PERSISTENCE AND SURVIVAL IN EQUILIBRIUM STEP FLUCTUATIONS

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REFERENCES:


• Physical Review E 69, 022101 (2004); 69, 061608 (2004); 71, 021602 (2005); 73, 011602 (2006).

OUTLINE

1. Introduction
   - Dynamics of steps on a vicinal surface
   - Persistence and survival probabilities

2. Results (analytic, numerical and experimental)
   - Temporal persistence probability and the probability of persistent large deviations
   - Temporal survival probability
   - Effects of discrete sampling and finite size
   - Spatial persistence and survival probabilities

3. Conclusions
Step edges $\rightarrow$ fluctuating lines; interactions between steps neglected

[Pictures provided by Ellen Williams]
EQUILIBRIUM FLUCTUATIONS OF STEPS

- **High T**: Attachment-detachment of adatoms → Non-conserved dynamics
- **Low T**: Diffusion along step edge → Conserved dynamics
Fluctuations in step position can be measured in dynamic scanning tunneling microscopy.
CONTINUUM DESCRIPTION OF STEP FLUCTUATIONS

\( h(x, t) \): Position of step-edge at time \( t \)

\[
\mathcal{H}[h(x)] = K \int_{0}^{L} \left( 1 + |\partial h/\partial x|^2 \right)^{0.5} dx
\]

\[
\simeq K \frac{1}{2} \int_{0}^{L} |\partial h/\partial x|^2 dx + \text{constant}
\]

High temperatures: Nonconserved Langevin equation

\[
\frac{\partial h(x, t)}{\partial t} = \Gamma K \frac{\partial^2 h(x, t)}{\partial x^2} + \eta(x, t)
\]

\[
\langle \eta(x, t) \eta(x', t') \rangle = 2k_B T \Gamma \delta(x - x') \delta(t - t')
\]

**Edwards-Wilkinson Equation**
Average step position, \( \tilde{h}(k = 0, t) \) exhibits random walk in time → measure step position from its instantaneous spatial average.

Low temperatures: Conserved Langevin equation

\[
\frac{\partial h(x, t)}{\partial t} = -\tilde{\Gamma} K \frac{\partial^4 h(x, t)}{\partial x^4} + \eta(x, t)
\]

\[
\langle \eta(x, t)\eta(x', t') \rangle = -2k_B T \tilde{\Gamma} \frac{\partial^2}{\partial x^2} \delta(x - x') \delta(t - t')
\]

Conserved Edwards-Wilkinson Equation
Conserved Mullins-Herring Equation
EQUILIBRIUM CORRELATIONS

• \( \langle [h(x + x_0, t) - h(x_0, t)]^2 \rangle \propto x^{2\alpha} \) for \( x \ll L \), with \( \alpha = 1/2 \).

• Interface width \( W(L) \equiv \sqrt{\langle [h(x, t)]^2 \rangle} \propto L^\alpha \).

• \( \langle [h(x, t_0 + t) - h(x, t_0)]^2 \rangle \propto t^{2\beta} \) for \( t \ll L^z \), with \( z = 2(4) \) for nonconserved (conserved) dynamics, and \( \beta = \alpha/z \).

• \( \langle h(x, t_0 + t)h(x, t_0) \rangle \propto \exp[-t/\tau_c(L)] \) for large \( t \), with \( \tau_c(L) \propto L^z \).

Numerical work: Integration of the Langevin equations and simulations of equivalent atomistic models.
PERSISTENCE AND SURVIVAL PROBABILITIES

The Persistence Probability $P(t)$ is the probability that a characteristic property (e.g. the sign) of a fluctuating quantity does not change over time $t$.

(Temporal) Persistence probability $P(x; t_0, t_0 + t)$: Probability that sign[$h(x, t_0 + t') - h(x, t_0)$] remains the same for all $0 < t' \leq t$.

Average over $x$ and initial time $t_0$ in the steady state ($t_0 \gg L_z$): $P(x; t_0, t_0 + t) \to P(t)$.

The persistence probability $P(t)$ is closely related to the zero-crossing statistics of the stochastic variable $[h(x, t_0 + t) - h(x, t_0)]$. 
(Temporal) Survival probability $S(x, t_0, t_0 + t)$:
Probability that sign[$h(x, t_0 + t')$] remains the same for all $0 < t' \leq t$.

