THEORETICAL CONTINUOUS EQUATION DERIVED FROM THE MICROSCOPIC DYNAMICS FOR GROWING INTERFACES IN QUENCHED MEDIA

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Abstract

We present an analytical continuous equation for the Tang and Leschhorn model [Phys. Rev A 45, R8309 (1992)] derived from his microscopic rules using a regularization procedure. As well in this approach the nonlinear term $(\nabla h)^2$ arises naturally from the microscopic dynamics even if the continuous equation is not the Kardar-Parisi-Zhang equation [Phys. Rev. Lett. 56, 889 (1986)] with quenched noise (QKPZ). Our equation looks like a QKPZ but with multiplicative quenched and thermal noise. The numerical integration of our equation reproduce the scaling exponents of the roughness of this directed percolation depinning model.

PACS numbers: 47.55.Mh, 68.35.Fx
The investigation of rough surfaces and interfaces has attracted much attention for decades due to its importance in many fields, such as the motion of liquids in porous media, growth of bacterial colonies, crystal growth, etc. When a fluid wets a porous medium, a nonequilibrium self-affine rough interface is generated. The interface has been characterized through scaling of the interfacial width $w = \langle [h_i - \langle h_i \rangle]^2 \rangle^{1/2}$ with time $t$ and lateral size $L$. The result is the determination of two exponents, $\beta$ and $\alpha$ called dynamical and roughness exponents respectively. The interfacial width $w \sim L^\alpha$ for $t \gg t^\ast$ and $w \sim t^\beta$ for $t \ll t^\ast$, where $t^\ast = L^{\alpha/\beta}$ is the crossover time between these two regimes. Much effort has been done to understand the leading mechanisms of these processes and to try to explain how the dynamics affects the scaling exponents [1]. The formation of interfaces is determined by several factors, it is very difficult to discriminate theoretically all of them. The knowledge of the dynamical nonlinearities, the disorder of the media, and the theoretical model representing experimental results are difficult to overcome due to the complex nature of the growth. The disorder affects the motion of the interface and leads to its roughness. The discrete models provided an useful approach to obtain the exponents that allows its classification in universality classes. By extensively studying these models, one can obtain the scaling behaviors and the corresponding universality classes, and then associate the continuum stochastic equations with the given discrete growth models.

The most used method of establishing the correspondence between a continuum growth equation and a discrete model, is to numerically simulate the model and compare the obtained scaling exponents with those of the corresponding continuum equation. In this context attempts are being made to classify quenched disorder models in terms of universality classes based on equation of motion such as

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

where $F$ is the driving force responsible of the advance of the interface, $\xi(x,h)$ is the quenched disorder or pinning forces and $\eta(x,t)$ is the thermal noise. The noises are white. Eq. (1) is Kardar-Parisi-Zhang equation [2] with quenched noise (QKPZ). When $\lambda \to 0$ the quenched Edward-Wilkinson equation (QEW) [3] is recovered. In absence of quenched noise his thermal versions are recovered, named KPZ and EW respectively. Much effort has been done in order to classify discrete models and experiments in universality classes depending on the value of the coefficient $\lambda$ associated with the nonlinearity of the QKPZ. Numerical [4,5] studies indicate $\lambda$ is relevant at the depinning transition for discrete models in anisotropic media. These results only shows that the nonlinear term exist but they do not confirm that these models are represented by the QKPZ. However the exponents obtained by numerical simulation of Eq. (1), without thermal noise [3], agree very good with those of the model in anisotropic media.

