

Survival probability of a mobile particle in a fluctuating field

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We study the survival probability $P(t)$, up to time t , of a test particle moving in a fluctuating external field. The particle moves according to some prescribed deterministic or stochastic rules and survives as long as the external field that it “sees” at its own location does not change sign. This is a natural generalization of the “static persistence” (when the particle is at rest), which has generated considerable interest recently. Two types of particle motion are considered. In one case the particle adopts a strategy to live longer and in the other it just diffuses randomly. Three different external fields were considered: (i) the solution of diffusion equation, (ii) the “color” profile of the q -state Potts model undergoing zero-temperature coarsening dynamics, and (iii) spatially uncorrelated Brownian signals. In most cases studied, $P(t) \sim t^{-\theta_m}$ for large t . The exponent θ_m is calculated numerically, analytically by approximate methods, and in some cases exactly. It is shown in some special cases that the survival probability of the mobile particle is related to the persistence of special “patterns” present in the initial configuration of a phase-ordering system. [S1063-651X(98)10902-9]

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I. INTRODUCTION

Considerable interest has been generated recently in understanding the statistics of first passage events in spatially extended nonequilibrium systems. These systems include the Ising or Potts model undergoing zero-temperature phase-ordering dynamics [1–3], simple diffusion equation with random initial conditions [4,5], several reaction-diffusion systems [6–8], and fluctuating interfaces either in the steady states or approaching steady states starting from random initial configurations [9]. Typically one is interested in persistence, i.e., the probability $P_0(t)$ that at a fixed point in space, the quantity $\text{sgn}[\phi(x,t) - \langle \phi(x,t) \rangle]$ [where $\phi(x,t)$ is a fluctuating field, e.g., the spin field in the Ising model or the height of a fluctuating interface] does not change up to time t . In all the examples mentioned above, this probability decays as a power law $P_0(t) \sim t^{-\theta_0}$, where the exponent θ_0 is nontrivial. This nontriviality is due to the fact that the effective stochastic process in time at a fixed point in space becomes non-Markovian due to the coupling to the neighbors. For a non-Markovian process, calculation of any history-dependent quantity such as persistence is extremely hard barring a few special cases [10,11]. The exponent θ_0 has also been measured in a recent experiment on a liquid-crystal system that has the same dynamics as the $T=0$ Ising model in two dimensions [12]. The experimental value was in good agreement with the analytical prediction of θ_0 in two-dimensional (2D) Ising model [13]. The exponent θ_0 has also been measured in a recent experiment on two-dimensional soap froth [14].

In the above process, one studied the persistence of a *single* spin (e.g., in the Ising or Potts model) of the initial random configuration. A natural generalization of this would be to study the persistence of a *pattern*, and not just a single spin, present in the initial configuration. Persistent patterns are quite abundant in nature. Examples include persistent eddies and vortices in turbulence, the great red spot of Jupiter, and certain patterns of stock prices in financial markets.

Another example is the so-called activity-centered pattern in a self-organized system such as an interface in a random medium [15] and also in certain models of evolution [16]. A natural question then is, What is the probability that a given pattern survives up to time t ?

Such persistent patterns exist also in phase ordering systems such as the q -state Potts model. For example, one such pattern is an original domain of a specific color present in the random initial configuration of the Potts model. One can then ask, What is the survival probability of such a domain up to time t ? This quantity for the 1D Potts model has been studied recently by Krapivsky and Ben-Naim [17]. However, this can be a more general question for any fluctuating field such as the solution of diffusion equation with random initial configuration or a fluctuating interface approaching the steady state. In such examples, a domain would be a connected set of points where the sign of the fluctuating field is positive (or negative). Another example of “pattern” persistence would be to study the probability that two adjacent domains in the initial configuration both survive up to time t . In this paper we develop a general framework to study the persistence of patterns of a fluctuating field and discuss a few examples in detail where explicit results can be obtained.

The general framework to study some of these pattern persistence problems consists of monitoring the motion of an external test particle launched in the fluctuating field. The dynamics of the test particle is suitably chosen so that the particle evaluates where the specific pattern of the fluctuating field is and moves there. The persistence of the pattern is then precisely the survival probability of the test particle. This led us naturally to study a more general “persistence of a mobile particle in a field” problem (henceforth the PF problem), special cases of which correspond to the pattern persistence in the underlying field. In this paper we study in detail a few examples of this general PF problem and find very rich, though often nonuniversal, behavior.

The general PF problem can be defined as follows. Let us consider a field $\phi(x,t)$ that fluctuates in both space and time.

For example, the field $\phi(x,t)$ may be the solution of the simple diffusion equation $\partial_t \phi = \nabla^2 \phi$, the order parameter profile of the Ising model undergoing $T=0$ coarsening dynamics, the height profile of a fluctuating interface, or may even be spatially uncorrelated Brownian signal $\partial_t \phi = \eta$, where $\eta(x,t)$ is spatially and temporally uncorrelated Gaussian white noise. A test particle is launched at an arbitrary initial point at time $t=0$. The particle moves according to some prescribed deterministic or stochastic rules, which in general depend on the local field profile. We now ask the question, Given the dynamics of the particle, what is the probability $P(t)$ that the field “seen” by the particle at its own location does not change sign up to time t ?

The survival probability of a mobile particle in a field has been studied before in the context of heterogeneous reaction-diffusion systems [6,8] where the test particle was an external impurity diffusing through a homogeneous background. These studies dealt with a special case of our general PF problem, namely, when the test particle is a simple random walker and the field is the coarsening “color” field of the q -state Potts model at $T=0$ [6,8]. Among other studies on a similar line was the computation of the trapping time distribution of a diffusing tracer particle on a solid-on-solid surface [18]. In this paper we extend these studies to several other examples arising naturally in the context of our general PF problem.

In the PF problem one needs to specify the dynamics of the field as well as that of the test particle. For the field, we will consider three different cases, namely, when the fields are (i) the solution of diffusion equation, (ii) the spin profile of the Ising model or in general the color profile of the q -state Potts model undergoing $T=0$ coarsening dynamics, and (iii) spatially uncorrelated Brownian signals. The motion of the test particle, in general, consists of two separate moves. In the first part of the motion the particle sees the local field profile and then adopts a strategy to move in such a way so that it can live longer. This is the “adaptive” part of the motion that depends on the local field profile. In addition to this adaptive move the particle in general may be subjected to an external noise, which constitutes the second part of the motion. This “noisy” part consists of Brownian moves of the particle that is independent of the local field profile. While the motion consisting of both adaptive and noisy moves is more general, for the sake of simplicity we will restrict ourselves to two separate cases when the motion is either purely adaptive or purely noisy. In the first case, the survival probability is larger than the “static” case (when the particle is at rest) and in the second case it is smaller. In cases where survival probabilities in both the mobile and the static cases decay as power laws, the exponent inequality $\theta_{ad} \leq \theta_0 \leq \theta_{rw}$ holds, where θ_{ad} and θ_{rw} are the persistence exponents associated with the adaptive and the random walk motion of the test particle. The relationship between the survival probability of the test particle and the persistence of patterns in the underlying field is established wherever possible. In all these studies we will restrict ourselves to one dimension, although in most cases the generalizations to higher dimensions is quite straightforward.

