KPZ equation: Galilean-invariance violation, Consistency, and fluctuation–dissipation issues in real-space discretization

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Abstract. - Strong constraints are drawn for the choice of real-space discretization schemes, using the known fact that the KPZ equation results from a diffusion equation (with *multiplicative* noise) through a Hopf–Cole transformation. Whereas the nearest-neighbor discretization passes the consistency tests, known examples in the literature do not. We emphasize the importance of the Lyapunov functional as natural starting point for real-space discretization and, in the light of these findings, challenge the mainstream opinion on the relevance of Galilean invariance.

The KPZ equation is nowadays a paradigm as a stochastic-field description of a vast class of nonequilibrium phenomena, largely transcending the realm of surface growth processes in which it was originally formulated [**?**, **?**, **?**]. This stochastic nonlinear partial differential equation governs the evolution of a field $h(\mathbf{x},t)$, that describes the height of a fluctuating interface. For a one-dimensional (1D) homogeneous substrate of size L, the KPZ equation reads

$$\partial_t h = \nu\,\partial_x^2 h + \frac{\lambda}{2}\left(\partial_x h\right)^2 + F + \varepsilon\,\xi, \tag{1}$$

$\xi(x,t)$ being a Gaussian white noise with $\langle\xi(x,t)\rangle = 0$ and $\langle\xi(x,t)\xi(x',t')\rangle = 2\delta(x-x')\delta(t-t')$, F is an external constant driving force, ν determines the surface tension, and λ is proportional to the average growth velocity. As usual, periodic boundary conditions (pbc) are assumed.

There are two main symmetries associated with the 1D KPZ equation: Galilean invariance and the fluctuation–dissipation relation. On one hand, Galilean invariance has been traditionally linked to the exactness of the relation $\alpha + z = 2$ among the critical exponents, in any spatial dimensionality [the roughness exponent α, characterizing the surface morphology in the stationary regime, and the dynamic exponent z, indicating the correlation

length scaling as $\xi(t) \sim t^{1/z}$] [**?**]. However, this interpretation has been recently criticized in other nonequilibrium models [**?**, **?**]. On the other hand, the second symmetry essentially tells us that in 1D, the nonlinear (KPZ) term is not operative at long times.

Even recognizing the interesting analytical properties of the KPZ equation, it is clear that investigating the behavior of its solutions requires the (stochastic) numerical integration of a discrete version. Such an approach has been used e.g. to obtain the critical exponents in one and more spatial dimensions [**?**,**?**,**?**,**?**,**?**,**?**,**?**,**?**,**?**]. Although a pseudo-spectral spatial discretization scheme has been recently introduced [**?**, **?**, **?**], real-space discrete versions of Eq. (1) are still used for numerical simulations [**?**, **?**, **?**]. One reason is their relative ease of implementation and of interpretation in the case of non-homogeneous substrates like, e.g. a quenched impurity distribution [**?**].

This letter has several purposes: a) to point out that the choice of a real-space discretization scheme must obey two consistency conditions; b) to propose a consistent and highly accurate real-space discretization scheme, whose prescription is not more complex than known proposals in the literature; c) to advocate the usefulness of the Lyapunov functional as a safe starting point in the choice of spatial discretization schemes; d) to show that a consistent discretization scheme does not (essentially) violate the fluctuation–dissipation relation, peculiar of 1D; e) and the last but (obviously) not least, to reassess the value of Galilean invariance within the KPZ problem.

a) *Consistency*: We use the standard, nearest-neighbor discretization prescription as a benchmark to elucidate the constraints to be obeyed by any spatial discretization scheme, arising from the mapping between the KPZ and the diffusion equation (with multiplicative noise) through the Hopf–Cole transformation. As it is known [?], the (driven) diffusion equation with multiplicative noise

$$\partial_t \phi = \nu\, \partial_x^2 \phi + \frac{\lambda F}{2\nu}\phi + \frac{\lambda\varepsilon}{2\nu}\phi\,\xi, \tag{2}$$

where $\phi(x,t)$ can be interpreted as the restricted partition function of the directed polymer problem, is related to the KPZ equation [Eq. (1)] through the *Hopf–Cole transformation* [**?**]

$$\phi(x,t) = \exp\left[\frac{\lambda}{2\nu} h(x,t)\right]. \tag{3}$$

The standard spatially discrete version of Eq. (2) is

$$\dot{\phi}_j = \frac{\nu}{a^2}\,(\phi_{j+1} - 2\phi_j + \phi_{j-1}) + \frac{\lambda F}{2\nu}\phi_j + \frac{\lambda\varepsilon}{2\nu}\phi_j\xi_j, \tag{4}$$

