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Recent developments on the Kardar–Parisi–Zhang surface-growth equation

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The stochastic nonlinear partial differential equation known as the Kardar-Parisi-Zhang (KPZ) equation is a highly successful phenomenological mesoscopic model of surface and interface growth processes. Its suitability for analytical work, its explicit symmetries and its prediction of an exact dynamic scaling relation for a one-dimensional substratum led people to adopt it as a 'standard' model in the field during the last quarter of a century. At the same time, several conjectures deserving closer scrutiny were established as dogmas throughout the community. Among these, we find the beliefs that 'genuine' non-equilibrium processes are non-variational in essence, and that the exactness of the dynamic scaling relation owes its existence to a Galilean symmetry. Additionally, the equivalence among planar and radial interface profiles has been generally assumed in the literature throughout the years. Here—among other topics—we introduce a variational formulation of the KPZ equation, remark on the importance of consistency in discretization and challenge the mainstream view on the necessity for scaling of both Galilean symmetry and the one-dimensional fluctuation-dissipation theorem. We also derive the KPZ equation on a growing domain as a first approximation to radial growth, and outline the differences with respect to the classical case that arises in this new situation.

Keywords: growth dynamics; Galilean invariance; variational formulation; domain growth

1. Introduction

Phenomena far from thermodynamic equilibrium are ubiquitous in nature, a few examples being turbulence in fluids, interface and growth problems, chemical reactions, biological systems and economic and sociological spatio-temporal *Author for correspondence (wio@ifca.unican.es).

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patterns. During the last few decades, statistical physics has become mature enough to shift its focus towards non-equilibrium processes. Among those studies, the understanding of surface-growth kinetics at microscopic and mesoscopic levels constitutes a major challenge in physics and materials science [1–4]. In recent papers, the methods devised for static critical phenomena have been successfully applied to non-equilibrium interface-growth phenomena, to obtain scaling properties, symmetries, the morphology of pattern formation in a driven state, etc. [5–9].

It is a regrettable confusion enduring upto today to think that only 'gradient' (or 'variational') systems possess a Lyapunov function(al). This issue seemed to be already settled in standard references on pattern formation:

...Graham and co-workers have introduced a 'nonequilibrium potential' that is formally similar to a Lyapunov function but can be defined for an arbitrary dynamical system ... It is a single-valued functional in phase space ... that is constant on any attractor and decreases in any dynamics away from the attractors. It is defined formally as the solution of a complicated Hamiltonian-Jacobi equation and has an interesting interpretation in terms of the probability distribution of the system under the influence of weak external noise ...

([10], p. 868)

Whereas it is true that a non-equilibrium system exhibiting non-trivial spatiotemporal behaviour cannot be 'gradient' (or 'variational') in the sense of the first paragraph in this quotation, there exists in principle (albeit hard to find) a Lyapunov function(al) for arbitrarily complex dissipative dynamics. Examples of non-gradient dynamical systems for which the 'non-equilibrium potential' (NEP)—which plays an analogous role to the free energy in equilibrium systems [10]—is known can be found in Graham [11], Graham & Tél [12], Montagne et al. [13] and Izús et al. [14].

In a recent series of papers, we have reported on the obtaining of an NEP for scalar and non-scalar extended systems of the reaction—diffusion type—like activator—inhibitor systems and systems with local and non-local interactions—and exploited those results for the study of stochastic resonance in extended systems and other related phenomena [15–17].

The Kardar–Parisi–Zhang (KPZ) [18,19] equation is nowadays a paradigm as a stochastic-field description of a vast class of non-equilibrium phenomena, largely transcending the realm of surface-growth processes for which it was originally formulated [2,3]. This equation, which reads

$$\partial_t h(\mathbf{x}, t) = \nu \nabla^2 h(\mathbf{x}, t) + \frac{\lambda}{2} [\nabla h(\mathbf{x}, t)]^2 + F + \xi(\mathbf{x}, t), \tag{1.1}$$

describes the evolution of a field $h(\mathbf{x},t)$, corresponding to the height of a fluctuating interface on a d-dimensional substratum space. Here, $\xi(\mathbf{x},t)$ is a Gaussian white noise of zero mean, $\langle \xi(\mathbf{x},t) \rangle = 0$, and correlation $\langle \xi(\mathbf{x},t) \xi(\mathbf{x}',t') \rangle = 2\varepsilon \delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$, ν is the surface tension, and λ is proportional to the average growth velocity (it arises because the surface slope is parallel transported in the growth process). F indicates the deposition rate.