The paper is organized as follows. In Sec. II we consider the adaptive motion of the test particle. Three cases of the fields are considered. By suitably choosing the adaptive strat-

egy, the survival probability of the particle is related to that of a pattern (original domain in the Potts model or diffusion equation). An exact solution is presented for the special case when the motion of the adaptive particle is directed and the field is spatially uncorrelated Brownian signals. In Sec. III we consider the noisy motion of the test particle where it performs a simple random walk. Approximate analytical methods are developed to calculate the exponent characterizing the power-law decay of the survival probability of the particle. In Sec. IV a special case of the survival of the diffusive test particle in the 1D Potts model is shown to be related to the persistence of an initial pattern, namely, two adjacent original domains. This is also related to the fraction of *uncollided* domain walls at time t in the 1D Potts model, which we study by both numerical and analytical methods. Finally, we conclude with a summary, some suggestions for future directions, and possible experimental realizations or tests of our results. Some details about a variational calculation are presented in the Appendix.

II. ADAPTIVE MOTION OF THE TEST PARTICLE

In this section we consider the adaptive motion of the test particle in which the particle adopts a strategy to move in a way such that it can live longer. The model and the strategy is as follows. Consider a lattice with periodic boundary conditions for convenience. The field $\phi(i,t)$ evolves with time according to some prescribed dynamics. A test particle is launched at $t=0$, at an arbitrary site, say, the origin. Let us assume that at $t=0$ the sign of the field ϕ at the origin is positive (or negative). As time changes, the field $\phi(i,t)$ changes. As long as the sign of the field at the origin is positive (or negative), the particle does not move. When the sign changes at the origin, the particle looks for a nearest neighbor where the field is positive (or negative). If it finds such a neighbor it goes there. In case there is more than one neighbor with positive (or negative) fields, it chooses one of them at random. Then it waits there until the sign of ϕ at the new site changes and then again it moves to one of its current neighbors and so on. If at some stage the sign changes at the particle’s current site and it fails to find a neighbor with positive (or negative) field, then it dies. Then we ask, What is the probability $P_{ad}(t)$ that the particle survives up to time t ? Note that if the particle did not move at all and stayed put at one site only, then the survival probability $P_0(t)$ is the usual “static persistence.”

We first consider the case when the field $\phi(x,t)$ is the solution of the simple diffusion equation $\partial_t \phi = \nabla^2 \phi$, starting from a random initial configuration of ϕ . For this simple field, analytical computation of even the static persistence $P_0(t)$ turned out to be quite nontrivial [4]. In one dimension, it was found that $P_0(t) \sim t^{-\theta_0}$ for large t , where $\theta_0 = 0.1207 \pm 0.0005$ [4]. The reason for the nontriviality once again can be traced to the fact that the effective Gaussian process that a static particle sees in time is non-Markovian. Nevertheless, an “independent interval approximation” (IIA) was developed in [4], which produced analytical predictions for θ_0 for all dimensions that were extremely accurate.

In the case of the moving particle with the adaptive strategy, we carried out a numerical simulation. The results are

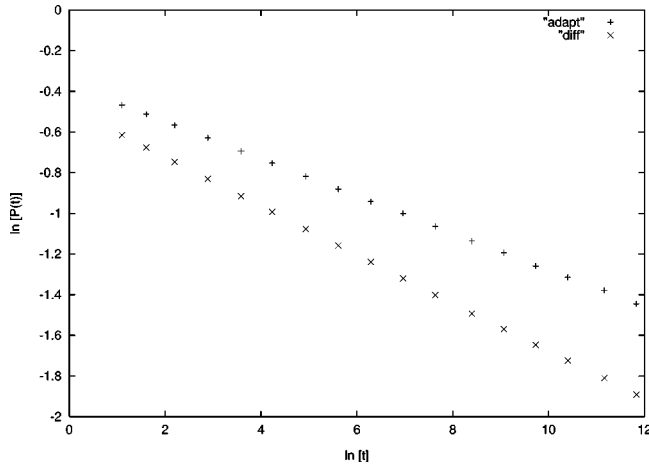


FIG. 1. A log-log plot of Monte Carlo simulations of the “adaptive” persistence $P_{ad}(t)$ (plus symbols) and “static” persistence $P_0(t)$ (cross) versus time t . The simulations were carried out on a periodic lattice of 100 000 sites and results were averaged over 20 samples. The best fit to the straight lines gives the exponent values $\theta_{ad}=0.091\pm 0.002$ and $\theta_0=0.12\pm 0.001$.

presented in Fig. 1. We find $P_{ad}(t)\sim t^{-\theta_{ad}}$ for large t , where $\theta_{ad}=0.091\pm 0.002$, compared to $\theta_0=0.12\pm 0.001$. Thus, the strategy adapted by the particle is “successful” in the sense that the exponent, and not just the amplitude, characterizing the decay of persistence decreases. Thus in the renormalization-group language, the adaptive strategy is a relevant perturbation.

It is clear from above that the strategy the particle adopts is basically to move towards the local maximum (or minimum) of the underlying field if the initial sign of the field that the particle sees is positive (or negative). By symmetry of the initial condition the survival probability of the particle does not depend on the initial sign of the field that it sees. Hence, without any loss of generality, it is sufficient to consider the case when the particle moves only towards a local maximum. This observation may be used to develop a possible continuum approach to this problem. Let $R(t)$ denote the position of the particle measured from a fixed point in space and x denote the coordinate of an arbitrary point in space measured from the location of the particle. Then the effective field $\psi(x,t)$ as seen by the particle is given by $\psi(x,t)=\phi(x+R(t),t)$. Note that $x=0$ denotes the position of the particle. Given that ϕ satisfies the diffusion equation, the equation of motion of $\psi(x,t)$ is given by $\partial_t\psi=\nabla^2\psi+\dot{R}(t)\partial_x\psi$. We now model the adaptive strategy (namely, that the particle tries to move towards the local maximum) by assuming that the velocity of the particle is proportional to the local slope of the field that the particle sees, i.e., $\dot{R}=\lambda\psi'(0,t)$, where ψ' denotes the derivative with respect to x and λ is a constant. The implication of this assumption is clear. If the local slope is positive the particle moves to the right and if the local slope is negative the particle moves to the left. Thus the particle always tries to move towards the local maximum. So the equation satisfied by $\psi(x,t)$ is

$$\partial_t\psi=\nabla^2\psi+\lambda\psi'(x,t)\psi'(0,t), \quad (2.1)$$

which is a nonlocal and nonlinear Kardar-Parisi-Zhang type of equation. Then the adaptive persistence in this formulation

is the probability that the local field $\psi(0,t)$ does not change sign up to time t . While a continuum formulation does not make it easier to compute the adaptive persistence exponent, it relates the problem to the more familiar problem of persistence of fluctuating interfaces [9]. However, we will not study this equation any further in the present paper and will defer its discussion to the future [19].

