

Survival Probability of a Gaussian Non-Markovian Process: Application to the $T = 0$ Dynamics of the Ising Model

Satya N. Majumdar^{1,*} and Clément Sire^{2,†}

¹*Department of Physics, Sloane Physics Laboratory, Yale University, New Haven, Connecticut 06520-8120*

²*Laboratoire de Physique Quantique (UMR C5626 du CNRS), Université Paul Sabatier, 31062 Toulouse Cedex, France*

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We study the decay of the probability for a *non-Markovian* stationary Gaussian walker not to cross the origin up to time t . This result is then used to evaluate the fraction of spins that do not flip up to time t in the zero temperature Monte Carlo spin flip dynamics of the Ising model. Our results are compared to extensive numerical simulations. [S0031-9007(96)00965-9]

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Gaussian processes are among the most widely studied stochastic processes in various branches of science [1]. However, there are still simple but important questions associated with a Gaussian process that are nontrivial to compute. One such question is the following: Consider a stationary Gaussian process $X(\tau)$ with zero mean and a prescribed correlator. What is the probability $P(\beta)$ that $X(\tau)$ does not cross the origin $X = 0$ between $\tau = 0$ and $\tau = \beta$? This quantity, although simple and natural, turns out to be quite nontrivial to compute [2]. Why is this so? A little thought shows that this quantity probes high order correlations in time of the dynamics, and it depends on the whole history of time evolution of the system. In this Letter, we would like to address this question. It turns out that the solution to this problem has very wide applications in various other problems in physics. For example, a related question arises naturally in the context of zero temperature Monte Carlo dynamics in any spin system: What is the probability that a spin does not flip up to time t [3–8]? Similar questions also arise in the study of the fraction of lattice sites that remain unvisited up to time t by a random walker or by chemical species in a generic reaction diffusion system [9,10].

In this Letter we restrict ourselves to one such application, namely, the simple case of the Ising model. In the zero temperature dynamics of the Ising model, domains of opposite spins grow with time. At late times, the system is characterized by a single length scale (typical size of a growing domain) $L(t) \sim t^{1/2}$ [11]. The fraction $P(t)$ of spins that remain unflipped up to time t decays as $P(t) \sim L(t)^{-\theta}$ for large time t [3], where θ is a universal, dimension dependent, nonequilibrium exponent. Analytical computation of θ seems to be extremely nontrivial. Even in $d = 1$, where the Glauber dynamics is exactly solvable, the calculation of θ turned out to be a real tour de force, achieved recently by Derrida *et al.* [3]. They found $\theta_{1d} = 3/4$. However, their technique is special to $d = 1$ and seems impossible to extend to higher dimensions, where only numerical estimates of θ are available [4–6]. Therefore it is highly desirable to obtain an ap-

proximate analytical method to determine θ , which we now present.

Let us start with a stationary Gaussian process $X(\tau)$, with zero mean and a correlator $\langle X(\tau_1)X(\tau_2) \rangle = f(\tau_1 - \tau_2)$. The probability $P(\beta)$ of not crossing the origin up to $\tau = \beta$ is expected to decay as $\exp(-\bar{\theta}\beta)$ for large β [at least when $f(\tau)$ decays exponentially for large τ]. We would like to calculate $\bar{\theta}$ since, as we will see later, $\bar{\theta}$ is related to the exponent θ of the Ising model. If the Gaussian process is Markovian, for which f is necessarily of the form $f(\tau) = \exp(-\bar{\lambda}|\tau|)/2\bar{\lambda}$ [13], it is possible to show by various methods [12–14] that $\bar{\theta} = \bar{\lambda}$ exactly (see below also). For any other form of f , the process is non-Markovian (i.e., history dependent) and $\bar{\theta}$ is hard to compute. In fact, $\bar{\theta}$ depends very sensitively on the full function $f(\tau)$ and not just on its asymptotic properties. Keeping the Ising problem in mind, we will restrict ourselves only to the class of non-Markovian processes for which (i) $f'(0^\pm) \neq 0$ and (ii) $f(\tau) \sim \exp(-\bar{\lambda}\tau)$ for large τ . For convenience, we will then normalize f , setting $f'(0^\pm) = \mp 1/2$ after a proper rescaling of X , such that its Fourier transform satisfies $\omega^2 f(\omega) \rightarrow 1$, for large ω .

