PHYSICAL REVIEW E **80**, 020101(R) (2009)

Work distributions for Ising chains in a time-dependent magnetic field

Mario Einax[1] and Philipp Maass[2]
[1]*Institut für Physik, Technische Universität Ilmenau, 98684 Ilmenau, Germany*
[2]*Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück, Germany*
(Received 24 June 2009; published 17 August 2009)

Master equations can be conveniently used to investigate many particle systems driven out of equilibrium by time-dependent external fields. This topic is of vital interest in connection with fluctuation theorems and the associated microscopic work and heat distributions. We present an exact Monte Carlo simulation algorithm, which allows us to study interaction effects on these distributions. The method is applied to an Ising chain with Glauber dynamics. We find that the distributions are characterized by δ and step functions with a smooth part in between. With decreasing sweeping rate of the external field or decreasing interaction strength, the singular part becomes less dominant and the Gaussian fluctuation regime is approached.

DOI: 10.1103/PhysRevE.80.020101 PACS number(s): 05.70.Ln, 05.10.−a, 05.40.−a

In nonequilibrium statistical physics work function theorems have received much attention recently, which connect nonequilibrium averages of microscopically defined work and heat quantities with equilibrium thermodynamic potentials (for reviews, see [1,2], and references therein). The perhaps most popular is the Jarzynski theorem [3],

$$\langle \exp(-\beta W) \rangle = \exp(-\beta \Delta F), \tag{1}$$

where W is the microscopic work for a given external protocol, which drives a system from an initial equilibrium state to another state during an observation time t, ΔF is the free-energy difference between the initial and target state, and $\beta = 1/k_B T$ is the inverse thermal energy. The averaging is performed over the work distribution $\rho(W,t)$ that can be sampled from the set of all trajectories under the given external protocol.

To determine $\rho(W,t)$ even for simple systems is a difficult task and so far not much is known of its form and possible generic features. Exact solutions have been obtained for a classical two-level system [4] and a forced quantum oscillator [5]. If the driving is quasistatic, such that the system's state is in thermodynamic equilibrium with respect to the instantaneous values of the external parameters, $\rho(W,t)$ is a delta function at the macroscopic (thermodynamic) work value W_{m}. If the system is driven slowly enough to be close to thermodynamic equilibrium, a Gaussian distribution with mean W_{m} is obtained.

Almost no investigations have been carried out yet for interacting systems since it is difficult to determine $\rho(W,t)$ with sufficient accuracy in simulations or experiments. Based on the time-evolution equation for $\rho(W,t)$, Imparato and Peliti succeeded to derive a mean-field solution by considering the coupling of an external driving field to a collective variable of an Ising-like system [6]. To go beyond such mean-field treatments one has to rely on simulations.

Conceptually simple for theoretical studies are stochastic processes governed by a master equation (as, e.g., the Ising model and its variants), where trajectories can by generated by kinetic Monte Carlo simulations. For transition rates with explicit time dependence in response to external fields, the question arises how to set up an efficient and exact algorithm. A straightforward extension of standard procedures is to discretize time in sufficiently small intervals. This procedure has been applied recently to calculate work distributions for the dynamics of a single spin system [7]. However, discrete time algorithms are always approximate and require very small time steps for rapid changes of the external fields.

In this Rapid Communication we present an exact rejection-free continuous-time Monte Carlo algorithm and demonstrate that it allows one to determine with high accuracy the work distribution for Ising spin systems driven by a time-varying external magnetic field. The algorithm is a generalization of the first reaction method (FRM) [8] to time-dependent transition rates by Jansen [9] who extended a similar approach developed already in 1978 by Gillespie [10]. The FRM and its high efficiency for time-dependent transition rates has not been exploited for the problem of calculating nonequilibrium work or heat distributions [11].

