

Generalized survival in equilibrium step fluctuations

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We investigate the dynamics of a generalized survival probability $S(t, R)$ defined with respect to an arbitrary reference level R (rather than the average) in equilibrium step fluctuations. The exponential decay at large time scales of the generalized survival probability is numerically analyzed. $S(t, R)$ is shown to exhibit simple scaling behavior as a function of system size L , sampling time δt , and the reference level R . The generalized survival time scale $\tau_s(R)$ associated with $S(t, R)$ is shown to decay exponentially as a function of R .

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Controlling the stability of nanostructures is an important fundamental issue in nanoscience. A key problem in this respect is the random stochastic interface dynamics associated with equilibrium nanometer scale thermal fluctuations unavoidably present in all nanosystems. Very interesting questions [1–5] have recently been addressed regarding the complex dynamics of fluctuating interfaces in the context of first-passage statistics, which seems to be the appropriate framework in investigating the time it takes for a nanodevice to first fluctuate into an unstable state. It turns out that useful dynamical quantities such as persistence probability $P(t)$ [1,2,4] (i.e., the probability that a stochastic variable does not return to its initial value over time t) and survival probability $S(t)$ [2,5] (i.e., the probability that a stochastic variable does not cross its average level up to time t) can be numerically and experimentally investigated for interfaces with dynamics governed by various kinetic mechanisms (such as high-temperature attachment/detachment of atoms at the step edge or low-temperature step edge diffusion of atoms) to gain insight into the stability issue.

Much work has been devoted [6,7] over the last decade in understanding equilibrium fluctuations on vicinal surfaces, mostly using the dynamic scaling approach. If $h(x, t)$ is the dynamical height (with respect to the chosen reference position which is defined to be the average position, i.e., the $h=0$ line) fluctuation of a thermally fluctuating step as a function of the lateral position x and time t (where t is also measured from an arbitrary time origin), then $h(t)$ at each value of x is a stochastic dynamical variable by virtue of equilibrium thermal fluctuations. Because of the spatially extended nature of the step fluctuations through its dependence on both x and t , the problem is non-Markovian, and persistence [8] and survival [5] concepts should be particularly relevant statistical tools in understanding the complex problem of surface fluctuations.

In this paper we introduce the concept of a generalized survival probability which enables us to probe deeper into the nature of the stochastic process of interface step fluctuations. The generalized survival probability is the probability $S(t, R)$ that a given lateral step position x with a height (i.e., step fluctuation measured from the equilibrium step position) $h(x, t)$ at time t never does cross a preassigned reference

level of the height R throughout the entire evolution. The particular case with $R=0$ [i.e., the probability of the dynamical step height not returning in time t to its average (“equilibrium”) $R=0$ level] has been studied recently [5] both analytically and experimentally, and it has been shown to exhibit an exponential decay at large times, $S(t) \propto \exp(-t/\tau_s)$, where τ_s is the survival time scale that provides information about the underlying kinetics. The resulting surface step fluctuation survival probability $S(t) = S(t, R=0)$ and the associated time scale τ_s have also recently been studied experimentally using dynamical scanning tunneling microscopy (STM) on different metallic systems: Al steps on Si (111) surface at high temperatures, and Ag and Pb (111) surfaces at relatively low temperatures [9]. In this paper we show numerically that $S(t, R)$ also has an exponential behavior at large time, $S(t, R) \propto \exp(-t/\tau_s(R))$, where $\tau_s(R)$ is the generalized survival time scale. Our study reveals the dependence of $\tau_s(R)$ on the system size L , sampling interval δt , and reference level position R , allowing us to establish the complete scaling form of $S(t, R)$. In particular, the sampling interval (i.e., the time between successive measurements) [10] turns out to be an essential ingredient inherent in any real experimental measurement procedure. Also the study of the dependence of the generalized survival time scale on the choice of the reference level R , which turns out to be exponential, should have particular importance for understanding the effect of thermal fluctuations at the nanoscale.

