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Complexity and Nonequilibrium Steady States: an Example

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1. Introduction

It is usual to find in Nature systems which are in states much more complex that the ones at equilibrium. Think, for example, of a large iron bar with both ends connected to heat reservoirs. When the temperature of the reservoirs is the same, the system evolves, after a while, to an equilibrium state. But when the temperature of each reservoir is different, it appears a continuous heat flux from the warmer reservoir to the cooler one. We say then that the system is in a *nonequilibrium stationary state.* This is nonequilibrium because there exist a net current of something through the system; it is stationary because the system properties do not change with time.

In contrast with the case of systems at equilibrium states, no general theory to study nonequilibrium stationary states exists. Therefore, one typically needs to develop specific approximate methods to deal with particular problems (McLennan, 1989). These theoretical approaches are usually inspired in the ones used for systems at equilibrium states, and it is generally

assumed that some concepts and techniques can be extrapolated to deal with systems at nonequilibrium steady states. We would like to illustrate in this paper that this attitude may be wrong in general, and that quite often the qualitative theoretical predictions are approximation-dependent. As an example, we refer to a simple, mathematically well-defined lattice model system: the *two-temperatures Ising model* (Garrido, Labarta, Marro, 1987; Garrido, Marro, 1994). We describe below its macroscopic behavior by means of an extensive Monte Carlo computer experiment. Furthermore, we use a mean field type of theoretical approach to solve the model. We will see that, under the latter approach, the system apparently behaves in a much more complex manner than observed in Monte Carlo experiments. We conclude that one should be careful when applying familiar theoretical approximations to systems in nonequilibrium states: It is not obvious at all that the qualitative results obtained are a characteristic of the corresponding system.

2. Definition of Model system

The *two-temperatures Ising model* was introduced by Garrido, Labarta and Marro (1987). Let us sketch its definition. At each site of a d-dimensional simple cubic lattice, $\underline{x} \in Z^d$, there is a spin variable, $s_{\underline{x}} = \pm 1$. Each configuration $\underline{s} = \{s_{\underline{x}}, \underline{x} \in Z^d\}$ has an interaction energy defined by

$$H(\underline{s}) = -J \sum_{|\underline{x}-\underline{y}|=1} s_{\underline{x}} s_{\underline{y}} \tag{2.1}$$

where $J > 0$ is the coupling constant. The evolution of the spin configuration has a stochastic nature: the probability of varying the configuration is i) a decreasing function of the increment of energy that the change implies, and ii) is independent on the previous evolution history (Glauber, 1963). Because of this type of dynamics, the function that carries the maximum information about the system evolution is the probability to find the system at a configuration $\underline{s}$ at time t, i.e., $P_t(\underline{s})$. This probability evolves with time according to a master equation, namely,

$$\frac{\partial P_t(\underline{s})}{\partial t} = \sum_{\underline{s}'} [c(\underline{s}' \to \underline{s}) P_t(\underline{s}') - c(\underline{s} \to \underline{s}') P_t(\underline{s})] \tag{2.2}$$

It is further assumed that each transition between consecutive configurations, $\underline{s} \to \underline{s}'$, just inverts (flips) the spin at a site, $s_{\underline{x}} \to -s_{\underline{x}}$, with probability $c(\underline{s} \to \underline{s}') = c(\underline{s}; \underline{x})$. The time evolution and the stationary properties of the

model depend on the particular analytical form of $c(\underline{s}; \underline{x})$. The *two-temperatures Ising model* is then defined by choosing:

$$c(\underline{s}; \underline{x}) = p\Phi(\beta_1 \Delta H(\underline{s}; \underline{x})) + (1-p)\Phi(\beta_2 \Delta H(\underline{s}; \underline{x})) \tag{2.3}$$

where $p \in [0, 1]$, $\Delta H(\underline{s}; \underline{x}) = 2Js_{\underline{x}} \Sigma_{\underline{y}; |\underline{x}-\underline{y}|=1} s_{\underline{y}}$ is the increment of energy that produces the flip of the spin at $\underline{x}$, and β_i, $i = 1, 2$, are two positive constants. $\Phi(\lambda)$ is any arbitrary positive function with the property: $\Phi(\lambda) = \Phi(-\lambda) \exp\{-\lambda\}$; for example: $\Phi(\lambda) = 1 - \tanh(\lambda/2) \equiv \Phi_G(\lambda)$ and $\Phi(\lambda) = \exp\{-\lambda/2\} \equiv \Phi_V(\lambda)$.