Let us consider a system, which can change its microstate k to a microstate l at time t with transition rate $w_{lk}(t)$. In the FRM a sequence of microstates $j_\alpha, j_{\alpha+1}, \ldots$ reached at times $t_\alpha, t_{\alpha+1}, \ldots$ is generated. Let the system be in state j_α at time t_α. The FRM then consists of the following steps:

(a) For each possible transition to a state k, draw a random "trial time" $\tau_k^{(\alpha)}$ from

$$\psi_k(\tau|t_\alpha) = -\frac{d}{d\tau}\exp\left(-\int_{t_\alpha}^{\tau} d\tau' w_{k,j_\alpha}(\tau')\right). \tag{2}$$

Note that $\psi_k(\tau|t_\alpha)$ is normalized if $w_{k,j_\alpha}(\tau) > 0$ for all times.

(b) Determine the transition to the state $j_{\alpha+1}$, which corresponds to the minimum of the set $\{\tau_k^{(\alpha)}\}$,

$$t_{\alpha+1} = \min_k \{\tau_k^{(\alpha)}\}. \tag{3}$$

(c) Advance the simulation time to $t_{\alpha+1}$ and perform the transition $j_\alpha \to j_{\alpha+1}$. Go back to step (a).

It is important that for short-range interactions, new random times in step (a) have to be drawn only for a few transitions. This is best illustrated for a single-flip dynamics of an Ising model, see Fig. 1. More generally, we can say: if for a state n accessible from state $j_{\alpha+1}$, a state m accessible from a state j_α exists, such that $w_{n,j_{\alpha+1}}(t) = w_{m,j_\alpha}(t)$ for $t > t_\alpha$, then

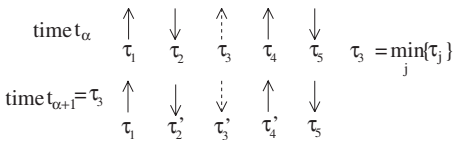

FIG. 1. Transition of an Ising spin configuration reached at time t_α to another configuration at time $t_{\alpha+1}$ for single-flip dynamics by applying the FRM: at time t_α, the "trial times" of spins $1,\ldots,5$ are $\tau_1,\ldots,\tau_5$. If τ_3 is smallest, the time is advanced from t_α to $t_{\alpha+1}=\tau_3$ and the spin 3 flipped. After the transition, new "trial times" τ_2', τ_3', and τ_4' have to be drawn only for those spins whose flip rates are affected by the flip of spin 3. The times τ_1 and τ_5 remain unchanged.

one can set $\tau_n^{(\alpha+1)}=\tau_m^{(\alpha)}$. This setting is justified since $\psi_n(\tau,t_{\alpha+1})\propto\psi_m(\tau,t_\alpha)$ from Eq. (2) [12]. For all other states k, $\tau_k^{(\alpha+1)}$ has to be drawn anew.

For the practical implementation of the FRM, we need to draw random numbers from $\phi(\tau)=\exp[-\int_{t_0}^{\tau}d\tau' w(\tau')]$ in an efficient manner. This is indeed possible for general forms $w(\tau)$: if $r\in[0,1[$ is a uniformly distributed random number, we obtain from the transformation method $1-r=\phi(\tau)$ or

$$f(\tau|t_0)=\int_{t_0}^{\tau}d\tau' w(\tau')=-\ln(1-r). \tag{4}$$

Since $w(\tau)$ is positive definite, $f(\tau|t_0)$ is a monotonously increasing function of τ. Hence $f(\tau|t_0)$ can be inverted with respect to τ, yielding the transformation formula

$$\tau=f^{-1}[-\ln(1-r);t_0]. \tag{5}$$

Dependent on the problem under study, the inversion can be carried out in different ways, e.g., by analytical means or a quick root finder.

As an example we consider the single spin-flip Glauber dynamics of an Ising chain of N spin variables $\sigma_i=\pm1$ with coupling constant J,

$$H(\sigma,t)=-J\sum_{i=1}^{N-1}\sigma_i\sigma_{i+1}-h(t)\sum_{i=1}^{N}\sigma_i, \tag{6}$$

where σ denotes the set of the σ_i and $h(t)$ is a time-dependent external field following a ramp protocol:

$$h(t)=\begin{cases}\dfrac{h_0}{t_h}t, & 0\le t\le t_h\\ h_0, & t>t_h.\end{cases} \tag{7}$$

The ith spin is stochastically flipped with the (detailed balanced) Glauber rates

$$w_i(\sigma(t),t)=\frac{\nu}{1+\exp[\beta\Delta H(t)]}, \tag{8}$$

where $\Delta H(t)$ is the energy difference between the state after and before the flip. We use the thermal energy and inverse attempt frequency as energy and time unit, respectively, i.e., $k_BT=\beta^{-1}=1$ and $\nu=1$.

