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Generalized Single-Spin Flip Dynamics for the Ising Model and Thermodynamic Properties

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We propose two different unifications of the Metropolis, the Glauber and the Heat–Bath dynamics for the Ising model. Both generalizations satisfy detailed balance. Computer simulations for the $d = 2$ Ising ferromagnet suggest that, in all cases , the correct magnetization, specific heat and susceptibility are recovered. The fundamental implications are discussed.

Key–Words: Ising dynamics; Detailed balance; Monte Carlo; Spread of damage

PACS Numbers: 05.50.+q , 05.20.Dd , 75.10.–b , 05.70.Ln

The thermostatistical approach of the dynamics to be associated with the Ising model persistently attracts attention since almost half a century. This interest has been greatly enhanced nowadays. This is due, on one hand, to the dissemination of computational facilities, and, on the other, to the usefulness of this model for studying a variety of systems (spin glasses and other magnetic models, neural networks, immunology models, cellular automata) and concepts (spread of damage, dynamical critical phenomena). Quite a number of different microscopic dynamics have been specially devised for the Ising model, essentially because of its simplicity. However, in some sense, this model is a peculiar one. Indeed, classical systems are characterized by two basic properties, namely that all the observables, (i) commute, and (ii) are continuous variables. The Ising model satisfies (i) but not (ii). This peculiarity is at the basis of the above mentioned proliferation of associated microscopic dynamics. These dynamics can be <u>stochastic</u> or <u>deterministic</u>, <u>single-spin</u> flip or <u>multi-spin</u> flip. To the stochastic/single-spin class belong the Metropolis [1-3], the Glauber [4] and the Heat-Bath [3] dynamics. To the stochastic/multi-spin class belong the Kawasaki dynamics [5], the Swendsen and Wang dynamics [6], its generalizations by Kandel and co-workers [7] and the Wolff dynamics [8]. To the deterministic/single-site class belong the Q2R [9] and the Creutz [10] dynamics, and finally, a deterministic/multi-spin flip dynamics has been obtained by Creutz [11], through a convenient generalization of his single-site dynamics. Let us finally mention that: (i) each one of these dynamics refers to a specific ensemble (microcanonical, canonical); (ii) the spin updating within all these dynamics can be <u>sequential</u> or <u>parallel</u>. One should say, at this point, that it is possible to define generalized dynamics which unify some of those defined above, either within a given class (e.g., Glauber and Heat-Bath [12]), or else, belonging to distinct classes (e.g., Glauber and Kawasaki [13]).

In the present paper, we focus attention to the three most frequently used dynamics, namely the Metropolis (M), Glauber (G) and Heat–Bath (HB) ones. We propose two different unifications (referred to as the arithmetic (a) and geometric (g) dynamics), both preserving detailed balance . Our primary aim is to see how these two generalized dynamics lead to the correct thermodynamics of the Ising model. To check this we calculate, through $L \times L$ sized computational simulations, the spontaneous magnetization m , specific heat C and susceptibility χ of the square–lattice Ising ferromagnet. Our results suggest that the correct thermodynamics is indeed recovered, in the $L \to \infty$ limit, in all cases .

We denote by P^{-+} the probability that the i–th spin becomes +1 at time t+1 if it was –1 at time t; we define analogously P^{+-} , P^{++} and P^{--} . These quantities satisfy $P^{+-} + P^{++} = P^{-+} + P^{--} = 1$. Let us now remind that

$$P_M^{+-} = \min\{1 , \exp(-\Delta E_i/k_B T)\} \quad , \tag{1.a}$$

$$P_M^{-+} = \min\{1 , \exp(\Delta E_i/k_B T)\} \quad , \tag{1.b}$$

for the Metropolis dynamics, and

$$P_G^{+-} = P_{HB}^{+-} = \{1 + \exp(\Delta E_i/k_B T)\}^{-1} \quad , \tag{2.a}$$

$$P_G^{-+} = P_{HB}^{-+} = \{1 + \exp(-\Delta E_i/k_B T)\}^{-1} \quad , \tag{2.b}$$

for both Glauber and Heat–Bath dynamics, with

$$\Delta E_i = E_i^- - E_i^+ \quad , \tag{3}$$

where E_i^- (E_i^+) is the energy of the system with the i-th spin down (up).

