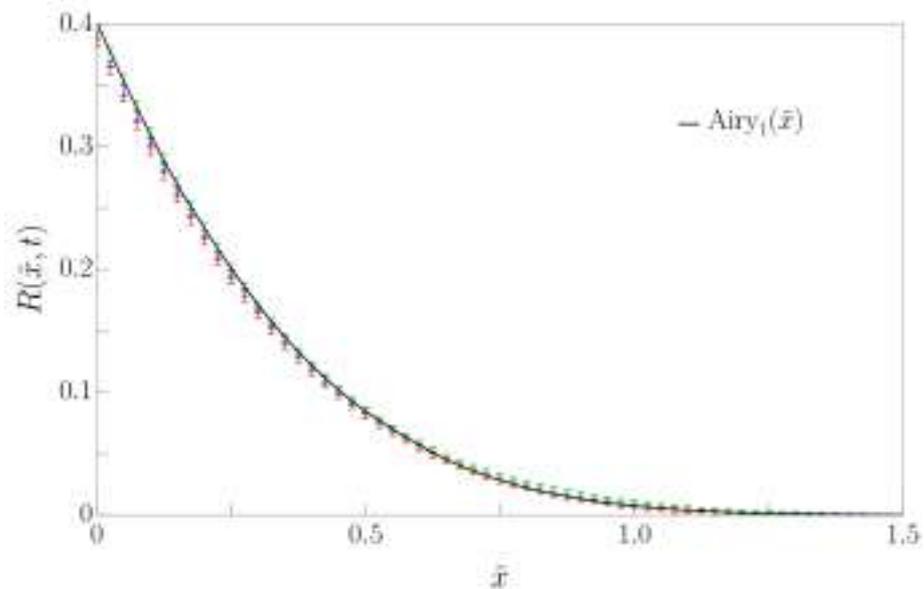
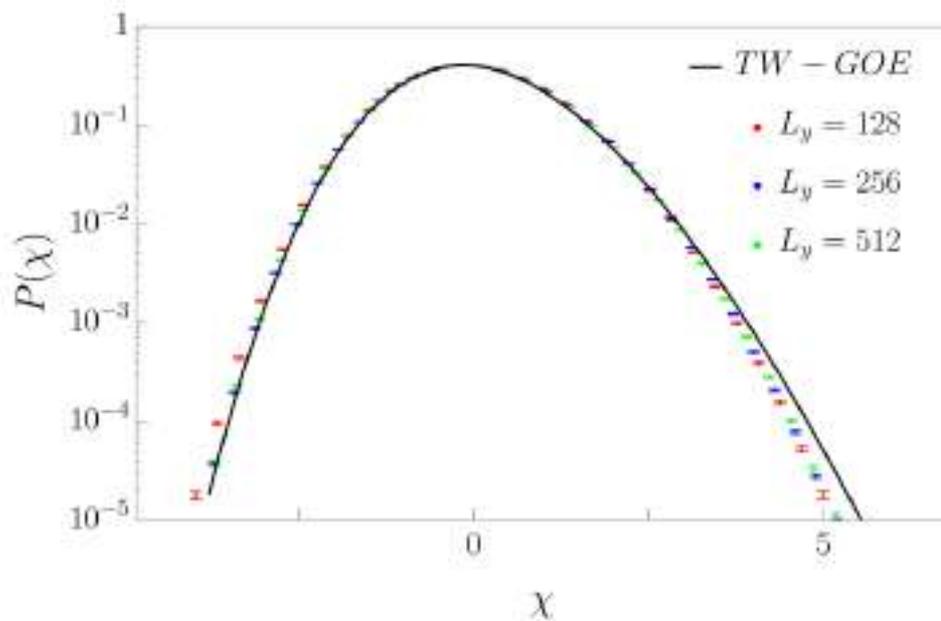
$$\alpha = 0.89 \quad z = 3.3$$