For Eqs. (7) and (8) the inversion in Eq. (5) can be done analytically with the following result:

(i) If $t_\alpha<t_h$,

$$\tau_i=\begin{cases}-\dfrac{1}{a_i}\ln[C_i(t_\alpha)(1-r)^{a_i}-A_i], & r<r_h\\ t_h-\dfrac{C_i(t_h)}{e^{-a_it_h}}\ln\left[\left(\dfrac{C_i(t_\alpha)}{C_i(t_h)}\right)^{a_i}(1-r)\right], & r_h\le r,\end{cases} \tag{9}$$

where $a_i=\sigma_i(t_\alpha)h_0/t_h$, $\ln A_i=2J\sigma_i(t_\alpha)[\sigma_{i-1}(t_\alpha)+\sigma_{i+1}(t_\alpha)]$ [we formally set $\sigma_0(t)=\sigma_{N+1}(t)=0$], $C_i(t)=A_i+\exp(-a_it)$, and $r_h=1-[C_i(t_h)/C_i(t_\alpha)]^{1/a_i}$.

(ii) If $t_\alpha\ge t_h$,

$$\tau_i=t_h-\frac{C_i(t_h)}{e^{-a_it_h}}\ln(1-r). \tag{10}$$

We start from a thermalized set of spin configurations at time $t_0=0$ and sample the microscopic work $W(t)=\int_0^t dt'\,\partial_{t'}H(\sigma(t'),t')$. For $t\le t_h$ in particular, we have $W(t)=-(h_0/t_h)\{\sum_{\alpha=0}^{(\alpha_\star-1)}M(t_\alpha)(t_{\alpha+1}-t_\alpha)+M(t_{\alpha_\star})(t-t_{\alpha_\star})\}$, where $M(t)=\Sigma_i\sigma_i(t)$ and $t_{\alpha_\star}$ is the largest transition time smaller

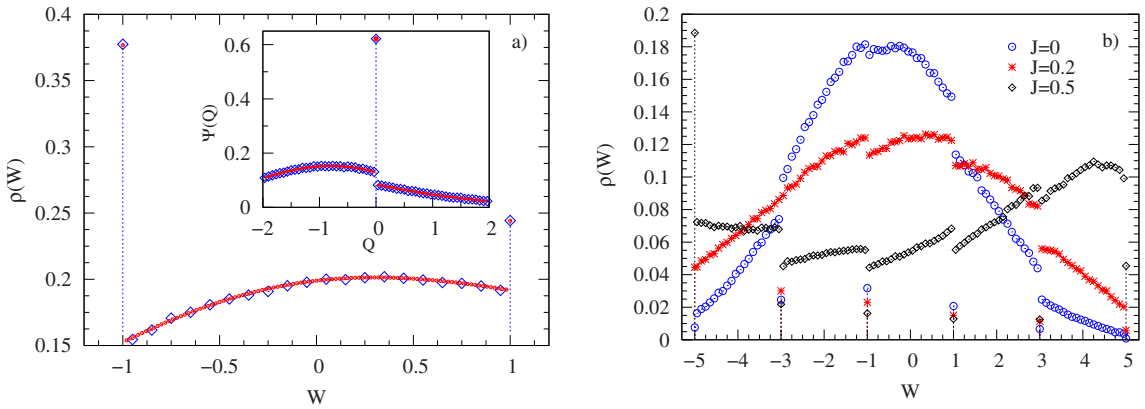

FIG. 2. (Color online) Work distributions $\rho(W)$ for $\omega=1$ sampled over $N_{tr}=10^6$ trajectories: (a) the simulated data are compared with the exact analytical solution (full line) for a single spin system. The inset shows the corresponding heat distribution $\Psi(Q)$; (b) simulated $\rho(W)$ for $N=5$ and three different interaction strengths J (dotted lines mark the δ functions).