We now turn to the case when the field is the color field of the q -state Potts model undergoing $T=0$ temperature dynamics. At each site of a lattice, the field can take q possible colors. One starts from a random initial configuration of colors. A site is chosen at random and its color is changed to one of its neighbors. This is how the color field evolves. A test particle is launched as usual and it waits at its initial site until the color of that site changes. Then it tries to find a neighbor with the same color and if succeeds it goes to that neighboring site. When it does not find any neighbor of its own color the particle dies. Then the question is as before, What is the probability $P_{ad}(t)$ that the particle survives up to time t ? The corresponding static persistence exponent has been calculated exactly for all q recently [2].

Our job for calculating the adaptive persistence for the q -state Potts model is simplified by making the observation that the test particle survives as long as the original domain of the Potts model that contained the test particle at $t=0$ survives. Thus the adaptive persistence is precisely the survival probability of an “original domain” that has been studied recently both numerically and analytically within an IIA for all q by Krapivsky and Ben-Naim [17]. In fact, even for the diffusion equation, adaptive persistence is also the survival probability of an original domain. However, the IIA developed in [17] for the Potts model cannot be easily extended to the diffusion equation for the following reason. The evolution of the Potts model is particularly simple in terms of the domain walls where the field changes color in space. These domain walls perform independent random walks (the rates of which do not depend on the local spins) and when two walls meet, they either annihilate [with probability $1/(q-1)$] or aggregate [with probability $(q-1)/(q-2)$]. Therefore, for the Potts model it is quite simple to write down an evolution equation for $P(n,m,t)$ (probability that a domain of length n contains m original domains) within the IIA [17] and thereby calculate the domain survival probability. However, writing down a similar evolution equation for the diffusion equation does not seem to be easy as the domain walls in the diffusion equation (i.e., the zeros of the diffusive field) undergo complicated motion that depends upon the local field profile.

However, we want to stress that the concept of adaptive persistence is more general than just being equivalent to the persistence of a pattern, e.g., the domain survival probability in the case of the Potts model or diffusion equation. In fact, it does not necessarily require that the evolving field has domain structures coarsening in time. For example, even in the simplest case where at each site of the lattice there is an independent Brownian signal (completely uncorrelated spatially), one can define the adaptive persistence and has a nontrivial exponent, as we will show below via an exact solution. In cases when the evolving field has a structure of coarsening domains, the adaptive persistence is equivalent to the domain survival probability.

We now turn to the last case for which we present an exact solution of the adaptive persistence. In this case, the field is spatially uncorrelated Brownian signal at each lattice site $\partial_t \phi(i, t) = \eta(i, t)$, where $\eta(i, t)$ is spatially uncorrelated Gaussian white noise with zero mean and $\langle \eta(i, t) \eta(j, t') \rangle = 2D \delta_{i,j} \delta(t-t')$, where D is a constant. A test particle is launched as usual at $t=0$ at the origin. Let us assume that the signal at the origin at $t=0$ is positive. The particle does not move as long as the sign of the signal ϕ at the origin does not change sign. When it does, the particle either dies with probability $1-p$ or survives with probability p and then tries to jump to its neighbor on the *right-hand side*. If the sign of the signal at that neighbor is positive at the time of jumping, the particle stays there until the signal is positive there and so on. Finally, if it does not find a right neighbor with a positive signal at the moment of jumping, the particle dies. Note the two different aspects in this problem from before. A survival factor p is introduced. $p=1$ is the fully adapted case considered earlier for the diffusion equation or the Potts model. $p=0$ will correspond to the static persistence. The second aspect is that the motion of the particle is *directed*, in contrast to the *undirected* case considered for the diffusion equation or the Potts model. This assumption of *directedness* turns out to be important for exact solution and thus serves as a useful exactly solvable toy model of adaptive persistence. It turns out, as we show below, that the exponent θ_{ad} can be calculated exactly and depends on the parameter p continuously.

Let $P_0(t, t_0)$ denote the probability that a Brownian signal at a given site does not change sign from time t_0 to time t . This is the usual static persistence, which can be readily computed since it is a Markovian process [10,20]. The conditional probability $Q(\phi, t | \phi_0, t_0)$ for a Brownian signal to assume the value ϕ at time t given that its value was ϕ_0 at t_0 ($< t$) is obtained by solving the diffusion equation

$$Q(\phi, t | \phi_0, t_0) = \frac{1}{\sqrt{4D\pi(t-t_0)}} \exp\left[-\frac{(\phi-\phi_0)^2}{4D(t-t_0)}\right]. \tag{2.2}$$

The method of images [20] may be used to express the probability Q^+ that the signal changes from ϕ_0 to ϕ *without changing sign* in the form $Q^+(\phi, t | \phi_0, t_0) = Q(\phi, t | \phi_0, t_0) - Q(\phi, t | -\phi_0, t_0)$, where ϕ_0 and ϕ have the same sign. To obtain the probability that the process is positive throughout the interval (t_0, t) one multiplies Q^+ by the probability $Q(\phi_0, t_0 | 0, 0)$ that the process takes the value ϕ_0 at t_0 and integrates over positive values of ϕ_0 and ϕ ; the persistence probability also contains a symmetric contribution from the process always being negative, yielding finally

$$P_0(t, t_0) = 2 \int_0^\infty d\phi \int_0^\infty d\phi_0 Q^+(\phi, t | \phi_0, t_0) Q(\phi_0, t_0 | 0, 0) = \frac{2}{\pi} \sin^{-1}(\sqrt{t_0/t}). \tag{2.3}$$

Let $F_0(t_0, t)$ denote the probability that the signal crosses zero for the first time at time t . Then clearly $F_0(t_0, t) = -dP_0/dt$. Then the probability of no zero crossing $P(t_0, t)$ for the adaptive particle is given by the convolution

$$P(t_0, t) = P_0(t_0, t) + (p/2)F_0 * P_0 + (p/2)^2 F_0 * F_0 * P_0 + \dots, \tag{2.4}$$

where $F_0 * P_0 = \int F_0(t_0, t_1) dt_1 P_0(t_1, t)$ and so on. The first term is the probability that the sign of the signal at the starting site did not change up to time t and hence the particle did not jump at all. The second term denotes the probability that the particle jumped once. The parameter p is the survival factor and $1/2$ is the probability that the sign of the signal of the right neighbor (to which the particle jumps) is positive. The third term denotes the probability that the particle jumped twice and so on.