A powerful method of establishing the correspondence between a continuum growth equation and a discrete model is to derive the continuum equation from a given discrete model analytically. Among them, a systematic method proposed by Vvedensky et al. [7], where the continuum equations can be constructed directly from the growth rules of the discrete model based on the master-equation description, has been applied to the derivation of growth
equations for some discrete models \[7\] with thermal noise. This method has proved to be useful to derive continuous equation from the microscopic ones with the advantage that the sources of the terms of the Langevin equation can be identified and their magnitude related to the microscopic dynamics. While the method described by thses authors can be applied to general case it is more easy to achieve the same results using a microscopic equation based on rules for the evolution of the height. The derivation of continuous equations from discrete models is an interesting subject which has not been addressed in the context of growth in presence of quenched media.

The aim of this work is to obtain the continuous equation from the microscopic dynamics of a model with quenched noise in order to establish if it is related in some way with the QKPZ equation. The main goal of our paper is to have obtained analytically the differential equation which describe the dynamics of the Tang and and Leschhorn (TL) model \[10\]. To our knowledge this is the first time that a Langevin equation is obtained from the microscopic growing rules for the evolution of the height at this site due that a site \(G_k\) with cells of size \(a\) represents the mean size of a pore. For a given applied pressure \(p > 0\), we can divide the cells into two groups, those with \(g(r) \leq p\) (free or active cells), and those with \(g(r) > p\) (blocked or inactive cells). Denoting by \(q\) the density of inactive cells on the lattice we have \(q = 1 - p\) for \(0 < p < 1\) and \(q = 0\) for \(p \geq 1\). In this model the critical pressure is \(p_c = 0.461\). Periodic boundary conditions are used. We consider the evolution of the height of the \(i\)-th site in this model. Let us denote by \(h_i(t)\) the height of the \(i\)-th generic site at time \(t\). The set \(\{h_i, i = 1, \ldots, N\}\) where \(N = L/a\), defines the interface between wet and dry cells. Given a site, chosen between \(N\), say the site \(j\), the height in the site \(i\) is increased by \(a\) with probability (i) \(1\) if \(j = i \pm 1\) and \(h_{i+1} \geq h_i + 2a\) and \(h_i < h_{i+2}\), (ii) \(1/2\) if \(j = i \pm 1\) and \(h_{i+1} \geq h_i + 2a\) and \(h_i = h_{i+2}\), (iii) \(1\) if \(j = i\) and \(h_i < \min(h_{i-1}, h_{i+1}) + 2a\) and \(F_i(h_i + a) = 1\). Otherwise no growth happens. \(F_i(h_i + a) = \Theta(p - g_i(h_i + a))\) is called the activity function \[13\] and \(\Theta(x)\) is the unit step function defined as \(\Theta(x) = 1\) for \(x \geq 0\) and equals to 0 otherwise, \(p\) is the microscopic driving force and \(g_i(h_i + a)\) is the quenched noise just above the interface distributed in the interval \([0, 1]\). Notice that the activity function \(F\) is the competition between the driving force and the quenched noise, so \(F\) is also a “noise”. Provided that the system size is large and that the intrinsic fluctuations are not too large \[7\], the evolution equation for the height in a site \(i\), in a short lapse \(\tau\), is

\[
\frac{\partial h_i}{\partial t} = \frac{a}{\tau} G_i + \eta_i ,
\]

where \(\tau\) is the mean lapse between successive election of any site and \(G_i\) \[13\] are the microscopic growing rules for the evolution of the height at this site due that a site \(j\) is chosen at time \(t\). Here \(\eta_i\) is a Gaussian “thermal” noise with zero mean and covariance

\[
\langle \eta_i(t)\eta_j(t') \rangle = \frac{a^2}{\tau} G_i \delta_{ij} \delta(t - t') .
\]

Notice that in the notation of \[7\] the transition rate from from a configuration \(H\) to another \(H'\) is \(W(H, H') = \frac{1}{\tau} \sum_k \delta(h'_k, h_k + a)G_k \prod_{j \neq k} \delta(h'_j, h_j)\). So the first moment is \(\frac{1}{\tau} \sum_{H'} \langle h'_k -
\[ h_k W(H, H') = \frac{2}{7} G_k. \] As a consequence of the fact that subsequent configurations differ only in the height at one site all the moments are diagonal and proportional to the first moment [4].