with $1 \le j \le N \equiv 0$, because of the assumed pbc (the implicit sum convention is not meant in any of the discrete expressions). Here a is the lattice spacing. Then, using the discrete version of Eq. (3)

$$\phi_j(t) = \exp\left[\frac{\lambda}{2\nu} h_j(t)\right], \tag{5}$$

we get

$$\dot{h}_j = \frac{2\nu^2}{\lambda a^2}\left(\mathrm{e}^{\delta_j^+ a} + \mathrm{e}^{\delta_j^- a} - 2\right) + F + \varepsilon\,\xi_j, \tag{6}$$

with $\delta_j^{\pm} \equiv \frac{\lambda}{2\nu a}(h_{j\pm1} - h_j)$. By expanding the exponentials up to terms of order of a^2, and collecting equal powers of a (observe that the zero-order contribution vanishes) we retrieve

$$\dot{h}_j = \frac{\nu}{a^2}\,(h_{j+1} - 2h_j + h_{j-1}) + \frac{\lambda}{2}\frac{1}{2a^2}\left[(h_{j+1} - h_j)^2 + (h_j - h_{j-1})^2\right] + F + \varepsilon\,\xi_j. \tag{7}$$

As we see, the first and second terms on the r.h.s. of Eq. (7) are *strictly* related by virtue of Eq. (5). In other words, the discrete form of the Laplacian in Eq. (6) constrains the discrete

form of the nonlinear term in the transformed equation. Latter we show again, in another way, the tight relation between the discretization of both terms. As will be discussed in a forthcoming paper [**?**], where the general real-space discretization scheme will be stated, known proposals [?, ?] fail to comply with this natural requirement.

An important feature of the Hopf–Cole transformation —Eqs. (3), (5)—is that it is *local*, i.e. it involves neither spatial nor temporal transformations. An effect of this feature is that the discrete form of the Laplacian is the same, regardless of whether it is applied to ϕ or h.

The *deterministic* part of Eq. (2), namely the diffusion term, admits a local Lyapunov functional. In other words, for $\varepsilon = 0$, Eq. (2) can be written in the following variational form

$$\partial_t \phi = -\frac{\delta \mathcal{F}[\phi]}{\delta \phi}, \text{ with } \mathcal{F}[\phi] = \frac{\nu}{2} \int \mathrm{d}x \left((\partial_x \phi)^2 - \frac{\lambda}{2\nu^2} F \phi^2 \right).$$

The aforementioned criterion dictates the following discrete form, thus Lyapunov function for any finite N (for simplicity we adopt $F = 0$)

$$\begin{aligned} \mathcal{F}[\phi] &= \frac{\nu}{2} \sum_{j=1}^{N} a \left((\partial_x \phi)^2 \right)_j \\ &= \frac{\nu}{4a} \sum_{j=1}^{N} \left[(\phi_{j+1} - \phi_j)^2 + (\phi_j - \phi_{j-1})^2 \right]. \end{aligned} \tag{8}$$

It is a trivial task to verify that the Laplacian is $(\partial_x^2 \phi)_j = -a^{-1} \partial \mathcal{F}[\phi] / \partial \phi_j$. Now, the obvious fact that this functional can also be written as

$$\mathcal{F}[\phi] = \frac{\nu}{2\,a} \sum_{j=1}^{N} (\phi_{j+1} - \phi_j)^2,$$

serves to illustrate a fact that for a more elaborate discretization requires explicit calculations: the Laplacian does not *uniquely* determine the Lyapunov function [?].

Summarizing, due to the *locality* of the Hopf–Cole transformation: i) the discrete form of the KPZ term cannot be prescribed independently of that of the Laplacian; ii) the discretization being an operation on space, should be independent of the field to which it is applied.

b) *An accurate consistent discretization*: Since the proposals of Refs. [?, ?] already involve next-to-nearest neighbors, one may seek a prescription that minimizes numerical error. An interesting choice for the Laplacian is [**?**]

$$\frac{1}{12\,a^2} \left[16(\phi_{j+1} + \phi_{j-1}) - (\phi_{j+2} + \phi_{j-2}) - 30\,\phi_j \right], \tag{9}$$

which has the associated discrete form for the KPZ term

$$(\partial_x \phi)^2 = \frac{1}{24\,a^2} \left\{ 16 \left[(\phi_{j+1} - \phi_j)^2 + (\phi_j - \phi_{j-1})^2 \right] - \left[(\phi_{j+2} - \phi_j)^2 + (\phi_j - \phi_{j-2})^2 \right] \right\} + O(a^4). \tag{10}$$

