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An approach to characterize metastability and critical droplets in stochastic Ising models

by

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ABSTRACT. – This note is an account of the present state of and of possible direction of research on an approach to characterize metastability and the role of critical droplets for some stochastic Ising models, by considering a limit in which the temperature vanishes. The emphasis lies in the identification of typical paths of the processes, as proposed in [CGOV].

Key words : Ising model, Glauber dynamics, metastability, critical droplets, limit of zero temperature, pathwise approach.

RÉSUMÉ. – Cet article rend compte de l'état actuel des connaissances et des directions possibles de recherche sur un programme dont le but est de caractériser la métastabilité et le rôle des gouttelettes critiques de certains modèles stochastiques d'Ising, en considérant la limite de température nulle. L'accent est porté sur l'identification des trajectoires typiques du processus, comme proposé dans [CGOV].

Classification A.M.S. : 60 K 35, 82 A 05

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In this note I give a short account of a line of research – the study of metastability and critical droplets for stochastic Ising models in the limit as the temperature vanishes – in which I am engaged, in collaboration with Eduardo Jordão Neves. I will also indicate some directions of present and future research. For more details and proofs the reader is refered to [NS1], [NS2] and [N]. I do not intend to write here a review on the subject of metastability and refer the reader to the nice survey [PL] and in particular its update added to the new edition. Nevertheless, in the next paragraphs I provide a brief overview of the sources of the problem, and some previous work on it, [PL] can be consulted for more details and for references to the literature.

The original motivation for the theoretical study of metastability came from a phenomenon reported in the physics literature: the metastable states in which some thermodynamic systems may enter instead of undergoing a phase transition. For instance, consider a vapor inside a container submitted to increasing pressures at fixed temperature. At a certain point the vapor should condensate into a liquid. But if this procedure is done carefully, in a smooth enough fashion, the vapor may not condensate at all and instead enter into a state called metastable. It continues to show properties of a gas, but may suddenly decay to the true equilibrium liquid state.

Phenomenologically this fact has been explained as being essentially kinetic. For the vapor to condensate, droplets of the liquid must be formed that grow until the whole system reaches this states. But small droplets have a large ratio of surface area per volume, which causes them to tend to lose molecules and to shrink. Only a droplet with a size larger than a critical one will grow. Such droplet will appear because of a random fluctuation in the metastable vapor in which small droplets are constantly being formed and shrinking. To give to this picture a more quantitative flavor one attributes a surface "free energy" to the droplets which competes with their bulk "free energy", causing the total free energy of the droplet to vary with its radius, increasing until the critical size is reached and then decreasing. This gives rise to a "free energy barrier" that has to be overcome for a large droplet to be formed

There is a vast literature devoted to finding more rigorous explanations for the phenomenon, at least in the context of some simple model systems. As a general rule the results can only be considered satisfatory for the mean-field models, in which each component of the system interacts with an average field caused by the other components. On the other hand this sort of interaction in not very realistic and several attempts have been made to provide rigorous results indicating the presence of metastability effects in model with short range interactions. This is also the case of our work.

As in many other papers we consider the nearest neighboor ferromagnetic Ising models with Glauber type of dynamics (stochastic Ising models). These models are caricatures of ferromagnetic materials evolving in time coupled to heat reservoirs (*i.e.*, at fixed temperatures). Metastable effects are expected to appear here when the system is initially in a state magnetized in one direction and an external field is turned on in the opposite direction. The new equilibrium state would be magnetized in the direction of the external field, but for it to be reached, first "droplets" of this phase have to be formed inside the opposite phase. The interface between a droplet and the background produces a positive energy proportional to its area, while the bulk of a droplet, parallel to the external field, produces a negative energy proportional to its volume. For such reasons it is a common idea that stochastic Ising models must present in a precise sense the features associated to metastability, including the characterization of critical droplets. Heuristic arguments and computer simulations have supported this view. Also related rigorous results have been obtained (*see* [PL] and references therein), but to our knowledge the rigorous results obtained so far do not provide the full picture of metastability and especially the role of critical droplets, as described above.