In order to understand the meaning of the parameters introduced above, we can do the substitution $p = 0(1)$ in (2.3). In those cases, it is straightforward to show that the stationary solution of the master equation (2.2), $\partial_t P_{st}(\underline{s}) = 0$, is the equilibrium Boltzmann distribution with the Ising Hamiltonian (2.1) and the inverse temperature $\beta_{2(1)}$, i.e.,

$$P_{st}(\underline{s}) \propto \exp\{-\beta_{2(1)} H(\underline{s})\} \tag{2.4}$$

Then, the dynamics in equation (2.3) may be interpreted assuming that the spin flip at each site $\underline{x}$ is attempted with probability p as if it were in contact with a thermal bath at temperature $T_1 = \beta_1^{-1}$ and with probability $1-p$ as if the temperature of the bath inducing the transition were $T_2 = \beta_2^{-1}$. Obviously, when $T_1 = T_2 = T$, one recovers the equilibrium distribution (2.4) with temperature T for any value of $p \in [0, 1]$.

Beyond the above simple limiting cases, when $T_1 \neq T_2$ and $p \in (0, 1)$, we are unable to find, in general, the master equation stationary solution $P_{st}(\underline{s})$. The competition of both temperatures generate nonequilibrium stationary states in general. In particular, we will see that the steady state depends on the function Φ we choose in (2.3) (in contrast with the equilibrium case $p = 0, 1$ where no such a dependence occurs).

3. Monte Carlo simulations

Before we begin to attack the theoretical problem of how to obtain information from these equations, let us show by means of a Monte Carlo computer simulation the *real* system behavior in two dimensions.

In addition to some preliminary numerical work by Garrido et al. (1987), the macroscopic behavior of the two-temperatures Ising model in 2-dimensions has been studied more systematically by simulation of the time evolution of square lattices of $N = 64 \times 64$ sites. In particular, we have considered a fixed value of $p = 50000/2^{16} = 0.7629\ldots$, a range of T_1 and T_2 values (in units where $J/K_B = 1$), and two different dynamics, namely, $\Phi_G(\lambda) = 1 - \tanh(\lambda/2)$, and $\Phi_V(\lambda) = \exp(-\lambda/2)$. It has required about

