

Relaxation to Equilibrium in Non-Conservative Lattice Systems.

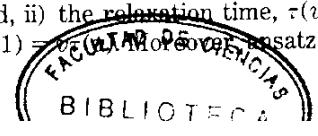
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Abstract. - We present a new approach to study relaxation towards equilibrium of lattice model systems with non-conserved order parameter and spatial homogeneity in time. The theory is mainly based on a simple scaling relation for the relaxation time. This relation, when true, implies that the system time-probability distribution has a Gibbsian form when it is near the final equilibrium state. We apply the theory to the study of the q -state Potts model in one dimension. Besides, we present a Monte Carlo computer-simulation study that provides a direct strong justification of the hypothesis and results of the theory.

It is well known that a system in contact with a thermal bath and otherwise isolated will relax, from an arbitrary initial state, towards an equilibrium final one. The study of this kind of processes is interesting because relaxation towards equilibrium is present everywhere in Nature. Moreover, the physics involved is non-equilibrium statistical mechanics, which is a subject strongly in need of a systematic effort that closes it to the level of development that equilibrium statistical mechanics has today. New theoretical treatments for relaxation processes, as the one reported here, are helpful contributions to the construction of that theory. In this letter, we will present a new approach designed for spatially homogeneous dynamical processes in which the order parameter is not conserved. To study these processes, we construct a new dynamical mechanism composed by the competition of the original non-conserved dynamical process with a new dynamics that conserves the order parameter. For example, for the Ising model, this new dynamical mechanism could be the competition of a Glauber spin-flip dynamics [1] and an exchange Kawasaki dynamics [2], both acting simultaneously at the same temperature and with probability $v \in [0, 1]$ and $1 - v$, respectively. The approach we explain below is based on two main ansätze: i) when $v \rightarrow 0$, the system relaxes effectively following a sequence of quasi-equilibrium states each one characterized by some fixed value of the order parameter and, ii) the relaxation time, $\tau(v)$, for the new dynamical mechanism, has the scaling property: $\tau(1) = \tau(v) \tau(v)^{-1}$ (ansatz i)



is expected to be true for systems at homogeneous states, far from critical points, where it is guaranteed that any local fluctuation could relax by diffusion in a microscopic time scale [3,4]. Therefore, our theory is mainly based on ansatz ii). We present below some arguments meant to convince the reader that this ansatz is essentially correct. Moreover, to reinforce such arguments, we have carried out an extensive Monte Carlo computer experiment for the one-dimensional Potts model and we have checked directly ii). Therefore, assuming that both ansatz are true, we may compute $\tau(1)$ as the limit: $\lim_{v \rightarrow 0} v\tau(v)$. Finally, we conclude that for all v and near the equilibrium state, the system relaxes by following a sequence of quasi-equilibrium states, and its characteristic relaxation time agrees with a well-known upper bound coming from Jensen's inequality [5].

Let us begin describing our model. In each node of a d -dimensional cubic lattice, $\mathbf{x} \in Z^d$, there is a state variable, $s(\mathbf{x})$, which can take a finite number of possible values. The system state configuration is given by $\mathbf{s} = \{s(\mathbf{x}), \mathbf{x} \in Z^d\}$, and its evolution is specified by means of a Markovian mechanism. Therefore, it is completely characterized by the probability measure of finding the state configuration \mathbf{s} at time t , say $P_t(\mathbf{s})$, which obeys the master equation

$$\frac{\partial P_t(\mathbf{s})}{\partial t} = \sum_{\mathbf{x}} \sum_{\sigma \neq s(\mathbf{x})} [c(\mathbf{s}^{\mathbf{x}, \sigma} \rightarrow \mathbf{s}) P_t(\mathbf{s}^{\mathbf{x}, \sigma}) - c(\mathbf{s} \rightarrow \mathbf{s}^{\mathbf{x}, \sigma}) P_t(\mathbf{s})] \equiv LP_t(\mathbf{s}), \quad (1)$$

where $\mathbf{s}^{\mathbf{x}, \sigma}$ stands for the configuration \mathbf{s} with the state at site \mathbf{x} changed by σ and $c(\mathbf{s} \rightarrow \mathbf{s}')$ is the transition probability per unit time from the state \mathbf{s} to \mathbf{s}' . To guarantee that the stationary state is an equilibrium Gibbsian one, we choose the rate $c(\mathbf{s} \rightarrow \mathbf{s}')$ having the so-called *detailed balance property*:

$$[c(\mathbf{s} \rightarrow \mathbf{s}') = c(\mathbf{s}' \rightarrow \mathbf{s}) \exp[\beta(H(\mathbf{s}) - H(\mathbf{s}'))], \quad (2)$$

where $H(\mathbf{s})$ is the system Hamiltonian. Let $f(\mathbf{s}, \mathbf{x})$ be a function of a finite number of state variables near \mathbf{x} , e.g. $f = s(\mathbf{x}), s(\mathbf{x})s(\mathbf{y}), \dots$. Its associated macroscopic observable, f_t , is defined by

$$f_t = \langle f(\mathbf{s}, \mathbf{x}) \rangle_t \equiv \sum_{\mathbf{s}} f(\mathbf{s}, \mathbf{x}) P_t(\mathbf{s}), \quad (3)$$

where we have omitted the space dependence because we are going to study only relaxation processes which are spatially homogeneous all over the time. The f_t functional dependence on t is usually quite complex but, for time large enough, it is expected to be of the exponential type [6]. The characteristic relaxation time for the process is consequently given by

$$\frac{1}{\tau} = \min_f \lim_{t \rightarrow \infty} \left[-\frac{1}{\tau} \ln(|f_t - f_e|) \right] > 0. \quad (4)$$

Let $m(\mathbf{s}, \mathbf{x})$ be one of the functions having smaller relaxation time. Let us define a new dynamical mechanism: with probability v the system evolves by using the non-conserved dynamics given by the operator L in eq. (1) and with probability $1 - v$ the evolution is done with a new dynamics L_m , which conserves the value $m = \sum_{\mathbf{x}} m(\mathbf{s}, \mathbf{x})$. L_m is built in such a form that the stationary state for this dynamical process is the one of L , i.e. an equilibrium state. The master equation associated to this new mechanism is

$$\frac{\partial P_t(\mathbf{s}; v)}{\partial t} = [vL + (1 - v)L_m] P_t(\mathbf{s}; v). \quad (5)$$

For $v = 1$ we obviously recover the description given by eq. (1). From eqs. (3) and (5) we may

write down the time differential equation for the evolution of $m_t(v)$:

$$\frac{dm_t}{dt} = v \left\langle \sum_{s'} [m(s'; \mathbf{x}) - m(\mathbf{s}; \mathbf{x})] c(\mathbf{s} \rightarrow \mathbf{s}') \right\rangle_t^v. \quad (6)$$

Our first assumption is that, as happens with $m_t(1)$, $m_t(v)$ still has slower relaxation time, $\tau(v)$, for all v . This point, which is not at all obvious, is, however, reasonable because the conservative dynamics is delaying the $m_t(v)$ evolution on the one hand, while favouring the system thermalization, on the other. This breaks correlations, and, therefore, makes the evolution easier. Assuming that this ansatz holds for large times and near the equilibrium final state, the evolution will be dominated by the $m_t(v)$ behaviour for times large enough. In this situation, our second assumption is that the relaxation time has the scaling property

$$\tau(1) = v\tau(v). \quad (7)$$

This is so because, if the system chooses to evolve under the conservative dynamics L_m , with probability $(1 - v)$, it is wasting time and not evolving. Then, only the fraction v of the total time evolution is really effective. Thus, in a time scale vt , the order parameter evolves as if the conservative part of the dynamics did not exist, implying that the relaxation time has the scaling property (7).

Therefore, to get the $\tau(1) \equiv \tau$ expression, we only need to find a single v for which we know how to solve eq. (6). This is the case when we rescale the time by v , i.e. $t' = vt$, and then we do the limit $v \rightarrow 0$ in the master equation (5). In this limit, and because the conservative part of the dynamics is infinitely faster than the original one, the system probability measure has an equilibrium type of structure when we are far from critical points, i.e.

$$P'_v(\mathbf{s}) = Z_v^{-1} \exp \left[-\beta H(\mathbf{s}) - \mu_v \sum_{\mathbf{x}} m(\mathbf{s}; \mathbf{x}) \right], \quad (8)$$

where

$$Z_v = \sum_{\mathbf{s}} \exp \left[-\beta H(\mathbf{s}) - \mu_v \sum_{\mathbf{x}} m(\mathbf{s}; \mathbf{x}) \right], \quad (9)$$

and μ_v is a chemical potential which fixes the global value of the order parameter to m_v , i.e.

$$m_v = \sum_{\mathbf{s}} m(\mathbf{s}; \mathbf{x}) P'_v(\mathbf{s}). \quad (10)$$