In this paper, we review some recent results we have obtained with regard to the KPZ equation. In §2, we recall some results from Wio [20] to show how an NEP is obtained for the KPZ case; next, we show how conjectures advanced by Hentschel [5] are fulfilled, exploiting its knowledge; finally, we extend the discussion to a

KPZ system including non-local contributions. In §3, we study the KPZ equation on a growing domain. Section 4 is devoted to discretization issues, stressing the value of consistency in numerical integrations and relativizing that of the one-dimensional fluctuation—dissipation theorem and Galilean invariance. Section 5 contains the conclusions and final remarks.

2. Non-equilibrium potential for the Kardar-Parisi-Zhang equation

(a) Derivation

We start from a general scalar reaction–diffusion equation with multiplicative noise

$$\partial_t \phi(\mathbf{x}, t) = \nu \nabla^2 \phi(\mathbf{x}, t) + \gamma \phi(\mathbf{x}, t) + \phi(\mathbf{x}, t) \eta(\mathbf{x}, t), \tag{2.1}$$

where $\eta(\mathbf{x}, t)$ is Gaussian, white, of zero mean and intensity σ , and we assume the Stratonovich interpretation. It is known that the deterministic part of the system in equation (2.1) has the following NEP:

$$\mathcal{F}[\phi] = \int_{\Omega} \left\{ -\frac{\gamma}{2} \phi(\mathbf{x}, t)^2 + \frac{\nu}{2} \left(\nabla \phi(\mathbf{x}, t) \right)^2 \right\} d\mathbf{x}, \tag{2.2}$$

where Ω indicates the integration range. In fact,

$$\partial_t \phi(\mathbf{x}, t) = -\frac{\delta \mathcal{F}[\phi]}{\delta \phi(\mathbf{x}, t)} + \phi(\mathbf{x}, t) \eta(\mathbf{x}, t), \tag{2.3}$$

where the contribution from the boundaries is null, owing to the variation $\delta \phi$ being fixed (=0) at these boundaries, as usual. As shown in previous works [16], it also fulfils the Lyapunov condition $(d/dt)\mathcal{F}[\phi] \leq 0$ (note that this condition is only strictly valid in a weak noise limit).

Exploiting the Hopf-Cole transformation, we now define a new field, $h(\mathbf{x}, t)$, that, as indicated before, corresponds to an interface height,

$$h(\mathbf{x}, t) = \frac{2\nu}{\lambda} \ln \phi(\mathbf{x}, t), \tag{2.4}$$

whose inverse is $\phi(\mathbf{x}, t) = \exp[(\lambda/2\nu)h(\mathbf{x}, t)]$. Since $\phi(\mathbf{x}, t) \ge 0$, $h(\mathbf{x}, t)$ is always well defined. The transformed equation reads

$$\partial_t h(\mathbf{x}, t) = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \frac{\lambda}{2\nu} \gamma + \xi(\mathbf{x}, t), \tag{2.5}$$

which is equation (1.1) if $F = (\lambda/2\nu)\gamma$ and $\varepsilon = (\lambda/2\nu)^2\sigma$. The noise term, which had a multiplicative character in equation (2.1), becomes additive in equation (1.1). If we now apply the same transformation to the NEP indicated in equation (2.2), we obtain

$$\mathcal{G}[h] = \int_{\Omega} e^{(\lambda/\nu)h(\mathbf{x},t)} \frac{\lambda}{2\nu} \left[-F + \frac{\lambda}{4} (\nabla h(\mathbf{x},t))^2 \right] d\mathbf{x}. \tag{2.6}$$

It is easy to prove that this functional fulfils both the relation

$$\partial_t h(\mathbf{x}, t) = -\Gamma[h] \frac{\delta \mathcal{G}[h]}{\delta h(\mathbf{x}, t)} + \xi(\mathbf{x}, t)$$
 (2.7)

and the Lyapunov property $(d/dt)\mathcal{G}[h] \leq 0$, where $\Gamma[h] = (2\nu/\lambda)^2 \exp[-(\lambda/\nu) h(\mathbf{x}, t)]$. Hence, we have a *free-energy-like functional* from which the KPZ kinetic equation can be obtained through functional derivation. Clearly, the contribution to the variation coming from the boundaries is null again.