Our approach to the problem is based on the consideration of a different limit than the one usually taken. In order to obtain sharp results, to idealize large systems and to disregard boundary effects, one takes (when studying equilibrium properties of statistical mechanics models) the thermodynamic limit, in which the volume goes to infinity, keeping a fixed density. But for a system with short interactions, the intuitive picture of metastability sketched above does not survive this limit. If the volume is as large as we want, then critical droplets, which appear as local fluctuations, will appear somewhere almost instantaneously. In fact a growing density of them will appear, and grow and the system will evolve in a smooth way to the equilibrium regime. Instead of the thermodynamic limit, we consider the volume (and external field) as fixed and take the limit as the temperature vanishes. In this limit and for some stochastic Ising models to be specified below, flips of the spins that cause the energy to grow become unlikely and play the role of a weak noise perturbing a system in which rectangular droplets would neither grow nor shrink. Only in a time scale that diverges as the temperature vanishes one can see the droplets evolve. In such a situation it is not surprising, that the evolution of a droplet will be dictated by the energy of nearby configurations. And so the heuristics which indicates the existence of critical droplets because of the competition between the surface and bulk energies should indeed lead to correct results. We do obtain results of this sort which will be stated more precisely below, but first we must clarify the meaning of the results that we obtain under the limit in which the temperature goes to zero. We are not at all studying the system at zero temperature, but at very low stricty positive temperature. We prove that in the limit the probabilities of certain patterns of evolution converge to one, and this means simply that at low enough temperature these patterns are very likely to be observed. In other words, we are identifying typical sorts of behavior, as precisely as we can, for the system at low enough strictly positive temperatures. This, of course, is similar to what can be said about other limit theorems as those obtained in equilibrium statistical mechanics in the thermodynamic limit. There one obtains the typical behavior of systems that are not infinite, but large enough and finite. In any one of these situations it is desirable to sharpen the results by estimating the errors in the limiting procedures. In other words, by saying in our case for a given system how low the temperature must be for the probability of a certain event to be larger than $1-\varepsilon$. Our estimates at that moment were not optimazed in this sense and for this reason we leave these questions for a future investigaticn.

We consider the system on a lattice $\Lambda=\{1, \ldots, N\}^d \subset \mathbb{Z}^d$, wrapped into a torus (periodic boundary conditions). At each site x there is a spin $\sigma(x)$ taking the values -1 or $+1$. The configurations with all spins down or up will be denoted respectively by $-\underline{1}$ and $+\underline{1}$. The energy corresponding to a configuration $\sigma \in \{-1, +1\}^\Lambda$ is given by

$$H(\sigma)=-\frac{1}{2}\sum_{\{x, y\} \in \mathbb{B}} \sigma(x)\sigma(y)-\frac{h}{2}\sum_{x \in \Lambda} \sigma(x),$$

where h is the external field, that we will here always assume as being positive and less than 1, and $\mathbb{B}$ is the set of neighboring sites in Λ with periodic boundary conditions, *i.e.*, $\{x, y\} \in \mathbb{B}$ in case x and y have $d-1$ coordinates in common and one coordinate which differs by 1 or $N-1$. For fixed inverse temperature β, the Gibbs probability measure μ is given by

$$\mu(\sigma)=Z^{-1}\exp(-\beta H(\sigma)),$$

where Z^{-1} is a normalization constant.

One constructs a corresponding stochastic Ising model by letting the spins change value in time in a stochastic fashion, with the spin at the site x flipping with rate $c(x, \sigma)$ when the configuration is σ. Formally this system is a continuous time Markov process with state space $\{-1, +1\}^\Lambda$ and generator L which acts on each function $f: \{-1, +1\}^\Lambda \to \mathbb{R}$ as

$$(Lf)(\sigma)=\sum_{x \in \Lambda} c(x, \sigma)(f(\sigma^x)-f(\sigma)),$$

where

$$\sigma^x(y)=\begin{cases}\sigma(y) & \text{if } y\neq x,\\ -\sigma(y) & \text{if } y=x.\end{cases}$$

The rates are supposed to satisfy the reversibility (detailed balance) condition

$$\mu(\sigma)\,c(x,\sigma)=\mu(\sigma^x)\,c(x,\sigma^x).$$

This assures that μ is the only invariant measure for the process and moreover the stationary process obtained by starting with this measure is time-reversible.