Equations (8), (9) and (10) give us a closed set of equations in which the only unknown is m_t . From it we can get the order parameter relaxation time in the limit $\tau' \equiv \lim_{v \rightarrow 0} v\tau(v)$. Then, after applying the scaling relation (7), we find the relaxation time for the original problem by means of $\tau = \tau'$. Notice that for large times and for all v , the distribution $P_t(\mathbf{s}; v) = P'_{vt}(\mathbf{s})$ plugged into (6) gives us $\tau(v)$ with the scaling property (7). Therefore, we may conclude that for any v the system evolves through a sequence of quasi-equilibrium states when it is near equilibrium. Moreover, it is a matter of algebra to check that the τ obtained agrees with a well-known upper bound coming from Jensen's inequality [5] (we thank a referee for pointing out this fact).

Let us apply the above scheme to check whether or not the scaling relation (7) holds for the one-dimensional q -state Potts model in order to find its relaxation time τ . The model Hamiltonian is

$$H(\mathbf{s}) = -J \sum_{\mathbf{x}} \delta(s(x), s(x')), \quad (11)$$

where $s(x) = 1, 2, \dots, q$, and $\delta(z, y)$ is the Kronecker delta. We choose a well-known family of local dynamics given by

$$c(s \rightarrow s') = \Phi(\beta[H(s') - H(s)]), \quad (12)$$

where $\Phi(\lambda)$ is an arbitrary function with the property: $\Phi(\lambda) = \exp[-\lambda]\Phi(-\lambda) > 0$. Usual choices for Φ are: $\Phi(\lambda) = \min(1, \exp[-\lambda])$ [7], $\Phi(\lambda) = 1 - \text{tgh}(\lambda/2)$ [1], and $\Phi(\lambda) = \exp[-\lambda/2]$ [8]. We assume for this model: $m(s; x) = s(x)$, as a natural extrapolation from the well-known exact analytic time behaviour for the one-dimensional Ising model ($q = 2$) with the Glauber rate. Using eqs. (4), (6) and (8), we get

$$\tau' = \tau(1) = \tau = \frac{(s + q - 1)^2(2s - 2 + q)}{q^2[2\Phi(-2\beta J) + 4(q - 2)\Phi(-\beta J) + (q - 2)^2 + 2s]}, \quad (13)$$

where $s = \exp[\beta J]$ and we have taken $\Phi(0) = 1$. The latter expression at high temperatures, i.e. ($\beta \rightarrow 0$), behaves as

$$\tau = \frac{1}{q} + \frac{2\beta J}{q^2} + O(\beta^2), \quad (14)$$

where we have assumed that $\Phi(\lambda)$ is an analytic function around zero. At infinite temperature ($\beta = 0$), the system needs q -jumps between different states to forget the initial one, implying $\tau = q^{-1}$. Notice that at first order in β , the behaviour is independent of the dynamics and if the coupling constant J is ferromagnetic ($J > 0$), the decay is slower than in the antiferromagnetic case ($J < 0$). This phenomenon is related with the space homogeneous initial conditions: since initially we have a non-zero value for the order parameter, during the evolution, the ferromagnetic couplings tend to conserve it, while the antiferromagnetic ones tend to destroy it. We have also studied the behaviour of τ at low temperatures, but we expect to publish those results in a future paper.

Because all the theory and results depend essentially on the scaling assumption (7), we wanted to check the latter and the τ analytical expression (13) by means of a Monte Carlo computer experiment for the one-dimensional Potts model. Our procedure is essentially the usual in Monte Carlo computer simulations. A site x in a given lattice is randomly chosen to attempt a process. This can be a change of the state of the site, or, alternatively, an exchange of this state with one of its neighbours chosen at random; being v the probability for the first process, and $1 - v$ the probability for the exchange. The probability of occurrence for any of these processes is given by $\Phi(\Delta H)$, where ΔH is the energy difference between the final and initial states. This algorithm is repeatedly iterated to obtain the evolution of the system. Most of the computer simulations have been done on a linear chain with 3600 sites, periodic boundary conditions and all the points in the same state as the initial configuration. Some simulations were done on systems with 1200 sites in order to study finite size effects, and they did not reveal any relevant correction to the results. We also considered the case when not all the particles were initially in the same state, finding the same relaxation time as before in all cases. For each case we did 500 evolutions with the same initial condition, but with different sequences of random numbers. We averaged them to get a smooth function and we fitted an exponential behaviour, getting τ from it. We have carried out computer simulations with $v = \{0.05, 0.1, 0.2, 0.4, 0.7, 1\}$, $|\beta J| = \{1/8, 1/4, 1/3, 1/2, 3/4, 1\}$ with $J > 0$ and $J < 0$, with the Metropolis [7], Glauber [1] and van Beijeren and Schulman (VBS) [8] rates, and with $q = 2$ and 3. Some of the results are shown in fig. 1-3. From these figures it is clear that: a) the τ scaling behaviour with v holds for all the dynamics, temperatures, coupling constants, and q studied, and b) the analytic solution given by eq. (13) fits the