For this model [13,14],

\[ G_i(h_{i-1}, h_i, h_{i+1}) = W_{i+1} + W_{i-1} + F_i(|h_i| + 1) W_i, \tag{4} \]

where \(|h_i| \equiv \left\lfloor \frac{h_i}{a} \right\rfloor\) denotes the integer part of \(h_i\) in units of \(a\). This definition is meaningless if \(a\) is taken as one, as in the discrete model. We shall show below that in the continuous limit, it means that \(F\) is taken as a constant inside a pore. In Eq. (4),

\[ W_{i\pm 1} = \frac{1}{2} \left[ 1 - \Theta(H_i^{i+2} + H_i^{i+2}) + \Theta(H_i^{i\pm 2}) \right] \Theta(H_i^{i\pm 1} - 2), \tag{5} \]

where \(H_i^s = (h_s - h_i)/a\) and \(U_i = \frac{1}{a}[h_i - \min(h_{i+1}, h_{i-1})]\). Notice that all the heights are in units of \(a\) in order to keep the arguments of the step function without units. For \(W_{i\pm 1}\) the \(\delta\) Kronecker function has been taken as

\[ \delta(x, y) = \Theta(x - y) + \Theta(y - x) - 1. \tag{6} \]

Using the fact that \(\min(x, y) = \frac{1}{2}[(x + y) - (x - y)[\Theta(x - y) - \Theta(y - x)]\} \) and with a more compact notation

\[ U_i = \frac{1}{2}\left[H_i^{i+1} + H_i^{i-1} + H_i^{i+1}[\Theta(H_i^{i+1}) - \Theta(H_i^{i-1})]\right]. \tag{7} \]

The representation of the step function can be expanded as \(\Theta(x) = \sum_{k=0}^{\infty} c_k x^k\) providing that \(x\) is smooth. Our focus is on properties of the surface on large length scales so we kept the expansion of the step function to first order in his argument. The best choice for the representation of the \(\Theta\) function is the shifted hyperbolic tangent [4], defined as \(\Theta(x) = \{1 + \tanh[C(x + b)]\}/2\), where \(b\) is the shift and \(C\) is a parameter that allows to recover the \(\Theta\) in the limit \(C \to \infty\). We choose \(b = 1/2\). The reason of our choices is that it allows us to define the \(\delta\) function as Eq. (3). The coefficients fulfill

\[ c_0 = \frac{1}{2} \left[ 1 + \tanh\left(\frac{C}{2}\right) \right] \quad \text{and} \quad c_1 = \frac{C}{2} \cosh^{-2}\left(\frac{C}{2}\right). \tag{8} \]

We shall show bellow the qualitative information that can be obtained from these coefficients assuming this regularization scheme. The next step is to regularize the height defining an interpolating function. This is done by expanding the height \(h_{i+\ell} \equiv h(x_i + x_\ell)\) around \(x_i = ia\). Retaining only the leading terms in the expansion, the adimensional difference of heights is

\[ H_{i+m}^{i+\ell} = (\ell - m) \partial_x h \big|_{x_i} + \frac{1}{2}(\ell^2 - m^2) \partial_x^2 h \big|_{x_i} a + \mathcal{O}(a^2), \tag{9} \]

where \(\partial^j_x h = \partial^j h/\partial x^j\).