(b) Some properties

In Hentschel [5], the fact that equations for relaxational self-affine surface growth are invariant under the Abelian group of global shift transformations, $h(x,t) \to h(x,t) + l$, was used to bound the form of nonlinear terms and related kinetic coefficients. In Wio [20], the relations found in Hentschel [5] are easily seen to follow from the invariance properties of $\mathcal{G}[h]$ itself. In fact, if l is an arbitrary (constant) shift,

$$\mathcal{G}[h+l] = K[l]\mathcal{G}[h], \quad \Gamma[h+l] = K[l]^{-1}\Gamma[h]$$

$$K[l] = e^{(\lambda/\nu)l} = \left(\frac{2\nu}{\lambda}\right)^2 \Gamma[l]^{-1}.$$
(2.8)

and

In order to prove other conjectures advanced in Hentschel [5], we introduce the free energy-like density $\tilde{\mathcal{G}}[h, \nabla h]$, defined by $\mathcal{G}[h] = \int dx \, \tilde{\mathcal{G}}[h, \nabla h]$, namely

$$\tilde{\mathcal{G}}[h, \nabla h] = \frac{\lambda}{2\nu} \mathrm{e}^{(\lambda/\nu)h(\mathbf{x},t)} \left[-F + \frac{\lambda}{4} \left(\nabla h(\mathbf{x},t) \right)^2 \right].$$

The relations we refer to are

$$\tilde{\mathcal{G}}[h, \nabla h] = e^{sh} \tilde{\mathcal{G}}_1[(\nabla h)^2]$$
 and $\Gamma[h, \nabla h] = e^{-sh} \Gamma_1[(\nabla h)^2].$ (2.9)

According to the form of $\tilde{\mathcal{G}}[h, \nabla h]$, the first relation above results obviously true, while for the second relation we have that $\Gamma[h, \nabla h] = e^{-sh(\mathbf{x},t)}\Gamma_0$, where $\Gamma_0 = 1$ and $s = \lambda/\nu$, as $\Gamma[h]$ is not a function of ∇h . Invariance under the nonlinear Galilei transformation, as discussed in Fogedby [7], follows also from the NEP.

From the *free-energy*-like functional (equation (2.6)) for the KPZ kinetic equation and through functional differentiation, we have obtained a form (equation (2.7)) that resembles a (relaxation) 'model A' according to the classification in Hohenberg & Halperin [21]. However, since here the regime is far from equilibrium, its behaviour is highly non-trivial and we have no *a priori* intuition as to what its dynamics could be. Clearly, this is a point to keep in mind when suggesting ansätze for the temporal behaviour.

(c) About non-locality

In Wio [20], it was shown that the functional including a non-local contribution (for simplicity we adopt F = 0),

$$\mathcal{G}[h] = \int_{\Omega} \left\{ \left(\frac{\lambda^2}{8\nu} \right) (\nabla h)^2 + e^{-(\lambda/2\nu)h(\mathbf{x},t)} \int_{\Omega} d\mathbf{x}' G(\mathbf{x},\mathbf{x}') e^{(\lambda/2\nu)h(\mathbf{x}',t)} \right\} e^{(\lambda/\nu)h(\mathbf{x},t)} d\mathbf{x},$$
(2.10)

leads, after a functional derivation, to a generalized KPZ equation

$$\partial_t h(\mathbf{x}, t) = \nu \nabla^2 h(\mathbf{x}, t) + \frac{\lambda}{2} [\nabla h(\mathbf{x}, t)]^2$$
$$- e^{-(\lambda/2\nu)h(\mathbf{x}, t)} \int_{\Omega} d\mathbf{x}' G(\mathbf{x}, \mathbf{x}') e^{(\lambda/2\nu)h(\mathbf{x}', t)} + \xi(\mathbf{x}, t). \tag{2.11}$$

Let us assume that the non-local kernel has translational invariance, that is $G(\mathbf{x}, \mathbf{x}') = G(\mathbf{x} - \mathbf{x}')$, and also that it is of (very) 'short' range. Hence, we can expand it as

$$G(\mathbf{x} - \mathbf{x}') = \sum_{n=0}^{\infty} A_{2n} \delta^{(2n)}(\mathbf{x} - \mathbf{x}'), \qquad (2.12)$$

with $\delta^{(n)}(\mathbf{x} - \mathbf{x}') = \nabla_{\mathbf{x}'}^n \delta(\mathbf{x} - \mathbf{x}')$, and symmetry properties are taken into account. Exploiting this form of the kernel, we arrive at the following contributions in equation (2.11):

$$e^{-(\lambda/2\nu)h(\mathbf{x},t)} \int_{\mathcal{Q}} d\mathbf{x}' G(\mathbf{x} - \mathbf{x}') e^{(\lambda/2\nu)h(\mathbf{x}',t)} \approx \left\{ A_0 + A_2 \left[\left(\frac{\lambda}{2\nu} \right)^2 (\nabla h)^2 + \frac{\lambda}{2\nu} \nabla^2 h \right] + A_4 \left[\left(\frac{\lambda}{2\nu} \right)^4 (\nabla h)^4 + 6 \left(\frac{\lambda}{2\nu} \right)^3 (\nabla h)^2 \nabla^2 h + 2 \left(\frac{\lambda}{2\nu} \right)^2 \nabla^2 (\nabla h)^2 - \left(\frac{\lambda}{2\nu} \right)^2 (\nabla^2 h)^2 + \frac{\lambda}{2\nu} \nabla^4 h \right] + A_6 \dots \right\},$$
(2.13)