$$\alpha_{\text{loc}} = 0.46$$

Non-KPZ exponents: $\alpha + z \neq 2$



Precursor spreading: fluctuation statistics

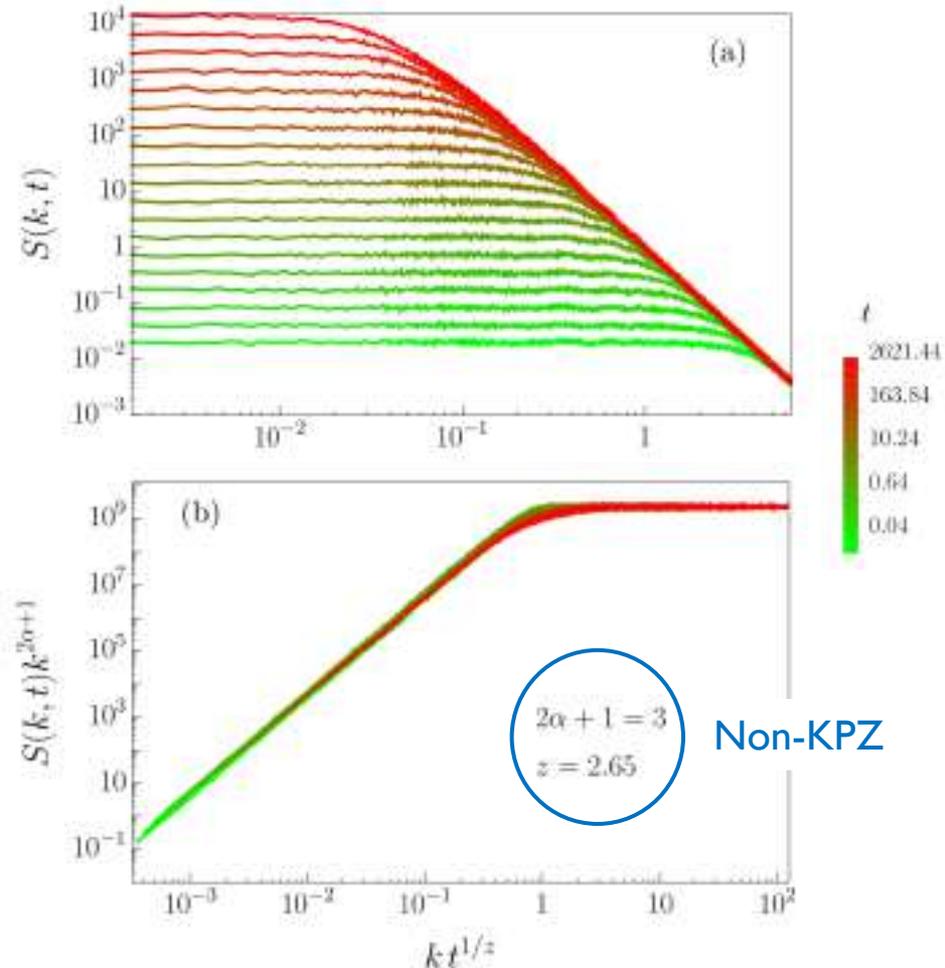
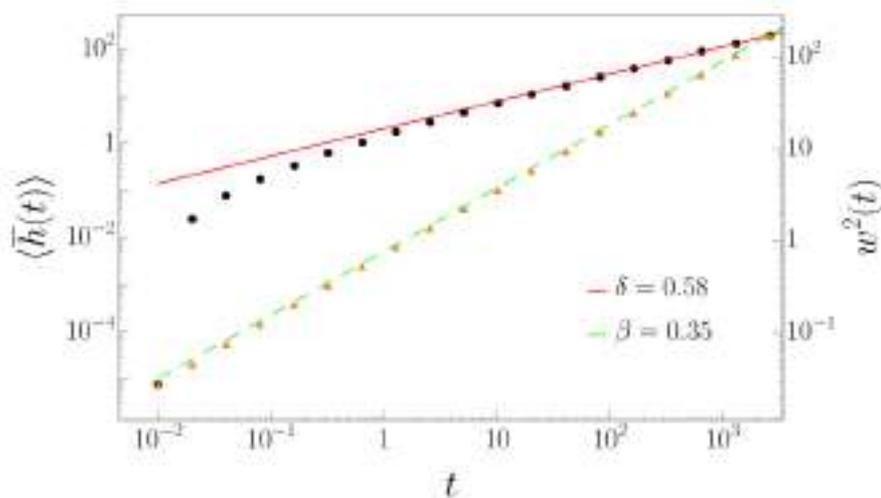


