

2 Work distribution functions for Hysteresis loops in a single spin system.

2.1 Introduction

Consider a magnetic system in a time-dependent magnetic field. Assume that the magnetic field is varied periodically. Then plotting the magnetization of the system against the instantaneous magnetic field we get the well-known hysteresis curve. The area enclosed by the hysteresis loop gives the work done on the system by the external field and this leads to heating of the magnet. In the usual picture, that one has of hysteresis, one expects that the work done is positive. However if the magnetic system is small (*i.e* contains small number of magnetic moments) then this is no longer true. For a small magnet, one finds that the work is a fluctuating quantity, and in a particular realization of the hysteresis experiment one could actually find that the magnet cools and does work on the driving force.

In general, for a small system driven by time-dependent forces whose rates are not slow compared to relaxation times, one typically finds that various non-equilibrium quantities, such as the work done or the heat exchanged, take values from a distribution. Recently there has been a lot of interest in the properties of such distributions. Part of the reason for the interest is that it leads us to examine the question as to how the usual laws of thermodynamics, which are true for macroscopic systems, need to be modified when we deal with mesoscopic systems [1].

For instance in our example of the magnet with a small number of spins, there is a finite probability that all the spins could suddenly spontaneously flip against the direction of the

field by drawing energy from the heat bath. Intuitively this gives one the feeling that there has been a violation of the second law. In fact historically early observers of Brownian motion had the same feeling when they saw the “perpetual” motion of the Brownian particles [2]. However if one looks at the precise statement of the second law one realizes that there is no real violation. The second law is a statement on the most probable behavior while here we are looking at fluctuations about the most probable values. These become extremely small for thermodynamic systems. On the other hand, for small systems these fluctuations are significant and a study of the properties of these fluctuations could provide us with a better understanding of the meaning of the second law in the present context. This will be necessary for an understanding of the behavior of mesoscopic systems such as molecular motors, nanomagnets, quantum dots etc. which are currently areas of active experimental interest.

Much of the recent interest on these non-equilibrium fluctuations has focused on two interesting results on the distribution of the fluctuations. These are (1) the Jarzynski relation [3–6] and (2) the fluctuation theorems [7 – 17]. A large number of studies, both theoretical and experimental [19 – 24] have looked at the validity of these theorems in a variety of systems and also their implications. At a fundamental level both these theorems give some measure of “second law violations”. At a practical level the possibility of using these theorems to determine the equilibrium free energy profile of systems using data from non-equilibrium experiments and simulations has been explored [25 – 29].

In this chapter we will be interested in the fluctuations of the area under a hysteresis loop for a small magnet. We look at the simplest example, namely a single Ising spin in a time-dependent magnetic field and evolving through Glauber dynamics. Hysteresis in kinetic Ising systems have been studied earlier [30 – 33] where the main aim was to understand various features such as dependence of the average loop area on sweeping rates and amplitudes, system size effects and dynamical phase transitions . The area distribution was also studied in [33] but the emphasis was on different aspects and so is quite incomplete from our present viewpoint.

A two state model with Markovian dynamics was earlier studied by Ritort *et al.* [34] to analyze experiments on stretching of single molecules. Systems with more than two states have also been studied [35] in the context of single-molecule experiments. However, the detailed forms of the work-distributions have not been investigated and that is the main aim of this study. These distributions are of interest since there are only a few examples where the explicit forms of the distributions have actually been worked out [37 – 40]. Most of the experiments so far, for example those in the RNA stretching experiments of Liphardt *et al.* [19] or the more recent experiment of Douarche *et al.* [25] on torsionally driven mirrors, are in regimes where the work-distributions are Gaussian.

We perform Monte-Carlo simulations to obtain the distributions for different driving rates. We consider different driving protocols and look at the two cases corresponding to the transient and the steady state fluctuation theorems. It is shown that the limiting cases of slow and fast driving rates can be solved analytically. We also point out that the problem of computing work-distributions is similar to that of computing residence-time distributions.

2.2 Definition of model and dynamics

Consider a single spin, with magnetic moment μ , in a time-dependent magnetic field $h(t)$. The Hamiltonian is given by

$$H = -\mu h \sigma \quad \sigma = \pm 1 \quad (2.1)$$

We assume that the time-evolution of the spin is given by the Glauber dynamics. Let us first consider a discretized version of the dynamics. Let the value of the magnetic field at the end of the $(n - 1)$ th time step be h_{n-1} and let the value of the spin be σ_{n-1} . The discrete dynamics consists of two distinct process during the n th time step:

1. The field is changed from h_{n-1} to $h_n = h_{n-1} + \Delta h_n$. During this step an amount of work $\Delta W = -\mu \sigma_{n-1} \Delta h_n$ is done on the system.

2. The spin flips with probability $p(e^{-\beta \mu h_n \sigma_{n-1}} / Z)$ where $Z = e^{\beta \mu h_n} + e^{-\beta \mu h_n}$ is the equilibrium partition function at the instantaneous field value. The factor p is a parameter that is required

when we take the continuum time limit and whose value will set equilibration times. At the end of this step the spin is in the state σ_n . During this step the system takes in an amount of heat $\Delta Q = -\mu h_n(\sigma_n - \sigma_{n-1})$ from the reservoir.

Given the microscopic dynamics we can derive time-evolution equations for various probability distributions. These are standard results but we reproduce them here for completeness.

Time-evolution equation for spin distribution: First let us consider the spin configuration probability $P_n(\sigma)$ which gives the probability that at time n the spin is in the state σ . We write the field in the form $h_n = h_0 f_n$ where f_n is dimensionless and let us define $\epsilon = \beta \mu h_0$. Then we get the following evolution equation:

$$\begin{pmatrix} P_{n+1}(\uparrow) \\ P_{n+1}(\downarrow) \end{pmatrix} = \begin{pmatrix} 1 - p \frac{e^{-\epsilon f_n}}{Z} & p \frac{e^{\epsilon f_n}}{Z} \\ p \frac{e^{-\epsilon f_n}}{Z} & 1 - p \frac{e^{\epsilon f_n}}{Z} \end{pmatrix} \begin{pmatrix} P_n(\uparrow) \\ P_n(\downarrow) \end{pmatrix}$$

To go to the continuum-time limit we take the limits $p \rightarrow 0$, $\Delta t \rightarrow 0$, with $p/\Delta t \rightarrow r$ and $f_n \rightarrow f(t)$, $P_n(\sigma) \rightarrow P(\sigma, t)$. Using the dimensionless time $\tau = rt$ we then get:

$$\begin{aligned} \frac{\partial \hat{P}}{\partial \tau} &= -\mathcal{T} \hat{P} \quad \text{where} \\ \hat{P} &= \begin{pmatrix} P(\uparrow, \tau) \\ P(\downarrow, \tau) \end{pmatrix}, \quad \mathcal{T} = \begin{pmatrix} \frac{e^{-\epsilon f(\tau)}}{Z} & -\frac{e^{\epsilon f(\tau)}}{Z} \\ -\frac{e^{-\epsilon f(\tau)}}{Z} & \frac{e^{\epsilon f(\tau)}}{Z} \end{pmatrix}. \end{aligned} \tag{2.2}$$

The magnetization $m(\tau) = \langle \sigma(\tau) \rangle = 2P(\uparrow, \tau) - 1$ thus satisfies the equation

$$\frac{dm(\tau)}{d\tau} = -m(\tau) + \tanh[\epsilon f(\tau)] \tag{2.3}$$

whose solution is

$$m(\tau) = e^{-\tau} m(0) + \int_0^\tau d\tau' e^{-(\tau-\tau')} \tanh[\epsilon f(\tau')]. \tag{2.4}$$