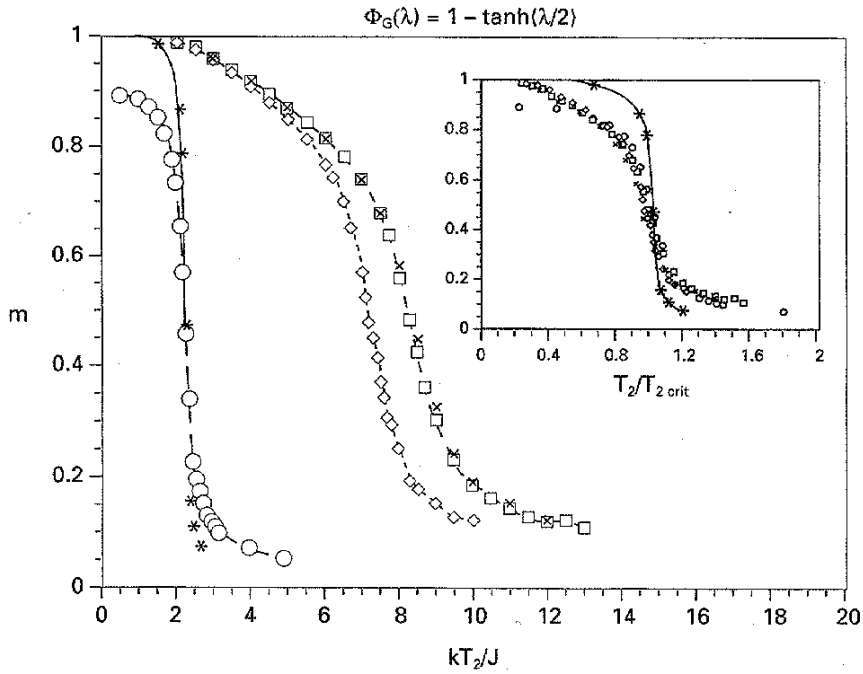

Figure 1. Magnetization m versus $T_2 = \beta_2^{-2}(J/k = 1)$ for the rate: $\Phi_G(\lambda) = 1 - \tanh(\lambda/2)$ and $p = 0.7629...$ The symbols are: $T_1 = \beta_1^{-1} = 0.25$ (×), 0.5 (⊔), 1 (◇) and 2.3 (○). The solid line is the Onsager equilibrium solution for the Ising model and (∗) are the results for the Monte Carlo simulation in order to show the finite size effects. The inset shows the same data but with T_2 scaled according to the critical temperature for each case.

$2.5 \times 10^5 - 5 \times 10^5$ MCS to stabilize the system and to obtain good statistics. One of the relevant macroscopic magnitudes we have measured in the experiment is the *magnetization*:

$$m = \frac{1}{N} \sum_{\underline{x}} s_{\underline{x}}$$

Figures 1 and 2 depict its behavior. We see how the increasing of T_1 decreases the critical temperature. Also, the magnetization tends to 1 when T_2 goes to zero if the dynamics is Φ_V, and whenever $T_1 < T_0^{(c)}$ for Φ_G ($T_0^{(c)}$ is the critical temperature for the ordinary Ising model). When $T_1 > T_0^{(c)}$ for Φ_G, the magnetization does not saturate to 1. In any case we always obtain a second order phase transition.

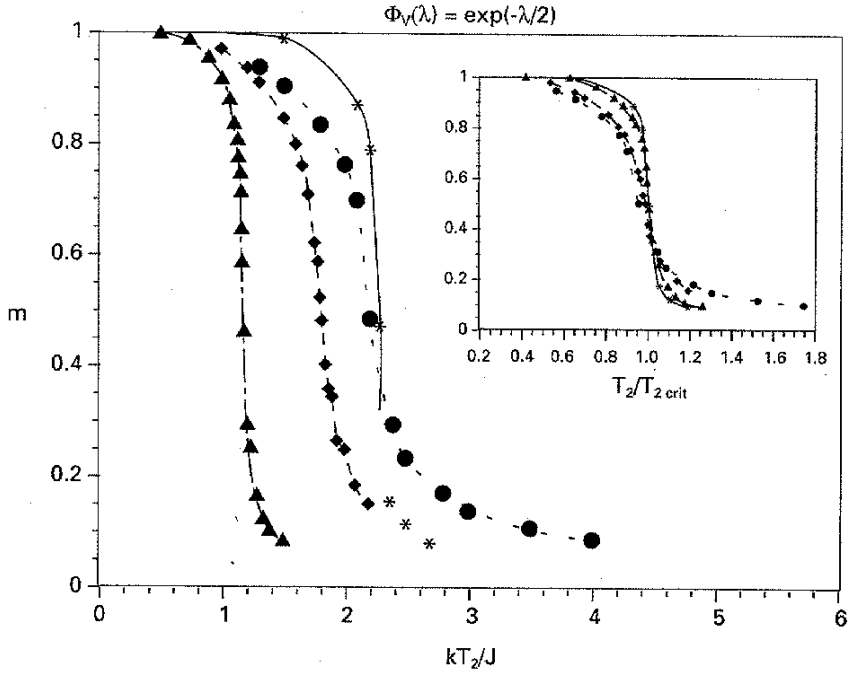

Figure 2. The same as Figure 1 for the rate $\Phi_V(\lambda)=\exp(-\lambda/2)$. The symbols are here: $T_1=2.3$ (●), 2.5 (◆) and 3.5 (▲).

4. Some theory

A simple theoretical approach one may think of to study this class of systems is a kind of mean-field approximation (Muñoz and Garrido, 1993). For systems at equilibrium states this kind of approaches is well defined; they usually consist of neglecting the system fluctuations around its *most probable path* in phase space and/or in breaking down some of the system correlations. If well done, the final results are qualitative similar to the actual system behavior, and they may be improved in a controlled manner by taking into account more fluctuations and/or correlations.