Let us now unify these three dynamics as follows:

$$P_a^{+-} = xP_M^{+-} + yP_G^{+-} + zP_{HB}^{+-} \quad , \tag{4.a}$$

$$P_a^{-+} = xP_M^{-+} + yP_G^{-+} + zP_{HB}^{-+} \quad , \tag{4.b}$$

where a stands for arithmetic and $x + y + z = 1$ $(0 \le x,y,z \le 1)$; see Fig. 1. We can straightforwardly verify that Eqs. (1), (2) and (4) lead to

$$\frac{P_a^{+-}}{P_a^{-+}} = \exp(-\Delta E_i/k_B T) \quad , \tag{5}$$

i.e., detailed balance is satisfied for arbitrary (x,y,z). Since Eqs. (2) hold for both Glauber and Heat-Bath dynamics, it is clear that, at this level, there is no need to work with a ternary composition (a binary composition with weights x and 1-x suffices). Nevertheless, we shall maintain the (x,y,z) notation for reasons that will become clear later on.

Along the same lines, a second unification can be proposed. Suppose we have D different dynamics characterized by (P_1^{+-}, P_1^{-+}), (P_2^{+-}, P_2^{-+}), ... , (P_D^{+-}, P_D^{-+}) such that detailed balance is satisfied for all of them, i.e.,

$$P_k^{+-} / P_k^{-+} = \exp(-\Delta E_i/k_B T) \qquad (k = 1,2, \ldots , D) \quad .$$

We define

$$P_g^{+-} = \prod_{k=1}^{D} (P_k^{+-})^{x_k} \quad , \tag{6.a}$$

$$P_g^{-+} = \prod_{k=1}^{D} (P_k^{-+})^{x_k} \quad , \tag{6.b}$$

where g stands for <u>geometric</u> and $\sum_{k=1}^{D} x_k = 1$ $(0 \le x_1, x_2, \ldots, x_D \le 1)$. It is trivially verified that

$$\frac{P_g^{+-}}{P_g^{-+}} = \exp(-\Delta E_i/k_B T) \quad , \tag{7}$$

i.e., the geometric dynamics <u>also</u> satisfies detailed balance for <u>arbitrary</u> $\{x_k\}$. By choosing $D = 3$ into the present problem we have

$$P_g^{+-} = (P_M^{+-})^x \, (P_G^{+-})^y \, (P_{HB}^{+-})^z \quad , \tag{8.a}$$

$$P_g^{-+} = (P_M^{-+})^x \, (P_G^{-+})^y \, (P_{HB}^{-+})^z \quad . \tag{8.b}$$

In our numerical simulations of the Ising ferromagnet we have used an $L \times L$ square lattice with periodic boundary conditions, and the updating has been done in the typewriter sequence. The ensemble averages have been performed by repeating $N_{exp} \approx 100$ independent realizations of the system $(L = 20,40)$. In order to accelerate the thermalization process, we have chosen, for all temperatures, initial conditions $(t = 0)$ such that the magnetization is close to a reasonable expectation. Before starting measuring thermodynamic quantities we have dropped a transient time of the order of L^2. The time averages have been performed along a time of the order of $L^2/2$ after the transient. Finally, the approximative spontaneous magnetization has been obtained through the usual procedure, i.e., by averaging $|m(t)|$ instead of $m(t)$. It is important to stress at this point that this (standard) procedure makes the finite L Monte Carlo thermodynamic results to resemble the $L \to \infty$ limit ones, which is the only limit where symmetry can be broken strictly speaking. In other words, one has to keep in mind that only the $L \to \infty$ extrapolated numerical results are physically meaningful.