Time-evolution equation for Work distribution: The total work done at the end of the n th time step is given by:

$$W = -\mu \sum_{l=1}^n \sigma_{l-1} \Delta h_l \tag{2.5}$$

To write evolution equations for the work-distribution it is necessary to first define $Q_n(W, \sigma)$,

the joint probability that at the end of the n th step the spin is in the state σ and the total work done on it is W . Then $Q_n(W, \sigma)$ will satisfy the following recursions:

$$\begin{aligned} Q_{n+1}(W, \uparrow) &= (1 - p \frac{e^{-\epsilon f_{n+1}}}{Z_{n+1}}) Q_n(W + \mu \Delta h_n, \uparrow) + p \frac{e^{\epsilon f_{n+1}}}{Z_{n+1}} Q_n(W - \mu \Delta h_n, \downarrow) \\ Q_{n+1}(W, \downarrow) &= p \frac{e^{-\epsilon f_{n+1}}}{Z_{n+1}} Q_n(W + \mu \Delta h_n, \uparrow) + (1 - p \frac{e^{\epsilon f_{n+1}}}{Z_{n+1}}) Q_n(W - \mu \Delta h_n, \downarrow). \end{aligned}$$

We take the limits $\Delta t \rightarrow 0$, $p \rightarrow 0$ with $p/(\Delta t) \rightarrow r$, $h_n \rightarrow h(t)$ and $\Delta h_n/(\Delta t) \rightarrow \dot{h}$. Then using the dimensionless variable τ defined earlier, and the total work done upto time τ , $w = \beta W = -\epsilon \int_0^\tau d\tau' \sigma(\tau') df/d\tau'$ we finally get

$$\begin{aligned} \frac{\partial \hat{Q}}{\partial \tau} &= -\mathcal{T} \cdot \hat{Q} + \epsilon \frac{df}{d\tau} \sigma_z \cdot \frac{\partial \hat{Q}}{\partial w} \quad \text{where} \\ \hat{Q} &= \begin{pmatrix} Q(w, \uparrow, \tau) \\ Q(w, \downarrow, \tau) \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned} \quad (2.6)$$

From Eq. (2.6) we get the following equation for $Q(w, \tau) = Q(w, \uparrow, \tau) + Q(w, \downarrow, \tau)$:

$$\frac{\partial^2 Q}{\partial \tau^2} + (1 - \frac{\ddot{f}}{\dot{f}}) \frac{\partial Q}{\partial \tau} = \epsilon \dot{f} \tanh(\epsilon f) \frac{\partial Q}{\partial w} + (\epsilon \dot{f})^2 \frac{\partial^2 Q}{\partial w^2} \quad (2.7)$$

We have not been able to solve these equations analytically except in the limiting cases where the rate of change of the magnetic field is very slow or very fast. In a recent study done by Chvosta *et al.* [38, 39], this kind of evolution equation for a two level system is solved analytically, and their results match with our simulation results.

In the next two sections we will first present results from Monte-Carlo simulations which give accurate results for any rates and then discuss the special cases.

2.3 Results from Monte-Carlo simulations

We have studied three different driving processes:

(A) The system is initially in equilibrium at zero field and the field ($\beta\mu h$) is then increased linearly as a function of time from 0 to ϵ . The total time duration of the process is t_m (or τ_m in dimensionless units). By changing τ_m while keeping ϵ fixed we can control the rate at which the magnetic field sweep takes place.

(B) The system is initially in equilibrium and the field, which is taken to be piecewise linear, is changed over one cycle. The total time duration of the cycle is $4\tau_m$ for a symmetric cycle and is $2(\tau_m + \tau_n)$ for an asymmetric cycle.

(C) The system is run through many cycles till it reaches a non-equilibrium steady state. We measure work fluctuations in this steady state.

In cases (A) and (B) we will be interested in testing the transient fluctuation theorem (TFT) while in case (C) we will look at the steady state fluctuation theorem (SSFT). Let us briefly recall the statements of these theorems for work distributions in systems with Markovian dynamics.

Crooks' Fluctuation Theorem: Let us quickly recall the various definitions of the fluctuation theorems with our present notation. Consider our spin system, initially in thermal equilibrium and then external magnetic field $h(t)$, is changed from an initial value h_i , at time $t = 0$, to a final value h_f in a finite time t_m . Suppose the work done on the system during this process is W and the change in equilibrium free energy is ΔF . Let the dissipated work $W_d = W - \Delta F$, have a distribution $Q(W_d)$. Now consider a time-reversed path for the external field $h_R(t) = h(t_m - t)$ for which the work distribution is $Q_R(W_d)$. The fluctuation theorem of Crooks' then states:

$$\frac{Q(W_d)}{Q_R(-W_d)} = e^{\beta W_d}. \quad (2.8)$$

For Gaussian processes it can be shown that $Q_R(W_d) = Q(W_d)$ [15] and hence we get the usual form of the transient fluctuation theorem (TFT)

$$\frac{Q(W_d)}{Q(-W_d)} = e^{\beta W_d}. \quad (2.9)$$

Another situation where TFT is satisfied is the case where the field is kept constant or if the process is time-reversal symmetric. Finally we note that the Jarzynski relation

$$\langle e^{-\beta W_d} \rangle = \int dW_d e^{-\beta W_d} Q(W_d) = 1 \quad (2.10)$$

follows immediately from Crooks' theorem Eq. (2.8) and so will be satisfied in all cases

where Crooks' holds.

In the following sections we will verify that Crooks' FT is always satisfied but that TFT does not hold whenever the distributions are non-Gaussian processes and the process does not have time-reversal symmetry. We will also test the validity a particular version of the steady state fluctuation theorem (SSFT), which differs from the Cohen-Gallavotti theorem in that we consider a finite time τ . Thus, this version of SSFT has the same form as Eq. (2.9) with the difference that the initial state is chosen from a non-equilibrium steady state distribution instead of an equilibrium distribution.

In the simulations we used the discrete time dynamics specified in the beginning of Sec. (2.2). To get results corresponding to the continuum time limit we took the parameter values $\Delta t = t_m/10000$ and $p = \Delta t$. The distribution functions for a given rate were obtained by generating 2×10^6 realizations.

2.3.1 Field increased linearly from 0 to ϵ

In this case $f(\tau) = \tau/\tau_m$ and we have chosen $\epsilon = 0.5$. We note that with a static field, the equilibrium relaxation time is given by $t_r = 1/r$ or $\tau_r = 1$. The rate of change of magnetic field $\sim 1/t_m$ and comparing this with the relaxation time we find that slow and fast rates correspond, respectively, to large and small values for $t_m/t_r = \tau_m$. In Fig. (2.1) we plot the work distributions for various values of τ_m . We have plotted the distribution of the dissipated work $w_d = w - \beta\Delta F$ (Here $\beta\Delta F = -\ln \cosh \epsilon$). In Fig. (2.2) we plot the average magnetization as a function of field, again for different rates. Some interesting features of the work-distributions are:

(i) The distributions are in general broad. This is true even at the slowest driving rates where the average magnetization (Fig. (2.2)) itself is close to the equilibrium prediction. Note that the allowed range of values of w_d is $[-\epsilon - \beta\Delta F, \epsilon - \beta\Delta F] \approx [-0.38, 0.62]$. Also we see that the probability of negative dissipated work is significant.