There are infinitely many choices of the rates $c(x,\sigma)$ that satisfy the reversibility condition. Most of our results ([NS1], [N]) were obtained for the so called Metropolis dynamics, which corresponds to

$$c(x,\sigma)=\begin{cases}1 & \text{if } \Delta_x \mathrm{H}(\sigma)\leqq 0,\\ \exp(-\beta(\Delta_x \mathrm{H}(\sigma))) & \text{otherwise,}\end{cases}$$

where $\Delta_x \mathrm{H}(\sigma)=\mathrm{H}(\sigma^x)-\mathrm{H}(\sigma)$ is the increment in energy caused by flipping the spin at the site x. In Theorem 1 of [NS1] we prove that in two dimensions for this dynamics the heuristics about critical droplets has in fact a rigorous counterpart. The energy of a configuration with a single square droplet $l\times l$ of spins $+1$ in a sea of spins -1 is $\mathrm{H}(-\underline{1})+4l-hl^2$, which has a single maximum at $l=2/h$. We prove that indeed a rectangular droplet of spins $+1$ in a sea of spins -1 is likely to grow if both its sides are larger than $2/h$, while it is likely to shrink if one of these sides is less than $2/h$. In the former case the time for the doplet to cover the whole system is of the order of $\exp(\beta(2-h))$, while in the latter case the time for the doplet to disappear is of the order of $\exp(\beta h(l-1))$, l being its smallest side. The results, as observed above, are of the form $\lim_{\beta\to\infty} \mathrm{P}(\mathrm{E})=1$, where $\mathrm{P}(\mathrm{E})$ is the probability in each case that an event E describing the typical behavior (skrinking or growing in a time of the correct order) occurs.

In [NS2] this result was extended to a class of rates in the two-dimensional case. This class is characterized by the fact that for fixed temperature each rate $c(x,\sigma)$ depends only on the increment in energy caused by the flip of the spin at x, $\Delta_x \mathrm{H}(\sigma)$, in a monotone non-increasing way. We observed also in [NS2] that the monotonicity of the rates in this condition is crucial, since otherwise we can find examples that violate the conclusion of the theorem (for instance with the critical lenght being 1 instead of $2/h$). This shows that in spite of the similarly between the heuristic and rigorous results, their contents are not really the same.

In more than two dimensions our results are at the present much less satisfactory. In [NS2] we showed (for the same class of dynamics with monotone rates) that in every dimension small enough droplets are likely to shrink while large enough droplets are likely to grow. But both bonds on the size of the droplet are far from the threshold expected heuristically. The difficulties lie mostly in the fact that while in two dimensions only rectangular droplets are local minima of the energy, in higher dimensions much more complicated shapes of droplets have this property (take for instance a small cube on top of a larger one). Even heuristically, we expect that not only the smallest, but in fact all but the largest sides of a doplet are relevant to determine its probable fate. For instance, in three dimensions consider a doplet with sides $P \leqq Q \leqq R$. We expect it to be subcritical in case the removal of a two-dimensional slice $P \times Q$ (which causes R to change to $R-1$) decreases the energy, and to be supercritical in case this removal increases the energy. The first conjecture (on subcritical droplets) was proved by Eduardo J. Neves in his thesis [N], in a long tour de force, in which he classified different local minima of the energy according to their stability and analysed their role in different time scales. His methods may potentially be used to prove also the second conjecture (on supercritical droplets), but at this moment this project is still not completed.

Once the typical behavior of single droplets had been identifyed for a class of stochastic Ising models in two dimensions, we used these results to study the evolution of the system $(\sigma_t^{-\underline{1}}, t \geqq 0)$ starting from $-\underline{1}$, until it hits $+\underline{1}$. Let $T = \inf\{t \geqq 0 : \sigma_t^{-\underline{1}} = +\underline{1}\}$ be the random time needed for this decay. In [NS1] and [NS2] we proved the following results, always as $\beta \to \infty$:

(*a*) $T/E(T)$ converges in distribution to a unit mean exponential random variable.