where the final dots indicate contributions of order $n \ge 3$ (2n = 6). These contributions have the same form as the ones arising in several previous works, where scaling properties, symmetry arguments, etc., have been used to discuss the possible contributions to a general form of the kinetic equation [5,22,23]. Clearly, the different contributions that arose in equation (2.13) are tightly related to several of other previously studied equations, like the Sun–Guo–Grant equation [24], and others [5,9].

(d) Non-locality in Kardar-Parisi-Zhang

From the above expression, we can extract a new form of NEP for the KPZ equation. Let us only retain the contribution that comes from the n=1 term. We define the functional

$$\tilde{G}[h] = \int_{\Omega} d\mathbf{x} \int_{\Omega} d\mathbf{x}' e^{(\lambda/2\nu)h(\mathbf{x},t)} G(\mathbf{x} - \mathbf{x}') e^{(\lambda/2\nu)h(\mathbf{x}',t)}$$
(2.14a)

and

$$G(\mathbf{x} - \mathbf{x}') = A_2 \delta^{(2)}(\mathbf{x} - \mathbf{x}'). \tag{2.14b}$$

The functional derivative of $\tilde{G}[h]$ yields

$$\frac{\delta \tilde{G}[h]}{\delta h(\mathbf{y})} = A_2 \frac{\lambda}{2\nu} \left[e^{(\lambda/2\nu)h(\mathbf{y})} \int_{\Omega} d\mathbf{x} \delta^{(2)}(\mathbf{y} - \mathbf{x}) e^{(\lambda/2\nu)h(\mathbf{x})} + e^{(\lambda/2\nu)h(\mathbf{y})} \int_{\Omega} d\mathbf{x} e^{(\lambda/2\nu)h(\mathbf{x})} \delta^{(2)}(\mathbf{x} - \mathbf{y}) \right]
= 2 A_2 \frac{\lambda}{2\nu} e^{(\lambda/2\nu)h(\mathbf{y})} \int_{\Omega} d\mathbf{x} \delta^{(2)}(\mathbf{y} - \mathbf{x}) e^{(\lambda/2\nu)h(\mathbf{x})}
= 2 A_2 \frac{\lambda}{2\nu} e^{(\lambda/2\nu)h(\mathbf{y})} \left[\left(\frac{\lambda}{2\nu} \right)^2 (\nabla_{\mathbf{x}} h)^2 + \left(\frac{\lambda}{2\nu} \right) \nabla_{\mathbf{y}}^2 h \right] e^{(\lambda/2\nu)h(\mathbf{y})}.$$
(2.15)

Recalling that $\Gamma[h] = (2\nu/\lambda)^2 \exp[-(\lambda/\nu)h(\mathbf{x})]$, and adopting $A_2 = -(\nu/2)$, the deterministic part of the KPZ equation results from

$$-\Gamma[h] \frac{\delta \tilde{G}[h]}{\delta h(\mathbf{x})} = \nu \nabla_{\mathbf{x}}^2 h + \frac{\lambda}{2} (\nabla_{\mathbf{x}} h)^2.$$
 (2.16)

The above indicated results allow us to define

$$\Phi_{2}[h] = -\int d\mathbf{x} \int^{h(\mathbf{x})} d\psi \, \frac{\delta \Gamma[\psi]}{\delta \psi} \, \tilde{\mathcal{G}}[\psi]
= -\int d\mathbf{x} \int d\mathbf{x}' \frac{2\nu^{2}}{\lambda} \int^{h(\mathbf{x})} d\psi \, e^{(-\lambda/2\nu)\psi(\mathbf{x})} \, \delta^{(2)}(\mathbf{x} - \mathbf{x}') \, e^{(\lambda/2\nu)\psi(\mathbf{x}')}, \qquad (2.17)$$

which yields

$$\partial_t h(\mathbf{x}, t) = -\frac{\delta \Phi_2[h]}{\delta h} + \xi(\mathbf{x}, t). \tag{2.18}$$

Hence, $\Phi_2[h]$ is another representation of the NEP for KPZ. It has a very interesting form that could allow for a nice way to approximately evaluate the NEP.