Notice that in any discrete model there is in principle an infinite number of nonlinearities, but at long wavelengths the higher order derivatives can be neglected using scaling arguments, since one expect affine interfaces over a long range of scales, and then one is usually concerned with the form of the relevant terms.
Replacing Eq. (9) in Eqs. (5) and (7), using the expansion of the step function and retaining the leading terms to order $O(a)$, Eq. (2) can be written as

$$\frac{\partial h(x_i, t)}{\partial t} = \frac{a}{\tau} \left[ W(x_i + a) + W(x_i - a) + W(x_i) F(x_i, |h(x_i)| + 1) \right] + \eta(x_i, t),$$

with

$$W(x + a) + W(x - a) = (c_0 - 2c_1) + 4c_1^2 (\partial_x h)^2 + ac_1 \left[ \frac{1}{2} + 4(c_0 - 2c_1) \right] \partial_x^2 h,$$  

$$W(x) = 1 - (c_0 - 2c_1) - 4c_1^2 (\partial_x h)^2 + \frac{1}{2}ac_1 \partial_x^2 h.$$  

Notice that the argument of $F = \Theta(p - g(x_i, |h(x_i)| + 1))$ is not smooth, so his expansion is meaningless. For the activity function $F$ we define an interpolation function

$$\tilde{F}(x_i, h(x_i)) = F(x_i, |h_i|) + \frac{\delta h}{a} [F(x_i, |h_i| + 1) - F(x_i, |h_i|)] + O(\delta h^2),$$

with $0 \leq \delta h \leq a$ that measures the departure of the height from the low pore. Then $\tilde{F}$ is a smooth function taking continuous values in the interval $[0, 1]$. With this definition we ensure that the characteristic size of the correlation between pores is of the order of the pore size. In real materials there always exist a typical size of the inhomogeneities in the disordered media which plays the role of the lattice constant $a$.

The final step is a coarse-grained spatial average of the variables in order to obtain smooth continuous functions at a macroscopic level. In this way we obtain the stochastic continuous equation for this model,

$$\frac{\partial h}{\partial t} = \mu(\tilde{F}) + \nu(\tilde{F}) \partial_x^2 h + \lambda(\tilde{F}) (\partial_x h)^2 + \eta(x, t),$$

where

$$\mu(\tilde{F}) = \left[(c_0 - 2c_1)(1 - \tilde{F}) + \tilde{F} \right] \frac{a}{\tau},$$

$$\nu(\tilde{F}) = c_1 \left[ \frac{1}{2} (1 + \tilde{F}) + 4(c_0 - 2c_1) \right] \frac{a^2}{\tau},$$

$$\lambda(\tilde{F}) = 4c_1^2 (1 - \tilde{F}) \frac{a}{\tau}.$$  

and $\tilde{F} \equiv F(x, h)$ as was defined in Eq. (13). Notice that $\mu(\tilde{F})$ is now the effective competition between the driving force and the quenched noise.

Equation (14) shows that the nonlinearity arises naturally as a consequence of the microscopic model.

This explains the previous numerical results obtained by Amaral et al. [4], that studied the effects of an effective coefficient $\lambda_{eff}$ from a tilted interface showing that the nonlinear term must exist. Our result is also in agreement with those of Réka et al. [5] that obtained numerically a parabolic shape of the local velocity as function of the gradient for the DPD model near above the criticality for different reduced forces ($p/p_c - 1$). Now, let us consider for a moment the restrictions we have imposed over the coefficients $c_0$ and $c_1$ in the expansion of the representation of the $\Theta$ function. When the conditions (8) are satisfied, the
coefficient $\nu$ is always positive. The coefficient $\lambda$ is greater or equal to zero independently of the representation of the step function. On the other hand $\mu$ can be positive or negative depending of the value of $\tilde{F}$. In Fig. 1 we show $\tilde{F}$ as function of $C$ for $\lambda = \nu$ (upper curve) and $\nu = 0$ (lower curve). We can distinguish three regions. In the region $\mu < 0$ and $\lambda > \nu > 0$, the function $\tilde{F}$ takes values close to zero. Notice that in the discrete model, as we approach to the critical value $F$ is mostly zero because the interface gets pinned by long chains of inactive sites [13,14]. In the continuous model near the criticality $\mu$ mostly becomes negative braking the advance of the interface and $\tilde{F}$ is close to zero. Then regions of small gradients will be halted by the effective driving force $\mu$. In these case the main responsible of the nonlinearities is the lateral contribution [see Eq. (11)]. This explain why this contribution enhances the roughness at the criticality as was predicted by Braunstein et al. [13].