In this study we consider the case of the high-temperature step fluctuations dominated by atomistic attachment and detachment (AD), where the step edge is known [6] to be well described by the coarse-grained second-order nonconserved linear Langevin equation, also known as the Edwards–Wilkinson (EW) equation [11]

$$\frac{\partial h(x, t)}{\partial t} = \nabla^2 h(x, t) + \eta(x, t), \quad (1)$$

where ∇^2 refers to the spatial derivative (with respect to x , the lateral position along the step), $\eta(x, t)$ with $\langle \eta(x, t) \eta(x', t') \rangle = 2D \delta(x-x') \delta(t-t')$ is the usual uncorrelated random Gaussian noise corresponding to the nonconserved white noise associated with the random AD process,

and D is the noise strength. The AD process, thought to be extremely important for relatively high-temperature step fluctuations, has been extensively studied in the literature using the EW equation [7].

For equilibrium step fluctuations, we define the generalized survival probability with respect to the height reference level R , $S(t, R)$, as the probability for the height variable to remain consistently *above* a certain preassigned value “ R ” over time t :

$$S(t, R) \equiv \text{Prob}\{h(x, t') > R, \quad \forall t_0 \leq t' \leq t_0 + t\}, \quad (2)$$

where $h(x, t)$ is the dynamical height of the interface at a fixed lateral position x at time t , and t_0 is the initial time of the measurement. Although the above definition involves the dynamical variable $h(x, t)$ defined for a particular lateral position x , we take a statistical ensemble average over all lateral positions to obtain a purely time dependent stochastic dynamical quantity $S(t, R)$. Obviously, another quantity that can be measured is the probability for the height stochastic variable to remain *below* the reference level up to time t . Since in our case the dynamics of the interface fluctuations obeys a linear stochastic equation, the interface preserves the up-down symmetry along the direction perpendicular to the step edge. As a consequence, in what follows we consider the average of the probabilities of remaining always above R and below $-R$, with $R \geq 0$.

The generalized survival probability function, $S(t, R)$, defined in Eq. (2) above, leads to a hierarchy of generalized survival time scales, $\tau_s(R)$, if the steady-state decay of $S(t, R)$ in time follows an exponential trend, $S(t, R) \sim e^{-t/\tau_s(R)}$. As we show below, this indeed is obtained for Edwards–Wilkinson equilibrium step fluctuation phenomena, allowing us to define and measure the nontrivial survival time scale $\tau_s(R)$, $0 \leq R \leq R_{max}$, that varies between $\tau_s(R=0)$ and $\tau_s(R_{max})$, where $\tau_s(R=0)$ is the usual survival time scale and $\tau_s(R_{max})$ is the survival time with respect to the highest reference level R_{max} that can be defined for a model with finite roughness (i.e., rms fluctuations of the height variable with respect to the average). R_{max} is limited by the maximum value of the height fluctuation amplitude. Obviously, $S(t, R)$ and $\tau_s(R)$ are natural generalizations of the survival probability $S(t)$ and the survival time scale τ_s , respectively, to the more complex concept of distribution of generalized survival times with limiting behavior (i.e. $R=0$) providing the usual survival time.

The exponential decay at large time of $S(t, R)$ that we find numerically is not surprising. The generalized survival probability with respect to the reference level R can be regarded as the probability $Z(t)$ of no zero crossing of the new stochastic variable $H(x, t) = h(x, t) - R$. What we are looking for is the probability for the stochastic variable $H(x, t)$ to remain positive up to time t [or, equivalently, the probability for $H(x, t) + R$ to remain negative over time t]. This type of question for the Gaussian stationary processes with zero mean has been addressed by mathematicians for a long time [12]. The no zero crossing probability is traditionally investigated in conjunction with the autocorrelation function, $C_H \equiv \langle H(x, t_1)H(x, t_2) \rangle$ [where $\langle \dots \rangle$ represents an average over all realizations of $H(x, t)$ arising from the thermal noise

source]. It is known [13] that for a stationary Gaussian process [i.e., $C_H = f(|t_1 - t_2|) \equiv f(t)$] with an autocorrelation function decaying faster than $1/t$ at large t , the asymptotic behavior of the no zero crossing probability is exponential, $Z(t) \propto \exp(-\mu t)$. The autocorrelation function $C_H(t)$ itself has been shown [5] to be stationary at late times and to decay exponentially. This, along with the exponential decay of $Z(t)$, ensures an exponential decay for $S(t, R)$.