To illustrate the explicit history dependent nature of the non-Markovian process, it is useful to write its associated Langevin equation:

$$\frac{dX}{d\tau} = -\bar{\lambda}X + \eta + \int_{-\infty}^{\tau} J(\tau - \tau')\eta(\tau')d\tau', \quad (1)$$

where $\eta(\tau)$ is a Gaussian white noise with $\langle \eta(\tau)\eta(\tau') \rangle = \delta(\tau - \tau')$, and J is a causal [$J(\tau) = 0$, for $\tau < 0$] and integrable function. The history dependence is explicitly encoded in the kernel J . For $J = 0$, Eq. (1) describes a Markov process with $f(\tau) = \exp(-\bar{\lambda}|\tau|)/2\bar{\lambda}$ as stated above. In Fourier space, Eq. (1) amounts to $X_\omega = \eta_\omega[1 + J(\omega)]/(i\omega + \bar{\lambda})$, which allows us to relate the Fourier transform of f to that of J : $f(\omega) = |1 + J(\omega)|^2/(\omega^2 + \bar{\lambda}^2)$, with the correct large ω behavior, since $J(\omega) \rightarrow 0$ in this limit.

We now proceed to a variational and perturbative calculation of $\bar{\theta}$, which will be tested by simulating Eq. (1), before applying these results to the spin flip problem.

$P(\beta)$ can be written as the ratio of two path integrals, the first one Z_1 over, say, positive trajectories $X(\tau)$, the second one Z_0 over unrestricted trajectories:

$$P(\beta) = \frac{2 \int_{X>0} \mathcal{D}X(\tau) \exp[-S]}{\int \mathcal{D}X(\tau) \exp[-S]} = \frac{Z_1}{Z_0}, \quad (2)$$

where $S = \frac{1}{2} \int_0^\beta \int_0^\beta X(\tau_1) G(\tau_1 - \tau_2) X(\tau_2) d\tau_1 d\tau_2$, and $G(\tau_1 - \tau_2)$ is the inverse matrix of $f(\tau_1 - \tau_2)$. $\bar{\theta}$ is then calculated from $P(\beta)$ by taking the limit, $\bar{\theta} = -\lim_{\beta \rightarrow \infty} \beta^{-1} \ln P(\beta)$. We impose periodic boundary conditions, $X(0) = X(\beta)$, for the paths, which should not affect the value of $\bar{\theta}$ in the limit of large β . We notice that the Gaussian weight in Eq. (1) then becomes $S = \frac{1}{2\beta} \sum_n G(\omega_n) |X(\omega_n)|^2$, where $G(\omega_n) = 1/f(\omega_n)$ and $\omega_n = 2\pi n/\beta$ are Matsubara frequencies. First consider a Markov process for which $G(\omega) = \omega^2 + \bar{\lambda}^2$. We recognize the action in imaginary time (β is then the inverse temperature) of a harmonic oscillator of frequency $\bar{\lambda}$, $S = \int_0^\beta \mathcal{L}(X(\tau)) d\tau$, with $\mathcal{L}(X) = \frac{1}{2}[(\frac{dX}{d\tau})^2 + \bar{\lambda}^2 X^2]$. Thus $P(\beta)$ is the ratio between the partition function of an oscillator with a infinite wall at $X = 0$ and that of the same oscillator without the wall. For large β , it goes as $\exp[-\beta(E_1 - E_0)]$, where E_1 (E_0) is the ground state energy of the oscillator with (without) a wall. Thus $E_0 = \bar{\lambda}/2$, and $E_1 = 3\bar{\lambda}/2$, as the eigenstates of the problem with a hard wall at the origin are the odd states of the unrestricted oscillator. This gives the Markovian result $\bar{\theta} = \bar{\lambda}$.

For non-Markovian processes, unfortunately, S is no longer a classical action with an associated quantum problem. The denominator Z_0 can, however, still be computed exactly, and we find after taking $\beta \rightarrow \infty$,

$$E_0 = \frac{1}{2\pi} \int_0^\infty \ln\left(\frac{G(\omega)}{\omega^2}\right) d\omega. \quad (3)$$

As a check, one can verify that for an oscillator, for which $G(\omega) = \omega^2 + \bar{\lambda}^2$, one recovers $E_0 = \bar{\lambda}/2$. The most difficult part is to evaluate the ‘‘ground state energy’’ $E_1 = -\lim_{\beta \rightarrow \infty} \ln Z_1/\beta$ of the problem with a wall at the origin. One way of computing Z_1 will be to perturb around a classical action, for instance, that of harmonic oscillator of frequency ω_0 (or that of a particle in a box as we also did in [14]). We adopt a variational method, by choosing a trial inverse correlator $G_0(\omega) = \omega^2 + \omega_0^2$, corresponding to that of an oscillator (with a hard wall at the origin), whose frequency ω_0 is going to be our variational parameter. We have the general variational inequality, $E_1 \leq 3\omega_0/2 + \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \langle S - S_0 \rangle_w$, where the average is performed using the action of the hard wall oscillator. The second term of the inequality requires evaluating the propagator $\langle |X(\omega_n)|^2 \rangle_w$ of the hard wall