$$\alpha = 0.89 \quad z = 3.3$$

$$\alpha_{loc} = 0.46$$

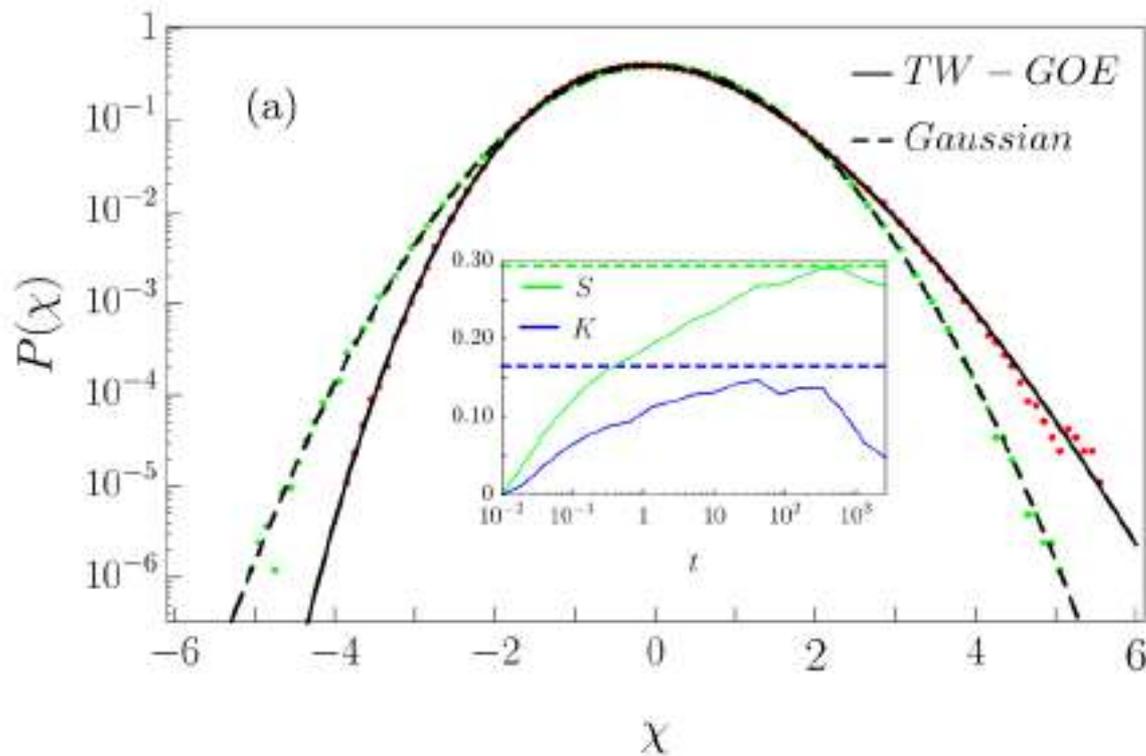
Precursor spreading: continuum model

$$\partial_t \hat{h}_k(t) = -\nu |k|^3 \hat{h}_k(t) + \frac{\lambda}{\sqrt{t}} \hat{\mathcal{F}}_k[(\partial_y h)^2] + \hat{\eta}_k(t)$$



Precursor spreading: continuum model

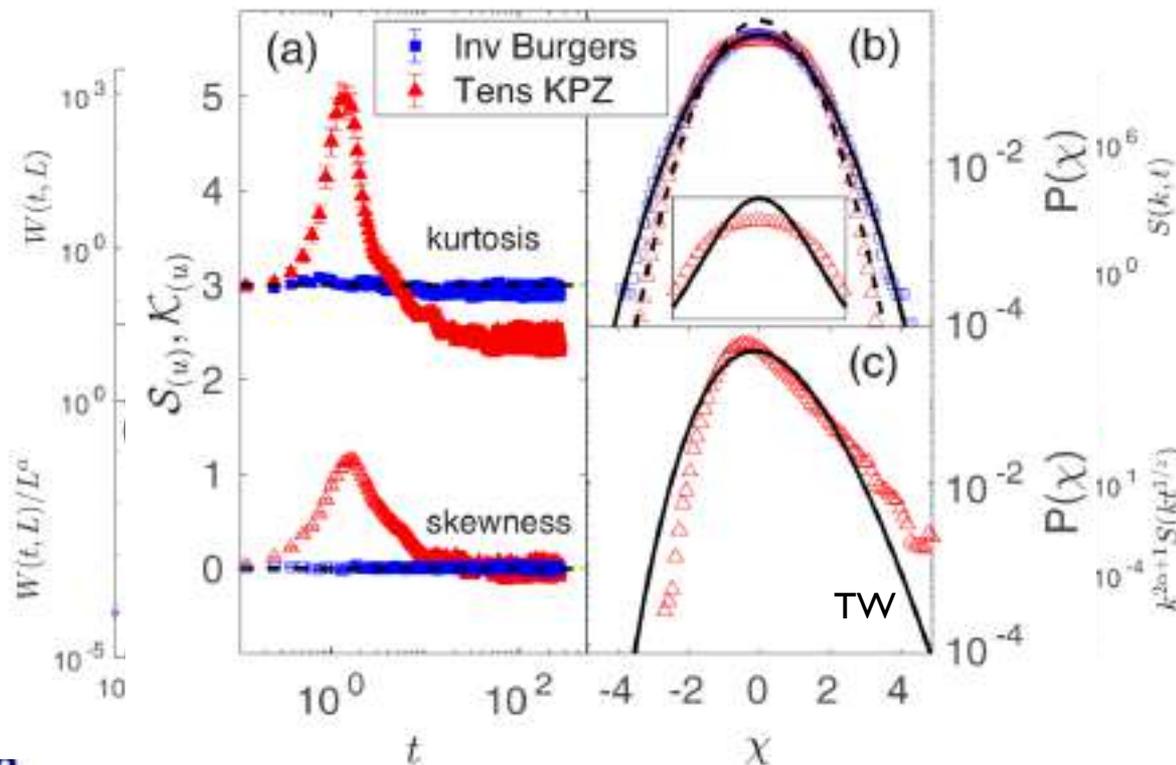
$$\partial_t \hat{h}_k(t) = -\nu |k|^3 \hat{h}_k(t) + \frac{\lambda}{\sqrt{t}} \hat{\mathcal{F}}_k[(\partial_y h)^2] + \hat{\eta}_k(t)$$