The survival probability $S(x, t_0, t_0 + t)$ is related to the zero-crossing statistics of the stochastic variable $h(x, t)$.

Average over $x$ and initial time $t_0$ in the steady state:
$S(x, t_0, t_0 + t) \to S(t)$.

Spatial persistence and survival probabilities $P(x)$ and $S(x)$ are defined in a similar way from zero-crossings of the stochastic variables $[h(x + x_0, t_0) - h(x_0, t_0)]$ and $h(x, t_0)$, respectively, as functions of $x$. 
WHY IS THIS IMPORTANT?

• Several aspects of first-passage properties of step fluctuations are non-trivial and poorly understood.

• Theoretical predictions can be directly compared with experimental observations.

• Understanding of first-passage properties of fluctuating edges is necessary for assessing the stability of nanoscale devices. For example, in a nanoscale device with two edges separated by a small gap, it would be useful to have an estimate of the probability that the two edges do not come into contact through fluctuations in a given time interval.
RESULTS
A. Temporal persistence probability:

Main result: $P(t) \propto t^{-\theta}$ at long times, with $\theta = 1 - \beta$, where $\beta = 1/4(1/8)$ for the nonconserved (conserved) EW equation.

Numerical integration of nonconserved EW equation in 1d
Experiment on Al on Si(111) surface

Persistence probabilities at 3 temperatures,
\( P(t) \propto t^{-\theta} \), \( \theta = 0.78 \pm 0.03 \).
B. Temporal survival probability

For step dynamics described by the linear Langevin equations, \( h(x, t) \) is a stationary Gaussian Process with exponentially decaying autocorrelation function.

Newell and Rosenblatt (1962): \( S(t) \propto \exp(-t/\tau_p) \) with \( \tau_p/\tau_c = c < 1 \).

Numerical integration of nonconserved EW equation in 1d
Experiment on Al on Si(111) surface

Survival probabilities at 3 temperatures and fits to exponential decay.
C. Probability of persistent large deviations


\[ P(t, s = 1) = P(t), \text{ the usual persistence probability.} \]

\[ P(t, s = -1) = 1 \text{ for all } t. \]

\[ P(t, s) \propto t^{-\theta(s)t} \text{ for all } s? \]

Infinite family of exponents \( \{\theta(s)\} \), characterizing the probability of persistent large deviations.

\[ S(t) = \text{sign}[h(x, t + t_0) - h(x, t_0)] \]

\[ S_{av}(t) = \frac{1}{t} \int_0^t S(t')dt' \]

\[ P(t, s): \text{ Probability that } S_{av}(t') \geq s \text{ for all } 0 < t' \leq t, -1 \leq s \leq 1. \]
Numerical and Experimental Results for $P(t, s)$


Experiment on steps on Al/Si(111) surface at 970K, and simulation of 1d nonconserved EW equation.

Similar agreement between experimental results for steps on Ag(111) surface at 320K and simulation results for the 1d conserved EW equation.
Baldassarri \textit{et al.}, PRE 59, R20 (1999): Analytic calculation of $\theta(s)$ for a spin model in which the intervals between successive spin-flips are uncorrelated.

$\theta(s)$ is completely determined by $\theta(s = 1)$.

The assumptions in this model do not hold for the dynamics of step fluctuations.
D. Effects of discrete sampling and finite system size

In simulations and experiments, the step position $h(x, t)$ is measured at discrete intervals of a sampling time $\delta t$. System size $L$ is finite in simulations (and also in experimental studies of the survival probability!)

The measured persistence and survival probabilities depend on the values of $\delta t$ and $L$ [Majumdar et al., Phys. Rev. E 64, 015101(R) (2001)].

Scaling relations:

\[ P(t, \delta t, L) = f_p(t/\delta t) \text{ for } t \ll L^z. \]
\[ S(t, \delta t, L) = f_s(t/L^z, \delta t/L^z). \]

Scaling relations verified from results of experiments and simulations [PRB 71, 045426(2005); PRE 71, 021602 (2005)].
Persistence probability: experiment on Al/Si(111) and simulation of 1d conserved EW equation

![Persistence probability graphs](image-url)
Survival probability: simulation of 1d EW equation

Plots of $S(t, \delta t, L)$ vs. $t/L^z$ collapse to a single curve only if $\delta t/L^z$ is held constant [Phys. Rev. E 69, 022102 (2004)].
In experimental measurements of $S(t)$, the finiteness of the total observation time $T$ leads to a finite “effective sample size” $L_{eff} \propto T^{1/z}$.

