Chapter 1

Escape from Metastable States in a Nonequilibrium Environment

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We review in this paper some results on metastability in a two-dimensional Ising ferromagnet relaxing toward a nonequilibrium steady state. Nucleation in this case may be understood in terms of a nonequilibrium free energy, which predicts Noise Enhanced Stability of the metastable state for low temperature in a nonequilibrium environment. This is a consequence of the anomalous, non-monotonous temperature dependence of the nonequilibrium surface tension. In addition, when subject to both open boundaries and nonequilibrium fluctuations, the metastable system decays via well-defined avalanches. These exhibit power-law size and lifetime distributions. We expect some of these results to be verificable in actual (impure) specimens.

1.1 Introduction and Model Definition

Many natural phenomena are characterized by the presence of metastable states slowing down the dynamics.[1, 2] Metastability is a dynamic phenomenon not included in ensemble formalism,[1] and its microscopic understanding still raise many fundamental questions. Studying simple models is therefore most useful. In particular, the two-dimensional Ising model has been subject to a number of analytical and numerical studies regarding metastability.[1, 2, 3] All these studies concern systems relaxing toward an equilibrium steady state. However, most interesting is the case in which the system converges toward a *nonequilibrium* stationary state.[4] Nonequilibrium conditions are more likely found in nature, and they characterize the evolution of most real systems. In particular, metastability in a nonequilibrium environment is relevant to the behavior of real magnetic particles, where impurities dominating the particle behavior cause break-up of detailed balance.[5]

We study in this paper metastability in a *nonequilibrium* Ising model. Consider a two-dimensional square lattice of side L with periodic boundary conditions. We define on each of its nodes $i \in [1, N \equiv L^2]$ a spin variable $s_i = \pm 1$. Spins interact among them and with an external magnetic field h via the Hamiltonian function $\mathcal{H} = -\sum' s_i s_j - h\sum_{i=1}^{N} s_i$, where the first sum runs over all nearest-neighbors pairs. In addition, we endow this model with a stochastic single spin-flip dynamics with transition rate,

$$\omega(\mathbf{s} \rightarrow \mathbf{s}^i) = p + (1-p)\frac{\mathrm{e}^{-\beta\Delta\mathcal{H}_i}}{1+\mathrm{e}^{-\beta\Delta\mathcal{H}_i}} \quad , \tag{1.1}$$

where $\mathbf{s}$ and $\mathbf{s}^i$ stand for the system configuration before and after flipping the spin at node i, respectively, $\Delta\mathcal{H}_i$ is the *energy* increment in such flip, and $\beta = 1/T$. For any $0 < p < 1$ two different heat baths compete in (1.1), and a nonequilibrium steady state sets in asymptotically, characterized by a non-Gibbsian measure.[4] This is the simplest way of inducing nonequilibrium behavior in simple lattice systems,[4] and it is assumed that this kind of stochastic, non$-$canonical perturbation for $p > 0$ may actually occur in Nature due to microscopic disorder and/or impurities, etc.[5] The zero-field model exhibits a second-order phase transition at a critical temperature $T_c(p) < T_c(p=0) \equiv T_{ons}$, where $T_{ons} \approx 2.2691$, between a low-temperature ordered phase and a high-temperature disordered one. Order disappears for $p > p_c \approx 0.17$ even for $T = 0$. On the other hand, for $p = 0$ we recover the usual *equilibrium* Ising model with Glauber dynamics.

1.2 Escape from Metastable States

For small $h < 0$ and $T < T_c(p)$, an initial state with all spins up, $s_i = +1$ for $i = 1, \ldots, N$, is metastable. It eventually decays toward the stable state, which corresponds now to a state with magnetization $m = N^{-1}\sum_{i=1}^{N} s_i < 0$. In order to characterize this metastable state, we measured its mean lifetime for values of T and p such that $T < T_c(p)$ and a magnetic field $h = -0.1$. We define the mean lifetime of the metastable state, $\tau(T, p, h)$, as the mean first-passage time (in Monte Carlo steps per spin, MCSS) to $m = 0$. The simulations reported here required in practice using the *s-1 Monte Carlo with absorbing Markov chains*

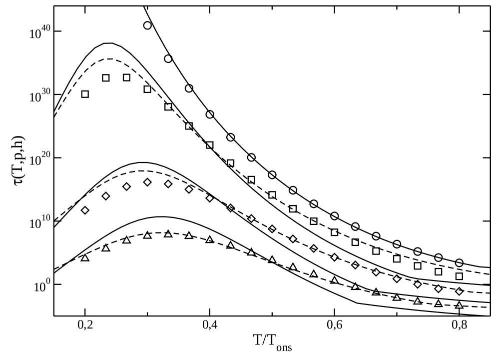

Figure 1.1: Metastable lifetime results as a function of T for $L = 53$, $h = -0.1$ and, from top to bottom, $p = 0$, 0.001, 0.005 and 0.01. The n^{th} curve (from top to bottom) is rescaled by a factor $10^{-2(n-1)}$. Points are Monte Carlo results obtained after averaging over $N_{exp} = 1000$ experiments. Full lines are predictions based on necleation theory (see main text). Dashed lines are predictions derived using the 1-parameter deformed $\mathcal{F}'(R) = \alpha(p)\mathcal{F}(R)$, with $\alpha(p) = 1, 0.85, 0.77, 0.65$ from top to bottom.