In order to numerically simulate the process described by Eq. (1), we have used discrete stochastic Monte Carlo simulations of the corresponding atomistic solid-on-solid model, the extensively studied Family model [6], which belongs asymptotically to the Edwards–Wilkinson universality class [1]. The Family model in (1+1)-dimensions (i.e., one spatial variable and one temporal variable) is characterized by $\beta = 1/4$, $\alpha = 1/2$, and $z = \alpha/\beta = 2$ [6], where the growth exponent β is the rate of change of interface width (or roughness) in the transient regime [$w(t) \sim t^\beta$], the roughness exponent α shows the saturation of the width for a system with fixed size L in the steady state regime [$w(L) \sim L^\alpha$] and z is the dynamical exponent. This model involves the traditional random deposition (at a rate of one complete monolayer during one unit of time) and surface relaxation such that the adatoms are searching for the sites with the minimum local height. We have taken the relaxation length to be the lattice constant and we have applied the usual periodic boundary conditions. Typical sizes (i.e., number of lattice sites) used in this numerical work are 100–900, and the averaging procedure implies a number of at least 10^5 independent runs. All the measurements correspond to the steady state regime where the interface roughness has reached a time-independent equilibrium value [i.e., $t_0 \gg L^z$ in Eq. (2)]. We also mention that the smallest value for the sampling time is 1. We emphasize that our use of Family model is just a matter of convenience in simulating the EW equation [6]; our results are simply an exact discrete stochastic simulation of the EW equation.

Our results for the generalized survival probability and the associated time scale are presented in Figs. 1 and 2. $S(t, R)$ is simply computed as the fraction of sites which, starting above (below) the level R ($-R$) at time t_0 , have not crossed the reference level up to a later time $t_0 + t$. In Fig. 1 we show that, as expected, the generalized survival with respect to an arbitrary reference level R follows an exponential decay at large times. The only varying parameter in Fig. 1 is the reference level R . We have considered six values for R , $R=0, 1, \dots, 5$ [only the first four curves are displayed due to the limitations imposed by the quality of the statistics, since as R increases it is less probable to have a reasonable number of lattice sites with height variables above (below) R ($-R$)]. The dashed lines are fits of the long-time data to an exponential form, $S(t, R) \propto \exp(-t/\tau_s(R))$. The upper curve has $R=0$ and corresponds to the usual survival probability previously studied in Ref. [5]. However, all the other curves are new and they prove that the generalized survival probability decays exponentially in the long-time limit, with an associated time scale $\tau_s(R)$, which decreases with the reference level value. As shown in the inset of Fig. 1, the dependence of $\tau_s(R)$ on R is exponential, but clearly more work is needed in order to understand this trend.

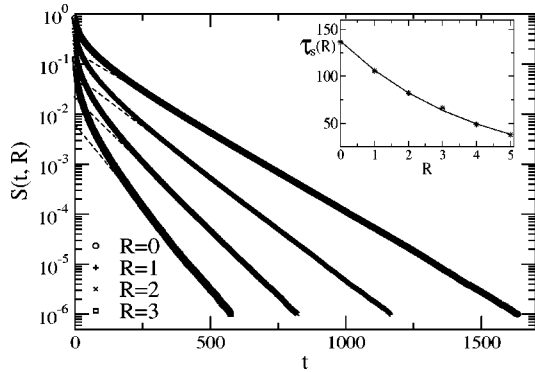


FIG. 1. The generalized survival probability, $S(t, R)$, for the discrete Family model. The dashed lines are fits of the long-time data to an exponential form. The system size is $L=100$, the sampling time is $\delta t=1.0$ and the reference level R takes four different values: 0, 1, 2, and 3 (from top to bottom). The inset shows the dependence of the generalized survival time scale $\tau_s(R)$ on the reference level value (up to $R=5$). The continuous curve represents a fit to an exponential decay of the generalized time scale vs. R .