To perform the convoluted integrals in Eq. (2.4) we make a change of variable $T_i = \ln(t_i/t_0)$. In this new variable the effective process that the particle sees, though not Gaussian, becomes stationary. One can then use the Laplace transforms to solve Eq. (2.4). Let $\tilde{P}(s)$, $\tilde{P}_0(s)$, and $\tilde{F}_0(s)$ denote the respective Laplace transforms of $P(T)$, $P_0(T)$, and $F_0(T)$. Then, by taking the Laplace transform of Eq. (2.4), one gets

$$\tilde{P}(s) = \frac{\tilde{P}_0(s)}{1 - \frac{p}{2} \tilde{F}_0(s)}. \tag{2.5}$$

Using the relation $F_0(T) = -dP_0/dT$, one further gets $\tilde{F}_0(s) = 1 - s\tilde{P}_0(s)$. This enables us to write $\tilde{P}(s)$ entirely in terms of $\tilde{P}_0(s)$,

$$\tilde{P}(s) = \frac{\tilde{P}_0(s)}{1 - \frac{p}{2} + \frac{ps}{2} \tilde{P}_0(s)}. \tag{2.6}$$

We expect $P(t_0, t)$ to decay as $t^{-\theta_{ad}}$ for large t . This means that in the variable $T = \ln(t/t_0)$, $P(T) \sim \exp(-\theta_{ad}T)$ for large T . This implies that the Laplace transform $\tilde{P}(s)$ will have a pole at $s = -\theta_{ad}$, i.e., the denominator of the right-hand side of Eq. (2.6) will have a zero at $s = -\theta_{ad}$. Using $P_0(T) = (2/\pi) \sin^{-1}(e^{-T/2})$, one therefore sees that the exponent θ_{ad} is given by the positive root of

$$1 - \frac{p}{2} - \frac{p\theta_{ad}}{\pi} \int_0^\infty \sin^{-1}(e^{-T/2}) e^{\theta_{ad}T} dT = 0. \tag{2.7}$$

This integration can be evaluated by parts and one finally gets

$$B[1/2, 1/2 - \theta_{ad}] = \frac{2\pi}{p}, \tag{2.8}$$

where $B[m, n]$ is the usual Beta function. It is clear that in the limit $p \rightarrow 0$ one recovers the usual static persistence exponent $\theta_0 = 1/2$. For the fully adapted model ($p = 1$), we get $\theta_{ad} = 0.3005681\dots$, which agrees very well with our numerical simulations. It is also clear that for any nonzero p , the adaptive exponent $\theta_{ad} < \theta_0 = 1/2$ as expected.

The reason that the exponent θ_{ad} is exactly soluble for the directed case is that the effective process seen by the test particle is Markovian. In the undirected case this is not so because the particle can jump back to a site already visited

TABLE I. Estimates of the persistence exponents of a diffusing tracer particle through an external field evolving via diffusion equation. For different values of the ratio $c = D_p/D_f$ as shown in column 1, exponents are obtained in column 2 by direct Monte Carlo simulation of the process (θ_{MC}), in column 3 by simulating a Gaussian stationary process with the correlator $f(T) = [\cosh(T/2) + c \sinh(|T|/2)]^{-1/2}(\theta_{GS})$, in column 4 by using the variational estimate θ_{var} for the above Gaussian stationary process with correlator $f(T)$, and in column 5 by using the rigorous upper bound θ_{max} for the above Gaussian process. Monte Carlo simulations were carried out on a periodic lattice of 100 000 sites and the results were averaged over 20 samples.

c	$\theta_d(\text{MC})$	$\theta_d(G)$	θ_{var}	θ_{max}
0.5	0.20 ± 0.01	0.190 ± 0.005	0.189	0.210
1.0	0.26 ± 0.01	0.25 = 1/4	1/4	1/4
2.0	0.35 ± 0.01	0.325 ± 0.005	0.319	0.350
3.0	0.42 ± 0.01	0.389 ± 0.005	0.363	0.442
4.0	0.48 ± 0.01	0.439 ± 0.005	0.396	0.528
5.0	0.53 ± 0.01	0.496 ± 0.005	0.422	0.611
6.0	0.58 ± 0.01	0.527 ± 0.005	0.444	0.688
7.0	0.62 ± 0.01	0.579 ± 0.005	0.463	0.776
8.0	0.65 ± 0.01	0.628 ± 0.005	0.479	0.839
9.0	0.69 ± 0.01	0.694 ± 0.005	0.493	0.912
10.0	0.73 ± 0.01	0.723 ± 0.005	0.505	0.984

before and therefore the probability that the signal is positive there at the time of current jumping is conditioned by the fact that the signal had crossed zero there at some earlier time. Therefore, it is difficult to compute θ_{ad} exactly for the undirected case.

III. NOISY MOTION OF THE TEST PARTICLE

In the preceding section we considered the adaptive motion of the test external noise. In this section we consider the other case when there is only noise and no adaptation. In this case the particle just moves randomly through the medium in which a field $\phi(x, t)$ is evolving according to its own prescribed dynamics. As before, the test particle is launched at the origin at $t=0$ where the sign of the field is positive (say) at $t=0$. The particle then performs a Brownian motion $\dot{R} = \eta(t)$, where $\eta(t)$ is a Gaussian white noise with zero mean and the correlator $\langle \eta(t) \eta(t') \rangle = 2D_p \delta(t-t')$. Here $R(t)$ denotes the position of the particle from some fixed reference point. The motion of the field and that of the particle are completely uncorrelated. The particle dies when the field that it sees changes sign. Then we ask, What is the probability that the particle survives up to time t ?