(MCAMC) algorithm, and the *slow forcing approximation*.[6] Fig. 1.1 shows $\tau(T,p,h)$ as a function of T for $L = 53$ and $p \in [0, 0.01]$. Rather amazing, we observe that the nonequilibrium metastable lifetime exhibits non-monotonous temperature dependence: $\tau(T, p > 0, h)$ *increases* with temperature at low T for a fixed $p > 0$, showing a maximum at a non-trivial temperature $T_{max}(p)$, and then decreasing as temperature drops. That is, the local stability of the metastable state at low T and $p > 0$ (nonequilibrium environment) is enhanced by the addition of thermal noise. This behavior resembles the Noise-Enhanced Stability (NES) phenomenon reported in experiments on unstable systems.[7] On the other hand, adding *nonequilibrium noise* (increasing p) for a fixed T results always in a shorter τ, so only *thermal* NES is observed.

In order to understand this result, let us first point out that, in equilibrium ($p = 0$), the escape from the metastable state is a highly inhomogeneous process triggered by large, compact stable-phase fluctuations or droplets, which grow or shrink into the metastable sea depending on the competition between their surface, which hampers droplet growth, and their bulk, which favours it. For $p = 0$, the evolution of a stable-phase droplet of radius R and volume $V = \Omega(T)R^2$ is controled by its free energy, $\mathcal{F}(R) = 2\Omega(T)R\sigma_0(T) - \Omega(T)R^2 2m_s(T)|h|$,[2, 8] where $\sigma_0(T)$ is the zero-field surface tension along a primitive lattice vector, $m_s(T)$ is the zero-field spontaneous magnetization, and $\Omega(T)$ is the droplet form factor. In this way, there exists a critical droplet size $\mathcal{R}_c$ such that small (*subcritical*) droplets (with large surface/volume ratio) tend to shrink, while large (*supercritical*) droplets tend to grow.

In principle, under nonequilibrium conditions ($p > 0$), no free energy may be defined. However, direct inspection of escape configurations confirms for $p > 0$ that droplet picture (characterized by the surface-bulk competition) is still valid here. That is, the relevant excitations responsible of the metastable-stable transition are the same is essence for both the nonequilibrium and equilibrium cases. This allows us to assume that the nonequilibrium demagnetization process is controled by a droplet *nonequilibrium free energy*,

$$\mathcal{F}(R) = 2\Omega(T,p)R\sigma_0(T,p) - \Omega(T,p)R^2 2m_s(T,p)|h|, \tag{1.2}$$

where $\sigma_0(T,p)$, $m_s(T,p)$ and $\Omega(T,p)$ are the nonequilibrium counterparts of the above-defined observables. This plausible, although unjustified, hypothesis allows us to apply homogeneous nucleation theory[2] to this far-from-equilibrium system, and projects the metastability problem into the more tractable exercise of calculating how nonequilibrium conditions affect both the surface and the bulk in this spin model. This has been addressed in a recent series of papers.[9] The interfacial properties of our model, and in particular the nonequilibrium surface tension, $\sigma_0(T,p)$, have been studied using an extended Solid-On-Solid (SOS) approximation. This approach shows that $\sigma_0(T,p>0)$ is a non-monotonous function of temperature. Homogeneous nucleation theory[2, 8] then predicts that most relevant observables associated to metastability, and in particular the mean lifetime of metastable states, inherit the non-monotonous behavior of $\sigma_0(T,p>0)$. Fig. 1.1 shows theoretical expectations based on droplet theory, using the SOS estimation for $\sigma_0(T,p>0)$ and $\Omega(T,p)$, and a mean field approximation for $m_s(T,p)$.[9] As observed, agreement is very good. This good agreement extends also to other observables, such as the droplet critical radius, $\mathcal{R}_c(T,p,h)$, etc. Hence, the observed Noise Enhanced Stability of nonequilibrium metastable states at low T is derived from the non-monotonous temperature dependence of the nonequilibrium surface tension, and the hypothesis of a nonequilibrium free energy controling the escape from the metastable region turns out to be sensible to correctly describe the metastable-stable transition in a nonequilibrium environment.

