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Level crossing analysis of growing surfaces

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Abstract

We investigate the average frequency of positive slope ν_{α}^+ , crossing the height $\alpha=h-\bar{h}$ in the surface growing processes. The exact level crossing analysis of the random deposition model and the Kardar–Parisi–Zhang equation in the strong coupling limit before creation of singularities is given.

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1. Introduction

Due to the technical importance and fundamental interest, a great deal of effort has been devoted to understanding the mechanism of thin-film growth and the kinetic roughening of growing surfaces in various growth techniques. Analytical and numerical treatments of simple growth models suggest, quite generally, that the height fluctuations have a self-affine character and their average correlations exhibit a dynamic scaling form [1–6]. It is known that to derive the quantitative information of the surface morphology one may consider a sample of size L and define the mean height of growing film \bar{h} and its roughness w by [1]

$$\bar{h}(L,t) = \frac{1}{L} \int_{-L/2}^{L/2} dx \, h(x,t) \tag{1}$$

and

$$w(L,t) = (\langle (h-\bar{h})^2 \rangle)^{1/2} \tag{2}$$

where $\langle \cdots \rangle$ denotes an averaging over different realization (samples). Starting from a flat interface (one of the possible initial conditions), it was conjectured by Family and Vicsek [7] that a scaling of space by a factor b and of time by a factor b^z (z is the dynamical scaling

exponent), re-scales the roughness w by a factor b^{χ} as follows: $w(bL, b^z t) = b^{\chi} w(L, t)$, which implies that

$$w(L,t) = L^{\chi} f(t/L^{\zeta}). \tag{3}$$

If for large t and fixed $L(t/L^z \to \infty)$, w saturates then $f(x) \to \text{const}$, as $x \to \infty$. However, for fixed large L and $1 \ll t \ll L^z$, one expects that correlations of the height fluctuations are set up only within a distance $t^{1/z}$ and thus must be independent of L. This implies that for $x \ll 1$, $f(x) \sim x^{\beta}$ with $\beta = \chi/z$. Thus dynamic scaling postulates that $w(L, t) \sim t^{\beta}$ for $1 \ll t \ll L^z$ and $\sim L^{\chi}$ for $t \gg L^z$. The roughness exponent χ and the dynamic exponent z characterize the self-affine geometry of the surface and its dynamics, respectively.

Here we introduce the level crossing analysis in the context of surface growth processes. In the level crossing analysis, we are interested in determining the average frequency (in spatial dimension) of observing a definite value for height function $h - \bar{h} = \alpha$ in growing thin films, ν_{α}^{+} , from which one can find the averaged number of crossing the given height in a sample with size L. The average number visiting the height $h - \bar{h} = \alpha$ with positive slope will be $N_{\alpha}^{+} = \nu_{\alpha}^{+}L$. It can be shown that ν_{α}^{+} can be written in terms of joint probability distribution function (PDF) of $h - \bar{h}$ and its gradient. Therefore the quantity v_{α}^{+} carries the whole information of surface lying in joint PDF of height and its gradient fluctuations. This work aims to study the frequency of positive slope crossing (i.e. v_{α}^{+}) in time t for the growing surface on a substrate with size L. We also introduce a quantity N_{tot}^+ which is defined as $N_{\text{tot}}^+ = \int_{-\infty}^{+\infty} v_{\alpha}^+ d\alpha$ to measure the total number of crossings of the surface with positive slope. This quantity is proportional to the length of the path constructed by growing surface. For example, for a given growth process, with finite correlation length parallel to the substrate, the number of crossings within a system size L is proportional to the roughness of the surface, so it is expected that N_{α}^+ grows as t^{β} , such that N_{tot}^+ scales as $t^{2\beta}$. In the stationary regime we expect N_{tot}^+ to saturate as $L^{2\chi}$. But for the random deposition (RD) model, in which there is no correlation length, the N_{α}^{+} is time independent and the total number of the crossings should grow as t^{β} and never saturate.