Faraway above the criticality the nonlinear term becomes less relevant. In the limit $p \to 0$ ($p \to 1$) we recover the KPZ (EW) equation with thermal noise. However the fact that these limits are recovered is a specific characteristic of this particular model.

In Figs. 2 we show the temporal scaling behavior of the roughness $w$ obtained from the numerical integration of Eq. (14). At the criticality a slope $\beta = 0.67 \pm 0.05$ was obtained. Above the threshold we recover a crossover between the exponent $\beta = 0.67 \pm 0.05$ and the $\beta_m \simeq 1/3$ as was obtained by Leschhorn [3] by means of the numerical integration of the QKPZ equation and by his automaton version. In Fig. 3 we show the scaling behavior of the correlation function $C_2(r, t) = \langle [h_{i+r}(t) - h_i(t)]^2 \rangle^{1/2}$. The exponent obtained was $\alpha = 0.641 \pm 0.07$ in agreement with the DPD models. The numerical integration was made in short lattices. The results in large systems and the details of the integration will be published elsewhere. Notice that even if the exponents from our equation are very similar that the one obtained from the QKPZ one, our equation is very different. The main difference is that the coefficient of the nonlinear term in our equation is strongly affected by the local characteristic of the substratum. Another great difference is that the global velocity of the interface is affected by the coefficient of the Laplacian term. The study of these differences requires a great computational effort that is not in the aim of the present work.

How our results could be used in order to explain the role played by the disordered media in the experiments? In the experiments the advancement of the interface is determinated by the coupled effect of the random distribution of the capillary sizes, the surface tension and the local properties of the flow, so it is not surprising that all these effect give rise to a multiplicative noise in any evolution equation that intends to represent an experimental growth with disordered media.

Summarizing, we derive the continuous equation from the microscopic one for the TL model. In our work the nonlinear term arises naturally as consequence of the microscopic dynamics. The numerical integration of our equation reproduces very accurately the scaling exponents of the roughness. However these results show that the DPD model is not described by a QKPZ equation with additive noise even if the exponents of the roughness are very similar. Our equation also allows to explain that the lateral growth contribution is the main responsible of the roughness near the criticality. Finally, we hope that this framework can be used in other growing models with quenched noise.
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FIGURES

FIG. 1. $\tilde{F}$ as function of $C$ for $\mu(\tilde{F}) = 0$ (dashed line) and $\lambda(\tilde{F}) = \nu(\tilde{F})$ (solid line). In the first region (I) $\lambda(\tilde{F}) > \nu(\tilde{F}) > 0$ and $\mu(\tilde{F}) < 0$, in the second region (II) $\lambda(\tilde{F}) > \nu(\tilde{F}) > 0$ and $\mu(\tilde{F}) > 0$ and in the third region (III) $0 < \lambda(\tilde{F}) < \nu(\tilde{F})$ and $\mu(\tilde{F}) > 0$

FIG. 2. log-log plot of the square roughness $w^2$ vs time for $C = 1.3$. In (a) $p = 0.1$, for this value of $C$ the critical pressure is $p_c \simeq 0.1$. In circles we shows the results obtained from the numerical integration of Eq. (14). The dashed line is used as a guide and as exponent $2\beta = 1.34$. In (b) $p = 0.3$, the dashed line has slope $2\beta = 1.34$ and the solid line has slope $2\beta_m = 0.66$. The numerical integration has been done with $L = 1024$ and over 30 independent samples.

FIG. 3. log-log plot of $C_2(r)$ as function of $r$ for $p = 0.1$ and $C = 1.3$. The dashed line that is used as a guide has slope $2\alpha = 1.28$