In Fig. 2 we present our results for m, C and χ for both $L = 20$ and $L = 40$ for six different dynamics, namely $x = 0$ (i.e., Glauber or, equivalently, Heat-Bath), $x = 1$ (i.e., Metropolis), arithmetic $x = 1/3$ and $x = 1/2$, and geometric $x = 1/3$ and $x = 1/2$. We remark: (i) for fixed L, the magnetization practically independs from x and from the dynamics being either arithmetic or geometric; (ii) for fixed L, the specific heat and susceptibility exhibit a moderate trend to monotonously increase while x varies form 0 to 1, and this for both a and g dynamics; (iii) for increasing L, the already small discrepancy between the curves associated with the six different dynamics decreases. These remarks, put together with the well known fact that the Metropolis, the Glauber and the Heat-Bath dynamics yield (in the $(L,t) \to (\infty,\infty)$ limit) the correct Ising thermodynamics, very strongly suggest that the same happens with the intermediate dynamics (i.e., arbitrary (x,y,z)) for both arithmetic and geometric unifications. This large set of dynamics share one important fact: they all satisfy detailed balance. It is well known that this condition suffices for recovering the correct equilibrium thermodynamics [15] (at least for sequential updating of the dynamic variables), in the $(L,t) \to (\infty,\infty)$ limit. However, in numerical simulations (performed for limited values of L and t), finite-size effects and relaxation times could differ when we change the dynamics. Our results suggest that equilibrium thermodynamics properties are quite insensitive to variations in the (x,y,z) parameters (i.e., different dynamics), even for small L and t.

It is in the realm of non-equilibrium properties that the present proposal of two infinite classes of dynamics could be used to provide distinct and interesting results for different values of (x,y,z). In what folllows, we present two possible fields of research where these generalized dynamics could be useful.

If we start from a given global initial condition, different dynamics will make a physical system to evolve through different paths in the phase space; such evolution is being intensively studied nowadays. One privileged tool for doing this is the "spread of damage" between two different copies of the system. More precisely, the two copies are (slightly of appreciably) different at $t = 0$, and, by using a given dynamical prescrition (which includes the <u>same</u> sequence of random numbers), the "distance" in phase space (e.g., the Hamming distance $D(t)$) between the two copies is followed as time goes on (with particular interest in the asymptotic behavior in the $t \to \infty$ limit). The system is said to be "chaotic" if $D(\infty) \neq 0$, because it is sensitive to the initial conditions. This method is well illustrated through the Ising ferromagnet. Indeed, with the Heat-Bath dynamics, chaos tends to appear at <u>low</u> temperatures ($T < T_c$) [16], whereas with the Metropolis and Glauber dynamics, it tends to appear at <u>high</u> tempertaures ($T > T_c$) [12,17-19]. As we see, Glauber and Heat-Bath dynamics yield <u>qualitatively</u> different spread of damage, in spite of the fact that they share the same transition probabilities (as expressed in Eqs. (2)). This discrepancy is due to the different use that is done, in these two dynamics, of the random number corresponding to time t (see [12,18,20]). Because of this subtle difference, the Glauber and the Heat-Bath dynamics yield the <u>same</u> result when only <u>one</u> copy of the system is followed (as it is the case when we study its equilibrium thermodynamics), but yield <u>different</u> results when <u>two</u> copies are followed (as it is the case for the study of the spread of damage). It is for this reason that we mantained, in the present work, the notation (x,y,z), thus individually treating each one of these three dynamics. In fact, the study of the spread of damage corresponding to the unifications introduced in the present paper is in progress.

Finally, it is clear that the relaxation process towards thermodynamical equilibrium depends upon the particular dynamics which is used. Consequently, quantities such as relaxation time and amplitude should depend on (x,y,z). In other words, the present unifications provide also a tool for adjusting (within certain limits) these relaxation quantities.