KPZ nonlinearity with non-KPZ exponents & fluctuations + anomalous scaling: tensionless KPZ equation

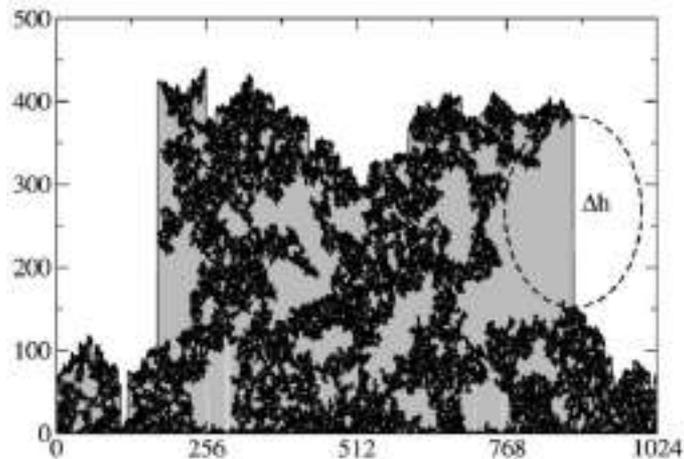
C. Cartes, E. Tirapegui, R. Pandit & M. Brachet PTRSA **380**, 2021009 (2021)
C. Fontaine, F. Vercesi, M. Brachet & L. Canet PRL **131**, 247101 (2023)

$$\partial_t h = \frac{\lambda}{2} (\partial_x h)^2 + \eta(x, t)$$



$\alpha = 1$
(b) Steady state $\alpha = 2$
 $z = 1$
(c) Growth regime
 $\alpha_s = 1/2$

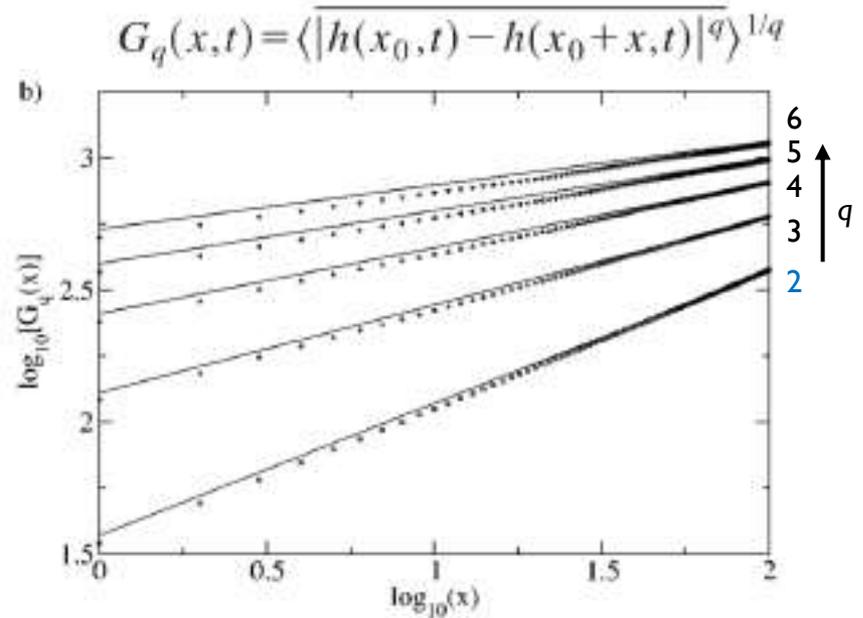
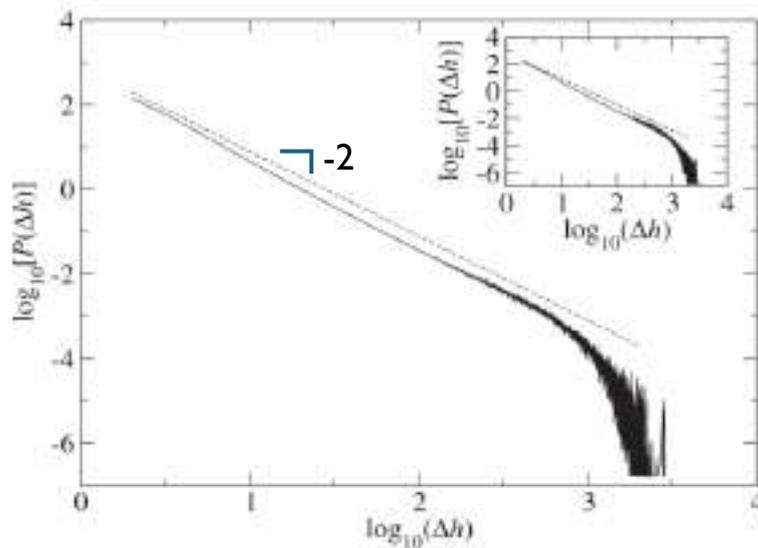
TKPZ universality class? Invasion percolation w/o trapping