Replacing this into the first line of Eq. (8), we obtain Eq. (9). Since this discretization scheme fulfills the consistency conditions, is accurate up to $\mathcal{O}(a^4)$ corrections, and its prescription is not more complex than other known proposals, we expect that it will be the convenient one to use when high accuracy is required in numerical schemes [?].

c) *Lyapunov functional for the KPZ equation*: In Ref. [**?**], a variational formulation has been introduced for the KPZ equation. As it was shown, Eq. (1) can be written as (with $F = 0$)

$$\partial_t h(x,t) = -\Gamma(h) \frac{\delta \mathcal{G}[h]}{\delta h(x,t)} + \varepsilon\, \xi(x,t); \tag{11}$$

where

$$\mathcal{G}[h] = \int_\Omega \mathrm{e}^{\frac{\lambda}{\nu}h(x,t)} \frac{\lambda^2}{8\nu} \left[\partial_x h(x,t)\right]^2 \mathrm{d}x, \tag{12}$$

and $\Gamma(h) = \left(\frac{2\nu}{\lambda}\right)^2 \mathrm{e}^{-\frac{\lambda}{\nu}h}$. The way in which the functionals $\mathcal{F}[\phi]$ and $\mathcal{G}[h]$ are related is also shown in Ref. [?]. It is also easy to prove that the functional $\mathcal{G}[h]$ fulfills the Lyapunov property $\partial_t \mathcal{G}[h] \leq 0$. According to the previous results, we can write the discrete version of Eq. (12) as

$$\mathcal{G}[h] = \frac{\lambda^2}{8\nu} \frac{1}{2\,a} \sum_j \mathrm{e}^{\frac{\lambda}{\nu}h_j} \left[(h_{j+1}-h_j)^2 + (h_j - h_{j-1})^2\right].$$

Introducing this expression into Eq. (11), and through a simple algebra, we obtain Eq. (7). This reinforces our previous result, and moreover indicates that the discrete variational formulation naturally leads to a consistent discretization of the KPZ equation.

d) ***The fluctuation–dissipation relation*** is, together with Galilean invariance, another fundamental symmetry of the one-dimensional KPZ equation. It is clear that both symmetries are recovered when the continuum limit is taken in any reasonable discretization scheme. Thus, an accurate enough partition must yield suitable results.

The stationary probability distribution for the KPZ problem in 1D is known to be [?, ?]

$$\mathcal{P}_{\mathrm{stat}}[h] \sim \exp\left\{\frac{\nu}{2\,\varepsilon}\int \mathrm{d}x \left(\partial_x h\right)^2\right\}.$$

For the discretization scheme in Eq. (7) (with $F = 0$), this is

$$\sim \exp\left\{\frac{\nu}{2\varepsilon}\frac{1}{2a}\sum_j \left[(h_{j+1}-h_j)^2 + (h_j - h_{j-1})^2\right]\right\}. \tag{13}$$

Inserting this expression into the stationary Fokker–Planck equation, the only surviving term has the form

$$\frac{1}{2a^3}\sum_j \left[(h_{j+1}-h_j)^2 + (h_j - h_{j-1})^2\right] \times \left[h_{j+1} - 2h_j + h_{j-1}\right]. \tag{14}$$

The continuum limit of this term is $\int \mathrm{d}x \left(\partial_x h\right)^2 \partial_x^2 h$, that is identically zero [?]. A numerical analysis of Eq. (14) indicates that it is several orders of magnitude smaller than the value of the exponents' pdf [in Eq. (13)], and typically behaves as $\mathcal{O}(1/N)$, where N is the number of spatial points used in the discretization. Moreover, it shows an even faster approach to zero if expressions with higher accuracy [like Eqs. (9) and (10)] are used for the differential operators. In addition, when the discrete form of $\left(\frac{\partial h}{\partial x}\right)^2$ from [?, ?] is used together with its consistent form for the Laplacian, the fluctuation–dissipation relation **is not** exactly fulfilled. This indicates that the problem with the fluctuation–dissipation theorem in $1+1$, discussed in [?, ?] can be just circumvented by using more accurate expressions.

e) ***Galilean invariance*** means that the transformation

$$x \to x - \lambda v t \quad , \quad h \to h + v x \quad , \quad F \to F - \frac{\lambda}{2} v^2,$$

where v is an arbitrary constant vector field, leaves the KPZ equation invariant. The equation obtained using the classical discretization

$$\partial_x h \to \frac{1}{2\,a}(h_{j+1} - h_{j-1}), \tag{15}$$

is invariant under the discrete Galilean transformation

$$ja \to ja - \lambda v t, \quad h_j \to h_j + vja, \quad F \to F - \frac{\lambda}{2} v^2. \tag{16}$$

However, the associated equation is known to be numerically unstable [?], at least when a is not small enough.