In this paper, we determine the time and height dependence of v_{α}^{+} for two exactly solvable models, random deposition model and (1+1)-dimensional Kardar–Parisi–Zhang (KPZ) equation in the zero tension limit with short-range forcing and before creation of singularities (sharp valleys) [10]. It is shown that the RD model and KPZ equation, in the mentioned regime have different v_{α}^{+} ; however, N_{tot}^{+} scales as $t^{1/2}$ in both models which shows that for time scales less than the characteristic time for the creation of the singularities, KPZ process is like RD growth. We expect that for time scales much larger than the time scale of singularity formation and much less than saturation time, the scaling behaviour of N_{tot}^{+} crosses over to $t^{2/3}$. In section 2, we discuss the connection between v_{α}^{+} and underlying probability distribution functions of growing surfaces. Exact expression of v_{α}^{+} for the RD model with short-range forcing is given in section 3. In section 4, we derive the integral representation of v_{α}^{+} for the KPZ equation in 1+1 dimensions and in the strong coupling limit (zero tension limit) before the creation of singularities. We summarize the results in section 5.

2. The level crossing analysis of growing surface

Consider a sample function of an ensemble of functions which make up the homogeneous random process h(x,t). Let n_{α}^+ denote the number of positive slope crossings of $h(x) - \bar{h} = \alpha$ in time t for a typical sample size L (see figure 1) and let the mean value for all the samples be $N_{\alpha}^+(L)$ where

$$N_{\alpha}^{+}(L) = E[n_{\alpha}^{+}(L)]. \tag{4}$$

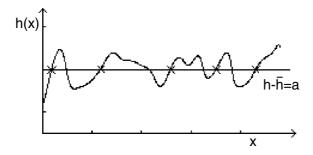


Figure 1. Positive slope crossing of the level $h - \bar{h} = \alpha$.

Since the process is homogeneous, if we take a second interval of L immediately following the first, we shall obtain the same result, and for the two intervals together we shall therefore obtain

$$N_{\alpha}^{+}(2L) = 2N_{\alpha}^{+}(L) \tag{5}$$

from which it follows that, for a homogeneous process, the average number of crossings is proportional to the space interval L. Hence

$$N_{\alpha}^{+}(L) \propto L$$
 (6)

or

$$N_{\alpha}^{+}(L) = \nu_{\alpha}^{+}L \tag{7}$$

where v_{α}^{+} is the average frequency of positive slope crossing of the level $h - \bar{h} = \alpha$. We now consider how the frequency parameter v_{α}^{+} can be deduced from the underlying probability distributions for $h - \bar{h}$. Consider a small length dl of a typical sample function. Since we are assuming that the process $h - \bar{h}$ is a smooth function of x, with no sudden ups and downs, if dl is small enough, the sample can only cross $h - \bar{h} = \alpha$ with positive slope if $h - \bar{h} < \alpha$ at the beginning of the interval location x. Furthermore, there is a minimum slope at position x if the level $h - \bar{h} = \alpha$ is to be crossed in interval dl, depending on the value of $h - \bar{h}$ at location x. So there will be a positive crossing of $h - \bar{h} = \alpha$ in the next space interval dl if, at position x,

$$h - \bar{h} < \alpha$$
 and $\frac{\mathrm{d}(h - \bar{h})}{\mathrm{d}l} > \frac{\alpha - (h - \bar{h})}{\mathrm{d}l}$. (8)

Actually what we really mean is that there will be high probability of a crossing in interval dl if these conditions are satisfied [8, 9].