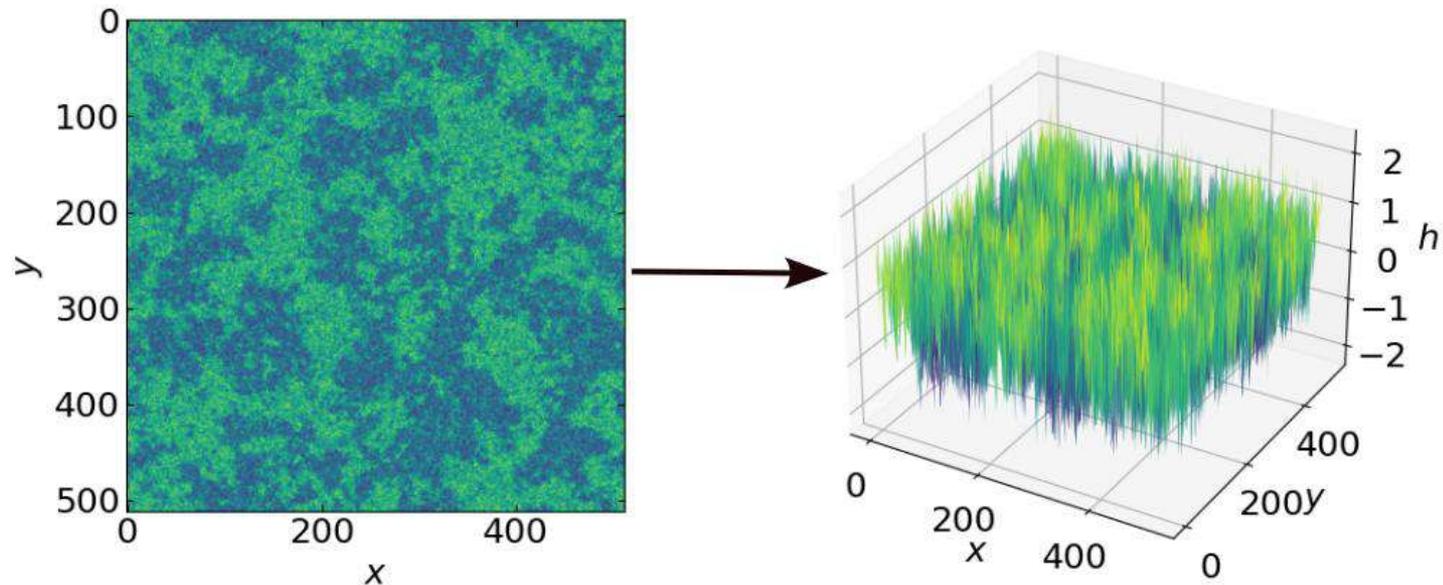
$$\alpha = 1$$

$$z = 1 \quad \alpha + z = 2$$

$$\alpha_s = 1/2$$



Critical ($T=T_c$) Ising model as a rough surface



$$S(k) \sim \frac{1}{k^{2-\eta}} = \frac{1}{k^{2\alpha+d}} \Rightarrow \alpha = \frac{2-d-\eta}{2}$$