oscillator, leading finally to

$$E_1^{(2)} = \omega_0 \left[\frac{3}{2} + \frac{2}{\pi} \left(\frac{G(0)}{\omega_0^2} - 1 \right) + \frac{2}{\pi} \int_0^\infty dx \left(\frac{G(x\omega_0)}{\omega_0^2} - x^2 - 1 \right) \times \sum_{n=1}^\infty \frac{nc_n}{x^2 + 4n^2} \right], \quad (4)$$

where the numbers c_n can be evaluated using properties of Hermite polynomials and are given by

$$c_n = \frac{4}{\pi 2^{2n} (2n+1)!} \left[\frac{(2n)!}{n!(2n-1)!} \right]^2. \quad (5)$$

One can then differentiate Eq. (4) with respect to ω_0 to obtain an equation for ω_0 , which minimizes $E_1^{(2)}$. This equation can then be easily solved numerically. In principle, the value of E_1 can be improved by summing higher terms of the cumulant expansion around the trial action [14]. The superscript (2) denotes that we have kept only the first two terms of this expansion. To perform a systematic order by order cumulant expansion, one should also keep only the first two terms in E_0 [even though E_0 can be evaluated exactly to all orders from Eq. (3)]. This gives

$$E_0^{(2)} = \omega_0 \left[\frac{1}{2} + \frac{1}{2\pi} \int_0^\infty dx \left(\frac{G(x\omega_0)}{\omega_0^2(x^2+1)} - 1 \right) \right]. \quad (6)$$

We can then define $\bar{\theta}^{(2)}$ as $\bar{\theta}^{(2)} = \min_{\omega_0} (E_1^{(2)} - E_0^{(2)})$, remembering that $\bar{\theta}_v = \min_{\omega_0} E_1^{(2)} - E_0$ is an exact (presumably bad) bound of $\bar{\theta}$.

When $J(\omega)$ is small [see Eq. (1) and below], and using Eqs. (4)–(6), one can perform a straightforward perturbative calculation around the Markov process $J = 0$ to first order in $K(\omega) = J(\omega) + J(-\omega)$,

$$\bar{\theta} = \bar{\lambda} \left[1 - \frac{2}{\pi} K(0) - \frac{1}{2\pi} \int_0^\infty K(x\bar{\lambda}) V(x) dx \right], \quad (7)$$

where $V(x) = 4(x^2 + 1)S(x) - 1$, and $S(x)$ is the same series that appears in Eq. (4). In fact, an infinite number of terms of the perturbation theory can be resummed by using a novel technique (for details, see [14]), leading to

$$\bar{\theta} = \frac{4}{\pi} \sqrt{G(0)} + \frac{1}{2\pi} \int_0^\infty W[G(\omega)/\omega^2] d\omega, \quad (8)$$

$$W(x) = \sum_{n=1}^\infty \frac{c_n}{n} \ln[1 + 4n^2(x-1)] - \ln(x). \quad (9)$$

This expression is valid provided $G(\omega)/\omega^2 \geq 1$, which is always the case for (and close to) a Markovian process. We have tested Eq. (8), by comparing its prediction to the direct simulation of Eq. (1), with $f(\tau) = \varepsilon \exp(-\tau)/2 + (1 - \varepsilon) \exp(-2\tau)/4$, interpolating between two Markovian processes with $\bar{\lambda} = 2$ and $\bar{\lambda} = 1$. Note that ε must be positive to ensure $f > 0$, and that for $\varepsilon > 4/3$, one can

find ω such that $G(\omega)/\omega^2 < 1$, and Eq. (8) is not reliable any more. The results for some representative values of $\varepsilon \neq 0, 1$ (for which $\bar{\theta} = 2$ and $\bar{\theta} = 1$) are displayed in Table I, showing a very good agreement between Eq. (8) and numerical simulations.

We now turn to the $T = 0$ dynamics of the Ising model starting from a random (high temperature) initial configuration. We would like to show that calculating the fraction of unflipped spins up to time t in the Ising model reduces to calculating the survival probability of a Gaussian process in the framework of Gaussian closure approximation (GCA), introduced by Mazenko [15,16]. But before we make this connection, a few facts about the $T = 0$ dynamics of the Ising model would be relevant.