(ii) For slow rates the distributions are Gaussian and this can be understood in the following way. Imagine dividing the time range into small intervals. Because the rate is slow, there

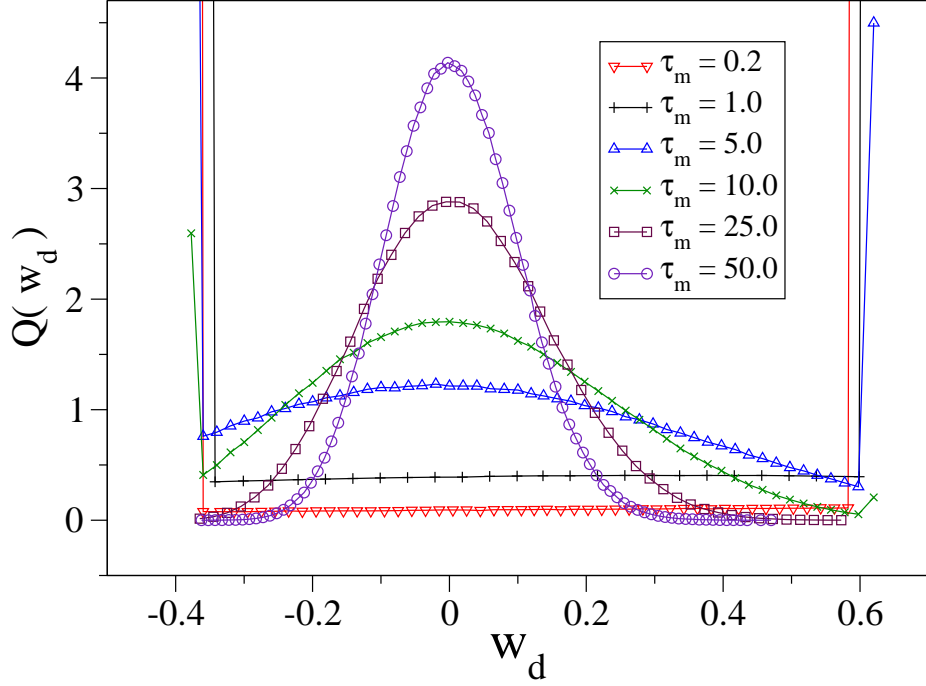


Figure 2.1: Distributions of the work done in driving a magnet at different rates when magnetic field is changed linearly.

are a large number of spin flips within each such interval, and so the average magnetization from one interval to the next can be expected to be uncorrelated. Since the work is a weighted sum of the magnetization over all the time intervals we can expect it to be a Gaussian.

(iii) For fast rates we get δ -function peaks at $w = \pm\epsilon$. This again is easy to understand since the spin doesn't have time to react and stays in its initial state. In Sec. (2.4) we will work out analytic expressions for the the work distributions by considering probabilities of 0-spin flip and 1-spin flip processes.

For slow rates we have verified (see Fig. (2.3)) that the fluctuation theorem is satisfied. For faster rates we see that the probability of negative work processes is higher than what is predicted by the TFT.

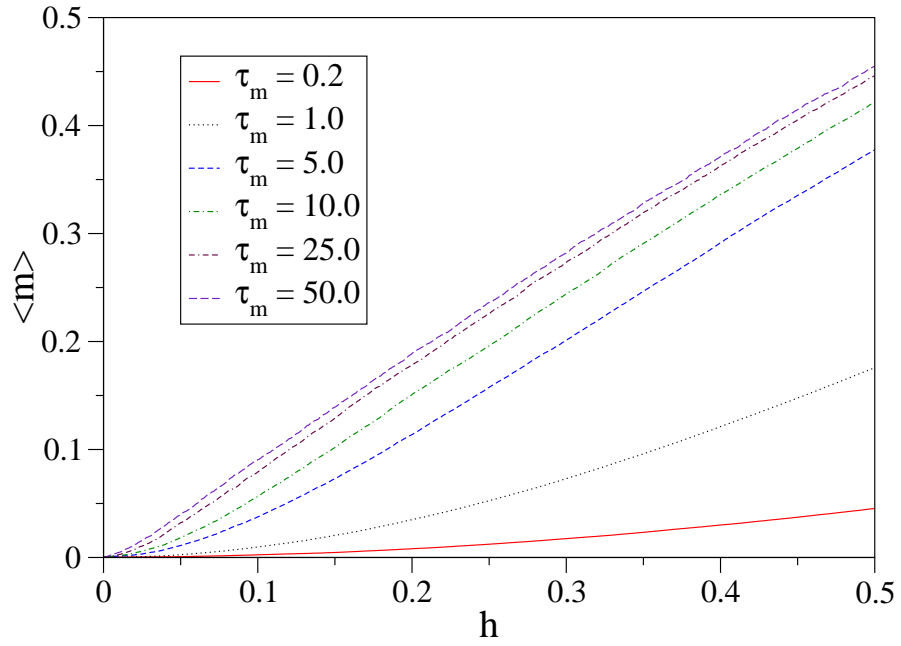


Figure 2.2: Average magnetization $m(\tau)$ for different rates, when magnetic field is changed linearly.

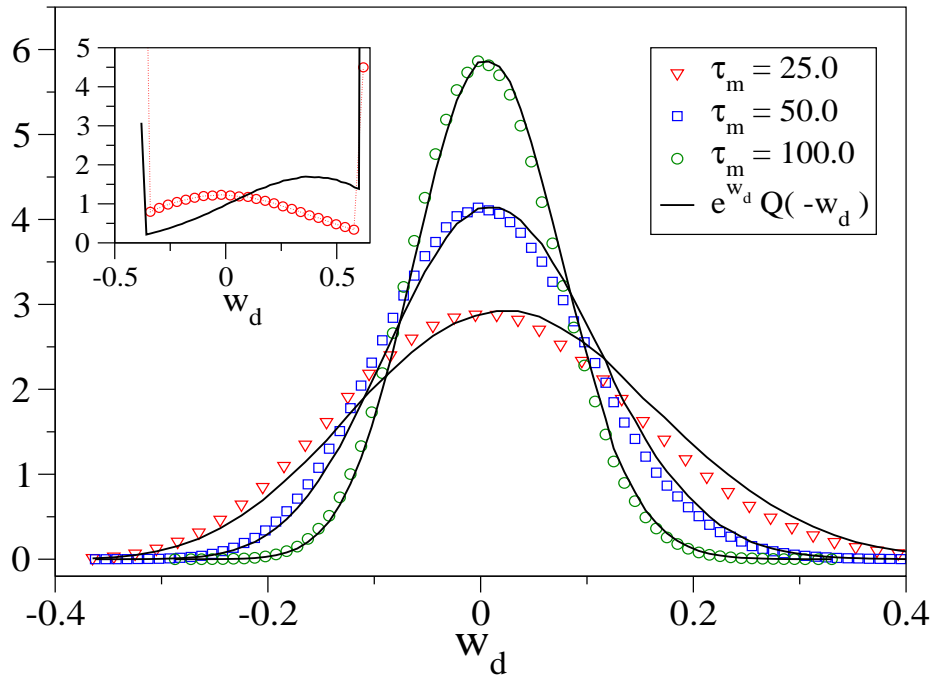


Figure 2.3: Plot shows that the fluctuation theorem is valid for slow processes with Gaussian work-distributions. Inset shows that for a fast rate ($\tau_m = 5.0$) the probability of negative work is much larger than that predicted by the FT.

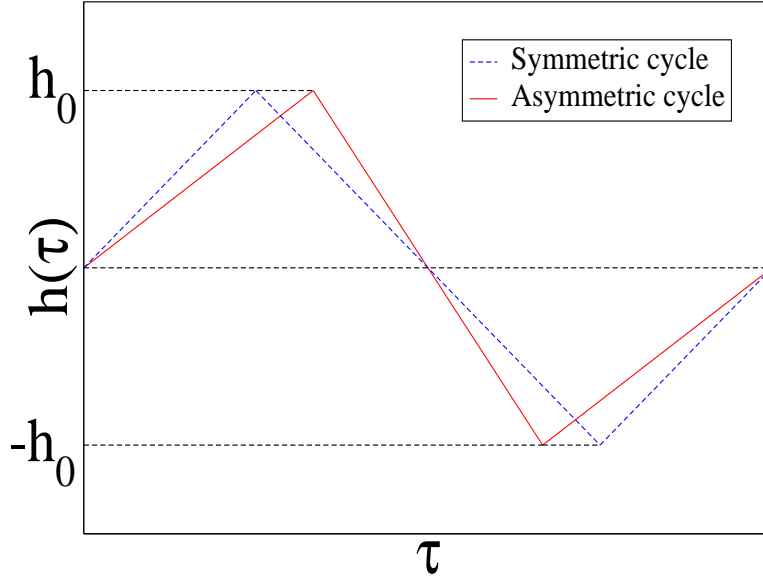


Figure 2.4: Magnetic field changed over a cycle. In the symmetric case the total cycle time is $4\tau_m$ while in the asymmetric case it is $2(\tau_m + \tau_n)$.