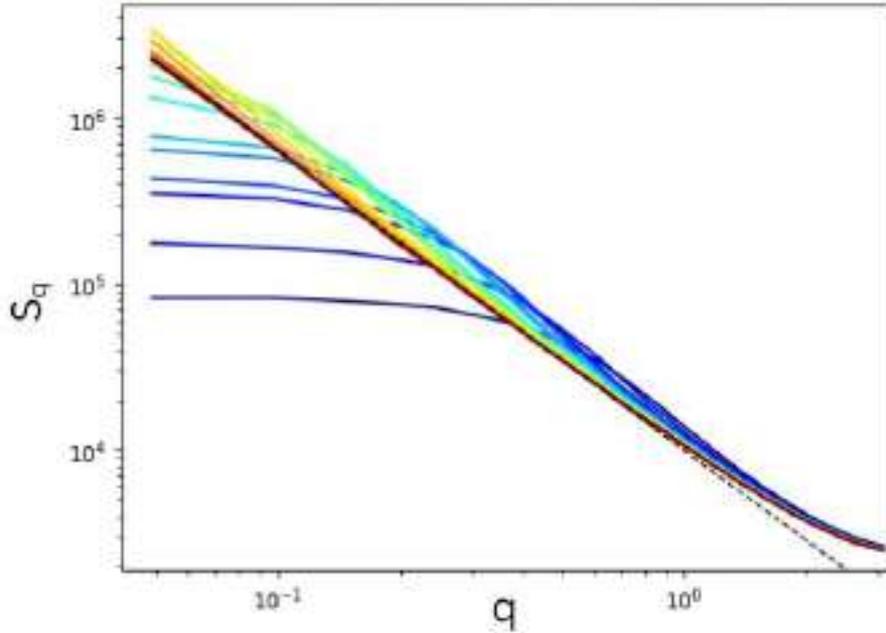
$$\eta_{\text{Ising2D}} = \frac{1}{4} \Rightarrow \alpha_{\text{Ising2D}} = -\frac{1}{8} = -0.125$$

$$z_{\text{Ising2D}} \approx 2 - 2\alpha_{\text{Ising2D}}(6 \ln(4/3) - 1) \simeq 2.18$$

Anomalous scaling in critical Ising dynamics

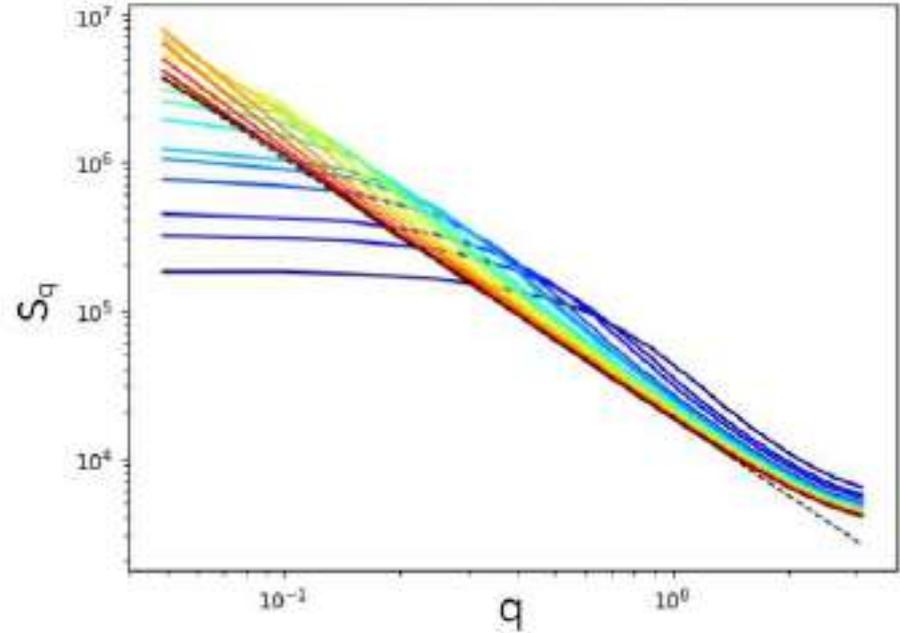
Critical quench from $T=\infty \rightarrow T_c$ $\phi(\mathbf{r}, t = 0) = 0$