In order to determine whether the above conditions are satisfied at any arbitrary location x, we must find how the values of $y=h-\bar{h}$ and $y'=\frac{\mathrm{d}y}{\mathrm{d}l}$ are distributed by considering their joint probability density p(y,y'). Suppose that the level $y=\alpha$ and interval $\mathrm{d}l$ are specified. Then we need only the region between the lines $y=\alpha$ and $y'=\frac{\alpha-y}{\mathrm{d}l}$ in the plane (y,y'), to find the probability of the positive slope crossing of $y=\alpha$ in $\mathrm{d}l$. Hence the probability of positive slope crossing of $y=\alpha$ in $\mathrm{d}l$ is

$$\int_0^\infty dy' \int_{\alpha - y'}^\alpha dy \ p(y, y'). \tag{9}$$

When $dl \rightarrow 0$, it is legitimate to put

$$p(y, y') = p(y = \alpha, y').$$
 (10)

Since at large values of y and y', the probability density function approaches zero fast enough, therefore equation (6) may be written as

$$\int_0^\infty dy' \int_{\alpha - y' \, dl}^\alpha dy \, p(y = \alpha, y') \tag{11}$$

in which the integrand is no longer a function of y so that the first integral is just: $\int_{\alpha-y'\mathrm{d}l}^{\alpha}\mathrm{d}y\ p(y=\alpha,y')=p(y=\alpha,y')y'\,\mathrm{d}l, \text{ so that the probability of slope crossing of }y=\alpha \text{ in }dl \text{ is equal to}$

$$dl \int_0^\infty p(\alpha, y') y' \, dy' \tag{12}$$

in which the term $p(\alpha, y')$ is the joint probability density p(y, y') evaluated at $y = \alpha$.

We have said that the average number of positive slope crossing in scale L is $\nu_{\alpha}^{+}L$, according to (7). The average number of crossings in interval dl is therefore $\nu_{\alpha}^{+}dl$. So, an average number of positive crossings of $y=\alpha$ in interval dl is equal to the probability of positive crossing of y=a in dl, which is only true because dl is small and the process y(x) is smooth so that there cannot be more than one crossing of $y=\alpha$ in space interval dl, Therefore we have $\nu_{\alpha}^{+}dl=dl\int_{0}^{\infty}p(\alpha,y')y'dy'$, from which we get the following result for the frequency parameter ν_{α}^{+} in terms of the joint probability density function p(y,y'),

$$v_{\alpha}^{+} = \int_{0}^{\infty} p(\alpha, y') y' \, \mathrm{d}y'. \tag{13}$$

In the following sections, we derive the ν_{α}^+ via the joint PDF of $h-\bar{h}$ and height gradient. To derive the joint PDF we use the master equation method [10]. This method enables us to find the ν_{α}^+ in terms of generating function $Z(\lambda, \mu, x, t) = \langle \exp(-\mathrm{i}\lambda(h(x, t) - \bar{h}) - \mathrm{i}\mu u(x, t)) \rangle$, where $u(x, t) = -\nabla h$.

3. The frequency of a definite height with positive slope for the random deposition model

In random deposition model, particles are dropped randomly over deposition sites, and stick to the top of the pre-existing columns on the site [1]. The height of each column thus performs an independent random walk. This model leads to an unrealistically rough surface whose overall width increases with the exponent $\beta = \frac{1}{2}$ without saturation. In the continuum limit, the random deposition model is described by the following equations.

$$\frac{\partial}{\partial t}h(x,t) = f(x,t) \qquad \frac{\partial}{\partial t}u(x,t) = f_x \tag{14}$$

where h(x, t) is the height field, $u(x, t) = \frac{\partial}{\partial x} h(x, t)$ and f(x, t) is a zero mean random force Gaussian correlated in space and white in time,

$$\langle f(x,t) f(x',t') \rangle = 2D_0 D(x-x') \delta(t-t') \tag{15}$$

where D(x) is the space correlation function and is an even function of its argument. It has the following form:

$$D(x - x') = \frac{1}{\sqrt{\pi}\sigma} \exp\left(-\frac{(x - x')^2}{\sigma^2}\right)$$
 (16)

where σ is the standard deviation of D(x-x'). The average force on the interface is not essential and can be removed by a simple shift of h (i.e., $h \to (h-\bar{F}t)$ where $\bar{F} = \langle f(x,t) \rangle$). Typically the correlation of forcing is considered as delta function for mimicking the short-range correlation. We regularize the delta function correlation by a Gaussian function. When

the standard deviation σ is much less than the system size, we would expect that the model would represent a short-range character for the forcing. So we would stress that our calculations are done for finite $\sigma \ll L$, where L is the system size. The parameter D_0 describes the noise strength.