(*b*) Modify the process $(\sigma_t^{-\underline{1}})$ by freezing it in $+\underline{1}$ when it first hits this configuration. Then the finite dimensional distributions of the process $(\sigma_{s E(T)}^{-\underline{1}}, s \geqq 0)$ converge to those of a pure jump Markovian process which stays in $-\underline{1}$ for a unit mean exponential time and then jumps to $+\underline{1}$, where it is trapped forever.

Intuitively, the system stays essentially in $-\underline{1}$ and eventually jumps to $+\underline{1}$; also the moment of the jump is close to unpredictable (exponential) at low temperature. We can not take more than the finite dimensional distributions in (*b*), since subcritical droplets are appearing and disappearing here and there from time to time before T. But the result above indicates that "most" of the time before T the system is in $-\underline{1}$. We will discuss later on ways in which (*b*) may be strengthened. Incidentally, in [NS1] we proved also that for Metropolis dynamics, in the time scale $E(T)$, one never sees a jump back from $+\underline{1}$ to $-\underline{1}$, so that (*b*) remains true also if we do not freeze the process in $+\underline{1}$. This should be true with much greater generality, but is a marginal issue for us, since we are mostly concerned with the behavior of the system before it hits $+\underline{1}$.

In (*b*) above we characterize typical paths of the process $(\sigma_t^{-\underline{1}})$ as looking like one would expect in a metastable situation. The idea of looking to metastability in this way was introduced by M. Cassandro, A. Galves, E. Olivieri and M. E. Vares in [CGOV], and further developed and applyed in several situations in [KN], [Sch], [NCK], [GOV], [COP], [MOS1], [EGJL] and [Bra]. Our work was very strongly influenced by this so called "pathwise approach to metastability", and may be considered as one more step in the direction of establishing the presence of metastability in this sense for reasonable and interesting model systems.

Looking back to the heuristic picture of droplets nucleating the decay of the metastable system and to the results above, one sees that there is much more that one would like to prove. For instance, in the passage from $-\underline{1}$ to $+\underline{1}$ one expects that the system passes through a configuration with a single critical droplet, that then grows and covers the whole lattice (instead of seeing several droplets growing simultaneously.) Also one would expect the magnitude of the nucleation time T to be asymptotically of the order of $\exp(\beta\Gamma(h))$, where $\Gamma(h)$ is an energy barrier which must be overcome to go from $-\underline{1}$ to $+\underline{1}$. In [NS1] we proved indeed such results for Metropolis dynamics in $d=2$. We proved also there that starting from any configuration the system is likely to relax to $+\underline{1}$ or $-\underline{1}$ in a time which is much shorter than the nucleation time.

In parallel to our work, F. Martinelli, E. Olivieri and E. Scoppola wrote a series of papers ([MOS2]-[MOS5]), in which they combined our results and techniques with others to prove exponential approach to equilibrium for some stochastic Ising models for small positive external field at low enough but fixed positive temperature. They also extended these results to the Swendsen-Wang cluster dynamics, a dynamics for the Ising model in which whole blocks of spins flip simultaneously.

I point out now directions in which we are going or plan to go.

1) Dealing with $d \geqq 3$ is not only a mathematical challange, but is also important for understanding the physical role of the complicated structure of the local minima and how to handle it. Here the ideas of E. J. Neves seem promissing, but see also item (5) below.

2) In parallel to (1) above, we plan to sharpen our control and understanding of the two-dimensional case, especially in the simplest case of Metropolis dynamics. For instance, we would like to be able to tell in more detail how is the typical evolution from the time the system leaves $-\underline{1}$ for the last time before hitting $+\underline{1}$ and the time it hits this configuration. Using the reversibility of the process we have some results in this direction. We also expect to identify a set of configurations which are "close" to $-\underline{1}$ in the sense that they are visited many times before the system hits $+\underline{1}$. For example, configurations with a single subcritical droplet, or with several droplets much smaller than the critical one. We

expect the system to "thermalize" in this set of configurations before it hits $+\underline{1}$, in the sense that for every η in this set

$$\exp(\beta(H(\eta)-H(-\underline{1})))\left[\frac{1}{T}\int_0^T \mathbf{1}_{\{\eta\}}(\sigma_t^{-\underline{1}})\,dt\right]\to 1$$

in probability as $\beta\to\infty$. Of course, all the η above must have energies larger than $H(-\underline{1})$, and hence the statement above would give the order of magnitude of the very small fraction of time that the system spends in each of these configurations before it is nucleated. These fractions of time would then roughly correspond to those observed in a system in equilibrium with a heat bath. Partial results in this direction have already been obtained.