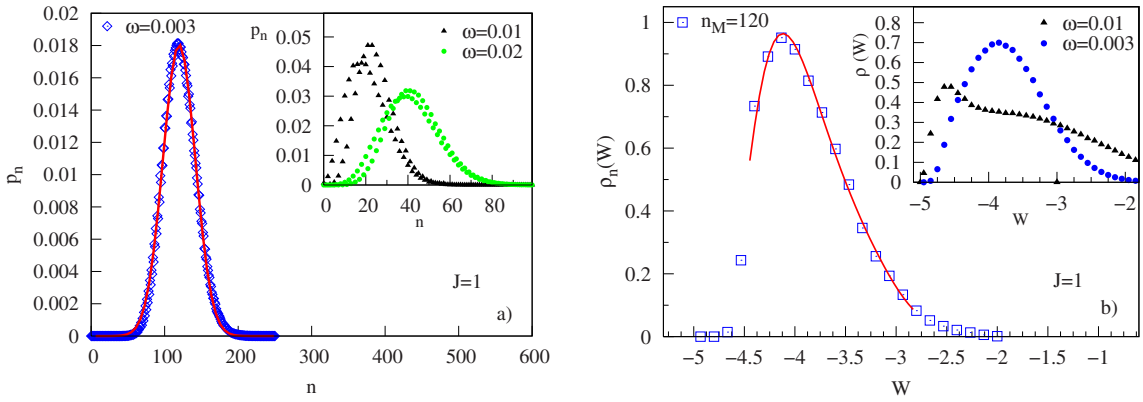

FIG. 3. (Color online) (a) Probability p_n of exactly n spin flips until $t_h=1$ for three different ω and fixed $N=5$; (b) work distribution $\rho_{n_M}(W)$ at the maximum $n_M=120$ of p_n for $\omega=0.003$. The inset shows the corresponding work distribution in comparison with that at $\omega=0.01$.

than t. Simultaneously we determine the values of microscopic heat $Q(t)=\Delta H(t)-W(t)$ transferred to the system, where $\Delta H(t)=H(t)-H(0)$ is the difference between the energies of the final and initial spin configuration. By sampling the values $W(t)$ and $Q(t)$ for a large number of trajectories N_{tr}, we determine the work and heat distributions $\rho(W,t)$ and $\Psi(Q,t)$, respectively.

The resulting work distributions $\rho(W,t)$ contain singularities consisting of delta functions and steps. The delta functions $A_\kappa\delta(W-W_\kappa)$ correspond to time evolutions, where the system remains in the same microstate in the time interval $[0,t]$. Since in our case the work depends only on $M(t)$, in total $N+1$ delta functions occur corresponding to the possible values of M_k for the 2^N spin configurations. The positions of the delta contributions are $W_\kappa=-M_\kappa h_0$ [13]. Their amplitudes satisfy $A_\kappa=\Sigma_j p_j^{\mathrm{eq}}\exp[-\int_0^t dt'\Omega_j(t')]$, where the sum runs over all spin configuration $\sigma^{(j)}$ with the same value $M_\kappa=\Sigma_i\sigma_i^{(j)}$; p_j^{eq} is the Boltzmann equilibrium probability and $\Omega_j(t)=\Sigma_i w_i(\sigma^{(j)},t)$ is the total spin flip rate in the configuration j. Since no heat is exchanged in the absence of transitions, each delta function in $\rho(W,t)$ gives a contribution to a delta function at $Q=0$ in the heat distribution, i.e., the singular part of $\Psi(Q,t)$ is given by $\Sigma_k A_k\delta(Q)$.