On the other hand, Eq. (7) is not invariant under the discrete Galilean transformation. In fact, the transformation $h \to h + vja$ yields an excess term which is compatible with the gradient discretization in Eq. (15); however this discretization does not allow to recover the quadratic term in Eq. (7), indicating that this finite-difference scheme is not Galilean-invariant.

Since Eq. (4) is invariant under the transformation indicated in Eq. (16), it is the non-linear Hopf–Cole transformation (within the present discrete context) which is responsible for the loss of Galilean invariance. Note that these results are independent of whether we consider this discretization scheme or a more accurate one.

Galilean invariance has been always associated with the exactness of the one-dimensional KPZ exponents, and with a relation that connects the critical exponents in higher dimensions [**?**]. If the numerical solution obtained from a finite-difference scheme as Eq. (7), which is not Galilean invariant, *yields the well known critical exponents*, that would strongly suggest that Galilean invariance is not a fundamental symmetry as usually considered.

Here we present some preliminary numerical analysis indicating that, using a consistent discretization scheme, the same critical exponents than with the standard one [Eq. (15)] are obtained. It is worth noting that the discretization used in Refs. [?, ?], which also violates Galilean invariance, yields the same critical exponents too.

The numerical analysis was done using the algorithmic model proposed in [**?**, **?**]to study the dynamics of 1d interfaces moving through heterogeneous media. It is basically a cellular automaton model, for which both space and time coordinates are discrete with the evolution happening on the plane (x, h). This model was proposed to analyze the zero temperature depinning transition at low dimensions. However, variations of this simple automaton model have also been employed to analyze the dynamics in presence of thermal fluctuations [?]. Therefore, this model is adequate to simulate the KPZ dynamics.

We consider a semi-infinite square lattice $L \times \infty$, with the string position h_i at each point i taking integer values. The evolution of the model is as follows. Starting from a flat initial state, the function

$$v_i(t) = \nu L(h_j) + \frac{\lambda}{2} Q(h_j) + \sqrt{T}\,\varepsilon_i(t) \tag{17}$$

is evaluated at time $t > 0$ for all sites $i = 1, \cdots, L$. Here, $v_i = \dot{h}_i$, and L and Q indicates the linear and nonlinear operators' parts respectively. Site i moves forward, $h_i(t+1) \to h_i(t)+1$, if and only if $v_i(t) > 0$, otherwise it remains pinned. Periodic boundary conditions in the substrate direction are used. After evaluation of Eq. (17) for all i the update is carried out in parallel for the whole front.

On the left of Fig. (1) we observe that, when the alternative discretization scheme Eq (7) is considered, the dynamic falls into the KPZ universality class. The global width, that concerns the fluctuations of the growth height around its mean value, scales according to the Family-Vicsek Ansatz [?] as

$$W(L,t) = t^{\beta} f(t/t_{\times}) = t^{\beta} f(t/L^{z}) \ , \tag{18}$$

where the scaling function $f(u)$ is defined as

$$f(u) \sim \begin{cases} \text{const} & \text{if } u \ll 1, \\ u^{-\beta} & \text{otherwise.} \end{cases} \tag{19}$$

Correlations can be analyzed in the reciprocal space by means of the structure factor

$$S(k,t) = \langle \widehat{h}(\mathbf{k},t)\widehat{h}(-\mathbf{k},t)\rangle, \tag{20}$$

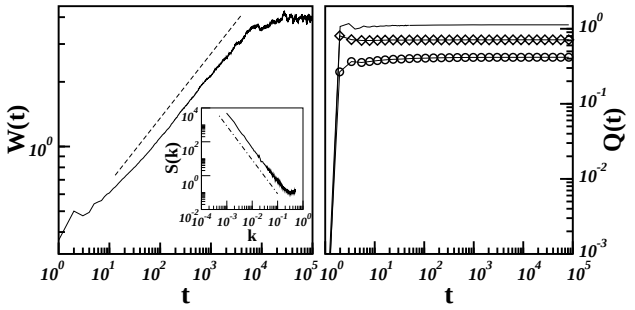

Fig. 1: Numerical results obtained for a system of size $L = 1024$ and $\lambda = 8$ when the alternative discretization scheme Eq.(7) is considered. *Left:* Global width and structure factor (*inset*) are consistent with the KPZ scaling. Lines are plotted as a guide with exponent $\beta = 0.3$ (*dashed*) and $-(2\alpha+1) = 2$ (*dot-dashed*). *Right:* Time dependence of the nonlinear contribution. We also depict the Galilean contribution (circles) and the excess of fluctuations (diamonds). Numerical results show that the later contribution is comparable with the former one.

where $\widehat{h}(\mathbf{k},t) = \frac{1}{L^{d/2}} \sum_x \Delta h(\mathbf{x},t) \exp[-i(\mathbf{kx})]$ is the Fourier transform of the string profile. According to the previous scaling Ansatz, $S(k,t)$ scales as $k^{-(2\alpha+1)}$ with the roughness exponent α. The fact that the results from such a discretization scheme are consistent with the KPZ scaling, with roughness and growth exponents $\alpha = 1/2$ and $\beta = 1/3$ respectively, is apparent.