1.3 Avalanches during Relaxation

The previous observations concern the *bulk* metastability. However, in real magnets, one needs in practice to create and to control fine grains, i.e., magnetic particles with *borders* whose size ranges from mesoscopic to atomic levels, namely, clusters of 10^4 to 10^2 spins, and even smaller ones. Though experimental techniques are already accurate for the purpose, the underlying physics is much less understood than for bulk properties. In particular, one cannot assume that such particles are neither *infinite* nor *pure.* That is, they have free borders, which results in a large surface/volume ratio inducing strong border effects, and impurities. Motivated by the experimental situation, we also studied a finite, relatively small two−dimensional system subject to open circular boundary conditions. The system is defined on a square lattice, where we inscribe a circle of radius r; sites outside this circle do not belong to the system and are set $s_i = 0$. We mainly report in the following on a set of fixed values for the model parameters, namely, $h = -0.1$, $T = 0.11T_{ons}$ and $p = 10^{-6}$. This choice is dictated

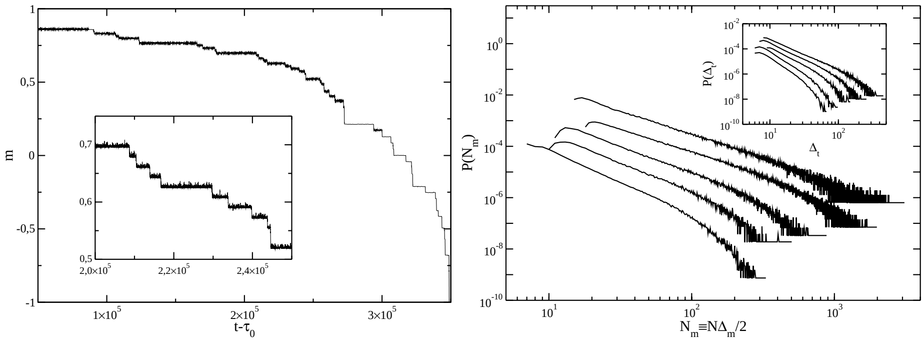

Figure 1.2: (a) Time variation of the magnetization showing the decay from a metastable state for a $r = 30$ particle; avalanches are seen here by direct inspection. Time is in Monte Carlo Steps per Spin (MCSS), and $\tau_0 \sim 10^{30}$ MCSS. The inset shows a detail of the relaxation. (b) Large avalanche size distribution $P(\Delta_m)$ for the circular magnetic nanoparticle and, from bottom to top, $r = 30$, 42, 60, 84 and 120. (For visual convenience, curves have been shifted vertically.) The inset shows the avalanche duration distribution for the same system sizes.

by simplicity and also because (after exploring the behavior for other cases) we came to the conclusion that this corresponds to an interesting region of the system parameter space, where many metastable states emerge slowing down the system relaxation, and where the effects of p and T are comparable and clusters are compact and hence easy to analize.

The effects of free borders on the metastable-stable transition have already been studied for equilibrium systems.[10] In this case, the system evolves to the stable state through the *heterogeneous* nucleation of one or several critical droplets which always appear at the system's border. That is, the free border acts as a droplet condenser. This is so because it is energetically favorable for the droplet to nucleate at the border. Apart from this, the properties of the metastable-stable transition in equilibrium ferromagnetic nanoparticles do not change qualitatively as compared to the periodic boundary conditions case.[10] In our nonequilibrium system we observe a similar behavior. However, the fluctuations or noise that the nonequilibrium metastable system shows as it evolves towards the stable state subject to the combined action of free borders and the nonequilibrium perturbation are quite unexpected.

As illustrated in Fig. 1.2.a, the relaxation of magnetization occurs via a sequence of well−defined abrupt jumps. That is, when the system relaxation is observed after each MCSS, which corresponds to a 'macroscopic' time scale, *stricktly monotonic changes of* $m(t)$ can be identified that we shall call *avalanches* in the following. To be precise, consider the avalanche beginning at time t_a, when the system magnetization is $m(t_a)$, and finishing at t_b. We define its *size* and *duration*, respectively, as $\Delta_m = |m(t_b) - m(t_a)|$ and $\Delta_t = |t_b - t_a|$. Our interest is on the histograms $P(\Delta_m)$ and $P(\Delta_t)$. Fig. 1.2.b shows the large avalanche size distribution $P(\Delta_m)$ for particle sizes $r = 30, 42, 60, 84$ and 120, after an extrinsic noise[11] (i.e. some trivial, exponentially distributed small avalanches) has been substracted. A power law behavior, followed by a cutoff is clearly observed. The measured power law exponents, $P(\Delta_m) \sim \Delta_m^{-\eta(r)}$, show size-dependent corrections to scaling of the form $\eta(r) = \eta_\infty + a_1 r^{-2}$, with $\eta_\infty = 1.71(4)$. The duration distribution also exhibits power law behavior, $P(\Delta_t) \sim \Delta_t^{-\alpha(r)}$, with a cutoff, and again $\alpha(r) = \alpha_\infty + a_2 r^{-2}$ with $\alpha_\infty = 2.25(3)$. Remarkably, size and duration cutoffs also scale algebraically with system size.[9] Similar finite size corrections have been also found in real experimental systems.[12, 13, 14] These power laws imply that avalanches are scale-free (up to certain maximum size and duration) in our nonequilibrium ferromagnet subjected to open boundary conditions. We also measured avalanches for $p = 0$ in the circular magnetic particle, and for $p \neq 0$ in the periodic boundary conditions system. In both cases only small avalanches occur and the distributions are exponential-like, thus indicating the absence of scale invariance. That is, the combined action of free boundaries and impurities is behind the large, scale-free avalanches.