In Fig. 2 we have used several lattice sizes, sampling times and reference levels in order to identify the scaling behavior of $S(t, R)$. In panel (a) we show the generalized survival with respect to level $R=1$, measured using $\delta t=1$, for two system sizes: $L=100$ and $L=200$. We observe that the underlying survival time scale increases rapidly with L . In fact, $\tau_s(R)$ for a fixed R is expected to grow proportionally to L^z [5]. However, we obtain that $\tau_s(R=1) \approx 103$ for $L=100$, and $\tau_s(R=1) \approx 429$ for $L=200$, so the measured generalized survival time exhibits a small deviation from the expected value of $103 \times 4 = 412$. We find that this small effect is due to the dependence of the generalized survival on sampling time δt . This is clearly seen in panel (b). It turns out that a system with a fixed size ($L=200$) is characterized by different values of $\tau_s(R)$ if the sampling time of the measurement is adjusted. We observe that $\tau_s(R)$ increases weakly as the sampling time is increased. One might argue that this effect is very small and could be neglected, but we have found that the effect of the sampling time on the measured generalized survival probability has to be taken into account in order to find the complete scaling function of $S(t, R)$. In addition, this effect is even stronger for systems with slower dynamics (i.e., larger z) [5]. Interestingly enough, we note that fixing the reference height level in the generalized survival probability problem introduces an additional length scale, that is related to the steady state value of the interface width, i.e. L^α . Indeed, in panel (c) we look at three different systems with $L=200$, 400, and 900, respectively, and the generalized survival curves are calculated for $R=1, 2$ and 3, respectively, i.e., the level R is varied proportionally to L^α , with $\alpha=1/2$ as appropriate for the EW equation. In addition, the sampling time for each of these three cases is also varied, $\delta t \propto L^z$ ($z=2$), so we have considered $\delta t=1$ for $L=100$, $\delta t=16$ for $L=400$, and $\delta t=81$ for $L=900$, respectively. A perfect collapse of the curves $S(t, R)$ vs t/L^z occurs when using $z=2.03$, which agrees with the expected value $z=2$, characteristic for the EW dynamics.

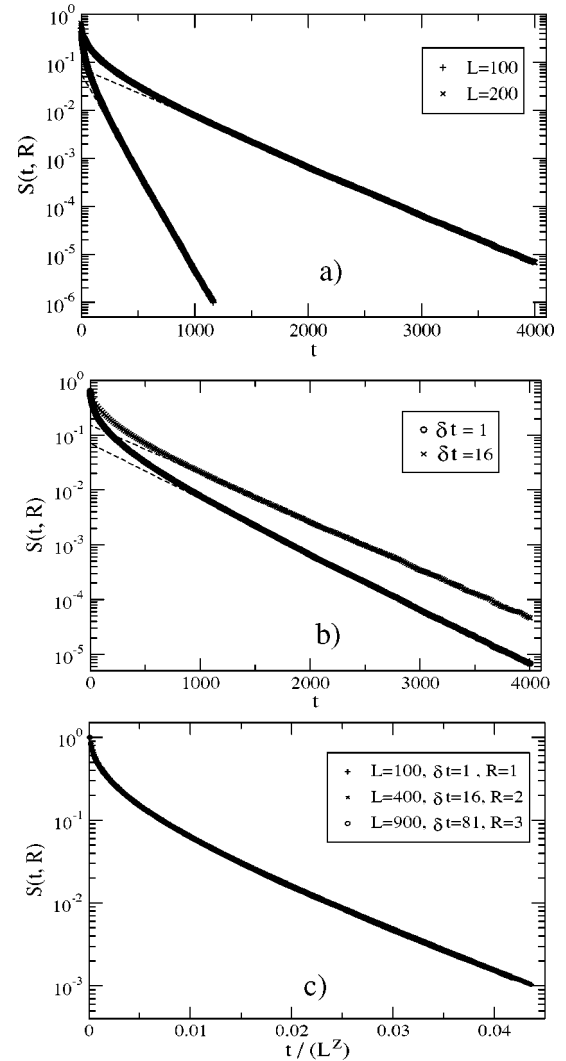


FIG. 2. The generalized survival probability $S(t, R)$ for the Family model. The dashed lines are fits of the long-time data to an exponential form. Panel (a): $L=100$ (lower curve) and $L=200$ (upper curve), using fixed sampling time $\delta t=1$ and reference level $R=1$. Panel (b): $\delta t=1$ (lower plot) and $\delta t=16$ (upper plot) with fixed system size $L=200$ and reference level position $R=1$. Panel (c): Scaling of $S(t, R)$ using three different system sizes with sampling times and reference levels varied such that $\delta t/L^z$ and R/L^α are kept constant [i.e., $\delta t/L^z=1/10\,000$ and $R/L^\alpha=1/\sqrt{100}$]. A perfect collapse of the curves with $L=100, 400$, and 900 , respectively, occurs when using $z=2.03$.