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Caption for Figures

Fig. 1 – Triangular representation of the arithmetic and geometric dynamics (M, G and HB respectively refer to Metropolis, Glauber and Heat-Bath dynamics).

Fig. 2 – Monte Carlo results corresponding to six different dynamics and two different sizes: (a) Spontaneous magnetization; (b) Specific heat; (c) Susceptibility. "Exact" refers to L. Onsager and C.N. Yang results (e.g., $k_B T_c/J = 2/\ln(1+\sqrt{2}) \approx 2.269$); "Nearly exact" is taken from [14]. $L = 20$: $x = 0$ ($*$), $x = 1$ ($\square$), arithmetic $x = 1/3$ ($\circ$), geometric $x = 1/3$ ($\triangle$), arithmetic $x = 1/2$ ($+$), geometric $x = 1/2$ (⊕); $L = 40$: $x = 0$ ($\times$), $x = 1$ ($\bullet$), arithmetic $x = 1/3$ ($\Diamond$), geometric $x = 1/3$ (✦), arithmetic $x = 1/2$ ($\blacksquare$), geometric $x = 1/2$ ($\circ$). At every chosen temperature and for all three m, C and χ , all <u>twelve</u> points have been computed, even if they are not graphically distinguishable. For fixed L , the highest relative discrepancy in both C and χ for the six different dynamics occurs at their peaks: $\Delta C/C \approx 0.12$ for $L = 20$ and 0.11 for $L = 40$, and $\Delta\chi/\chi \approx 0.27$ for $L = 20$ and 0.21 for $L = 40$. The non neglectable discrepancy between the (nearly) exact and finite-L susceptibility in the paramagnetic region has been already discussed in [3].