Another main result is that the reported power laws are in fact a finite sum of exponential contributions. This fact, together with the lack of any divergent correlation length in the system, rules out the presence of any underlying critical point, neither plain nor self-organized.[9] To prove the latter result, we followed the demagnetization process in a large circular particle. The main interest was in the interface between the rich and poor spin–up regions at low temperature. One observes curved interfaces due to the faster growth of the domain near the concave open borders. In fact, the critical droplet always sprouts at the free border.[10] Then, given that curvature costs energy, the large avalanches tend to occur at the curved domain walls which, consequently, transform into rather flat interfaces. We confirmed this by measuring $P(\Delta_m \mid C)$, the conditional probability that an avalanche of size Δ_m develops at an interface region of curvature C.[9] This distribution exhibits (stretched) exponential behavior, $P(\Delta_m \mid C) \sim \exp[-(\Delta_m/\bar{\Delta}_m)^\eta]$ with $\eta \approx 0.89$. That is, a wall of curvature C induces avalanches of typical size $\bar{\Delta}_m(C)$. This fact turns out most relevant because, due to the free borders and impurities, the interface tends to exhibit a broad range of curvatures with time. Therefore, what one really observes when averaging over time is a combination of many different avalanches, each with its typical well–defined (gap–separated) size and duration, which results in an *effective* distribution. The fact that this combination depicts several decades (more the larger the system is) of power–law behavior can be mathematically understood on simple grounds, studying finite superpositions of many exponential distributions.[9]

Scale-invariant (or $1/f$) noise has been found in many complex systems, ranging from electronic devices to superconducting vortices, human cognition, earthquakes and radiation from white dwarfs, to mention some. The hypothesis that some underlying mechanism is common to many situations is therefore appealing. Many possible generic mechanisms have been proposed in literature, most of them based on possible underlying critical phenomena. After much effort, there is no full agreement on a globally coherent explanation, however. We have seen here that a non-critical superposition of many different scales can give rise to $1/f$ noise. In addition, the properties of fluctuations in our oversimplified model are indistinguishable in practice from what one measures in many natural phenomena showing $1/f$ noise. For instance, size corrections similar to the ones observed here for $\eta(r)$ and $\alpha(r)$ have been reported in avalanche experiments on rice piles,[12] and our values for η_∞ and α_∞ are amazingly close to those reported in some magnetic experiments for *quasi-two dimensional systems*.[11] Moreover, our cutoff values follow the precise trend observed, for instance, in magnetic materials. All these facts (and other, not mentioned results[9]) indicate that the mechanism here proposed, namely the non-critical superposition of many different scales, is a good candidate to explain the origin and ubiquity of $1/f$ noise in many natural systems in which a series of transitions between many different, short-lived metastable states characterize the dynamics.

1.4 Conclusion

We have reviewed in this paper some results on the escape from metastable states in a two-dimensional Ising ferromagnet evolving toward a nonequilibrium steady state. Relaxation in this case is considerably enriched as compared to equilibrium. In particular, using periodic boundary conditions, we have shown that the stability of the metastable state at low T is enhanced by the addition of thermal noise. This Noise Enhanced Stability (NES) of the metastable state can be understood in terms of a nonequilibrium droplet free energy which controls the escape from the metastable region. Using this hypothesis, it can be shown that the observed NES is inherited from the non-monotonous temperature dependence of the nonequilibrium surface tension.[9]

We also observe that, under the action of both the nonequilibrium impurity and free borders, the metastable-stable transition proceeds by avalanches. These are power-law distributed, thus showing scale invariance (up to certain cutoffs). The origin of the observed scale invariance can be traced back to a non-critical superposition of many different scales, ruling out the presence of any underlying critical point. The striking similarities between the statistical properties of fluctuations in this model and those of avalanches observed in many real complex systems lead us to propose this mechanism as a generic explanation of $1/f$ noise in systems characterized by a rich, varied set of transitions between many short-lived metastable states.

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