We first consider the case when the field $\phi(x, t)$ is evolving according to diffusion equation $\partial_t \phi = D_f \nabla^2 \phi$. We performed numerical simulation to compute the survival probability of the test particle. This probability decays as a power law $P(t) \sim t^{-\theta_d}$ for large t , where the exponent θ_d is found to depend continuously on the ratio of the two diffusion constants $c = D_p/D_f$. The results are presented in the second column of Table I under the heading $\theta_d(\text{MC})$. It is clear from this table that for any nonzero c , $\theta_d(c) > \theta_0$, where θ_0 is the corresponding static persistence exponent, i.e., when $c=0$. This continuous nonuniversal dependence of θ_d

on c , however, is not very surprising for the following reason. The test particle dies whenever it crosses any ‘‘zero’’ of the field $\phi(x, t)$. Thus two zeros of the field on either side of the test particle act like two boundary walls. However, these walls are not static. They themselves are moving as the field $\phi(x, t)$ is evolving in time. In fact, since the typical distance between zeros of the diffusing field increases as \sqrt{t} , the walls bounding the test particle are therefore diffusing as \sqrt{t} . This particular case is known to be marginal [21] in the sense that the exponent, characterizing the power-law decay of survival probability of the particle, depends continuously on the ratio of the diffusion constants of the particle and the walls.

While this explains qualitatively why θ_d depends continuously on c , it does not give any quantitative estimate of the exponent. To make progress in that direction, we proceed as follows. Let x be the coordinate of an arbitrary point in space measured from the rest frame of the particle. Then the field $\psi(x, t) = \phi(x + R(t), t)$ as seen by the particle evolves as

$$\frac{\partial \psi}{\partial t} = D_f \nabla^2 \psi + \frac{\partial \psi}{\partial x} \eta(t). \quad (3.1)$$

The field ψ and the noise η are completely uncorrelated. Note that for a given realization of the noise process $\{\eta(t)\}$, the process $\psi(x, t)$ at a fixed x as a function of t is a Gaussian process. However, when the distribution of $\eta(t)$ is also taken into consideration, $\psi(x, t)$ at a fixed x no longer has a Gaussian distribution due to the multiplicative nature of the noise in Eq. (3.1). It is nevertheless useful to calculate the two-time correlator $C(t', t) = \langle \psi(0, t') \psi(0, t) \rangle$ that characterizes the temporal process at the location of the particle, i.e., at $x=0$. This can be easily performed in the k space where the solution is given by

$$\psi(k, t) = \psi(k, 0) e^{-D_f k^2 t} \exp\left(ik \int_0^t \eta(t') dt'\right). \quad (3.2)$$

We then compute $C(t', t) = \int dk \langle \psi(-k, t') \psi(k, t) \rangle$, where the average, denoted by angular brackets, is taken over both the initial conditions of ψ and the history of the noise η . The initial condition is taken to be random, so that $\langle \psi(k, 0) \psi(-k, 0) \rangle = \Delta$, where Δ is a constant. Since the noise η is Gaussian white noise, we use the property $\langle \exp(ik \int_{t'}^t \eta(t_1) dt_1) \rangle = \exp[-D_p k^2 |t-t'|]$. It is then easy to see that in $d=1$,

$$C(t', t) = \frac{1}{2\sqrt{\pi}} \frac{1}{\sqrt{D_f(t+t') + D_p|t-t'|}}. \quad (3.3)$$

The normalized autocorrelator $f(t', t) = C(t', t) / \sqrt{C(t', t')C(t, t)}$, when expressed in terms of the variable $T = \ln(t)$, becomes stationary, i.e., only a function of the time difference $|T - T'|$. Denoting, for convenience, this time difference by T , one finds that the stationary autocorrelator $f(T)$ is given by

$$f(T) = \frac{1}{\sqrt{\cosh(T/2) + c \sinh(|T|/2)}}, \quad (3.4)$$

where $c = D_p/D_f$ is the ratio of the two diffusion constants.

Note that for $c=0$, $f(T)$ reduces to the static autocorrelator $f_0(T)=[\cosh(T/2)]^{-1/2}$ [4]. However, there is an important difference between $c=0$ and $c\neq 0$ cases. For $c=0$, the stochastic stationary process, whose correlator is given by $f_0(T)$, is Gaussian. However, for $c\neq 0$, while the process is still stationary in the variable T , it is non-Gaussian, as mentioned earlier. This is evident from Eq. (3.2) since $\psi(k,t)$ is a product of two random variables $\psi(k,0)$ and $\exp[ikf\eta(t')dt']$ and hence is not clearly Gaussian, even though both $\psi(k,0)$ and $\eta(t)$ are individually Gaussian. Therefore, the approximate method developed [4] for the case $c=0$ to compute the asymptotic distribution of the interval between successive zero crossings $P_0(T)\sim\exp(-\theta_0 T)\sim t^{-\theta_0}$ for large t cannot be simply extended to the $c\neq 0$ case.

It is nevertheless useful to calculate θ_d by approximating the process by a Gaussian process having the same two-point correlator for two reasons. First, a comparison between θ_d obtained numerically for the actual process and that obtained for the corresponding Gaussian process will tell us how important the non-Gaussian effects are. Second, there have been some recent developments [13] in approximate analytical calculations of the exponent for Gaussian stationary processes that one can use in the present context. Therefore, in the following, our strategy would be to estimate the exponent $\theta_d(G)$ [which characterizes the exponential decay of the distribution of intervals between successive zero crossings $P(T)\sim e^{-\theta_d(G)T}$ for large T] for the Gaussian process with the correlator $f(T)$ as in Eq. (3.4) and then compare it with the θ_d for the actual process.

We first present the numerical results for $\theta_d(G)$ for the Gaussian process with the correlator as in Eq. (3.4). This is done by constructing a time series having the same correlation function. It is most convenient to work in the frequency domain rather than the time domain. Details of this simulation procedure can be found in Ref. [9]. The results of $\theta_d(G)$ for different values of c are presented in the third column of Table I. By comparing columns 2 and 3, it is evident that the non-Gaussian effects are indeed quite small and the Gaussian approximation seems to be quite good.