For systems in states away from equilibrium as the above two-temperatures Ising model, the situation is quite different. First, one lacks a general theory which allows for an *a priori* control of the mean-field approach. Second, as we show below, the qualitative results differ in some cases from the Monte Carlo ones.

The starting point is the Bragg-Williams approach to the Ising model. Let N be the number of lattice sites, and N_+ and N_- the total number of spins with values $+1$ and -1 respectively, with $N=N_++N_-$. The total

magnetization is then defined by $M=N_+-N_-=\Sigma_{\underline{x}}s_{\underline{x}}$, and the following relations hold:

$$N_+=\frac{1}{2}(N+M), \qquad N_-=\frac{1}{2}(N-M).$$

The mean-field Hamiltonian is build up by assuming that all lattice pairs interact *via* the same coupling strength, i.e., J/N. Therefore, one has

$$H_0(M)=-\frac{J}{N}\sum_{\underline{x}\underline{y}} s_{\underline{x}}s_{\underline{y}}=-JNm^2 \tag{3.1}$$

where $m=M/N$ is the system magnetization. The probability to find the system with the magnetization m when it is in equilibrium with a thermal bath at temperature β^{-1} is

$$Q_{eq}(m)=\binom{N}{\frac{N(1+m)}{2}}\exp\{\beta JNm^2\}$$

The two-temperatures Ising model in the Bragg-Williams approximation is then defined by equations (2.2) and (2.3) with the mean field Hamiltonian H_0 in (3.1). The master equation (2.2) is originally defined for spins and not for the magnetization. To set up the corresponding one for the magnetization, we define the probability to find the system with magnetization m at time t:

$$Q_t(m)=\sum_{\underline{s}}\delta\left(m-N^{-1}\sum_{\underline{x}}s_{\underline{x}}\right)P_t(\underline{s}), \tag{3.2}$$

where $P_t(\underline{s})$ obeys the Master Equation (2.2). Taking partial derivative with respect to time in both sides of equation (3.2), and using (2.2), we get

$$\frac{\partial}{\partial t}Q_t(m)=\sum_{\mu=\pm 1}\left[c\left(m+\frac{2\mu}{N}\to m\right)Q_t\left(m+\frac{2\mu}{N}\right)-c\left(m\to m+\frac{2\mu}{N}\right)Q_t(m)\right], \tag{3.3}$$

where

$$\begin{aligned} c\left(m+\frac{2\mu}{N}\to m\right)=\frac{N}{2}\left(1+\mu m+\frac{2}{N}\right)\left\{p\Phi\left[4\beta_1 J\left(\mu m+\frac{1}{N}\right)\right]+\right. \\ \left.+(1-p)\Phi\left[4\beta_2 J\left(\mu m+\frac{1}{N}\right)\right]\right\}. \end{aligned} \tag{3.4}$$

The master equation (3.3) can be solved explicitely for $N \to \infty$ (van Kampen, 1981):

$$Q_t(m) = \delta(m - m_t) \tag{3.5}$$

where m_t is the solution of the differential equation:

$$\partial_t m_t = - \sum_{\mu = \pm} (\mu + m_t) [p\Phi(4\beta_1 J \mu m_t) + (1-p)\Phi(4\beta_2 J \mu m_t)] \tag{3.6}$$

The stationary solutions, m_{st}, are found by equating to zero the right hand side of equation (3.6). However, it is more illuminating to write down the latter equation as the dynamics associated with a Hamiltonian system with a potential $U = U(m)$, i.e.

$$\partial_t m_t = - \partial m_t U(m_t) \tag{3.7}$$

where $U(m)$ is defined by integrating the right hand side of (3.6) with respect to m_t. The analytical integration obviously depends on the explicit form of $\Phi(\lambda)$ but we can integrate it by assuming that $\Phi(\lambda)$ admits an analytical expansion around zero. In this case we get:

$$U(m) = U_0 + \sum_{n=0}^{\infty} a_n m^{2n+2}, \tag{3.8}$$

where

$$a_n = \frac{1}{n+1} \left[\frac{\Phi^{(2n+1)}(0)}{(2n+1)!} w(2n+1) + \frac{\Phi^{(2n)}(0)}{(2n)!} w(2n) \right] \tag{3.9}$$