3. The Kardar-Parisi-Zhang equation on a growing domain

The KPZ equation has also been related to the biologically motivated Eden model [2]. This model was introduced as a simplified probabilistic description of a developing cell colony. For long time, it shows the propagation of a rough interface with an approximate radial symmetry. Numerical simulations suggested that the Eden model interface fluctuations belong to the KPZ universality class. As a first step in understanding radial interfaces [25,26], one can derive the KPZ equation in a growing domain [27]. The simplest possibility is applying the dilatation transformation $x \to (t/t_0)^{\gamma} x$ to the KPZ equation to find

$$\partial_t h = \nu \left(\frac{t_0}{t}\right)^{2\gamma} \nabla^2 h + \frac{\lambda}{2} \left(\frac{t_0}{t}\right)^{2\gamma} (\nabla h)^2 + \gamma F t^{\gamma - 1} + \left(\frac{t_0}{t}\right)^{d\gamma / 2} \xi(x, t), \tag{3.1}$$

where $\gamma > 0$ is the growth index that specifies the speed with which the domain grows. Note that this equation, in the absence of external fluxes (i.e. $\lambda = F = 0$), conserves the average density; in other words, this domain growth mechanism is responsible for a simultaneous mass dilatation. It is possible to derive a KPZ equation on a growing domain in such a way that the total mass is conserved. This is achieved by introducing a dilution term, which renders the KPZ equation [27]

$$\partial_t h = \nu \left(\frac{t_0}{t}\right)^{2\gamma} \nabla^2 h + \frac{\lambda}{2} \left(\frac{t_0}{t}\right)^{2\gamma} (\nabla h)^2 - \frac{d\gamma}{t} h + \gamma F t^{\gamma - 1} + \left(\frac{t_0}{t}\right)^{d\gamma / 2} \xi(x, t). \quad (3.2)$$

It is known that the dilution-free equation (3.1) presents memory effects that separate its behaviour from the one dictated by the Family-Vicsek scaling for large enough γ [27]. This implies a somehow paradoxical situation. As we have mentioned, there are two main symmetries associated with the d-dimensional KPZ equation: the Hopf-Cole transformation, which maps it onto the noisy diffusion equation [20], and Galilean invariance which have been traditionally related to the non-renormalization of the KPZ vertex at an arbitrary order in the perturbation expansion [19]. In the case of the no-dilution KPZ equation (3.1), both symmetries are still present. Indeed, this equation transforms under the Hopf-Cole transformation $u = \exp[\lambda h/(2\nu)]$ to

$$\partial_t u = \nu \left(\frac{t_0}{t}\right)^{2\gamma} \nabla^2 u + \frac{\gamma F \lambda}{2\nu} t^{\gamma - 1} u + \frac{\lambda}{2\nu} \left(\frac{t_0}{t}\right)^{d\gamma/2} u \,\xi(x, t), \tag{3.3}$$

which is again a noisy diffusion equation and it can be explicitly solved in the deterministic limit $\epsilon = 0$. We find in this case

$$u(x,t) = \frac{(1-2\gamma)^{d/2} \exp[F\lambda t^{\gamma}/(2\nu)]}{[4\pi t_0^{2\gamma} (t^{1-2\gamma} - t_0^{1-2\gamma})]^{d/2}} \int_{\mathbb{R}^d} \exp\left[-\frac{|x-y|^2 (1-2\gamma)}{4t_0^{2\gamma} (t^{1-2\gamma} - t_0^{1-2\gamma})}\right] u(y,t_0) \,\mathrm{d}y,$$
(3.4)

which corresponds to

$$h(x,t) = \frac{2\nu}{\lambda} \ln \left\{ \frac{(1-2\gamma)^{d/2} \exp[F\lambda t^{\gamma}/(2\nu)]}{[4\pi t_0^{2\gamma} (t^{1-2\gamma} - t_0^{1-2\gamma})]^{d/2}} \right\} + \frac{2\nu}{\lambda} \ln \left\{ \int_{\mathbb{R}^d} \exp\left[-\frac{|x-y|^2 (1-2\gamma)}{4t_0^{2\gamma} (t^{1-2\gamma} - t_0^{1-2\gamma})} + \frac{\lambda}{2\nu} h(y,t_0) \right] dy \right\},$$
(3.5)

for given initial conditions $u(x, t_0)$ and $h(x, t_0)$. If we consider the dilution KPZ equation (3.2), then applying the Hopf–Cole transformation, we find the nonlinear equation

$$\partial_t u = \nu \left(\frac{t_0}{t}\right)^{2\gamma} \nabla^2 u - \frac{d\gamma}{t} u \ln(u) + \frac{\gamma F \lambda}{2\nu} t^{\gamma - 1} u + \frac{\lambda}{2\nu} \left(\frac{t_0}{t}\right)^{d\gamma / 2} \xi(x, t) u, \tag{3.6}$$

which may be thought of as a time-dependent and spatially distributed version of the Gompertz differential equation. In this case, it is not evident how to find an explicit solution at the deterministic level for an arbitrary initial condition.