In order to analyze the excess of fluctuations that the discretization scheme Eq. (7) presents with respect to the standard discretization [Eq. (15)], we extract from the quadratic term of the equation of motion the Galilean invariant fluctuations. On the right of Fig. (1) we show the time dependence of such nonlinear contribution. We observe that the excess of fluctuations is comparable, or even larger, than the Galilean fluctuations.

These findings suggest that the role of Galilean invariance is not so determinant in fixing the KPZ scaling. Our numerical test, where we have not only considered the critical exponents but also the simultaneous quantitative computation of the violation of Galilean invariance supports the conjecture. A more detailed theoretical and numerical analysis will be present elsewhere [?].

The moral from the present analysis is clear:

- Due to the locality of the Hopf–Cole transformation [Eqs. (3) and (5)] the discrete forms of the Laplacian and the nonlinear (KPZ) term cannot be chosen independently; moreover, the prescriptions should be the same, regardless of the fields they are applied to. Equation (6) has also been written in [?], although with different goals than ours (their interest was to analyze the strong coupling limit via mapping to the directed polymer problem).

  The consequences of this analysis are general. In obtaining the discrete versions of any set of differential equations related through a local transformation, both the original (or leading) equation *and* the transformation rules should be taken into account.

  Regarding the recently introduced pseudospectral (PS) approach [**?**, ?, ?, ?] it has been already said that, when analyzing situations where defects or impurities are present, such methods do not apply and one must resort to real-space discrete forms of the differential operators [?, **?**]. Besides that, it has known advantages. One of them is related to the numerical instabilities in discrete growth models: whereas in [**?**], the problem has been tackled by introducing higher order contributions, in PS treatments of the same problem such an instability seems not to arise (or at least is delayed). In addition to those advantages, the PS approach seems to be in principle "transparent" to the question of consistency. Nonetheless, in a forthcoming paper [?] we establish a

relation between the real-space discretization schemes here discussed (of which more details are given) and the PS methods, in the limit where—in order to define a highly accurate discrete representation of the differential operators—we use all the N lattice points.

- A consistent discretization scheme, accurate up to $\mathcal{O}(a^4)$ corrections, and whose prescription is not more complex than other known proposals, has been proposed in this letter. Its ability to control (or at least to delay the appearance of) numerical instabilities found in previous works (see e.g. [?, ?] and references therein) will be the subject of further work.

- The results discussed here are general; although we have exposed them in 1D for the sake of simplicity, their extension to arbitrary dimensionality is straightforward. Moreover, they do not rely on variational representations; nonetheless, the recently introduced variational approach for KPZ [?] offers a natural framework for the consistent discretization of the KPZ equation.

- Regarding the two main symmetries associated with the one-dimensional KPZ equation, we have the following relevant results:
  ♣ Whereas the fluctuation–dissipation relation essentially tells that the nonlinearity is not operative for long times in 1D, our analysis indicates that the problem with the fluctuation–dissipation theorem in $1 + 1$, can be circumvented by improving the numerical accuracy.
  ♠ Galilean invariance has been always associated with the exactness of the one-dimensional KPZ exponents, and with a relation that connects the critical exponents in higher dimensions. However, it is worth remarking that this interpretation has been recently criticized [?, ?]. One of the main results of our analysis indicates that the numerical solution obtained with a non-Galilean-invariant finite-difference scheme yields the same critical exponents as the well known ones obtained with the standard discretization scheme [Eq. (15)]. Moreover, even the discretization used in [?, ?] (that in addition to not passing the consistency test, also violates Galilean invariance) gives the same critical exponents.

The emphasis in the present work has been on the constraints introduced by the local transformation on the discrete versions of the differential equations, as well as some of their consequences. A major point has been to call the attention to the true role of Galilean invariance in KPZ. Our purpose is not to compare alternative spatial discretization schemes with regard to specific KPZ features, nor to present concrete results concerning the violation of Galilean invariance. The study of such aspects will be the subject of further work.

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