Now assuming the homogeneity we define the generating function as

$$Z(\lambda, \mu, t) = \langle \exp(-i\lambda h(x, t) - i\mu u(x, t)). \tag{17}$$

Using equation (14) we can find the following equation for the evolution of $Z(\lambda, \mu, t)$:

$$\frac{\partial}{\partial t}Z(\lambda,\mu,t) = -\mathrm{i}\lambda\langle h_t(x,t)\exp(-\mathrm{i}\lambda h(x,t) - \mathrm{i}\mu u(x,t))\rangle
-\mathrm{i}\mu\langle u_t(x,t)\exp(-\mathrm{i}\lambda h(x,t) - \mathrm{i}\mu u(x,t))\rangle
= -\mathrm{i}\lambda\langle f(x,t)\exp(-\mathrm{i}\lambda h(x,t) - \mathrm{i}\mu f_x(x,t))\rangle
-\mathrm{i}\mu\langle u_t\exp(-\mathrm{i}\lambda h(x,t) - \mathrm{i}\mu u(x,t))\rangle
= -\lambda^2 D_0 D(0)Z + \mu^2 D_0 D_{xx}(0)Z.$$
(18)

The joint probability density function of h and u can be obtained by Fourier transform of the generating function

$$P(h, u, t) = \frac{1}{2\pi} \int d\lambda \, d\mu \, e^{i\lambda h + i\mu u} Z(\lambda, \mu, t)$$
 (19)

so by Fourier transformation of equation (18), we get the Fokker-Planck equation as

$$\frac{\partial}{\partial t}P = D_0 D(0) \frac{\partial^2}{\partial h^2} P - D_0 D_{xx}(0) \frac{\partial^2}{\partial u^2} P. \tag{20}$$

The solution of the above equation can be separated as $P(h, u, t) = p_1(h, t)p_2(u, t)$. Using the initial conditions $P_1(h, 0) = \delta(h)$ and $P_2(u, 0) = \delta(u)$ (starting from flat surface) it can be shown that

$$P(h, u, t) = \frac{1}{4\pi t \sqrt{-D_0^2 D(0) D_{xx}(0)}} \exp\left(-\frac{h^2}{4D_0 D(0)t} + \frac{u^2}{4D_0 D_{xx}(0)t}\right)$$
(21)

from which the frequency of repeating a definite height $(h(x, t) = \alpha)$ can be calculated as

$$\nu_{\alpha}^{+} = \int_{0}^{\infty} u P(\alpha, u) \, \mathrm{d}u = \frac{1}{2\pi} \sqrt{-\frac{D_{xx}(0)}{D(0)}} \exp\left(-\frac{\alpha^{2}}{4D(0)t}\right) = \frac{1}{2\pi\sigma} \exp\left(-\frac{\alpha^{2}}{4D_{0}D(0)t}\right). \tag{22}$$

The quantity v_{α}^+ in RD model has a Gaussian form with respect to α . The zero level crossing scales with σ as $v_{\alpha=0}^+ \sim \sigma^{-1}$. Also, using equation (22) it is found that $N_{\rm tot}^+ = D_0^{1/2} \pi^{-3/4} \sigma^{-3/2} t^{1/2}$. This shows that there is no stationary state for the RD model and the quantity $N_{\rm tot}^+$ diverges without saturation.