However, exact analytical calculation of $\theta_d(G)$ even for a Gaussian stationary process with a general correlator $f(T)$ is difficult and has remained an unsolved problem for many years [10,11]. Exact results are known only in a few special cases [10,11]. One such case is when $f(T)=e^{-\lambda_0|T|}$ for all T . In this case, the Gaussian process is a Markov process and one can show exactly that $P(T)\sim e^{-\theta T}$ for large T where $\theta=\lambda_0$. By looking at $f(T)$ in Eq. (3.4), we see that for $c=1$, $f(T)=e^{-|T|/4}$ for all T . Therefore, $\theta_d(G)=1/4$ for $c=1$. For c close 1, say, $c=1+\epsilon$, one can use a perturbation theory that has been developed recently to calculate θ_d for processes that are close to a Markov process [13,22]. According to this theory, if $f(T)=\exp(-\lambda|T|)+\epsilon f_1(T)$, where ϵ is small, then the exponent θ_d , to order ϵ , can be most easily expressed as

$$\theta_d(G)=\lambda\left(1-\epsilon\frac{2\lambda}{\pi}\int_0^\infty f_1(T)[1-\exp(-2\lambda T)]^{-3/2}dT\right). \quad (3.5)$$

In our case, expanding $f(T)$ in Eq. (3.4) around $c=1$, we get

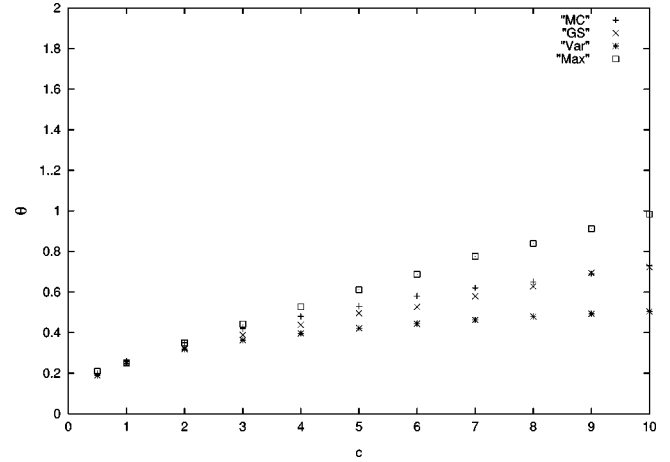


FIG. 2. Visual summary of the different measures of the exponent θ_d as given in Table I.

$\lambda=1/4$ and $f_1(T)=-1/2\sinh(T/2)\exp(-3T/4)$. Using this in Eq. (3.5) and performing the integration, we get, to order ϵ ,

$$\theta_d(G)=\frac{1}{4}+\epsilon\frac{3}{32}. \quad (3.6)$$

This perturbation theory may not give good estimates for $\theta_d(G)$ when c is far away from 1. However, one can use a variational estimate for $\theta_d(G)$ for general c . This variational method was developed recently in Ref. [13] by mapping the zero crossing problem to that of the evaluation of ground-state energy of a corresponding quantum problem. This method was used [13] to approximately calculate the static persistence exponent for the Ising model in both one and two dimensions. The results were in good agreement [13] with the exact result in one-dimension [2] and numerical simulations [23] as well as direct experiment [12] in two dimensions. This method works for class-1 Gaussian stationary processes, i.e., when $f(T)=1-a|T|+\dots$ for small T . Since in our present case $f(T)$ in Eq. (3.4) is class 1 for any nonzero c , one can estimate $\theta_d(G)$ by using this variational method. This method gives two estimates θ_{max} and θ_{var} for the exponent $\theta_d(G)$. While θ_{max} is a strict rigorous upper bound for $\theta_d(G)$, θ_{var} gives the best variational estimate. The salient features of the variational method and the expressions for θ_{max} and θ_{var} are given in the Appendix.

For the process being considered with the correlator as in Eq. (3.4), estimates θ_{var} and θ_{max} are presented, respectively, in columns 4 and 5 of Table I for different values of the parameter c . Comparing these with columns 2 and 3, it is clear that the variational approximation gets progressively worse as c increases. A visual summary of these different measures of the exponent is given in Fig. 2.

To summarize, we find that the exponent θ_d depends continuously on the ratio c of the diffusion constants. For any arbitrary nonzero c , $\theta_d>\theta_0$, where θ_0 is the corresponding static persistence exponent. Non-Gaussian effects are found to be quite small.

We now turn to the case when the fluctuating field is the spin field of the Ising model or, in general, the color field of the q -state Potts model undergoing $T=0$ coarsening dynamics starting from a random initial configuration. The tracer

particle once again moves diffusively through the medium with a diffusion constant D_p and whenever the field that the particle sees at its own location changes sign, the particle dies. As before, one is interested in calculating the survival probability $P(t)$ of the tracer particle.

In the q -state Potts model at $T=0$, the domain walls perform a random walk and whenever two domain walls meet, they either annihilate each other with probability $1/(q-1)$ or coagulate to form a single wall with probability $(q-2)/(q-1)$ [2,24]. The tracer particle dies whenever it crosses paths with any domain wall. One expects that the survival probability of the tracer particle will decay as $P(t) \sim t^{-\theta_p}$ for large t . The exponent $\theta_p(q, c)$ is expected, as in the diffusion case, to depend continuously on q and the ratio $c = D_p/D_f$, where D_p is the diffusion constant of the test particle and D_f is that of the domain walls.

This problem has been studied in some detail before [6,8]. Let us just summarize here the main results that are already known. In the limit $q \rightarrow \infty$, $\theta_p(\infty, c)$ can be computed exactly by noting that only two domain walls on either side of the tracer particle actually matter for the calculation of $P(t)$ [25]. One finds exactly $\theta_p(\infty, c) = \pi/\{2 \cos^{-1}[c/(1+c)]\}$ [25,6]. Note that for $c=0$ this reduces to the static persistence exponent $\theta_p(\infty, 0) = 1$ [2]. In the Ising limit $q=2$, however, there is no exact result for general c . An exact result is available only for $c=0$, $\theta_p(2, 0) = 3/8$ [2]. For general c and $q=2$, a mean-field Smoluchowski type of approach was developed [6], whose predictions $\theta_p(2, c) = \sqrt{(1+c)}/8$ were in good agreement with numerical simulations [6]. However, this Smoluchowski approach, when extended to the large- q limit, differed substantially [6] from the exact $q \rightarrow \infty$ result. Finally, a perturbation theory has been developed recently by Monthus [8] and the exponent $\theta_p(q, c)$ has been determined at first-order perturbation in $q-1$ for arbitrary c and at first order in c for arbitrary q .

We will not study this exponent $\theta_p(q, c)$ in its generality any further in this section. However, in the next section, we will study in some detail the special case $c=1$, as it turns out to be a particularly interesting case from the point of view of the pattern persistence problem of the Potts model.

IV. PERSISTENCE OF A SPECIFIC PATTERN IN THE 1D POTTS MODEL

In Sec. II we showed that the survival probability of an adaptive test particle is related to the persistence of a specific pattern, namely, an original domain in the $T=0$ dynamics of the Potts model. In this section, we show that the survival probability of a noisy or diffusive test particle (studied in Sec. III) is also related to the persistence of yet another pattern in the 1D Potts model, namely, the survival up to time t of two adjacent original domains present in the initial configuration.