As we have already explained, Galilean invariance means that the transformation indicated in equation (4.10) leaves the KPZ equation invariant. In the case of no dilution, this transformation can be replaced by

$$x \to x - \frac{\lambda}{1 - 2\gamma} v t_0^{2\gamma} t^{1 - 2\gamma}, \quad h \to h + v x \quad \text{and} \quad F \to F - \frac{\lambda}{2\gamma} v^2 t_0^{2\gamma} t^{1 - 3\gamma}, \quad (3.7)$$

which leaves equation (3.1) invariant. If we consider dilution, then it is not clear how to extend this transformation to leave equation (3.2) invariant. The main difficulty comes from the dilution term that yields a non-homogeneous contribution to the dynamics as a response to the tilt transformation $h \to h + vx$. So, in summary, we may talk of a certain sort of Galilean invariance that is obeyed by the no-dilution KPZ dynamics (3.1) and is lost when dilution is taken into account. If it were found that the dilution equation (3.2) obeys the traditional KPZ scaling (at least in some suitable limit), then that would put into question the role that Galilean invariance has in fixing the exponents. We have already mentioned that the KPZ roughness α and dynamical z exponents are believed to obey the scaling relation $\alpha + z = 2$ in all spatial dimensions, a relation that has been traditionally attributed to Galilean invariance [19], although this interpretation has been recently put into question [28]. Note that our numerical results on the KPZ equation precisely indicate the lack of control that Galilean invariance has on the critical exponents [29].

As we have already discussed, there is still another fundamental symmetry of the KPZ equation that manifests itself exclusively in one spatial dimension: the so-called fluctuation–dissipation theorem. It basically says that for long times, when saturation has already been achieved, the nonlinearity ceases to be operative and the resulting interface profile would be statistically indistinguishable from that created by this equation for $\lambda \equiv 0$. For fast domain growth, we know from the linear theory that the interface never becomes correlated, and it operates, in this sense, as if it were effectively in the short time regime for all times [26,27]. As a consequence, the fluctuation–dissipation theorem is not expected to play any role in this case. Of course, this result would be independent of whether we contemplated dilution or not.

4. Discretization issues, symmetry violation and all that

There are two main symmetries associated with the one-dimensional KPZ equation: Galilean invariance and the fluctuation–dissipation relation. On the 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 criticized in this and other non-equilibrium models [28,30]. On the other hand, the second symmetry essentially tells us that in one dimension, 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 behaviour of its solutions requires the (stochastic) numerical integration of a discrete version. Such an approach has been used, for

example, to obtain the critical exponents in one and more spatial dimensions [31–37]. Although a pseudo-spectral (PS) spatial discretization scheme has been recently introduced [38,39], real-space discrete versions of equation (1.1) are still used for numerical simulations [8,40]. One reason is their relative ease of implementation and of interpretation in the case of non-homogeneous substrates like, for example, a quenched impurity distribution [41].

We use the standard, nearest-neighbour 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.

The standard spatially discrete version of equation (2.1) (recalling that $\gamma = \lambda F/2\nu$) is

$$\dot{\phi}_j = \frac{\nu}{a^2} \left(\phi_{j+1} - 2\phi_j + \phi_{j-1} \right) + \frac{\lambda F}{2\nu} \phi_j + \frac{\lambda \varepsilon}{2\nu} \phi_j \xi_j, \tag{4.1}$$

with $1 \le j \le N \equiv 0$, because of the assumed periodic boundary conditions (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 the Hopf–Cole transformation (equation (2.4))

$$\phi_j(t) = \exp\left[\frac{\lambda}{2\nu}h_j(t)\right],$$
(4.2)

we get

$$\dot{h}_{j} = \frac{2\nu^{2}}{\lambda a^{2}} (e^{\delta_{j}^{+}a} + e^{\delta_{j}^{-}a} - 2) + F + \varepsilon \xi_{j}, \tag{4.3}$$

with $\delta_j^{\pm} \equiv (\lambda/2\nu a)(h_{j\pm 1} - h_j)$. By expanding the exponentials up to terms of order a^2 , and collecting equal powers of a (observe that the zero-order contribution vanishes), we retrieve (in order to simplify we adopt F = 0)

$$\dot{h}_{j} = \frac{\nu}{a^{2}} (h_{j+1} - 2h_{j} + h_{j-1}) + \frac{\lambda}{4 a^{2}} [(h_{j+1} - h_{j})^{2} + (h_{j} - h_{j-1})^{2}] + \varepsilon \xi_{j}.$$
 (4.4)

As we can see, the first and second terms on the right-hand side of equation (4.4) are *strictly* related by virtue of equation (4.2). In other words, the discrete form of the Laplacian in equation (4.3) constrains the discrete form of the nonlinear term in the transformed equation. Later we show again, in another way, the tight relation between the discretization of both terms. Known proposals [35] fail to comply with this natural requirement.