3) It is not hard to see that if we let the volume go to infinity slowly enough at the same time that the temperature goes to zero, then we obtain the same results that we proved for finite volume. In particular, a single critical droplet nucleates the decay of the metastable state. On the other hand, if in such a double limit the volume grows too fast, then the picture resembles that in the case of fixed temperature, and many droplets appear rapidly and nucleate the passage from $-\underline{1}$ to $+\underline{1}$ homogeneously. It would be interesting to see if one can identify a sharp threshold between the two sorts of regimes, or at least obtain upper and lower bounds with the same kind of dependence between β and N. Preliminary observations seem to indicate that the critical relation is of the form $\beta = C\log N$. This would be a nice result, in particular because it would tell us that even if N^d is of the order of Avogadro's number, β^{-1} may be a "reasonable" temperature for the metastable picture to hold.

4) The previous question is related but not identical to the problem already mentioned of estimating the errors in the limits. One may even want to be very concrete and ask things like how low the temperature must be for the probability that a square droplet of side 100 shrinks to be larger than 0.999, when $N=10^8$ and $h=10^{-3}$.

5) One can abstract the problem and consider a general finite graph whose vertices play the role of configurations and such that its edges generalize the notion of configurations which differ at a single site. Attributing energies to the vertices one can define a Metropolis dynamics on such a graph. This is in fact done in the optimization procedure known as simulated annealing but there the temperature is slowly decreased as the process evolves (*see* [KGV]). The question here is to state and prove results related to the structure of local minima of the graph, which may in particular be applied then to the case of the stochastic (Metropolis) Ising model. One may also try to explore the consequences of this point of view to simulated annealing. Such questions are closely related to the Freidlin-Wentzell theory on weakly perturbed dynamical systems [FW].

6) We argued already that for fixed β and h we do not expect a metastable behavior for large volume. But if we keep β fixed, larger than the critical value and take the thermodynamic limit and $h \to 0$ simultaneously and rapidly enough, then it it natural to expect metastable effects to appear. This is so because the size of the critical droplet grows as h vanishes and hence in this case the appearance of a critical droplet must still be the result of a large fluctuation. One may even extend the problem in item (3) above and consider the different behaviors of the system in the three-dimensional parameter space $N \times \beta \times h$. Technically these questions seem to be much harder to handle than those treated so far.

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REFERENCES

[Bra] S. Brassesco, *Tunelling for a Non-Linear Heat Equation with Noise*, preprint, 1989.

[CGOV] M. Cassandro, A. Galves, E. Olivieri, and M. E. Vares, Metastable Behavior of Stochastic Dynamics: A Pathwise Approach, *J. Stat. Phys.*, Vol. **35**, 1984, pp. 603-634.

[COP] M. Cassandro, E. Olivieri and P. Picco, Small Random Perturbation of Infinite Dimensional Dynamical Systems and Nucleation Theory, *Ann. Inst. Henri Poincaré Phys. Théor.*, Vol. **44**, 1986, pp. 343-396.

[EGJL] V. R. Eston, A. Galves, C. M. Jacobi and R. Langevin, *Dominance Switch Between Two Interacting Species and Metastability*, preprint, 1988.

[FW] M. I. Freidlin, A. D. Wentzell, *Random Perturbation of Dynamical Systems*, Springer, 1984.

[GOV] A. Galves, E. Olivieri and M. E. Vares: Metastability for a Class of Dynamical Systems Subject to Small Random Perturbations, *Ann. Probab.*, Vol. **15**, 1987, pp. 1288-1305.