More generally, the work distribution $\rho(W,t)$ can be decomposed as $\rho(W,t)=\Sigma_{n=0}^{\infty}p_n(t)\rho_n(W,t)$, where $p_n(t)$ is the probability that exactly n spin flips take place during time t [14] and $\rho_n(W,t)$ is the work distribution under the condition of exactly n spin flip. The $n=0$ contribution (no transitions) yields the δ functions discussed above. The $n=1$ contribution yields steps at the positions W_κ of the δ function (with the exception of two δ functions at minimum and maximum work). These steps can be explained as follows: to obtain a value $W(t)$ being infinitesimally different from W_κ, the spin flip has to occur shortly before time t in an initial spin configuration given rise to W_κ. The probability that this flip is in the down-up direction, leading to a $W(t)$ slightly larger than W_κ, is, however, different from the reversed up-down direction, which leads to a $W(t)$ slightly smaller than W_κ. Taking into account the possible ΔH, the corresponding steps can be seen in $\Psi(Q,t)$. For $n\geq 2$, the $\rho_n(W,t)$ yield smooth contributions to $\rho(W,t)$ without singularities.

We next discuss numerical results from our simulation method. To this end we will analyze the work distribution $\rho(W)\equiv\rho(W,t=t_h)$ at $t_h=1$ for different sweeping rates $\omega=h_0/t_h$ and interaction strength J [cf. Eq. (7)]. First we test the method by comparing $\rho(W)$ for a single spin dynamics with the analytical solution given in [4]. The excellent agreement of the simulated data with the analytical solution demonstrates the validity of the numerical procedure. As discussed above, two delta functions occur at $W=\pm 1$ with weights $A_1=0.38$ and $A_2=0.24$. In the inset we show the corresponding distribution of the heat. Based on the numerical procedure we are able to study also systems with many interacting spins. Figure 2(b) shows $\rho(W)$ for $N=5$ spins and $J=0$, 0.2, and 0.5. Again we can clearly identify the delta functions discussed above. With increasing J, the singular part becomes more pronounced.

In order to understand the influence of the sweeping rate at fixed interaction strength $J=1$, we analyze the results with respect to the contributions $\rho_n(W)\equiv\rho_n(W,t=t_h=1)$ described above. Figure 3(a) shows the corresponding weights p_n for three different sweeping rates. These weights approach a Gaussian shape with decreasing ω. For large $\omega\gtrsim 10^{-1}$, p_n decays nearly exponential with n (not shown). For intermediate sweeping rates $10^{-2}\lesssim\omega\lesssim 10^{-1}$, p_n decomposes into

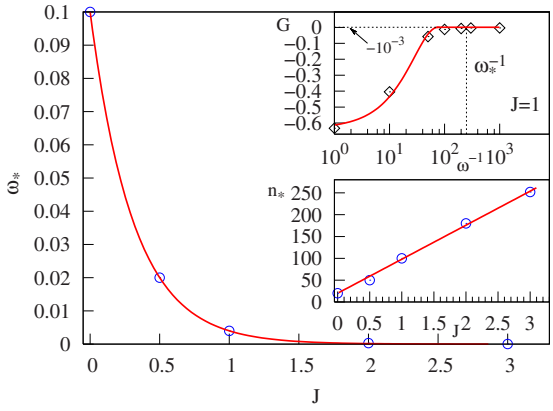

FIG. 4. (Color online) Onset frequency to the GFR as a function of J. The upper inset shows a representative curve of the non-Gaussian parameter G and the lower inset the mean number of spin flips to reach the GFR as a function of J.

two disjoint "smooth" parts for even and odd n, which both can be approximated by a Gaussian. As a result, the p_n has a shape alternating between these two Gaussians, as can seen from the inset of Fig. 3(a). For sufficiently small sweeping rates $\omega < 10^{-2}$ the two Gaussians approach each other so that the p_n can be effectively described by one Gaussian with a maximum at n_M. Looking at the dependence of $\rho_{n_M}(W)$ on W at this maximum n_M in Fig. 3(b), we find a single peaked function that close to its peak can again be approximated by a Gaussian. As a consequence, the total work distribution $\rho(W)$, being dominated by $p_{n_M}\rho_{n_M}(W)$, has a nearly Gaussian shape [see the circles in the inset of Fig. 3(b)]. By contrast, at large sweeping rates, $\rho(W)$ is very different from a Gaussian [see the triangles in the inset of Fig. 3(b)].