2.3.2 Field is taken around a cycle

As shown in Fig. (2.4) we consider two different cyclic forms for $f(\tau)$. One is a symmetric cycle and the other a asymmetric one. For these two cases the work-distributions are plotted in Fig. (2.5) and Fig. (2.6) respectively. For the symmetric cycle we plot the average magnetization as a function of the field in Fig. (2.7). This gives the familiar hysteresis curves.

As before we again find that the work-distributions are broad. For slow rates we get Gaussian distributions while for fast rates we get a δ -function peak at the origin which correspond to a 0-spin flip process. The slow and fast cases are treated analytically in Sec. (2.4).

As expected we can verify the transient fluctuation theorem for both the symmetric and asymmetric processes. That TFT should be satisfied follows from Crooks FT and noting that the time reversed process has the same distribution as the forward process because of the additional $h \rightarrow -h$ symmetry that we have in this case. We have also studied an asymmetric *half-cycle* for which $Q_R(w_d) \neq Q(w_d)$. Consequently we find that the usual TFT is not satisfied while the more general form of TFT of Crooks holds. We show this in Fig. (2.8) where we have plotted $Q(w_d)$, $e^{w_d}Q(-w_d)$ and $e^{w_d}Q_R(-w_d)$.

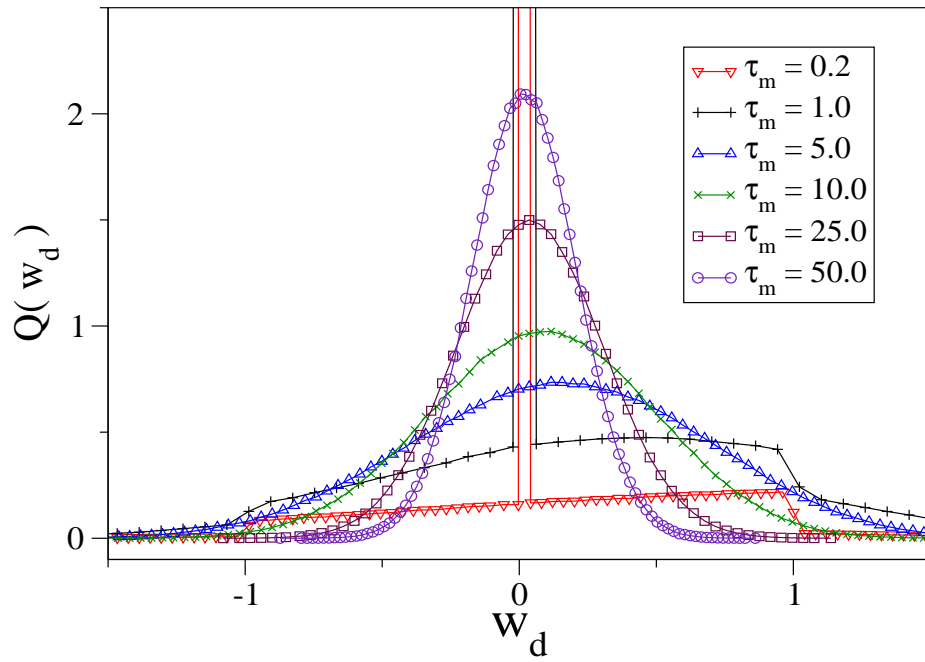


Figure 2.5: Plot of work-distributions for different driving rates when magnetic field is changed in a symmetric cycle.

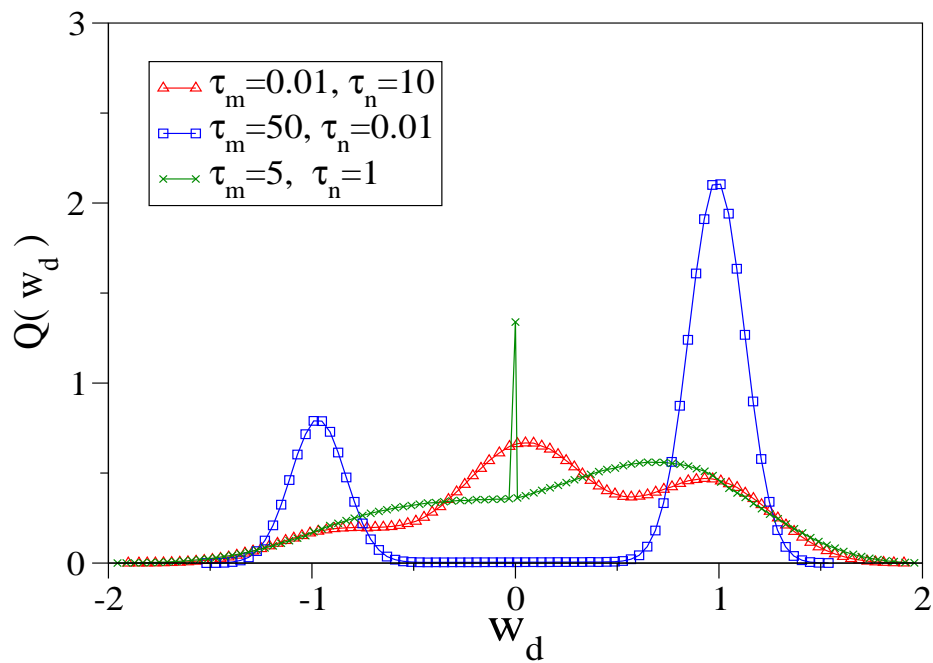


Figure 2.6: Plot of work-distributions obtained for different asymmetric cycles of the magnetic field.

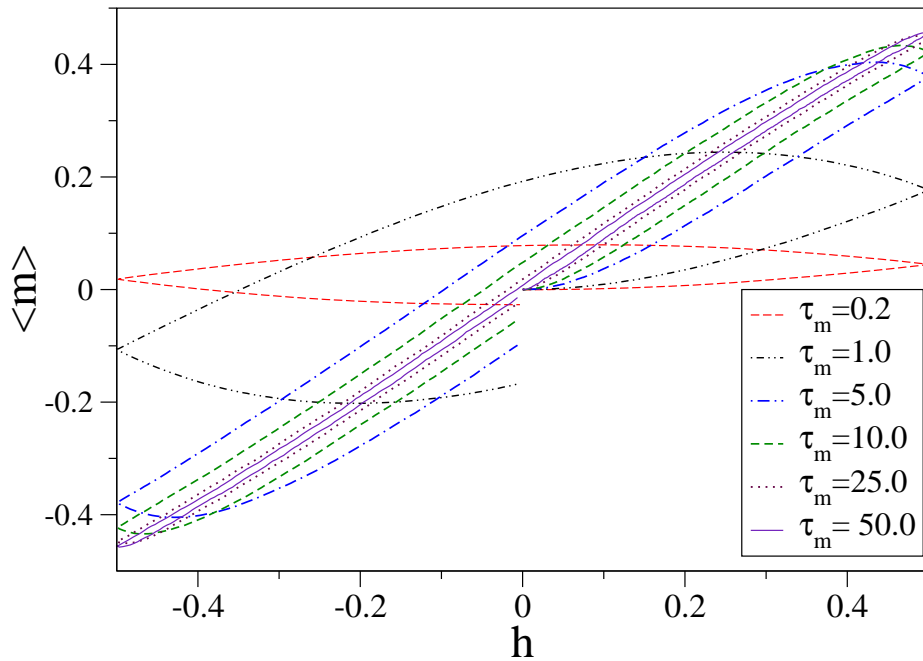


Figure 2.7: Hysteresis curves in driving a magnet at different rates when magnetic field is changed in a symmetric cycle and with the spin initially in equilibrium.