Let us consider the zero-temperature coarsening dynamics of the q -state Potts model starting from a random initial configuration. In an infinitesimal time interval dt , each spin changes its color to that of one of its neighbors selected at random. These dynamics can be equivalently formulated in terms of the motions of domain walls. The domain walls perform independent random walks and whenever two walls meet, they either annihilate with probability $1/(q-1)$ or ag-

TABLE II. Exponent θ_1 that characterizes the asymptotic decay $P_1(t) \sim t^{-\theta_1}$, the probability that a domain wall remains uncollided up to time t in the zero-temperature dynamics of the q -state Potts model. Exact values of θ_1 are quoted for $q=2$ and $q \rightarrow \infty$. For other values of q , θ_1 (column 2) is estimated from Monte Carlo simulations on a periodic lattice of 75 000 sites and results averaged over 20 different initial conditions. The estimated upper bounds for $\theta_1(q)$ (as explained in the text) are presented in column 3.

q	θ_1	$\theta_1(\text{max})$
2	1/2	
3	0.72 ± 0.01	$0.792481 \dots$
4	0.86 ± 0.01	0.91 ± 0.01
5	0.95 ± 0.01	1.00 ± 0.01
6	1.04 ± 0.01	1.06 ± 0.01
50	1.47 ± 0.01	
∞	3/2	

gregate to become a single wall with probability $(q-2)/(q-1)$ [3,24]. The static persistence then is the probability that a fixed point in space is not traversed by any domain wall. However, a somewhat more natural quantity in this domain wall representation is the probability $P_1(t)$ that a given domain wall remains uncollided up to time t . A little thought shows that this is precisely the survival probability of two adjacent domains present in the initial configuration. We show below that $P_1(t) \sim t^{-\theta_1}$ for large t , where $\theta_1(q)$ is a q -dependent exponent that is not obviously related to any other known exponent via scaling relations.

In Sec. III we considered the exponent $\theta_p(q, c)$ characterizing the decay of the survival probability of a diffusing test particle in the background of the diffusing domain walls of the Potts model. The parameter c is the ratio of the diffusion constant of the test particle to that of the domain walls. Let us consider the case $c=1$. In this case the test particle cannot be distinguished from the other diffusing domain walls. Since the test particle dies whenever any other domain wall touches it, it is clear that the survival probability of the test particle for $c=1$ is precisely the fraction of uncollided domain walls in the Potts model and hence $\theta_1(q) = \theta_p(q, c=1)$.

Clearly, θ_1 can be determined exactly in the two limits $q=2$ and $q \rightarrow \infty$. For $q=2$, since there is only annihilation upon contact between domain walls, the fraction of uncollided walls is the same as the density of domain walls that decays as $\sim t^{-1/2}$ for large t and hence $\theta_1(2) = 1/2$. In the $q \rightarrow \infty$ limit, by setting $c=1$ in the exact formula, $\theta_p(\infty, c) = \pi/\{2 \cos^{-1}[c/(1+c)]\}$ [25,6], one gets $\theta_1 = 3/2$. For intermediate values of q , we present numerical results in column 2 of Table II. It is clear that the exponent $\theta_1(q)$ increases monotonically with q .

The exponent θ_1 can be quite easily computed within mean-field theory. Let $N(t)$ and $N_1(t)$ denote, respectively, the total density of domain walls and density of uncollided walls at time t . Let $Q_1(t)$ denote the density of domains of size 1 (here 1 is the lattice spacing and hence the smallest interval size). Then $N(t)$ and $Q_1(t)$ are related via the exact relation

$$\frac{dN}{dt} = -\frac{q}{q-1}Q_1. \quad (4.1)$$

However, there is no such simple exact relationship between $N_1(t)$ and $Q_1(t)$. However, if one neglects correlations, it is easy to write such a relationship within mean-field theory,

$$\frac{dN_1}{dt} = -2\left(\frac{N_1}{N}\right)^2 Q_1 - 2\frac{N_1}{N}\left(1 - \frac{N_1}{N}\right)Q_1, \quad (4.2)$$

where the first term on the right-hand side represents the annihilation of two uncollided walls and the second the contribution from annihilation of an uncollided wall with a collided wall. Eliminating Q_1 from the two equations above, we get $N_1 \sim N^{2(q-1)/q}$. Using the result $N(t) \sim t^{-1/2}$, we finally obtain $\theta_1(q) = (q-1)/q$, within mean-field theory. While the mean-field answer is exact for $q=2$, it gets worse as q increases as evident by comparison with Table II. Presumably, the mean-field value forms a lower bound to the true exponent value, though we have not been able to prove it.

However, one can obtain rigorous upper bounds to $\theta_1(q)$ as follows. This can be done by generalizing the arguments used by Derrida [3] to obtain upper bounds to the static persistence exponent $\theta_0(q)$. The argument goes as follows. It was noted by Monthus [8] that the problem of a diffusing tracer particle moving among the domain walls of the Potts model can be mapped to a reaction diffusion problem where particles are generated from a source that is diffuse around and aggregate upon contact. The only difference from the static case [3] was that the source is now moving. In fact, the source diffuses with the same diffusion constant as the tracer particle. It is then possible to write the survival probability $P_1(t)$ as [8]

$$P_1(t) = \sum_1^{\infty} P(m,t)q^{1-m}, \quad (4.3)$$

where $P(m,t)$ is the probability of having m particles in the corresponding reaction diffusion problem. Writing the above equation for $q=q_2$ as ($a \geq 1$)

$$\frac{P_1(q_2)}{q_2} = \sum_{m=1}^{\infty} P(m,t)q_2^{-m} = \sum P(m,t)[q_1^{-m}]^{\ln q_2 / \ln q_1} \quad (4.4)$$

and then using Jensen's inequality ($\langle x^a \rangle \geq \langle x \rangle^a$ for $a \geq 1$ and x a positive random variable) as was used in the static case [3], we immediately obtain the inequality

$$\theta_1(q_2) \leq \theta_1(q_1) \frac{\ln q_2}{\ln q_1} \quad (4.5)$$

for $q_2 \geq q_1$. For example, using the exact result $\theta_1 = 1/2$ for $q=2$ and the above inequality we get

$$\theta_1(q) \leq \ln q / 2 \ln 2. \quad (4.6)$$

For $q=3$ this gives $\theta_1(3) \leq 0.792481\dots$, which should be compared with its numerical value 0.72 ± 0.005 . For higher values of q , one can have a numerical estimate of a tighter upper bound of $\theta_1(q)$ by using the numerical value of

$\theta_1(q-1)$ in the inequality (4.5). This would be an improvement over the exact bound (4.6) obtained by comparing with $q=2$. These improved numerical bounds $\theta_1(\max)$ are presented in column 3 of Table II.