An important feature of the Hopf–Cole transformation 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 aforementioned criterion dictates the following discrete form for $\mathcal{F}[\phi]$ given by equation (2.2), thus a Lyapunov function for any finite N:

$$\mathcal{F}[\phi] = \frac{\nu}{2} \sum_{j=1}^{N} a((\partial_x \phi)^2)_j = \frac{\nu}{4a} \sum_{j=1}^{N} [(\phi_{j+1} - \phi_j)^2 + (\phi_j - \phi_{j-1})^2]. \tag{4.5}$$

It is a trivial task to verify that the Laplacian is $(\partial_x^2 \phi)_j = -a^{-1} \partial_{\phi_j} \mathcal{F}[\phi]$. Now, the obvious fact that this functional can also be written as $\mathcal{F}[\phi] = (\nu/2 \ a) \sum_{j=1}^N (\phi_{j+1} - \phi_j)^2$ serves to illustrate a fact that a more elaborate discretization requires explicit calculations: the Laplacian does not *uniquely* determine the Lyapunov function [29].

(b) An accurate consistent discretization

Since the proposals of Lam & Shin [35] already involve next-to-nearest neighbours, one may seek a prescription that minimizes the numerical error. An interesting choice for the Laplacian is [42]

$$\frac{1}{12 a^2} [16(\phi_{j+1} + \phi_{j-1}) - (\phi_{j+2} + \phi_{j-2}) - 30 \phi_j], \tag{4.6}$$

which has the associated discrete form for the KPZ term

$$(\partial_x \phi)^2 = \frac{1}{24 a^2} \{ 16[(\phi_{j+1} - \phi_j)^2 + (\phi_j - \phi_{j-1})^2] - [(\phi_{j+2} - \phi_j)^2 + (\phi_j - \phi_{j-2})^2] \} + \mathcal{O}(a^4).$$
(4.7)

Replacing this into the first line of equation (4.5), we obtain equation (4.6). Since this discretization scheme fulfils 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 [29,43].

(c) Relation with the Lyapunov functional

In §2, we have indicated the form of the NEP for KPZ, and the way in which the functionals $\mathcal{F}[\phi]$ and $\mathcal{G}[h]$ are related [20]. According to the previous results, we can write the discrete version of equation (2.6) as

$$\mathcal{G}[h] = \frac{\lambda^2}{8\nu} \frac{1}{2 a} \sum_{j} e^{(\lambda/\nu)h_j} [(h_{j+1} - h_j)^2 + (h_j - h_{j-1})^2].$$

Introducing this expression into $\partial_t h_j = \Gamma_j \delta \mathcal{G}[h]/\delta h_j$, and through a simple algebra, we obtain equation (4.4). 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

This 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 one dimension is known to be [2,3]

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

For the discretization scheme in equation (4.4) (with F = 0), this is

$$\sim \exp\left\{\frac{\nu}{2\varepsilon} \frac{1}{2a} \sum_{j} \left[(h_{j+1} - h_j)^2 + (h_j - h_{j-1})^2 \right] \right\}.$$
 (4.8)

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

$$\frac{1}{2a^3} \sum_{j} \left[(h_{j+1} - h_j)^2 + (h_j - h_{j-1})^2 \right] \times [h_{j+1} - 2h_j + h_{j-1}]. \tag{4.9}$$

The continuum limit of this term is $\int dx (\partial_x h)^2 \partial_x^2 h$, which is identically zero [3]. A numerical analysis of equation (4.9) indicates that it is several orders of magnitude smaller than the value of the exponents' probability distribution function (in equation (4.8)), 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 equations (4.6) and (4.7)) are used for the differential operators. In addition, when the discrete form of $(\partial_x h)^2$ from Lam & Shin [35] 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 Lam & Shin [35] and Giada et al. [38], can be just circumvented by using more accurate expressions.