GL 128x128, dim: 2, $\Delta t: 0.1$, $r: 0.5$, $D: 0.835$



Continuous
STDGL equation

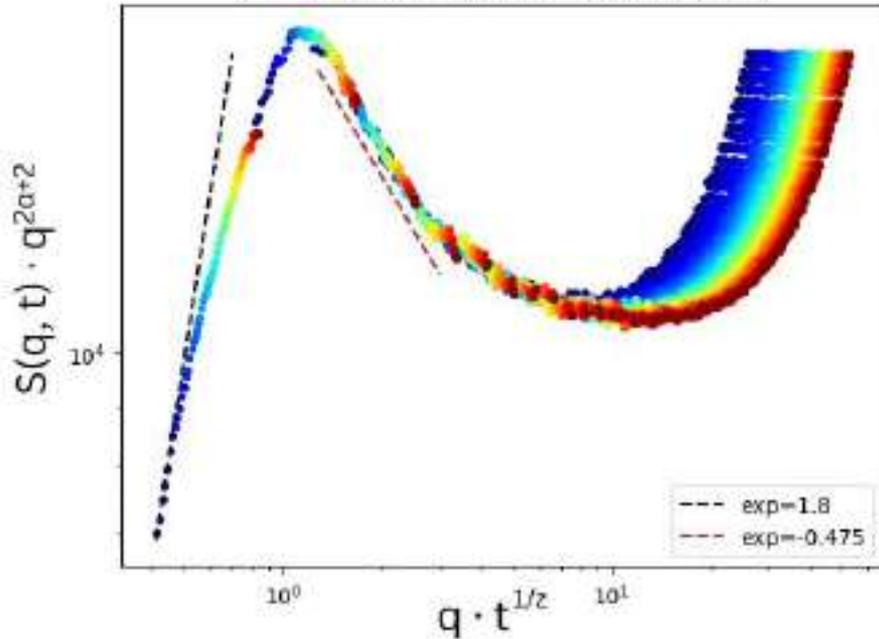
Glauber 128x128, $T = 2.277$



Discrete
Glauber dynamics

Quench crítico desde $T=\infty$ (overgrowth): $S(k,t)$

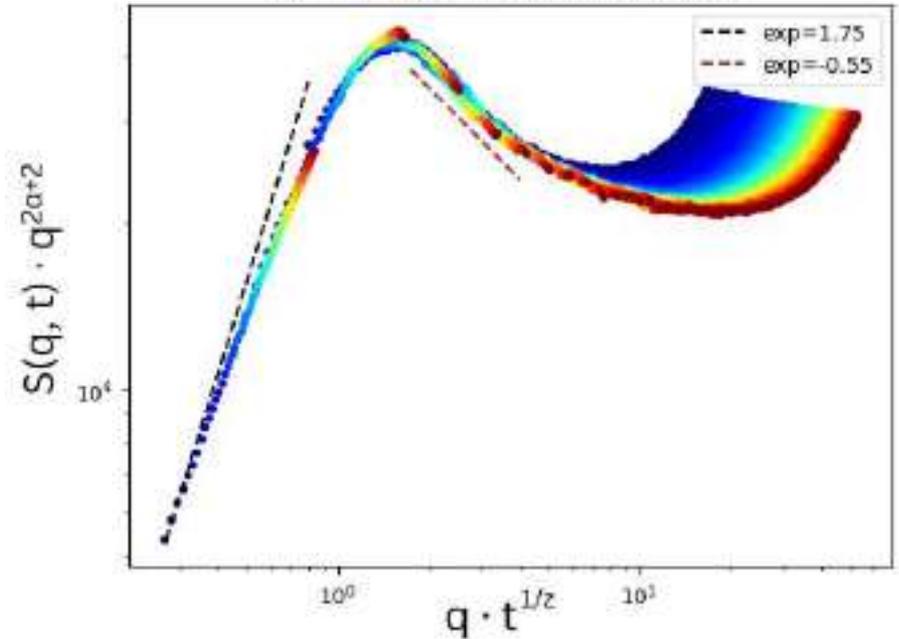
$\alpha = -0.125, z = 2.19, \text{time} : [105.0, 500.0]$