It was pointed out by Monthus [8] that carrying out the same formalism that led to the exact determination of the static persistence exponent $\theta_0(q)$ [2] is not as straightforward as computing the exact value of $\theta_p(q,c)$ for general c . However, one may hope that some special simplifications might occur for $c=1$, leading to the exact computation of the exponent $\theta_1(q)$, though we have not succeeded yet in that direction.

V. SUMMARY AND CONCLUSIONS

In this paper we have studied the persistence of some patterns present in the initial configuration of a fluctuating field. It was shown that some of these pattern persistence problems are related to the survival probability of a mobile particle launched into the field. By suitably adjusting the rules of the dynamics of the particle one can study the persistence of different patterns in the underlying field. This led us to study the PF problem in general. Several special cases were studied in detail and different results were derived.

It is clear from our study as well as others that there is a whole hierarchy of exponents associated with the decay of persistence of different patterns in the phase-ordering systems. It is not clear at present whether or not these exponents are independent of each other. While these exponents do not depend on the details of the initial configuration (as long as it is short ranged), it is not clear whether they can be considered universal and if so, in what sense. For example, if the diffusion constant of any single domain wall of the Potts model changes slightly, then the exponent θ_1 characterizing the decay of survival of the wall (probability that it remains uncollided) also changes. Clearly, in this respect the exponent is nonuniversal. So the important question that remains to be answered is, What are the criteria one should use to decide whether or not an exponent in the phase-ordering dynamics is universal?

One of the interesting extensions of the present work would be to study the PF problem when the fluctuating field is the height of an interface in or approaching the steady state. The static persistence for interfaces has been studied recently in some detail [9]. Also anomalous diffusive behavior of a tracer particle on a solid-on-solid surface was noted [18] and was attributed to the temporary trapping or burial of the particle in the bulk of the crystal. In addition, given that sophisticated techniques using scanning tunneling microscope already exist for determining temporal step fluctuations on crystal surfaces [26], it is not unreasonable to hope that such techniques may be refined in the future to measure the survival probabilities of the static as well as the mobile particle in a fluctuating interface.

Finally, it has been noted recently [27] that static persistence exponent for the diffusion equation may possibly be measured in dense spin-polarized noble gases (^3He and ^{129}Xe) using NMR spectroscopy and imaging [28]. In these systems the polarization acts like a diffusing field. With a slight modification these systems may possibly be used to measure the persistence of some patterns of the diffusive

field as discussed in the present paper.

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APPENDIX: THE VARIATIONAL METHOD

It was shown in [13] that the exponent $\theta_d(G)$ is exactly the ground-state energy difference $\theta_d(G) = E_1 - E_0$ between two quantum problems, one with a hard wall at the origin and the other without a wall. The energy E_0 (without a wall) can be determined exactly,

$$E_0 = \frac{1}{2\pi} \int_0^\infty \ln \left(\frac{G(\omega)}{\omega^2} \right) d\omega, \quad (\text{A1})$$

where $G(\omega) = 1/\tilde{f}(\omega)$ and $\tilde{f}(\omega)$ is the Fourier transform of the correlation function $f(T)$ of the Gaussian stationary process normalized such that $\tilde{f}(\omega) \sim \omega^{-2}$ for large ω . The energy E_1 (with a wall at the origin) is estimated variationally as it is hard to obtain exactly. For class-1 processes, one can use a harmonic oscillator with a wall as the trial state with the frequency ω_0 of the oscillator as the variational parameter. The variational energy $E_1(\omega_0)$ is given by the expression [13]

$$E_1(\omega_0) = \omega_0 \left[\frac{3}{2} + \frac{2}{\pi} \left(\frac{G(0)}{\omega_0^2} - 1 \right) + \frac{2}{\pi} \int_0^\infty dx \left(\frac{G(x\omega_0)}{\omega_0^2} - x^2 - 1 \right) S(x) \right], \quad (\text{A2})$$

where $S(x) = \sum_{n=1}^\infty n c_n / (x^2 + 4n^2)$ with c_n given by

$$c_n = \frac{4}{\pi 2^{2n} (2n+1)!} \left[\frac{(2n)!}{n!(2n-1)} \right]^2. \quad (\text{A3})$$

One then minimizes $E_1(\omega_0)$ with respect to ω_0 and uses this minimizing frequency ω_{min} to obtain the variational estimate

$\theta_{max} = E_1(\omega_{min}) - E_0(\omega_{min})$, which also is a rigorous upper bound to the true exponent $\theta_d(G)$ that characterizes the Gaussian process. However, as argued in [13], one can obtain a better estimate of $\theta_d(G)$ by using $\theta_{var} = E_1(\omega_{min}) - E_0^{(2)}(\omega_{min})$, where $E_0^{(2)}$ is given by

$$E_0^{(2)} = \omega_{min} \left[\frac{1}{2} + \frac{1}{2\pi} \int_0^\infty dx \left(\frac{G(x\omega_{min})}{\omega_{min}^2(x^2+1)} - 1 \right) \right]. \quad (\text{A4})$$

For numerical purposes, it is convenient to reformulate these expressions in terms of integrals in the time domain, in the form

$$E_1(\omega_0) = \omega_0 \left\{ \frac{3}{4} + \frac{2}{\pi \omega_0^2} \left[\frac{1}{\tilde{f}(0)} + \gamma \left(\frac{3\pi}{8} - 1 \right) \right] - \frac{1}{\omega_0^2} \int_0^\infty dT g(T) V(\omega_0 T) \right\}, \quad (\text{A5})$$

$$E_0^{(2)} = \frac{\omega_{min}}{4} + \frac{\gamma}{4\omega_{min}} - \frac{1}{2\omega_{min}} \int_0^\infty dT g(T) e^{-\omega_{min} T}, \quad (\text{A6})$$

where

$$V(x) \equiv \frac{4}{\pi} \left[-1 + \frac{3}{4} (1 - e^{-2x})^{1/2} + \left(\frac{e^{-x}}{2} + \frac{e^x}{4} \right) \sin^{-1}(e^{-x}) \right], \quad (\text{A7})$$

$$\gamma \equiv \lim_{\omega \rightarrow \infty} \left(\frac{1}{\tilde{f}(\omega)} - \omega^2 \right) = -2 \left. \frac{d^3}{dT^3} f(T) \right|_{T=0}, \quad (\text{A8})$$

and

$$g(T) \equiv \frac{1}{2\pi} \int_{-\infty}^\infty d\omega e^{-i\omega T} \left(\frac{1}{\tilde{f}(\omega)} - \omega^2 - \gamma \right). \quad (\text{A9})$$

Apart from the convenience of integrands with exponential rather than algebraic tails at large values of the integration variable, the real-space formulation has the bonus of not having to evaluate a sum at each point in the integration domain, as in Eq. (A2).

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