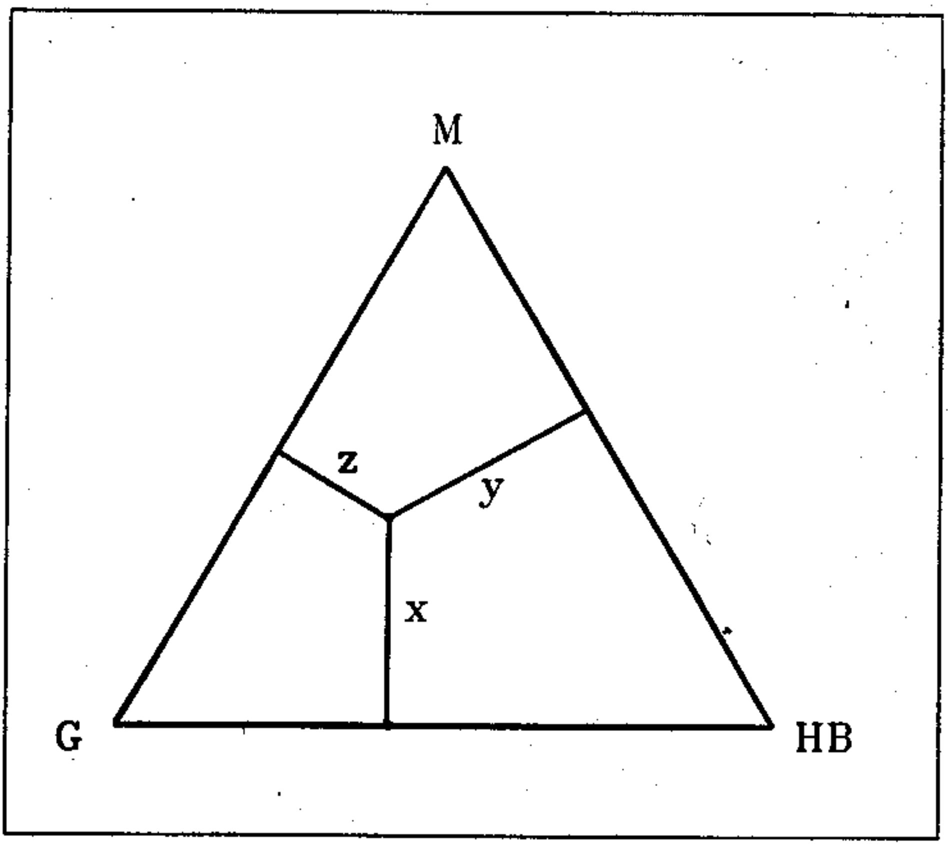

Fig. 1

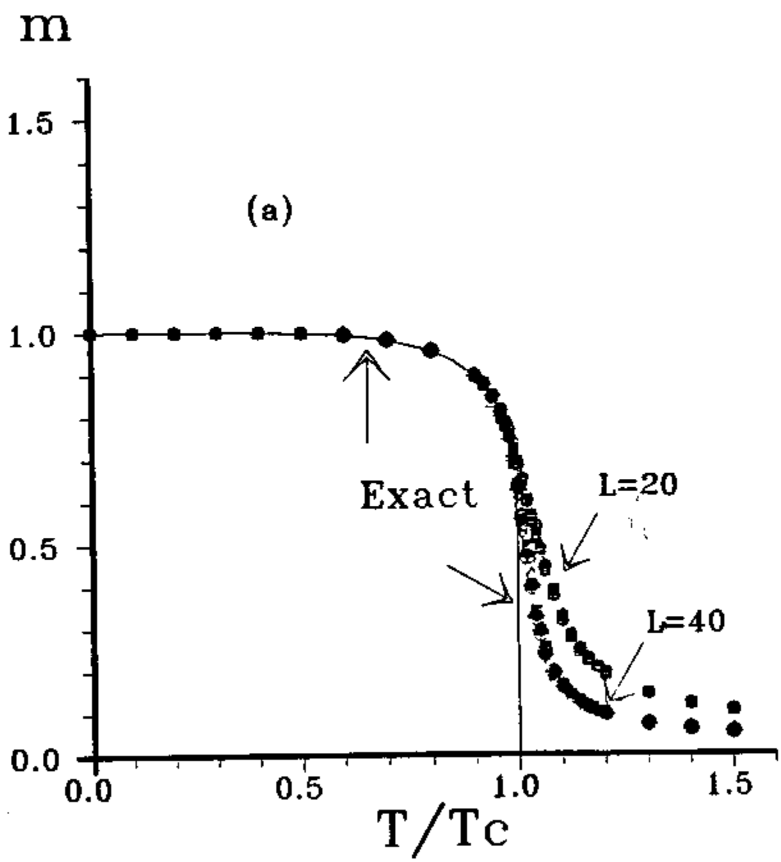

Fig. 2(a)

