Metastable lifetime of a kinetic Ising model with a transition dynamic algorithm

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We calculate the average lifetime $\langle\tau\rangle$ of the metastable state of a 2-d kinetic Ising model. The model evolves under what is called a transition dynamic (TDA), which assumes that the system in going from an initial to a final state, must pass through an intermediate state t, such that the transition rate has the form, $W(i \to j) = W(i \to t)W(t \to j)$. The results are obtained in two different ways. First, by calculating the first-passage time from the metastable to an absorbing state. Second, by the technique of absorbing Markov chains. Our calculations reproduce the standard result obtained in the low-temperature nucleation regime, $\langle\tau\rangle = Ae^{\Gamma/k_{\rm B}T}$. However, we find that A and Γ differ from the values calculated for the standard Glauber dynamics. These results are consistent with recent studies which indicate that, contrary to common belief, Γ is not simply the metastable energy barrier, but depends on the stochastic dynamics used.

Keywords: Metastable; nucleation; Kinetic Ising model.

Calculamos la vida media $\langle\tau\rangle$, del estado metastable de un modelo cinético de Ising en 2-dimensiones. La evolución del sistema viene dada por una dinámica de transición (TDA) que asume que el sistema para poder pasar de un estado inicial a uno final debe pasar por un estado intermedio t, tal que la probabilidad de transición es de la forma $W(i \to j) = W(i \to t)W(t \to j)$. Los resultados son obtenidos de dos formas distintas. Una del cálculo del tiempo que toma el sistema metaestable en pasar por primera vez a un estado absorbente. La otra utilizando la técnica de las cadenas absorbentes de Markov. Nuestros cálculos reproducen el resultado estandard que dice que, a bajas temperaturas, en el régimen de nucleación, $\langle\tau\rangle = Ae^{\Gamma/k_{\rm B}T}$. Sin embargo encontramos que A y Γ son distintos de los obtenidos para la dinámica estandard de Glauber. Estos resultados son consistentes con estudios recientes que prueban que, al contrario a lo que se creia, Γ no es simplemente la barrera de energía metastable sino que depende de la dinámica estocástica utilizada.

Descriptores: Metaestabilidad; nucleación; modelo cinético de Ising.

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Metastable states are very common in nature and occur in many systems ranging from supercooled fluids and vapors, quantum liquids, magnetic systems, to cosmological models. The decay of a metastable phase through nucleation and growth of droplets of a stable phase is a common feature of these processes. Kinetic Ising models have proven to be interesting and fruitful laboratories to study the decay of metastable states through a nucleation process [1, 2]. It is well known that in the regime of single droplet decay, the low-temperature limit of the the average waiting time to escape from a metastable phase, the known as lifetime $\langle\tau\rangle$, has the form [3]

$$\langle\tau\rangle = Ae^{\beta\Gamma}, \tag{1}$$

where $\beta = 1/k_{\rm B}T$. For the standard Glauber dynamic [4], Γ is equal to the energy difference between the saddle point and the metastable state [5]. Until recently, it was believed that this was a general result. However, recent work shows that both the prefactor A and Γ strongly depend on the stochastic dynamic selected [6].

In this paper we measure the lifetime of the metastable state of a two-dimensional nearest-neighbor Ising model.

$$\mathcal{H} = -\sum_{<nn>} \sigma_i\sigma_j - H\sum_i \sigma_i. \tag{2}$$

The system is prepared in a metastable state by initially setting all the spins up ($\sigma = +1$) and applying a static field of strength H directed opposite to the spins (downward). The transition rates are given by the transition dynamic algorithm (TDA) [7],

$$W(i \to f) = \frac{1}{(1 + e^{\beta(E_t - E_i)})(1 + e^{(\beta(E_f - E_t)})} \tag{3}$$

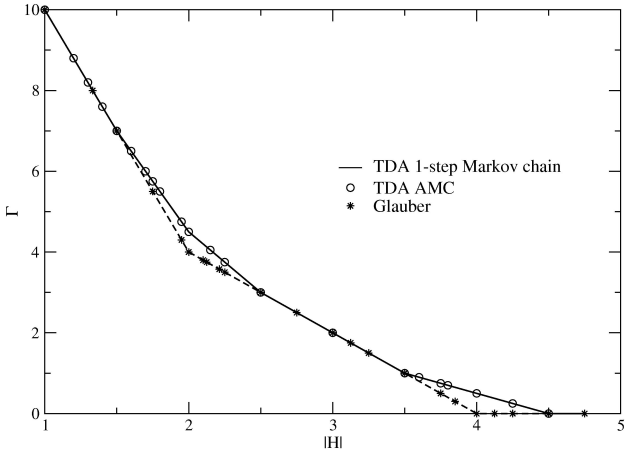

FIGURE 1. Γ factor calculated for the TDA dynamics with the one-step Markov chain approximation and with the absorbing Markov chain technique. For purposes of comparison we have included the results for the Glauber dynamics. Both dynamics give different results in the regions $2-\Delta<|H|<2+\Delta$ and $4-\Delta<|H|<4+\Delta$. Here $\Delta = 0.5$