4. Frequency of a definite height with positive slope for KPZ equation before the formation of the singularities

In the Kardar–Parisi–Zhang (KPZ) model (e.g., in one dimension), the surface height h(x, t) on the top of location x of one-dimensional substrate satisfies a stochastic random equation:

$$\frac{\partial h}{\partial t} - \frac{\alpha}{2} (\partial_x h)^2 = \nu \partial_x^2 h + f(x, t)$$
 (23)

where $\alpha \geqslant 0$ and f is a zero-mean, statistically homogeneous, white in time and Gaussian process with covariance as equation (16). The parameters ν , α and D_0 (and σ) describe surface

relaxation, lateral growth and the noise strength, respectively. Let us define the generating function $Z(\lambda, \mu, x, t)$ as

$$Z(\lambda, \mu, x, t) = \langle \exp(-i\lambda(h(x, t) - \bar{h}) - i\mu u(x, t)) \rangle.$$

Where $u(x, t) = -\partial_x h(x, t)$. Assuming statistical homogeneity, i.e. $Z_x = 0$, it follows from equation (23) that Z satisfies the following equation:

$$-i\mu Z_{t} = \gamma(t)\lambda\mu Z - \frac{\alpha}{2}\lambda\mu Z_{\mu\mu} + i\lambda^{2}\mu k(0)Z - i\mu^{3}k_{xx}(0)Z - i(\nu\lambda^{2} + i\alpha\lambda)Z_{\mu}$$
$$-\mu^{2}\nu\langle u_{xx}(x,t)\exp(-i\lambda\tilde{h}(x,t) - i\mu u(x,t))\rangle$$
(24)

where $k(x-x')=2D_0D(x-x')$, $\gamma(t)=\bar{h}_t$, $k(0)=\frac{D_0}{\sqrt{\pi}\sigma}$ and $k_{xx}(0)=-\frac{2D_0}{\sqrt{\pi}\sigma^3}$ and $\tilde{h}(x,t)=h(x,t)-\bar{h}$. Once we try to develop the statistical theory of the roughened surface, it becomes clear that the inter-dependency of the height difference and height gradient statistics would be taken into account. We are interested in the zero tension limit of the KPZ equation. The very existence of the nonlinear term in the KPZ equation with finite σ leads to development of the sharp valley singularities in a *finite time* and in the strong coupling limit (or zero tension limit), i.e. $\nu \to 0$. So one would distinguish between different time regimes, before and after singularity creation. Recently it has been shown that starting from the flat interface, the KPZ equation will develop sharp valleys singularity after time scale t*, where t* depends on the forcing properties as $t*=\left(\frac{1}{4}\right)^{4/3}(\pi)^{1/6}D_0^{-1/3}\alpha^{-2/3}\sigma^{5/3}$ [10]. This means that for time scales less than t*, the relaxation contribution tends to zero when $\nu \to 0$. In this regime, one can see that the generating function equation is closed. Solutions of the resulting equation are easily derived (starting from a flat surface, i.e. h(x,0)=0 and u(x,0)=0), and has the following form [10]:

$$Z(\mu, \lambda, t) = (1 - \tanh^{2}(\sqrt{2ik_{xx}(0)\alpha\lambda}t)) \exp\left[-\frac{5}{8}\ln(1 - \tanh^{4}(\sqrt{2ik_{xx}(0)\alpha\lambda}t))\right]$$

$$+ \frac{5}{4}\tanh^{-1}(\tanh^{2}(\sqrt{2ik_{xx}(0)\alpha\lambda}t)) - \lambda^{2}k(0)t$$

$$- \frac{1}{16}\ln^{2}\left(\frac{1 - \tanh(\sqrt{2ik_{xx}(0)\alpha\lambda}t)}{1 + \tanh(\sqrt{2ik_{xx}(0)\alpha\lambda}t)}\right)$$

$$- \frac{1}{2}i\mu^{2}\sqrt{\frac{2ik_{xx}(0)}{\alpha\lambda}}\tanh(\sqrt{2ik_{xx}(0)\alpha\lambda}t)\right]. \tag{25}$$