Following a quench to $T = 0$, interpenetrating domains of ± 1 phases grow with time. A scaling theory has been developed to characterize the morphology of the growing domains [11]. According to this theory, at late times, the system is characterized solely by the linear length of a growing domain $L(t)$. For the Ising model, $L(t) \sim t^{1/2}$ in all dimensions [however, in $d = 3$ cubic lattice at $T = 0$, it seems that $L(t) \sim t^{1/3}$ due to lattice effects [14,17], a fact which was underestimated in [5]]. Another prediction of the scaling theory relevant for us is that the on-site autocorrelation satisfies $\langle S(t)S(t') \rangle = F(L(t)/L(t'))$ for $t \geq t' \gg 0$, where $F(x) \sim x^{-\lambda}$ for large x [11,18]. The exponent λ is exactly 1 in $d = 1$, is close to 1.25 in $d = 2$ (from both simulations [18] and direct experiment [19]), is and close to 1.67 in $d = 3$ [11]. GCA has been particularly successful in calculating this exponent as it predicts $\lambda_{1d} = 1$, $\lambda_{2d} = 1.289$, and $\lambda_{3d} = 1.673$, this approach becoming asymptotically exact for large d . Recently, we have extended GCA to the q -state Potts model and calculated the q -dependent λ [20].

Without entering into the details of GCA, we simply mention that this method assumes that the spin at position \mathbf{x} and time t is essentially the sign of a continuous Gaussian stochastic variable $m(\mathbf{x}, t)$, which is physically interpreted as the distance to the nearest interface to the point \mathbf{x} [15]. We thus see that in the framework of GCA, *the probability that a spin does not change sign up to time t is equal to the probability that the associated Gaussian*

process $m(t)$ does not cross the origin $m = 0$ (for now we forget the label \mathbf{x} , as this probability does not depend on the considered site). The process $m(t)$ at a given site is Gaussian whose correlator $\langle m(t)m(t') \rangle$ can be calculated using the GCA scheme. However, $m(t)$ is not stationary since its correlation function depends explicitly on both t and t' , and we need to use the following trick before using the results of Eqs. (4)–(9). We define the variable $X(t) = m(t)/\sqrt{\langle m^2(t) \rangle}$, which is also Gaussian. Its correlator turns out to satisfy $\langle X(t)X(t') \rangle = g(L(t)/L(t'))$, where once again $g(x) \sim x^{-\lambda}$ for large x . If we now set $\tau = \ln[L(t)]$, we are left to study the survival probability of a stationary Gaussian process, with correlator $\langle X(\tau)X(\tau') \rangle = f(\tau - \tau')$, with $f(\tau) = g(\exp|\tau|)$. This completes the relation to the general problem studied in the first part of this Letter. For the Gaussian process, the survival probability $P(\tau) \sim \exp(-\bar{\theta}\tau) \sim L(t)^{-\bar{\theta}}$. Thus we get $\theta = \bar{\theta}$ in the framework of GCA. Note that for an ordinary Brownian walker $g(x) = x^{-1/2}$, or $f(\tau) = \exp(-|\tau|/2)$, which leads to the well-known result $P(t) \sim t^{-1/2}$.

By means of GCA (see [14] as these calculations are not the subject of this Letter), we have computed the functions f for $d = 1, 2, 3$. For instance, in $d = 1$, we got the (exact) result $f(\tau) = \sqrt{2}/(1 + \exp|2\tau|)$. We see that f is not a pure exponential and is thus non-Markovian. Knowing $f(\tau)$, we have computed the variational $\bar{\theta}^{(2)}$, and the associated frequency ω_0 . In Table II, these results are compared to $\bar{\theta}_{\text{NS}}$, extracted from numerical simulations of Eq. (1) (in Fourier space, then using an inverse fast Fourier transform), with the associated f . We also performed Ising simulations in $d = 2$ (800×800 lattice, 30 samples) confirming the results of [4–6], and in $d = 3$ ($100 \times 100 \times 100$ lattice, 60 samples). Note that the scaling of $P(t)$ is found to be much better as a function of $L(t)$ than as function of t [6,20].