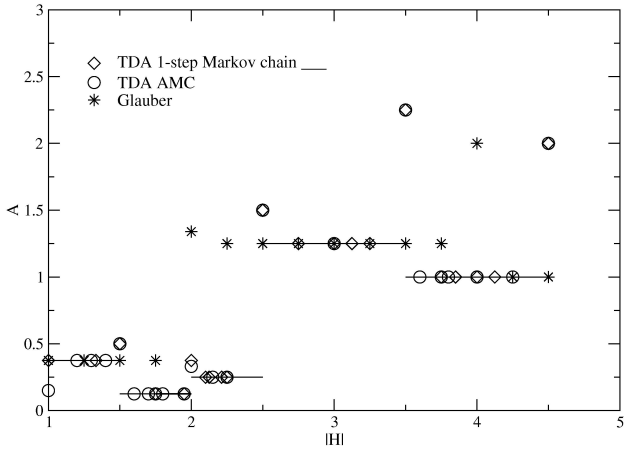

FIGURE 2. Prefactor A calculated for the TDA dynamics with the one-step Markov chain approximation and with the absorbing Markov chain technique. For purposes of comparison we have included the results for the Glauber dynamics. Both dynamics give different results in the regions $2-\Delta<|H|<2+\Delta$ and $4-\Delta<|H|<4+\Delta$. The A factor calculated with the Glauber dynamic is discontinuous at $|H| = 2, 4$, and the one calculated with the TDA at $H = 2-\Delta, 2, 2+\Delta, 4-\Delta$ and $4+\Delta$. Here $\Delta = 0.5$.

which is the product of the Glauber transition rates from i to an intermediate state t and from there to f. This kind of dynamic is frequently applied to study diffusion process on surfaces, where an energy barrier exists for the motion from one site to another. These transition probabilities describe explicitly the effect of an intermediate energy state in a diffusion process, which in the classical picture is the saddle point of the potential [8].

At very low temperatures, the critical droplet of a kinetic Ising model is a square of size $l_2 \times l_2$ with one row removed and a single overturned spin on one of the longest sides, where $l_2 = integer[2J/|H|] + 1$ [3].

Here, we calculate the average lifetime by two different analytical methods. First, in terms of the shrinking and growing probabilities of a droplet, by calculating the first-passage time from the metastable state to an absorbing state just beyond the saddle point, assuming that the path in the configuration space corresponds to a one-step Markov process [10].

In the single droplet regime the time, it takes the system to evolve from an initial state with no overturned spins to an absorbing state with I overturned spins is [6,9],

$$\langle \tau_I \rangle = \frac{N}{g_0} + \sum_{l=1}^{I-1} \frac{N}{g_l} \left(1 + \sum_{k=1}^{l} e^{\beta(E_l - E_{l-k})} \prod_{j=0}^{k-1} \frac{n_{l-j}^s}{n_{l-j-1}^g} \right). \quad (4)$$

where g_i is the rate at which the cluster grows from i to $i+1$ overturned spins, and n_i^s (n_{i-1}^g) are the number of lattice sites at which a single spin flip can shrink the cluster from i to $i-1$ (growth from $i-1$ to i). If I is greater than the number of overturned spins of the saddle point, then $\langle \tau = \rangle = \langle tau_I \rangle$. In the limit of $\beta \to \infty$, Eq.(4) is dominated by the terms with the largest exponential factor. When the external field is in the range $1 < |H| < 4$, the lifetime of the metastable states can be obtained by explicitly calculating the first four terms ($I = 4$) of Eq.(4).

$$\begin{aligned} \langle \tau_4 \rangle = & \frac{1}{p_1} + \frac{1}{4p_2}(N + e^{\beta(8-2|H|)}) \\ & + \frac{1}{4p_2}(N + \frac{N}{2}e^{\beta(4-2|H|)} + \frac{1}{2}e^{\beta(12-4|H|)}) \\ & + \frac{1}{p_3}(N + \frac{N}{2}e^{\beta(4-2|H|)} \\ & + \frac{N}{4}e^{\beta(8-4|H|)} + \frac{1}{4}e^{\beta(16-6|H|)}). \end{aligned} \quad (5)$$