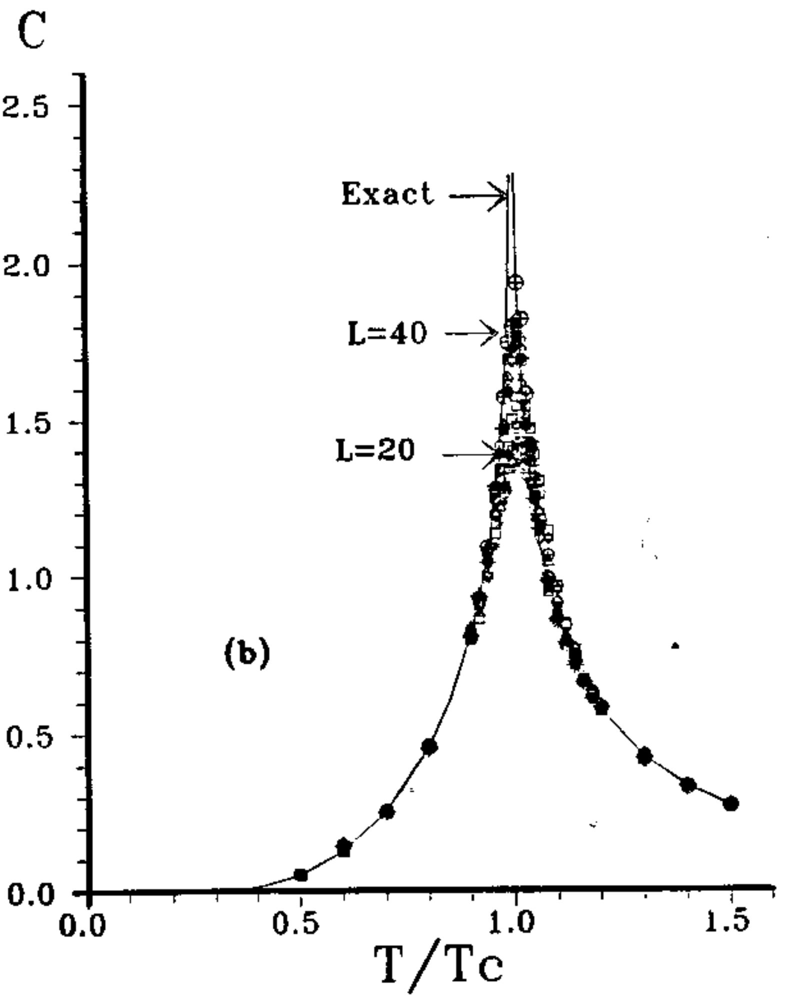

Fig. 2(b)

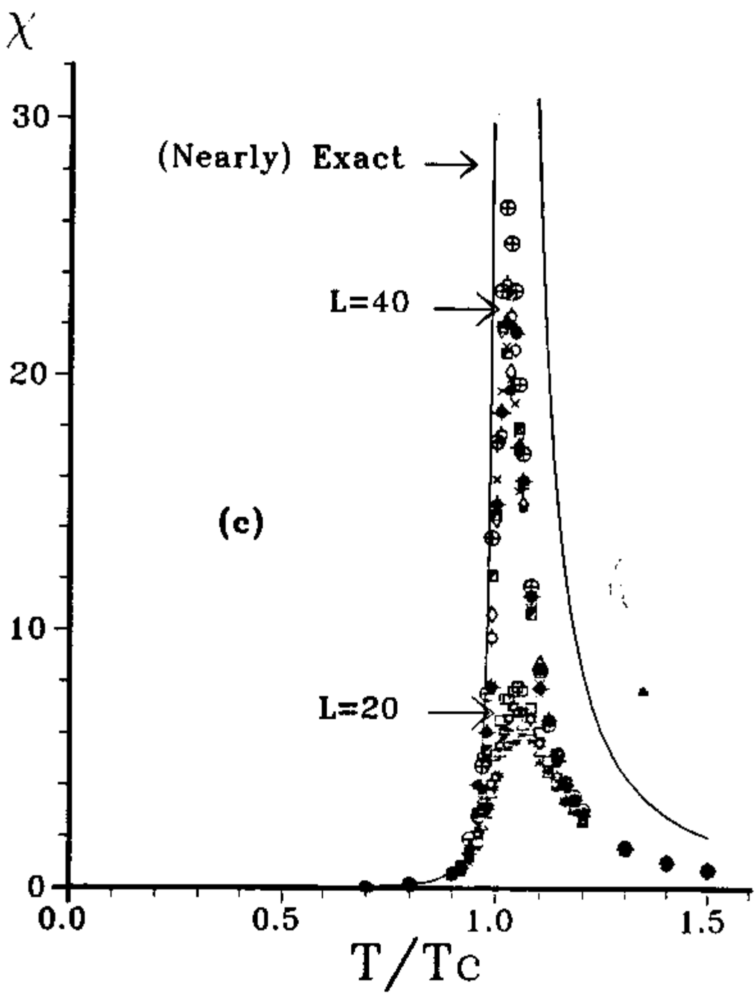

Fig. 2(c)

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