We note that the variational results are in good agreement with the simulations of Eq. (1), and with the Ising results in $d = 1$. However, the agreement in $d = 2, 3$ is not as good. To understand this, we have to remember that there are two possible sources of errors between the simulations of Eq. (1) and the Ising simulations: (i) the real variable $X(t) \sim m(t)$ is not truly Gaussian, and (ii) due to the use of GCA, the correlator f is not exact (except in $d = 1$, by accident). To illustrate the importance of the error due to (i), notice that although f is exact in $d = 1$, the Ising exact result $\theta = 3/4$ is bigger than the value 0.70 obtained by simulating Eq. (1), which is perfectly reproduced by our theory. Note that we got the exact bound for $\bar{\theta}$, $\bar{\theta}_v = 0.736$ in $d = 1$, whereas $\bar{\theta}_v$ is a bad bound for $d > 1$. In $d = 2, 3$, the main cause of error is presumably (ii), as f given by GCA is found to decrease faster than in the Ising simulations for $\tau < 2$ [14]. To check this, we computed $\bar{\theta}$ from Eq. (1) and $\bar{\theta}^{(2)}$ using for f a fit of the correlator obtained in the Ising simulations, leading to a clear improvement (see Table II). In $d = 3$, the

TABLE I. $\bar{\theta}_{\text{NS}}$ obtained from direct numerical simulations (NS) of Eq. (1) ($\tau_{\text{max}} \sim 1000$, $\Delta\tau \sim 10^{-3}$, 100 samples, uncertainties are $\Delta\theta = \pm 0.015$) is compared to the result of Eq. (8) as a function of ε , for $f(\tau) = \varepsilon \exp(-\tau)/2 + (1 - \varepsilon) \exp(-2\tau)/4$. We have reported the point $\varepsilon = 4/3$ [beyond which Eq. (8) must be regularized (see text)], which shows that θ can be less than the smallest inverse relaxation time (here 1). Note the remarkable accuracy of Eq. (8), up to its validity limit.

ε	0.10	0.25	0.5	0.75	1.33
$\bar{\theta}_{\text{NS}}$	1.72	1.47	1.22	1.09	0.91
$\bar{\theta}_{\text{Theory}}$	1.74	1.48	1.24	1.09	0.91

TABLE II. The four columns contain, respectively, (1) θ_{Ising} obtained in our Ising model numerical simulations for $d = 2, 3$; (2) $\bar{\theta}_{\text{NS}}$ obtained by simulating Eq. (1) ($\tau_{\text{max}} \sim 1000$, $\Delta\tau \sim 10^{-3}$, 500 samples); (3) $\bar{\theta}^{(2)}$ from Eqs. (7) and (8); (4) the optimal frequency $\omega_0 = \bar{\theta}^{(1)}$, which can be interpreted as the first term in the cumulant expansion. For $d = 2, 3$, we also give the same results using a fit of f taken from the Ising simulations, instead of GCA. In $d = 3$, θ depends on the nature of the fit (see text), and we only give typically obtained values (estimated uncertainty of order 0.05).

	θ_{Ising}	$\bar{\theta}_{\text{NS}}$	$\bar{\theta}^{(2)}$	$\bar{\theta}^{(1)}$
$d = 1$	3/4	0.70 ± 0.01	0.70	0.61
$d = 2$ (GCA)	0.45 ± 0.01	0.66 ± 0.01	0.58	0.43
$d = 2$ (fit of f)	...	0.49 ± 0.02	0.38	0.27
$d = 3$ (GCA)	0.52 ± 0.01	0.70 ± 0.02	0.47	0.30
$d = 3$ (fit of f)	...	~ 0.55	~ 0.4	~ 0.2

numerical $f(\tau)$ can be computed only up to a quite short time ($\tau < 1.5$), and θ is quite dependent on the way $f(\tau)$ is extended to large τ . Indeed, for such short times, the known asymptotics $f(\tau) \sim \exp(-\lambda\tau)$ is not reached yet. Finally, one can easily understand why the theoretical estimates in $d = 2, 3$ seem less accurate than in $d = 1$ or in Table I. It is possible to show [14] that for the Ising model f becomes *less and less Markovian* as d increases. An illustration of this is the fact that, as d increases, the relative difference between θ and λ strongly increases. In addition, the region for which $G(\omega)/\omega^2 < 1$ becomes wider as d increases, which is also a sign of strong “non-Markovianity,” and which prevented us from using Eq. (8) to evaluate θ . However, for large d , an alternate approach has been derived [14,21], which gives θ in excellent agreement with numerical simulations.

In summary, we have implemented variational and perturbative approaches to compute the survival probability of a Gaussian non-Markovian process, close enough to the Markovian limit associated to a quantum problem. These results were then used to calculate the fraction of unflipped spins in the zero temperature Monte Carlo dynamics of the Ising model within the framework of GCA. Further details of these calculations, the application to the calculation of the q -dependent θ for the q -state Potts model [4,6,20], numerics, and other approaches will be presented elsewhere [14]. Finally the related question of the probability that the *total* magnetization never flips after a quench at $T = T_c$ [22] or at $T = 0$ [14] is also the subject of further studies.

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*Electronic address: satya@cmphys.eng.yale.edu

†Electronic address: clement@irsamc2.ups-tlse.fr

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