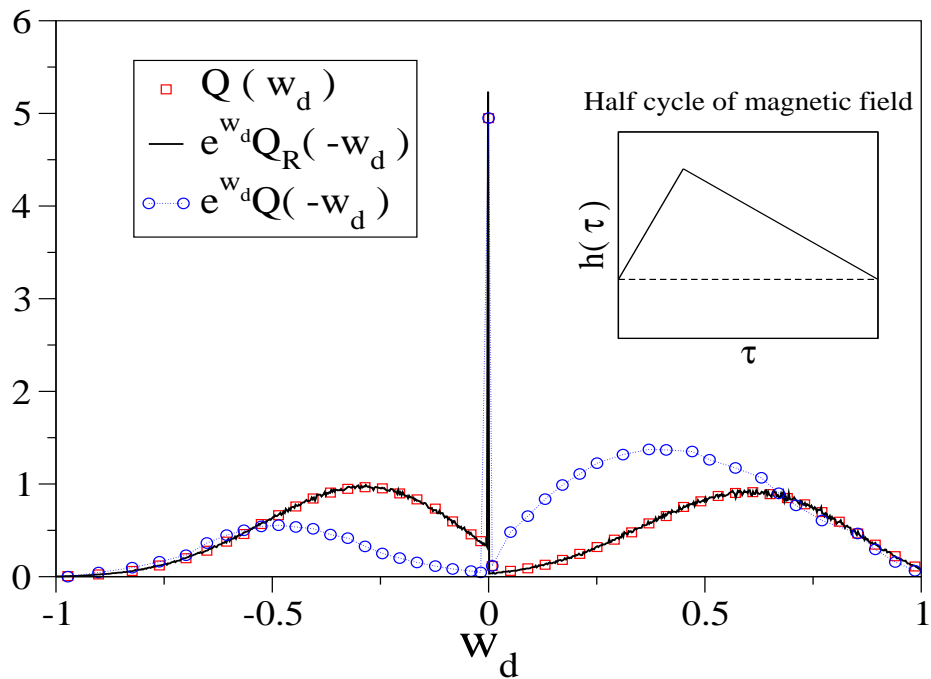


Figure 2.8: Plot showing the work-distribution for an asymmetric half-cycle and the validity of Crook's fluctuation theorem. Note that the probability of negative work processes is much higher than that predicted by usual TFT.

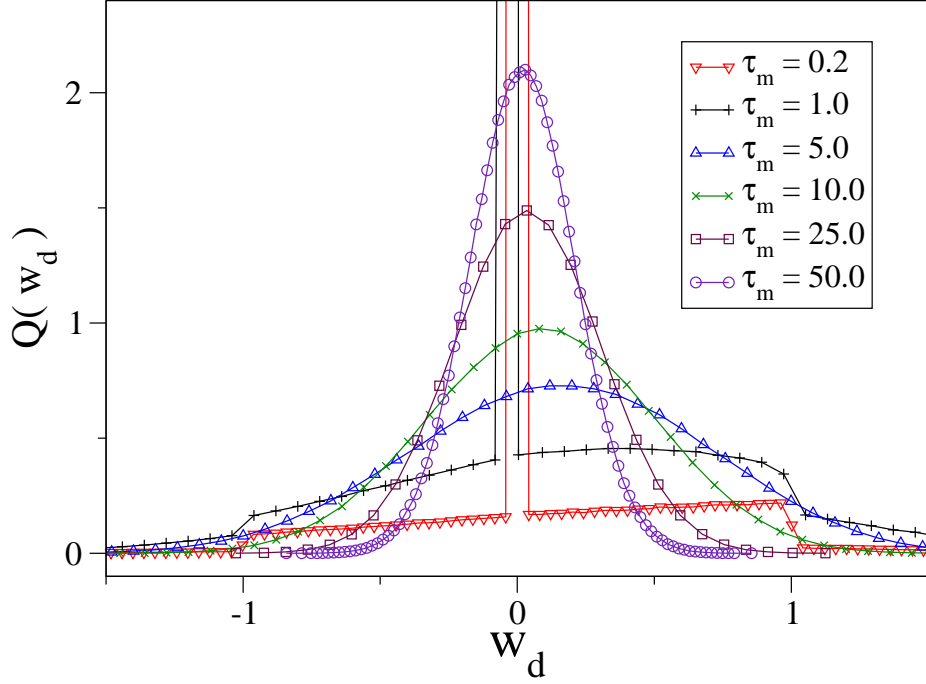


Figure 2.9: Work-distributions in the non-equilibrium steady state.

2.3.3 Properties in the non-equilibrium steady state

We now look at the case when the spin is driven by the oscillating field into a non-equilibrium steady state and we measure fluctuations in this steady state. In this case the work distributions (over a cycle) have the same forms as in the transient case (Fig. (2.9)). The joint distribution function $Q(w, \sigma, \tau)$ satisfies the same equation Eq. (2.6) but now the initial conditions are different. In Fig. (2.10) we plot the steady state hysteresis curves. Note that unlike the transient case the hysteresis curves are now closed loops.

Finally we test the validity of the steady state fluctuation theorem (SSFT). This theorem has been proved for dynamical systems evolving through deterministic equations but there exists no proof that a similar result holds for stochastic dynamics. From Fig. (2.11) it is clear that SSFT does not hold.

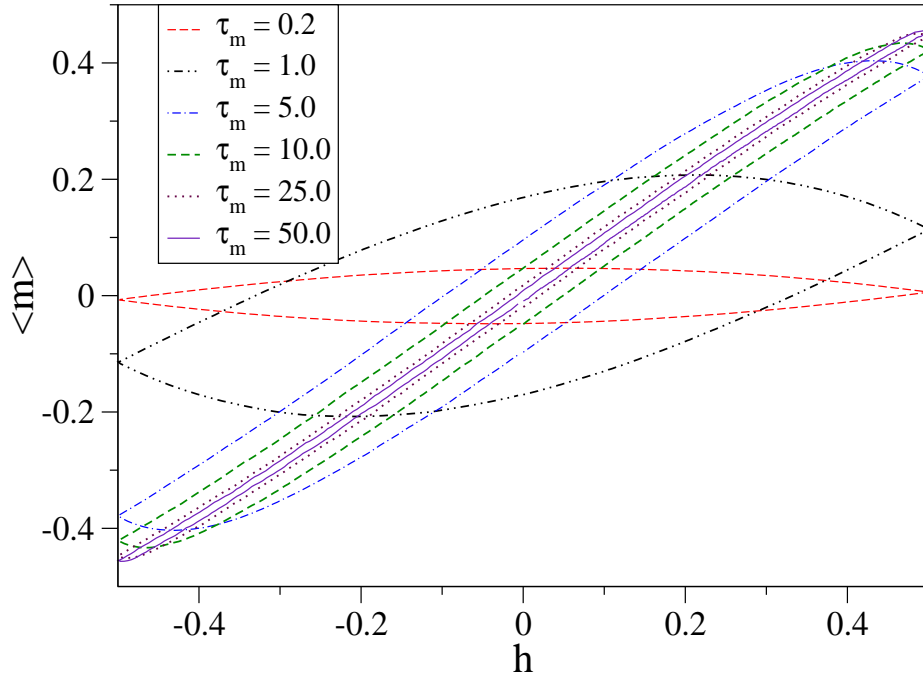


Figure 2.10: Hysteresis curves in the non-equilibrium steady state.