(e) Galilean invariance

This invariance means that the transformation

$$x \to x - \lambda v t$$
, $h \to h + v x$ and $F \to F - \frac{\lambda}{2} v^2$, (4.10)

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

$$\partial_x h \to \frac{1}{2a} (h_{j+1} - h_{j-1})$$
 (4.11)

is invariant under the discrete Galilean transformation

$$ja \to ja - \lambda v t$$
, $h_j \to h_j + v ja$ and $F \to F - \frac{\lambda}{2} v^2$. (4.12)

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However, the associated equation is known to be numerically unstable [34], at least when a is not small enough. Besides, equation (4.4) is not invariant under the discrete Galilean transformation. In fact, the transformation $h \to h + vja$ yields an excess term that is compatible with the gradient discretization in equation (4.11); however, this discretization does not allow us to recover the quadratic term in equation (4.4), indicating that this finite-difference scheme is not Galilean-invariant.

Since equation (4.1) is invariant under the transformation indicated in equation (4.12), it is the nonlinear Hopf–Cole transformation (within the present discrete context) that 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 always been associated with the exactness of the one-dimensional KPZ exponents, and with a relation that connects the critical exponents in higher dimensions [19]. If the numerical solution obtained from a finite-difference scheme as equation (4.4), which is not Galilean-invariant, yields the well-known critical exponents, this will be an indication that Galilean invariance is not strictly necessary to get the KPZ universality class. The numerical results presented in Wio et al. [29,43] clearly show that this is the case.

We will not discuss the simulation procedure here, but only indicate that to make the simulations h(x,t) was discretized along the substrate direction x with lattice spacing a=1, and that a standard second-order Runge–Kutta algorithm (with periodic boundary conditions) was employed (e.g. [44]). In Wio et al. [29,43] it was shown that all the cases (consistent or not) exhibit the same critical exponents. Moreover, we note that the discretization used in Lam & Shin [35,45], which also violates Galilean invariance, yields the same critical exponents too. Additionally, stochastic differential equations, which are not explicitly Galilean-invariant, have been shown to obey the relation $\alpha + z = 2$ [46]. Hence, our numerical analysis indicates that there are discrete schemes of the KPZ equation that, even not obeying Galilean invariance, show KPZ scaling.

The moral from the present analysis is clear: owing to the locality of the Hopf–Cole transformation, 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 (4.3) has also been written in Newman & Bray [34], although with different goals from ours (their interest was to analyse the strong coupling limit via mapping to the directed polymer problem).

5. Conclusions

The present work briefly reviews some new results in the study and analysis of the KPZ equation, which offer an alternative approach to other well-known techniques. We have here found the form of the Lyapunov functional or NEP for the KPZ equation, and have also devised a way to extend the procedure to derive it. From this NEP, and through a functional derivative, we have obtained the KPZ equation and have also shown that such an NEP fulfils global shift properties, as well as other ones anticipated for such an unknown functional [5].

Dynamic renormalization group techniques, being useful and powerful, in many cases only offer incomplete results, having no access to the strong coupling phase [2]. Hence, the need of alternative ways to analyse the KPZ and related problems is clear, as for instance the self-consistent expansion [47]. The present results open new possibilities for non-perturbational studies of the KPZ problem.

As a first approach to the understanding of radial growth, we have introduced the KPZ equation on a growing domain. This is justified on the grounds that the widespread Eden model, which is related to both biological growth and percolation, belongs to the KPZ universality class. It has been traditionally accepted that radial and planar interfaces behave analogously. However, we have seen that there are two natural ways of extending the KPZ equation to the growing domain setting. One causes the simultaneous growth of mass together with space, and the other keeps mass constant as the space dilates. The first of these generates memory effects that separate the interface fluctuations from the behaviour dictated by the Family-Vicsek ansatz, while the second is free from these memory effects. On the other hand, the first approach respects the Galilean invariance symmetry and the Hopf-Cole transformation to a linear equation, while the second one does not. This again suggests that some of the mathematical properties of the classical KPZ equation, which were intuitively related to the scaling of the surface fluctuations, are not necessary in order to define the universality class.

We have also discussed the implications of the NEP in the obtaining of consistent discrete representations of the KPZ equation. The fact that the KPZ equation is the result of a local transformation from a stochastic partial differential equation with multiplicative noise imposes some constraints in the discrete versions of the equation. A major point has been to call the attention to the true role of Galilean invariance in KPZ [29,43]. Our purpose was 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 consequences of such an analysis are general, as 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 PS approach [38,39] it has already been said that, when analysing 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 [41,48]. This drawback aside, it has advantages. One of them is related to the numerical instabilities in discrete growth models: whereas in Dasgupta et al. [49], 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, the PS approach seems to be in principle 'transparent' to the question of consistency. Nonetheless, in a recent paper [43] we established a relation between the real-space discretization schemes discussed here (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 used all the N lattice points.

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