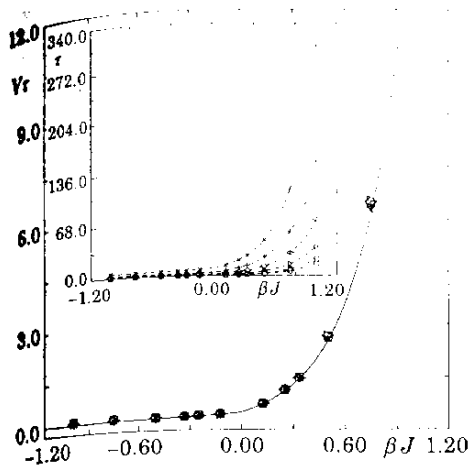


Fig. 1.

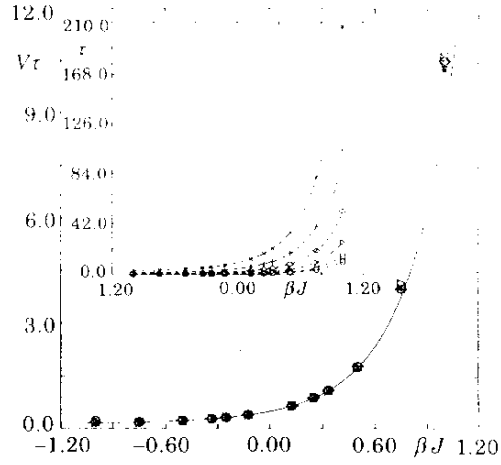


Fig. 2.

Fig. 1. - Scaled relaxation time $v\tau$ vs. the inverse temperature for the Metropolis dynamics, $\phi(\lambda) = \min(1, \exp[-\lambda])$, $q = 2$ and different v values: $\circ v = 1$, $\square v = 0.7$, $\triangle v = 0.4$, $\diamond v = 0.2$, $+ v = 0.1$ and $\times v = 0.05$. The theoretical function given by eq. (13) for this dynamics and q is represented by the solid line. The inset reproduces the very same data without τ scaling. The dashed lines joining the points are only guides to the eye.

Fig. 2. - The same as fig. 1 but for VBS dynamics, $\phi(\lambda) = \exp[-\lambda]$, and $q = 2$.

computer simulation results quite well in all cases. It is worthy to note that eq. (13) has no free parameters to be fitted.

In conclusion, we have presented a new approach to study relaxation to equilibrium in non-conservative lattice systems. The hypothesis on which our treatment is based: the quasi-equilibrium probability measure when $v \rightarrow 0$ and the scaling of the relaxation time with v , appear as good ansätze on the base of the analysis of the Monte Carlo computer experiment. As a result we conclude that, in general, the system relaxes to the equilibrium

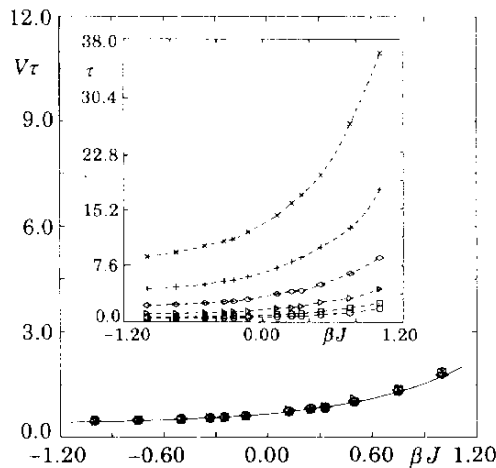


Fig. 3. - The same as fig. 1 but for VBS dynamics and $q = 3$.

by following those quasi-equilibrium states *for all v*. Our approach has a general formulation that, being independent of dimensionality, it allows the analytical computation of the relaxation time whenever the solution is known. This is a motivation for similar studies of more complex cases. In particular, we are actually working on the case of the two-dimensional Ising model. Some preliminary computer-simulation results confirm that the scaling behaviour still holds in this case. We hope that the theory presented here will be an useful alternative approach to deal with relaxation phenomena.

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