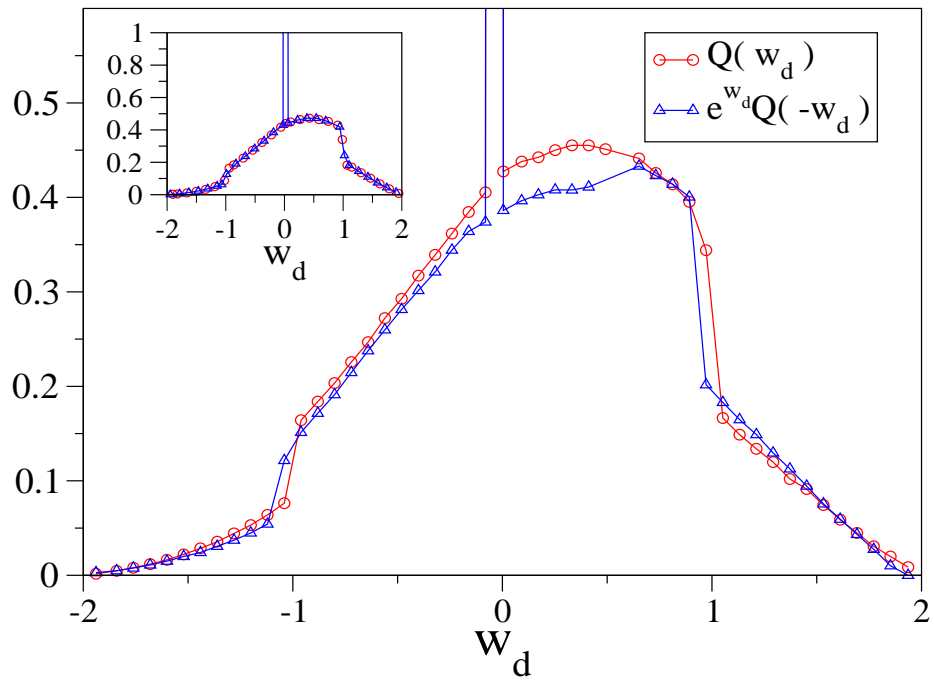


Figure 2.11: Violation of the fluctuation theorem for the steady state work-distribution corresponding to $\tau_m = 1.0$. Inset shows the same plots for the transient case where FT is clearly satisfied.

2.4 Analytic results for slow and fast rates

2.4.1 Field increased linearly from 0 to ϵ

(i) Slow case: $\tau_m \gg 1$

As argued in the previous section we expect that the work-distributions to be Gaussians which will be of the general form

$$Q(w) = \frac{1}{\sqrt{2\pi\sigma_w^2}} e^{-\frac{(w-\langle w \rangle)^2}{2\sigma_w^2}}. \quad (2.11)$$

where $\langle w \rangle$ and σ_w^2 are the mean and the variance of the distribution $Q(w)$. Since the distribution satisfies the Jarzynski equality, it follows at once that they are related by

$$\sigma_w^2 = 2(\langle w \rangle - \beta\Delta F). \quad (2.12)$$

Hence we just need to find the mean work done. The mean work done is given by $\langle w \rangle = -(\epsilon/\tau_m) \int_0^{\tau_m} d\tau m(\tau)$. In the strict adiabatic limit $\tau_m \rightarrow \infty$ we have $m_{ad}(\tau) = \tanh(\epsilon\tau/\tau_m)$ and the mean work done $\langle w \rangle = -\log(\cosh(\epsilon)) = \beta\Delta F$. For large τ_m we try the perturbative solution

$$m(\tau) = m_{ad}(\tau) + \frac{1}{\tau_m} g(\tau) \quad (2.13)$$

Substituting in Eq. (2.3) we get an equation for $g(\tau)$ whose solution gives

$$g(\tau) = -\frac{\epsilon}{\tau_m} \operatorname{sech}^2\left(\frac{\epsilon\tau}{\tau_m}\right) + O\left(\frac{1}{\tau_m^2}\right) \quad (2.14)$$

For the work done we then get

$$\langle w \rangle = \beta\Delta F + \frac{\epsilon}{\tau_m} \tanh(\epsilon) \quad (2.15)$$

In Fig. (2.12) we compare the simulations for slow rates with the analytic results.

(ii) Fast case: $\tau_m \ll 1$.

If we change the field very fast then the spin is not able to respond and so there are few spin flips during the entire process. At the lowest order there is no flip and this gives rise to

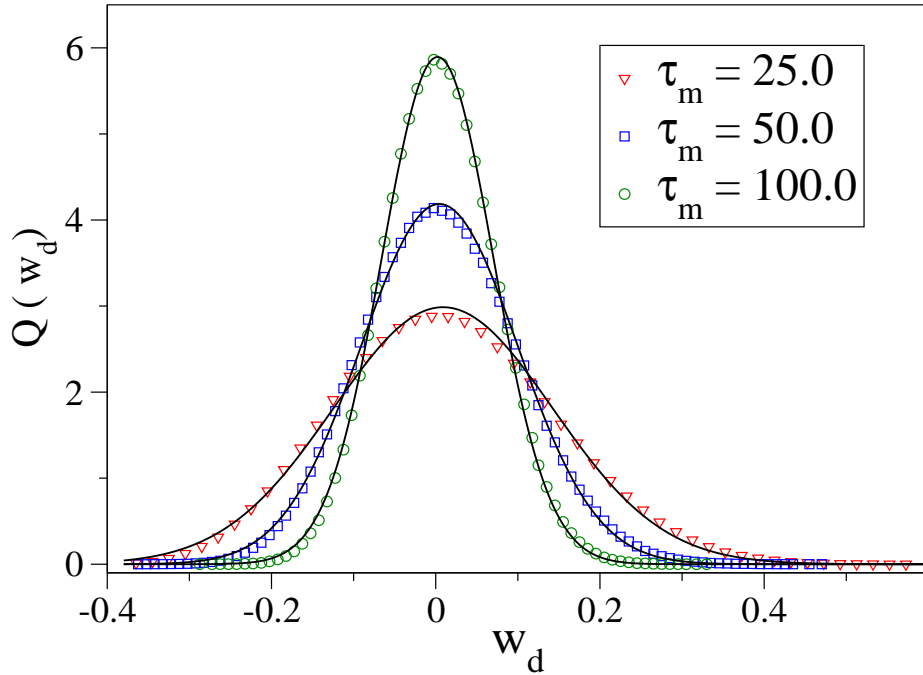


Figure 2.12: Comparison of work-distributions for slow rates obtained from simulations and from the analytic form. Solid lines show the analytic results.

the δ -functions peaks at $\pm\epsilon$ seen in the distribution. We now calculate the work-distribution by looking at contributions from 0-spin flip and 1-spin flip processes. Let $S(\uparrow, \tau_0, \tau)$ be the probability that, given that the spin is \uparrow at time τ_0 , it remains in the same state till time τ . It is easy to see that $S(\uparrow, \tau_0, \tau)$ satisfies the equation

$$\frac{\partial S(\uparrow, \tau_0, \tau)}{\partial \tau} = -\frac{e^{-\epsilon f(\tau)}}{Z} S(\uparrow, \tau_0, \tau) \quad (2.16)$$

Solving we get, for the linear case $f(\tau) = \tau/\tau_m$,

$$S(\uparrow, 0, \tau) = e^{-\int_0^\tau \frac{e^{-\epsilon \frac{\tau'}{\tau_m}}}{Z(\tau')} d\tau'} = e^{-\frac{\tau}{\tau_m}} \left(\cosh\left(\frac{\epsilon \tau}{\tau_m}\right) \right)^{\frac{\tau_m}{2\epsilon}} \quad (2.17)$$

Putting $\tau = \tau_m$ corresponds to the process for which the work done is $w = -\epsilon$. Hence, since the probability of the spin being initially in \uparrow state is $1/2$, we get

$$\text{Prob}(w = -\epsilon) = \frac{1}{2} e^{-\frac{\tau_m}{2}} [\cosh(\epsilon)]^{\frac{\tau_m}{2\epsilon}} \quad (2.18)$$

Proceeding in a similar fashion by starting with a \downarrow spin we get

$$Prob(w = \epsilon) = \frac{1}{2} e^{-\frac{\tau_m}{2}} (\cosh(\epsilon))^{-\frac{\tau_m}{2\epsilon}} \quad (2.19)$$