In experiments, one measures the step position $H(t)$, $0 \leq t \leq T$ and defines the average step position as $H_{av} = \frac{1}{T} \int_{0}^{T} H(t') dt'$, so that $h(t) = H(t) - H_{av}$.

$H_{av}$ is not the “true” average step position because $k$-modes with relaxation times $\tau_c(k) \propto 1/k^z$ much larger than $T$ do not equilibrate during the observation time.

This effect is similar to [Phys. Rev. B 71, 045426 (2005)] that of having a finite system of size $L_{eff} \propto T^{1/z}$.

“Finite-size” scaling relation:
$S(t, \delta t, T) = f_s(t/\delta t, \delta t/T)$
Scaling of the survival probability: experimental verification

Dougherty et al., PRE 71, 021602 (2005).
Two measurements of position of a step on Pb(111) at 320K,
$T = 19s$, $\delta t = 37$ ms in one run,
$T = 177s$, $\delta t = 0.346$ s in the other run.
$\delta t/T$ is the same in the two runs.
E. Spatial persistence and survival probabilities

Spatial persistence probability $P_s(x)$: Probability that $\text{sign}[h(x' + x_0, t_0) - h(x_0, t_0)]$ remains the same for all $0 < x' \leq x$, averaged over $x_0$ and $t_0 \gg L^z$.

Majumdar and Bray [Phys. Rev. Lett. 86, 3700 (2001)] showed that $P_s(x) \propto x^{-\theta_s}$ in a class of simple stochastic models for step fluctuations and surface growth.

These predictions have been verified and the scaling behavior of $P_s$ as a function of system size and sampling interval has been elucidated in Constantin et al., Phys. Rev E, 69, 051603 (2004).
Spatial survival probability for 1d nonconserved EW interface in the steady state

Spatial survival probability $S_s(x)$: Probability that $\text{sign}[h(x' + x_0, t_0)]$ remains the same for all $0 < x' \leq x$, averaged over $x_0$ and $t_0 \gg L^z$.

Dependence of $S_s(x)$ on $x$ is neither exponential nor power-law.

Numerical integration of 1d EW equation.

Results for different values of the sample size $L$ and the sampling interval $\delta x$, with $\delta x/L$ held constant.
Analytic calculation of $S_s(x)$ for 1d EW/KPZ interface


- Mapping of 1d EW interface to 1d Brownian motion
  $[h(x, t_0) \rightarrow X(t); \quad x \rightarrow t]$. 

- Periodic boundary condition,
  $h(x = 0, t_0) = h(x = L, t_0) \rightarrow$ the Brownian path returns to the starting point after time $T = L$ i.e. $X(t = 0) = X(t = T)$. “Brownian bridge”.

- $\int_0^L h(x, t_0)dx = 0$ [step position measured from its instantaneous spatial average] $\rightarrow$ “zero-area constraint”, $\int_0^T X(t)dt = 0$. 

Exact path integral formulation \( \rightarrow S_s(x, L) = f(x/L) \) where the function \( f(u) \) is expressed in terms of complicated integrals that can, in principle, be computed.

Simple “deterministic” approximation \( \rightarrow \) closed-form expression for \( f(u) \) which agrees quite well with simulation data.

With zero-area constraint Without the constraint
Comparison with experimental results (Ellen Williams, private communication)
CONCLUSIONS

• Persistence and survival probabilities provide an excellent way of characterizing equilibrium step fluctuations.

• Analytic understanding of several features observed in simulations and experiments.

• Elucidation of the effects of discrete sampling and finite system size on the measured persistence and survival probabilities (scaling behavior).

• Excellent agreement between theoretical predictions and results of experiments.
Questions for future study

- Analytic calculations for $\theta(s)$, the family of exponents for the probability of persistent large deviations, and for the dependence of persistence and survival probabilities on the size of the sampling interval.

- Persistence and survival probabilities for *nonlinear* equations describing surface growth and fluctuations. Positive and negative persistence exponents may be different in such cases [Constantin *et al.*, Phys. Rev. E 69, 061608 (2004)].

- Effects of interactions between steps.

- Generalization to interfaces in higher dimensions,...