Here,

$$w(n) = p(4\beta_1 J)^n + (1-p)(4\beta_2 J)^n, \tag{3.10}$$

and $\Phi^{(n)}(0)$ is value of the n-th derivative of Φ at zero. We see from equation (3.8) that $m = 0$ will always be the stationary solution of equations (3.6) or (3.7). There are other solutions nearby $m = 0$. For instance, if we consider the potential expansion (3.8) up to m^6, we find that

$$m_{st}^2 = \frac{-a_1 \pm \sqrt{a_1^2 - 3a_0 a_2}}{3a_2} \tag{3.11}$$

is a stationary solution of equation (3.7) whenever $a_1^2 \geqslant 3a_0 a_2$ and the right hand side of equation (3.11) is larger than zero. The local dynamical stability of these solutions is guaranteed by asking that the potential second derivative computed at m_{st} is larger than zero. Then, the stable solutions are:

$$
\begin{aligned}
&m_{st}=0 \quad \text{if} \quad a_0>0 \\
&m_{st}=\pm\left[\frac{-a_1+\sqrt{a_1^2+3|a_0|a_2}}{3a_2}\right]^{1/2} \quad \text{if} \quad a_0<0 \quad \text{and} \quad a_1>0 \\
&m_{st}=\pm\left[\frac{|a_1|+\sqrt{a_1^2+3a_0a_2}}{3a_2}\right]^{1/2} \quad \text{if} \quad a_0<\frac{a_1^2}{3a_2} \quad \text{and} \quad a_1<0
\end{aligned}
\tag{3.12}
$$

There are two different situations depending on the form of the dynamics Φ:

a) $\Phi^{(2)}(0)<1/6$: then, $a_1>0$ $\forall(p, \beta_1, \beta_2)$ wich implies that there is a second order phase transition on the parameter a_0. When $a_0>0$, there is a disordered phase characterized by the value $m_{st}=0$ of the order parameter. This disordered phase persist until $a_0=0$, where it appears continuously an ordered phase characterized by $|m_{st}|>0$. Then, any set of values (p, β_1, β_2) that are solution of the equation $a_0=2-w(1)=0$ define a critical point. It is interesting to remark that a_0 is independent on the explicit form of the dynamics Φ.

b) $\Phi^{(2)}(0)>1/6$: Then, the sign of a_1 can be positive or negative, depending on the values (p, β_1, β_2) choosen. When $a_1>0$, we have the same behavior as in case *a*), that is, a second order phase transition at the critical point defined by $a_0=0$. When $a_1<0$, there is a disordered phase when $a_0>a_1^2/3a_2$, an ordered phase $|m_{st}|>0$ when $a_0<0$, and the coexistence of both phases when $0<a_0<a_1^2/3a_2$. Obviously, this analysis is based on local dynamical stability. Global stability analysis is needed to known exactly which one of the solutions in the coexistence region is globally stable. Anyway, the order parameter in this case is discontinuous with respect to a_0. This behavior is characteristic of a first order phase transition. Finally, the values (p, β_1, β_2) that are simultaneous solution of the equations: $a_0=0$ and $a_1=0$ define a *tricritical point.*

It is also possible to extract the stationary solutions of equation (3.6) when $\beta_2\to\infty$ for a given value of (p, β_1). In order to study this, it is necessary to know the asymptotics of $\Phi(\lambda)$. In general, one can expect that $\Phi(\lambda)\to a\exp\{-b\lambda\}$ when $\lambda\to\infty$. Assuming this behavior, we can show that $m\to1$ if $b<1$, and $m\to m_0<1$ if $b\geqslant1$, when $\beta_2\to\infty$. That is, the order parameter saturates or not to unity depending on the assymptotic form of the dynamical function.

5. Conclusion

In order to compare the above results with the Monte Carlo experiment in section 3, we have solved the implicit equation $\partial_t m_{st}=0$ in (3.6) for the