One can construct $P(\tilde{h}, u, t)$ in terms of generating function Z as equation (19), from which the frequency of repeating a definite height $(h(x, t) - \bar{h} = \alpha)$ with positive slope can be calculated as $v_{\alpha}^+ = \int_0^{\infty} u P(\alpha, u) \, \mathrm{d}u$. In figure 2, we plot the v_{α}^+ for time scales before creation of singularity, t/t*=0.05, 0.15 and 0.25. In the KPZ equation, due to the nonlinear term there is no $h \to -h$ symmetry and one can deduce that the v_{α}^+ is also not symmetric under $h \to -h$. To derive the N_{tot}^+ let us express v_{α}^+ and N_{tot}^+ in terms of the generating function Z. It can be easily shown that the v_{α}^+ and N_{tot}^+ can be written in terms of the generating function Z as

$$v_{\alpha}^{+} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} -\frac{1}{\mu^{2}} Z(\lambda, \mu) \exp(i\lambda\alpha) d\lambda d\mu$$
 (26)

and

$$N_{\text{tot}}^{+} = \int_{-\infty}^{+\infty} -\frac{1}{\mu^2} Z(\lambda \to 0, \mu) \, \mathrm{d}\lambda. \tag{27}$$

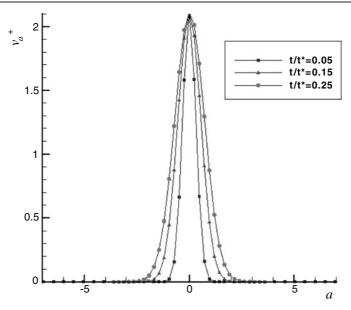


Figure 2. Plot of v_{α}^{+} versus α for the KPZ equation in the strong coupling and before the creation of sharp valleys for time scale t/t*=0.05, 0.15 and 0.25.

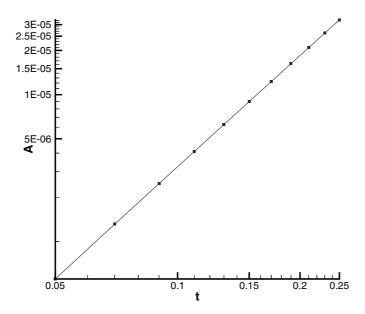


Figure 3. Log $-\log$ plot of N_{tot} (A) versus t for the KPZ equation in the strong coupling before the creation of sharp valleys.

Using equation (25), one finds $N_{\rm tot}^+ \sim \sigma^{-3/2} t^{1/2}$. We note that the expression of the v_{α}^+ for the RD model and KPZ equation before t* are different functions of α but $N_{\rm tot}^+$ scales as $\sim \sigma^{-3/2} t^{1/2}$ in both models. In figure 3 using the direct numerical integration of joint PDF of height and its gradient we plot the $N_{\rm tot}$ versus t. In this graph, $N_{\rm tot}$ scales as $t^{1/2}$ which is in agreement with the analytical prediction.

5. Conclusion

We obtained some exact results in the problems of RD model and KPZ equation in 1+1 dimensions with a Gaussian forcing which is white in time and short-range correlated in space. We determined the explicit expression of average frequency of crossing, i.e. ν_{α}^{+} of observing the definite value for height function $h - \bar{h} = \alpha$ in a growing thin film for the RD model, from which one can find the averaged number of crossing the given height in a sample with size L. It is shown that the ν_{α}^{+} is symmetric under $h \to -h$. An integral representation of ν_{α}^{+} is given for the KPZ equation in the strong coupling limit before the creation of sharp valleys. We introduced the quantity $N_{\text{tot}}^{+} = \int_{-\infty}^{+\infty} \nu_{\alpha}^{+} \, d\alpha$, which measures the total number of positive crossings of growing surface and show that for the RD model and the KPZ equation in the strong coupling limit and before the creation of sharp valleys, N_{tot}^{+} scales as $\sigma^{-3/2}t^{1/2}$. It is noted that for these models ν_{α}^{+} has different expression in terms of α . The ideas presented in this paper can be used to find the ν_{α}^{+} of the general Langevin equation with arbitrary drift and diffusion coefficients.

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