Here p_m is the rate of flipping a positive spin with $5-m$ positive nearest-neighbors, or more generally the probability of flipping a spin of class m in the classification scheme used to define the n-fold way advanced dynamical Monte Carlo algorithm [11,12]. These rates depend on the dynamic. For the transition dynamic algorithm defined in Eq. (3), we have the form,

$$p_m = \frac{1}{2} \frac{e^{\beta E_{fi}}}{(\cosh \beta E_{fi} + \cosh \beta \Delta)} \quad (6)$$

where $E_{fi} = (E_f - E_i)/2$, E_i is the initial energy of the spin in class m and E_f is the energy after the spin has been flipped. The term Δ is a measure of the barrier introduced by the transition state T,

$$\Delta = E_{fi} - E_t. \quad (7)$$

For the purpose of this work we choose $\Delta = 0.5$. We need to calculate the low-temperature limit of Eq. (6).

Comparing the dominant terms of $\langle \tau_4 \rangle$ at the low temperature limit with Eq.(1) we obtain the values of A and Γ.

We also calculate Γ and the prefactor A using absorbing Markov chains (AMC) with 13 transient states at the

limit $T \to 0$, allowing for multiple paths to the critical droplet [12].

In Fig. 1 we show the results for the Γ factor calculated from both techniques for the TDA dynamics, and also for the Glauber dynamics. Both methods give the same Γ values for the same dynamic. These results agree with previous studies that indicate that the values found for Γ are independent of the approximation used [6, 9], behaving piecewise linearly with $|H|$. For the Glauber dynamics there are 3 regimes with different slopes, $1 < |H| < 2$, $2 < |H| < 4$ and $|H| > 4$. For the TDA dynamics, there are 5 regimes where the slope changes ($\Delta < 1$), $1 < |H| < 2 - \Delta$, $2 - \Delta < |H| < 2 + \Delta$, $2 + \Delta < |H| < 4 - \Delta$, $4 - \Delta < |H| < 4 + \Delta$ and $|H| > 4 + \Delta$. The values of Γ found for the two dynamics are different in the regimes, $2 - \Delta < |H| < 2 + \Delta$ and $4 - \Delta < |H| < 4 + \Delta$. For both dynamics, Γ is zero in the strong-field limit, $|H| > 4 + \Delta$.

In Fig. 2 we show the results for the prefactor A. Again we see that, except at $|H| = 2$, both techniques give basically the same values for A , and that these values differ from those calculated for the Glauber dynamics in the regimes $2 - \Delta < |H| < 2 + \Delta$ and $4 - \Delta < |H| < 4 + \Delta$. As expected, the prefactor is discontinuous (for a discussion of prefactor discontinuities see [9]). For the Glauber dynamics the discontinuities appear at the values where $|H|/2$ is an integer [12], $|H| = 2$ and 4. For the TDA dynamics, they appear at $|H| = 2 - \Delta, 2, 2 + \Delta, 4 - \Delta$ and $4 + \Delta$.

Our results further confirm the fact that the factors Γ and A of the low-temperature metastable lifetime of a kinetic Ising model depend on the specific stochastic dynamic. In particular, Γ for the TDA dynamics is not everywhere equal to the energy barrier against nucleation.

1. F.F. Abraham, *Homogeneous Nucleation Theory* (Academic, New York, 1974).
2. M.A. Novotny, G. Brown, and P.A. Rikvold, *J. Appl. Phys.* **91** (2002) 6908; P.A. Rikvold and B.M. Gorman, in *Annual Reviews of Computational Physics I*, Ed. D. Stauffer (World Scientific, Singapure, 1994).
3. E. Jordao Neves and R.H. Schonmann, *Commun. Math. Phys.* **137** (1991) 209.
4. R.J. Glauber, *J. Math. Phys.* **4** (1963) 294.
5. V.A. Shneidman, *J. Stat. Phys.* **112** (2003) 293.
6. K. Park, P.A. Rikvold, G.M. Buendía, and M.A. Novotny, *Phys. Rev. Lett* (2003, in press).
7. T. Ala-Nissila, J. Kjoll, and S.C. Ying, *Phys. Rev B* **46** (1992) 846.
8. J. Kjoll, T. Ala-Nissila, and S.C. Ying, *Surface Sci* **218** (1989) L476; A.G. Naumovets and Yu.S. Vedula, *Surface Sci. Rep.* **4** (1985) 365.
9. K. Park, M.A. Novotny, and P.A. Rikvold, *Phys. Rev. E* **66** (2002) 056101.
10. N.G. Van Kampen, *Stochastic Processes in Physics and Chemistry*, 2nd Ed. (North-Holland, Amsterdam, 1992).
11. A.B. Bortz, M.H. Kalos, and J.L. Lebowitz, *J. Comput. Phys.* **17** (1975) 10.
12. M.A. Novotny, *Computer Phys. Commun.* **147** (2002) 659.