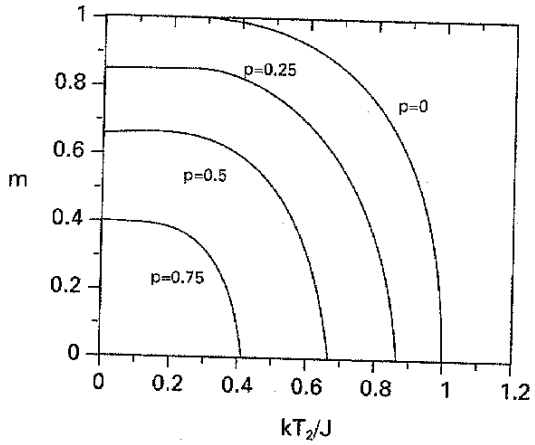

Figure 3. Numerical solution of m_{st} for the mean field equation (3.5) at stationary state, $\partial_t m_{st}=0$, $\Phi_G(\lambda)$, $T_1=2(J/k=1/2)$ and different p values.

two particular dynamics: $\Phi_G(\lambda)=1-\tanh(\lambda/2)$ and $\Phi_V(\lambda)=\exp(-\lambda/2)$. We see inmediately that Φ_G and Φ_V are representative of cases *a*) and *b*) respectively.

Figures 3, 4 and 5 represent the resulting magnetization m versus β_2^{-1} for some fixed values of β_1 and different values of p. In Figures 3 and 4 we observe the expected second order phase transition with a critical temperature of $\beta_{2,c}^{-1}=(1-p)/(1-\beta_1 p)$, which is independent of the dynamical function Φ. We see that $\beta_{1,c}^{-1}\to 0$ when $p\to 0$. It is also noticeable that $\beta_{1,c}^{-1}=1$ for any $\beta_2=1$. The asymptotic behavior of Φ_G guaranties that $m=m_0<1$ for

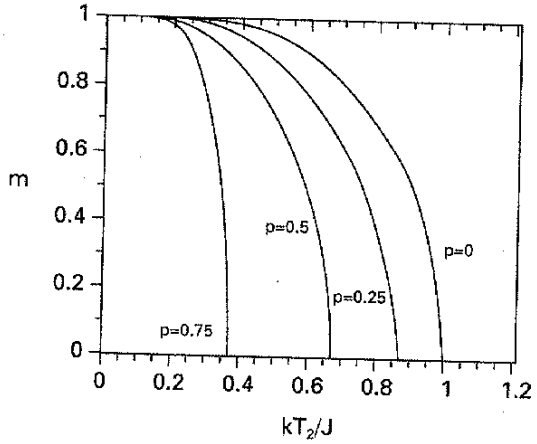

Figure 4. The same as Figure 3 for $\Phi_V(\lambda)$ and $T_1=2$.

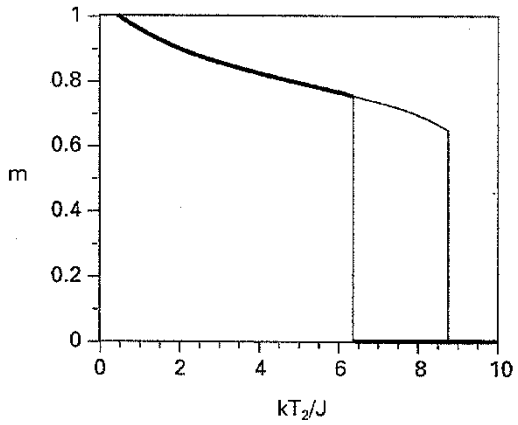

Figure 5. The same as Figure 3 for $\Phi_V(\lambda)$ and $T_1 = 0.25$.

$\beta_1^{-1} = 0$. The qualitative behavior depicted in the figures is similar to the one from the Monte Carlo simulation. However, there are some important differences:

1. The mean field theory predicts that no longer exists a second order phase transition below some critical value $T_1^{(c)} = p$. Instead, an ordered state appears for *all* T_2 values.
2. For the Φ_V dynamics, there exists a tricritical point and, therefore, a first order phase transition needs to occur in the parameter space of the system.

These two qualitative effects do not occur in the computer simulation, where only second order phase transitions are apparent for any values of p, T_1 and T_2.

Summing up, we have seen explicitely with this example that some of the theoretical results are qualitatively correct while others describe *new*, probably spurious phenomena. The *a priori* control of approximations when dealing theoretically with nonequilibrium systems is an open question in general. In fact mean field approximations may in some cases produce an incorrect description. This is probably related to the fact that fluctuations do not play in nonequilibrium systems the same role as in equilibrium, e.g., a fluctuation-dissipation relation may not hold, in general, away from equilibrium.

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