Continuous
STDGL equation

$$\alpha_S \approx 0.11$$

$\alpha = -0.125, z = 2.19, \text{time} : [40, 500]$

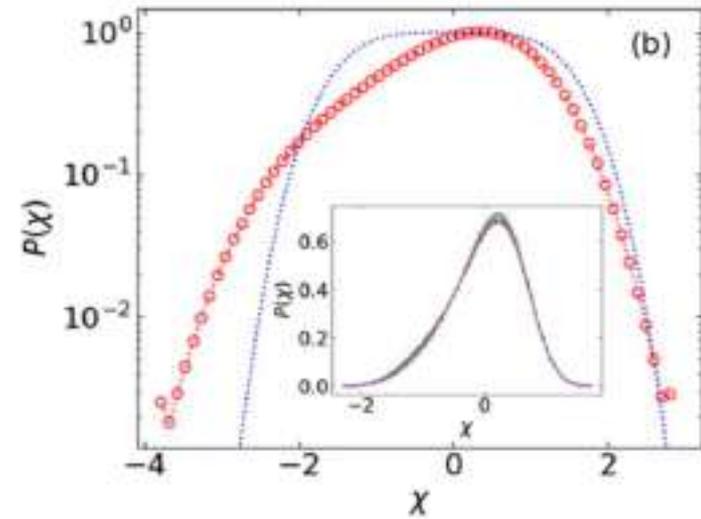
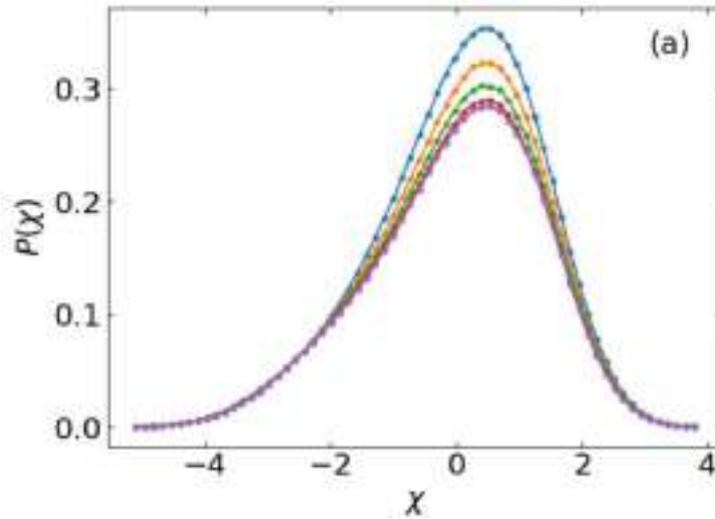


Discrete
Glauber dynamics

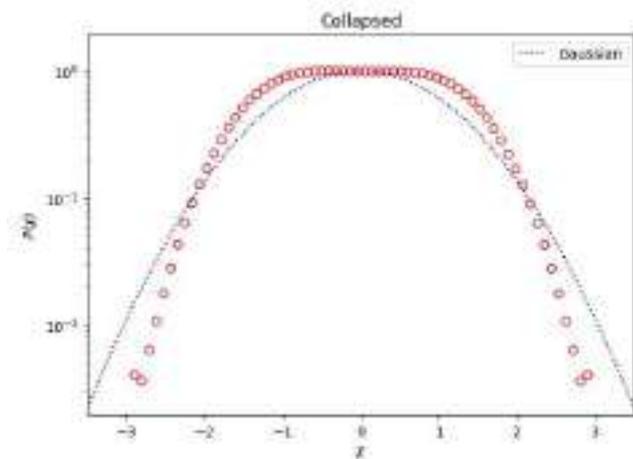
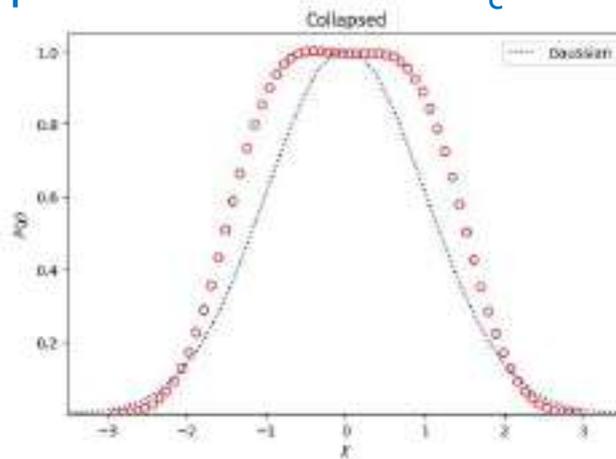
$$\alpha_S \approx 0.15$$

Prähofer-Spohn PDF collapse for critical Ising dynamics

Critical quench from $T=0 \rightarrow T_c$



Critical quench from $T=\infty \rightarrow T_c$



Conclusions/Outlook

- Rich behavior wrt the traits of kinetic roughening universality classes
- Additional factors (e.g. noise type) may induce subclasses
- TW one and two-point statistics with non-KPZ exponents
- TW statistics under anomalous dynamic scaling ansatz
- Non-KPZ behavior (PDF, exponents, scaling ansatz) with KPZ nonlinearity
- Analogous phenomena for other nonlinearities and/or universality classes
- Analogous phenomena for equilibrium universality classes
- Deeper understanding of anomalous scaling required
- Role of symmetries
- Higher dimensions

Thank you!



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Grant No. PID2024-159024NB-C21