This numerical analysis allows us to conclude that the scaling form of the generalized survival probability is

$$S(t, L, R, \delta t) = f(t/L^z, R/L^\alpha, \delta t/L^z), \quad (3)$$

where the function $f(x, y, z)$ decays exponentially for large values of x . The rate of this decay decreases rather rapidly as y is decreased and increases rather slowly as z is decreased. Note that for $y=0$ we recover the scaling form of the usual survival probability with $R=0$ [5].

To conclude, we have shown that the generalized survival probability of equilibrium step fluctuations on vicinal sur-

faces with Edwards-Wilkinson dynamics decays exponentially at long times. We have investigated the associated generalized survival time scale that depends on the system size L , sampling time δt , and the choice of the reference level R . In particular, the dependence of $\tau_s(R)$ on R , which based on our preliminary investigations seems to have an exponential trend, should be useful in understanding the stability of thermally fluctuating interfaces. We have also shown that the generalized survival probability exhibits simple scaling as a function of L , δt , and R . Our numerical results on $S(t, R)$ can be easily extended to fluctuating interfaces characterized by different dynamical evolutions (such as low-temperature step edge diffusion limited kinetics) belonging to different universality classes. Our goal here, using the example of the step fluctuations process characterized by the EW universality

class, is to establish the generalized survival probability as an important statistical concept in studying thermally fluctuating interfaces.

Finally, we mention that the generalized survival probability could be experimentally measured using dynamical STM step fluctuations data, opening the possibility for a direct approach to the crucial issue of interfacial stability. Our theoretical considerations for $S(t, R)$ should also be useful in understanding the dynamical evolution of other physical processes [14] where first-passage statistics have proven to be a useful concept.

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- [1] J. Krug *et al.*, Phys. Rev. E **56**, 2702 (1997).
[2] D. B. Dougherty *et al.*, Phys. Rev. Lett. **89**, 136102 (2002).
[3] M. Constantin, S. Das Sarma, C. Dasgupta, O. Bondarchuk, D. B. Dougherty, and E. D. Williams, Phys. Rev. Lett. **91**, 086103 (2003).
[4] D. B. Dougherty *et al.*, Surf. Sci. **527**, L213 (2003).
[5] C. Dasgupta, M. Constantin, S. Das Sarma, and S. N. Majumdar, Phys. Rev. E **69**, 022101 (2004).
[6] A.-L. Barabasi and H. E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, New York, 1995).
[7] H. Jeong and E. D. Williams, Surf. Sci. Rep. **34**, 171 (1999).
[8] S. N. Majumdar, Curr. Sci. **77**, 370 (1999).
[9] O. Bondarchuk *et al.* (unpublished).
[10] S. N. Majumdar *et al.*, Phys. Rev. E **64**, 015101(R) (2001); G. C. M. A. Ehrhardt *et al.*, *ibid.* **65**, 041102 (2002).
[11] S. F. Edwards and D. R. Wilkinson, Proc. R. Soc. London, Ser. A **381**, 17 (1982).
[12] D. Slepian, Bell Syst. Tech. J. **41**, 463 (1962).
[13] G. F. Newell and M. Roseblatt, Ann. Math. Stat. **33**, 1306 (1962).
[14] M. Marcos-Martin *et al.*, Physica A **214**, 396 (1995); W. Y. Tam *et al.*, Phys. Rev. Lett. **78**, 1588 (1997); B. Yurke *et al.*, Phys. Rev. E **56**, R40 (1997); G. P. Wong *et al.*, Phys. Rev. Lett. **86**, 4156 (2001); J. Merikoski *et al.*, *ibid.* **90**, 024501 (2003).