Next let us consider 1–spin flip processes which (for fast rates) are the major contributors to the part of the distribution between the two peaks. Let $S_1(\uparrow, \tau)d\tau$ be the probability that the spin starts in the \uparrow state, flips once between times τ to $\tau + d\tau$, and stays \downarrow till time τ_m . This is given by

$$S_1(\uparrow, \tau)d\tau = S(\uparrow, 0, \tau)(e^{-\epsilon\tau/\tau_m}/Z)d\tau S(\downarrow, \tau, \tau_m) \quad (2.20)$$

The work done during such a process is given by

$$w = -\frac{\epsilon}{\tau_m} (2\tau - \tau_m) \quad (2.21)$$

Similarly the case where the spin starts from a \downarrow state gives

$$S_1(\downarrow, \tau)d\tau = S(\downarrow, 0, \tau)(e^{\epsilon\tau/\tau_m}/Z)d\tau S(\uparrow, \tau, \tau_m) \quad (2.22)$$

and the work done in this case is

$$w = \frac{\epsilon}{\tau_m} (2\tau - \tau_m) \quad (2.23)$$

Adding this two contributions and plugging in the form of $S(\sigma, \tau_0, \tau)$ obtained earlier we get the following contribution to the work-distribution:

$$Q_1(w) = \frac{\tau_m}{8\epsilon} e^{-\frac{(\tau_m-w)}{2}} \left(\frac{e^{-\frac{\epsilon}{2}} (\cosh(\epsilon))^{\frac{\tau_m}{2\epsilon}}}{\cosh(\frac{\epsilon-w}{2})} + \frac{e^{\frac{\epsilon}{2}} (\cosh(\epsilon))^{-\frac{\tau_m}{2\epsilon}}}{\cosh(\frac{\epsilon+w}{2})} \right)$$

The full distribution is given by

$$Q(w) = \frac{1}{2} e^{-\frac{\tau_m}{2}} [\cosh(\epsilon)]^{\frac{\tau_m}{2\epsilon}} \delta(w + \epsilon) + \frac{1}{2} e^{-\frac{\tau_m}{2}} [\cosh(\epsilon)]^{-\frac{\tau_m}{2\epsilon}} \delta(w - \epsilon) + Q_1(w) \quad (2.24)$$

for $-\epsilon < w < \epsilon$, and zero elsewhere. In Fig. (2.13) we show a comparison of this analytic form with simulation results for $\tau_m = 0.01$. The strengths of the δ –functions at $w = \pm\epsilon$ are accurately given by Eqs. (2.18), (2.19).

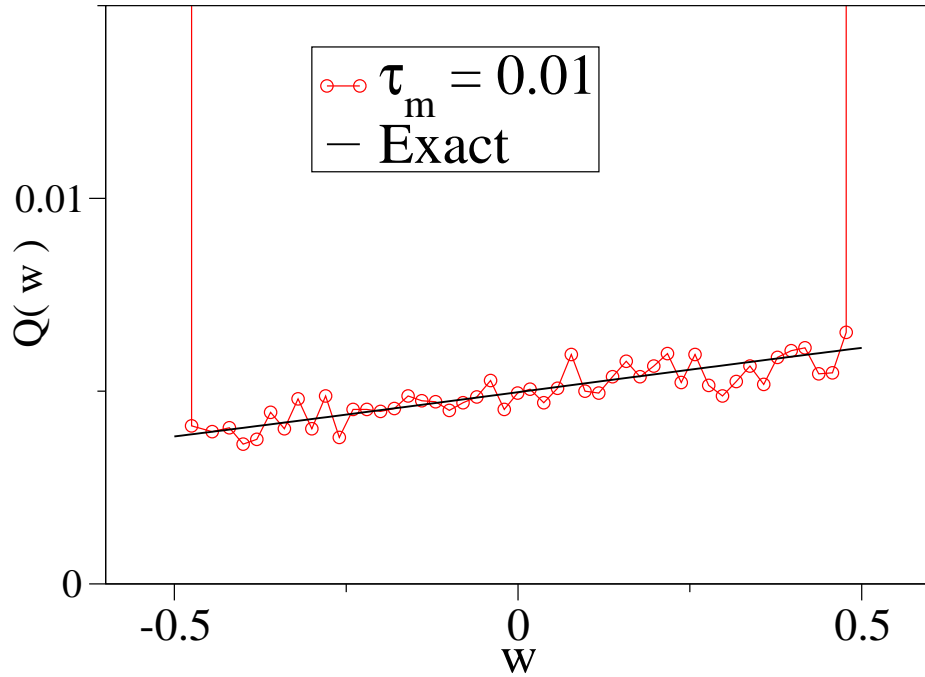


Figure 2.13: Comparison of work-distribution for a fast rate obtained from simulation and from the analytic form.

2.4.2 Field is taken around a cycle

(i) Slow case: $\tau_m \gg 1$

We again expect a Gaussian distribution and since $\Delta F = 0$ for a cyclic process, hence the mean and variance of the distribution are related by $\sigma_w^2 = 2\langle w \rangle$. As before we compute the mean work to order $1/\tau_m$ and find

$$\langle w \rangle = \frac{4\epsilon}{\tau_m} \tanh(\epsilon). \quad (2.25)$$

In Fig. (2.14) we show the comparison of analytical and simulation results.

(ii) Fast case: $\tau_m \ll 1$. In this case the work distribution gives a δ -function peak at the origin for 0-spin flip processes. To find the probability of this, we solve Eq. (2.16) with $f(\tau)$

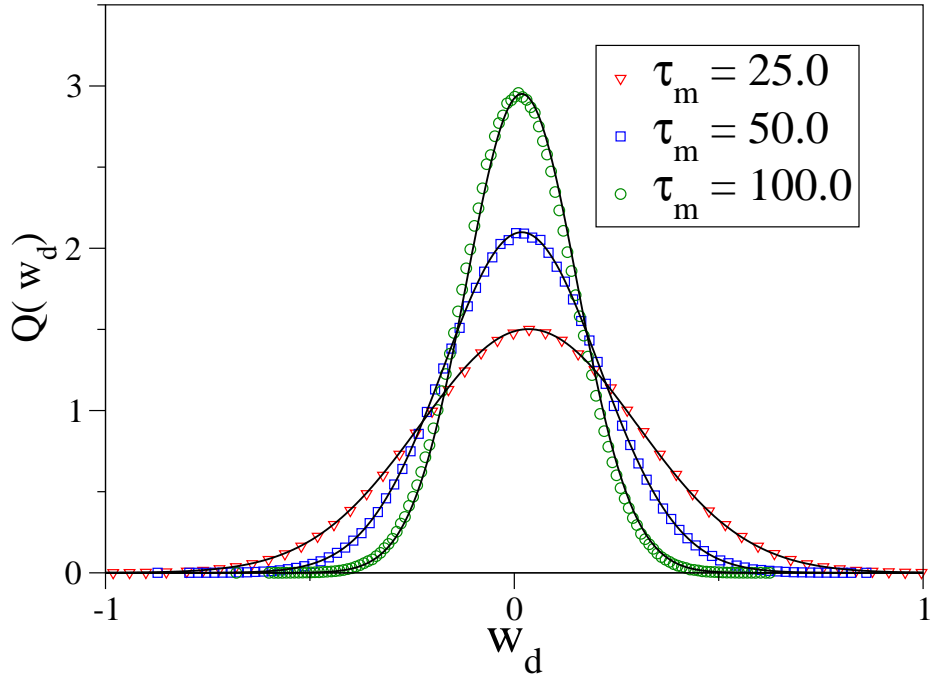


Figure 2.14: Comparison of work-distributions for slow rates obtained from simulations of the cyclic case and from the analytic form. Solid lines show the analytic results.