Finally we discuss, how, upon decreasing ω, the Gaussian fluctuation regime (GFR) is reached. To quantify the deviation from a Gaussian, we introduce the non-Gaussian parameter $G=\langle \delta W^4\rangle/[3\langle \delta W^2\rangle^2]-1$, $\delta W=W-\langle W\rangle$, and plot it as a function of ω^{-1} in the upper inset of Fig. 4. For small ω^{-1}, G is negative, and with increasing ω^{-1} eventually goes to zero. Let us define the onset frequency for entering the GFR by $G(\omega_\star)=10^{-3}$. As shown in Fig. 4, $\omega_\star$ decreases exponentially with J. This behavior can be understood from the corresponding mean total number of spin flips $n_\star$ necessary to enter the GFR, which increases linearly with J (see the lower inset of Fig. 4). This linear increase reflects longer range correlations with increasing J, which imply a larger number of total spin flips to rearrange spin configurations into states closer to thermal equilibrium. With a typical spin flip time $\tau \propto \exp(\gamma J)$ we obtain $\omega_\star^{-1} \propto n_\star \tau \propto J \exp(\gamma J)$, with $\gamma \approx 3.2$.

In summary, we presented an efficient method to study the work and heat distributions in nonequilibrium systems whose dynamics is governed by a master equation. Results were discussed for Glauber dynamics of an Ising chain during the switching of a magnetic field. These allowed us to gain insight into the structure of the distributions and its dependence on the rate of the external driving, on the number of degrees of freedom (spins), and on the interaction strength. In particular the transition from the behavior far from equilibrium to the GFR could be investigated in detail. We hope that our results will stimulate further research on these challenging problems.

We thank P. Chvosta for very valuable discussions.

[1] U. Seifert, Eur. Phys. J. B **64**, 423 (2008).
[2] F. Ritort, Adv. Chem. Phys. **137**, 31 (2008).
[3] C. Jarzynski, Phys. Rev. Lett. **78**, 2690 (1997); Phys. Rev. E **73**, 046105 (2006).
[4] E. Subrt and P. Chvosta, J. Stat. Mech.: Theory Exp. 2007, P09019 (2007).
[5] P. Talkner, P. S. Burada, and P. Hänggi, Phys. Rev. E **78**, 011115 (2008).
[6] A. Imparato and L. Peliti, Europhys. Lett. **69**, 643 (2005); Phys. Rev. E **72**, 046114 (2005).
[7] R. Marathe and A. Dhar, Phys. Rev. E **72**, 066112 (2005).
[8] D. T. Gillespie, J. Comput. Phys. **22**, 403 (1976).
[9] A. P. J. Jansen, Comput. Phys. Commun. **86**, 1 (1995).
[10] D. T. Gillespie, J. Comput. Phys. **28**, 395 (1978).
[11] Indeed, we developed the algorithm independently and thereafter became aware that the generalization to time-dependent rates was published already in the context of rate equations for chemical reactions [9]. That this algorithm was almost forgotten becomes clear also from the fact that Dall and Sibani published the FRM for time-independent rates as a new method in 2001 in the same journal, see Comput. Phys. Commun. **141**, 260 (2001). This algorithm was developed already one year after the widely used continuous-time Monte Carlo algorithm of A. B. Bortz *et al.*, J. Comput. Phys. **17**, 10 (1975).
[12] From Eq. (2) follows exactly $\psi_n(\tau|t_{\alpha+1})/\psi_m(\tau|t_\alpha) = \exp[\int_{t_\alpha}^{t_{\alpha+1}} d\tau' w_{m,j_\alpha}(\tau')]$, where the exponential factor guarantees the normalization.
[13] This information is important for a correct sampling of $\rho(W,t_h)$ in the simulation.
[14] These weights can be of interest in themselves as, e.g., discussed in connection with misfolding of DNA hairpins, see M. Manosas *et al.*, J. Stat. Mech.: Theory Exp. 2009, P02061 (2009).