for the cycle given by

$$\begin{aligned}
 f(\tau) &= \frac{\epsilon}{\tau_m} \tau, & 0 \leq \tau \leq \tau_m \\
 f(\tau) &= \frac{\epsilon}{\tau_m} (2\tau_m - \tau), & \tau_m \leq \tau \leq 3\tau_m \\
 f(\tau) &= \frac{\epsilon}{\tau_m} (\tau - 4\tau_m), & 3\tau_m \leq \tau \leq 4\tau_m
 \end{aligned}$$

This has the solution

$$S(\uparrow, 0, \tau_m) = e^{-2\tau_m} \quad (2.26)$$

Adding up an equal contribution from $S(\downarrow, 0, \tau_m)$, and since both initial conditions occur with probability half, we finally get

$$Prob(w = 0) = e^{-2\tau_m} \quad (2.27)$$

Next we look at the contribution of 1–spin flip processes. Let the spin flip occur between

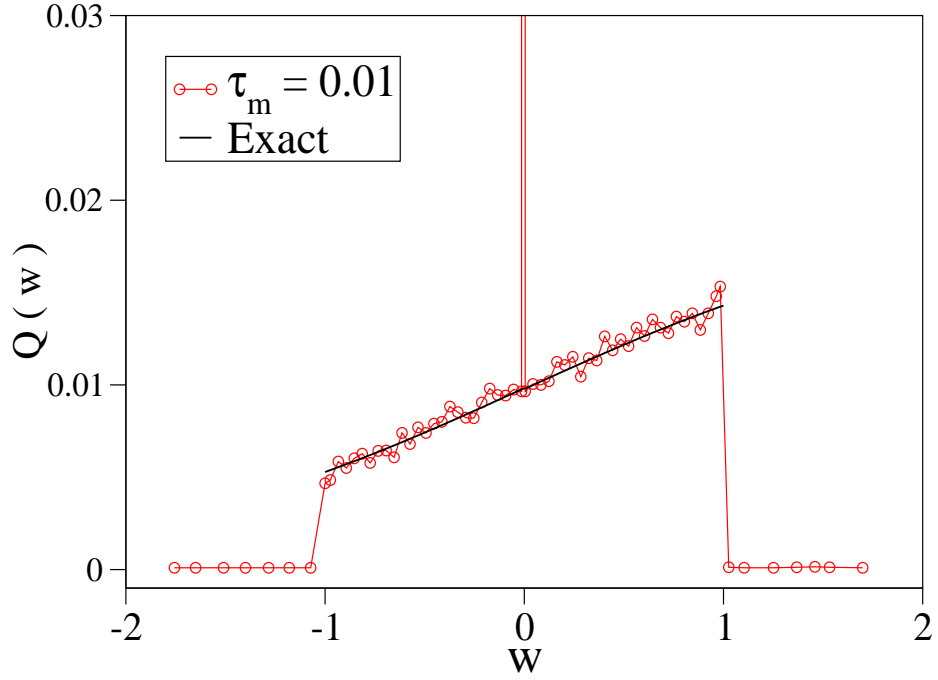


Figure 2.15: Comparison of work-distribution, for the symmetric cycle with a fast rate, obtained from simulations and from the analytic results.

times τ and $\tau + d\tau$. It is convenient to divide the total time $4\tau_m$ into four equal intervals, the dependence of w on τ being different in each of the intervals. Thus if we start with the spin initially in an \uparrow state then we have

$$\begin{aligned}
 w &= -\frac{2\epsilon\tau}{\tau_m} & , 0 < \tau < \tau_m \\
 &= \frac{2\epsilon}{\tau_m}(\tau - 2\tau_m) & , \tau_m < \tau < 2\tau_m \\
 &= \frac{2\epsilon}{\tau_m}(2\tau_m - \tau) & , 2\tau_m < \tau < 3\tau_m \\
 &= \frac{2\epsilon}{\tau_m}(\tau - 4\tau_m) & , 3\tau_m < \tau < 4\tau_m.
 \end{aligned}$$

The probabilities of each of these processes is again given by:

$$S_1(\uparrow, \tau)d\tau = S(\uparrow, 0, \tau)(e^{-\epsilon f(\tau)}/Z)d\tau S(\downarrow, \tau, 4\tau_m) \quad (2.28)$$

Using the relations between w and τ and summing up the four different possibilities we

finally get (for initial spin state \uparrow)

$$Q_1^\uparrow(w) = \frac{\tau_m}{8\epsilon} e^{-2\tau_m} e^{\frac{w}{2}} \left[\left(\cosh\left(\frac{W}{2}\right) \right)^{\frac{\tau_m}{\epsilon}-1} + \left(\cosh\left(\frac{W}{2}\right) \right)^{-\frac{\tau_m}{\epsilon}-1} (\cosh(\epsilon))^{\frac{2\tau_m}{\epsilon}} \right] \quad (2.29)$$

for $-1 < w < 1$ and zero elsewhere. Note that the allowed range of w is $[-2, 2]$ but single spin-flip processes only contribute to work in the range $[-1, 1]$. Similarly if we start with spin state \downarrow we get

$$Q_1^\downarrow(w) = \frac{\tau_m}{8\epsilon} e^{-2\tau_m} e^{\frac{w}{2}} \left[\left(\cosh\left(\frac{W}{2}\right) \right)^{-\frac{\tau_m}{\epsilon}-1} + \left(\cosh\left(\frac{W}{2}\right) \right)^{\frac{\tau_m}{\epsilon}-1} (\cosh(\epsilon))^{-\frac{2\tau_m}{\epsilon}} \right] \quad (2.30)$$

for $-1 < w < 1$. The full work-distribution (contribution from 1-spin flip processes) is thus:

$$Q(w) = e^{-2\tau_m} \delta(w) + Q_1^\uparrow(w) + Q_1^\downarrow(w) \quad (2.31)$$

In Fig. (2.15) we compare the analytic and simulation results. The strength of the δ -function at $w = 0$ is accurately given by Eq. (2.27).

2.5 Conclusions

We have computed probability distributions of the work done when a single spin, with Markovian dynamics, is driven by a time-dependent magnetic field. We find that work fluctuations are quite large (even for slow driving rates) and there is significant probability for processes with negative dissipated work. For slow driving the number of spin flips during the entire process is very large and the total work is effectively a sum of random variables. Hence the distributions are Gaussian with widths proportional to the driving rate. On the other hand for very fast driving the probability of flipping is low and we can compute the work-distributions perturbatively from probabilities of zero-flip, one-flip, etc. processes. While the two special cases of slow and fast rates can be solved, we have not been able to obtain a general solution valid for all rates even in this single particle problem. An exact solution of this problem was recently obtained by Chvosta *et al.* [38, 39].

Recently [40], work distribution functions for a charged colloidal particle placed in a time-dependent magnetic field has also been studied by Langevin equation approach. Where the

work distributions were Gaussian. Distributions of work and heat in a driven double well potential have been studied [41, 42] and also experimentally realised [43, 44], where non-Gaussian work distributions have been obtained. This system resembles to the two state Ising spin model discussed by us here.

We note that the problem of calculating the work-distribution is similar to that of calculating residence-time distributions in stochastic processes [43 – 45]. In fact for the case in Sec. (2.4.1) the work done is proportional to the average magnetization which is easily related to the residence time (time spin spends in \uparrow state). For stationary stochastic processes, such as the random walk, the residence time distribution can be obtained exactly. However for non-stationary processes this becomes difficult and no exact solutions are available [47]. In our spin-problem too it appears that the non-stationarity of the process makes an exact solution difficult.

For a system with N spins the total work done on the system is simply a sum of the work done on each of the spins. For the case where the spins are non-interacting we thus get a sum of N independent random variables. For large N the distribution will be a Gaussian with a mean that scales with N and variance as $N^{1/2}$. For interacting spins the properties of the work-distribution is an open problem. Especially of interest is the question as to what happens as we cross the transition temperature. This has been studied by Chatelain *et al.* [48], who found that the Jarzynski equality do hold in different temperature regions. Finally we note that the large fluctuations in the area under a hysteresis curve should be experimentally observable in nano-scale magnets.