Journal of Statistical Physics, Vol. 41, Nos. 1/2, 1985

Detailed Balance and Critical Slowing Down for Classical Lattice Systems

R. Alicki,[1,2] M. Fannes,[1,3] and A. Verbeure[1]

Received April 4, 1985; revision received May 28, 1985

For classical lattice systems we prove rigorously a relation between the fluctuations and the relaxation times for a dynamics given by a detailed balance semigroup. In particular we give a rigorous proof of the conventional theory of critical slowing down.

KEY WORDS: Detailed balance; fluctuations; critical slowing down; Ising systems.

1. INTRODUCTION

For the study of the approach to equilibrium in classical lattice models the Glauber dynamics[1] has become rather a theory than a model. Its essential feature is that it describes transitions from one state to another with a probability which is in correspondence to the one for its inverse transition. Mathematically this property of a Markovian semigroup evolution is expressed by its self-adjointness with respect to the equilibrium state, which means that the transition probabilities are proportional to the Boltzmann factor. This property is known as the condition of detailed balance.

The main interest in these processes comes from their property of describing the approach to equilibrium.[2] Here we are particularly interested in the characteristics of the relaxation to equilibrium under these processes. It is expected by the conventional phenomenological theories[3,4] that one has an exponential decay law to equilibrium.

---

[1] Instituut voor Theoretische Fysica, Universiteit Leuven, B-3030 Leuven, Belgium.

[2] On leave of absence from Institute of Theoretical Physics and Astrophysics, Gdansk University, Poland.

[3] Bevoegdverklaard Navoser NFWO, Belgium.

0022-4715/85/1000-0263$04.50/0

In this paper we prove a rigorous relation between the fluctuations and the decay rate of physical quantities for systems satisfying the detailed balance condition. The proof is given for a large class of classical lattice systems. In particular we prove that the lifetime of an observable is governed by the fluctuation of that observable. For equilibrium states of systems showing a phase transition this yields a rigorous relation between the critical exponents of the fluctuation and the lifetime.

As an illustration we sketch examples of evolutions generated by spin-flips and exchange of the spins, and examples of magnetization and energy fluctuations.

2. FORMULATION OF THE PROBLEM

We consider a classical system of particles attached to the sites of a countable set S. It includes the ordinary lattices with regular and irregular structure. At each site $j \in S$ we describe the particles by means of their phase space K, which we suppose to be a compact topological space. Given Λ a finite subset of S, denote by K_Λ the product $\prod_{j\in\Lambda} K_j$, where K_j is a copy of K attached to the site $j \in \Lambda$. The space K_Λ is the configuration space of the volume Λ. Denote by $C(K_\Lambda)$ the set of real-valued continuous functions on K_Λ. Then $C(K_S)$ represents the algebra of observables of our system, it is the uniform closure of the set $\cup_\Lambda C(K_\Lambda)$. The states of the system are given by the probability measures ω on K_S and we use the notation: $\langle f\rangle = \int_{K_s} f\, d\omega$.

Let Γ be a family $\{\Lambda\}$ of finite subsets Λ of S. For each $\Lambda \in \Gamma$, let L_Λ be a map of $C(K_S)$ into itself such that

$$\text{(i)}\quad L_\Lambda f = 0 \text{ for all } f \in C(K_{S\setminus\Lambda}) \tag{1}$$

$$\text{(ii)}\quad \text{For all } \Lambda,\ L_\Lambda \text{ is bounded.} \tag{2}$$

$$\text{(iii)}\quad L_\Lambda(f^2) \geqslant 2f L_\Lambda(f), \qquad f \in C(K_\Lambda) \qquad \text{(dissipativity)} \tag{3}$$

$$L_\Lambda(\mathbb{1}) = 0 \qquad \text{(unity preserving)}$$

$$\text{(iv)}\quad \forall i \in S\colon \sum_{\substack{\Lambda\in\Gamma\\ i\in\Lambda}} \|L_\Lambda\| < \infty \tag{4}$$

Now we define

$$L = \sum_{\Lambda\in\Gamma} L_\Lambda \tag{5}$$

on the domain $\mathscr{D}(L) = \{f \in C(K_S) \mid f \in C(K_\Lambda)$ for some finite $\Lambda\}$. If $f \in C(K_\Lambda)$, then

$$Lf = \sum_{\substack{\Lambda' \in \Gamma \\ \Lambda' \cap \Lambda \neq \phi}} L_{\Lambda'} f$$

and it is obvious that

$$\begin{aligned} \left\| \sum_{\substack{\Lambda' \in \Gamma \\ \Lambda' \cap \Lambda \neq \phi}} L_{\Lambda'} f \right\| &\leqslant \sum_{\substack{\Lambda' \in \Gamma \\ \Lambda' \cap \Lambda \neq \phi}} \|L_{\Lambda'} f\| \\ &\leqslant \sum_{\substack{\Lambda' \in \Gamma \\ \Lambda' \cap \Lambda \neq \phi}} \|L_{\Lambda'}\| \, \|f\| \\ &\leqslant \sum_{i \in \Lambda} \left(\sum_{\substack{\Lambda' \in \Gamma \\ i \in \Lambda'}} \|L_{\Lambda'}\| \right) \|f\| \end{aligned}$$

which is finite because of condition (4).

The map L is said to satisfy the *condition of detailed balance with respect to a* measure ω on K_S if for all $f, g \in C(K_S)$

$$\text{(v)} \quad \langle f L_\Lambda g \rangle = \langle (L_\Lambda f)\, g \rangle \tag{6}$$

holds for all $\Lambda \in \Gamma$.[5,6]

Let $\mathscr{H}_\omega = L^2(C(K_S), \omega)$ be the complex Hilbert space with a usual scalar product $(f, g) = \langle \bar{f} g \rangle$, then the map L, defined by (5), induces a symmetric, negative definite, densely defined operator $\hat{L}$. $\hat{L}$ is well defined because, let $f \in \mathscr{D}(L)$ such that $\langle |f|^2 \rangle = 0$ then by (6) $\langle |L_\Lambda f|^2 \rangle = \langle \bar{f} L_\Lambda^2 f \rangle \leqslant \langle |f|^2 \rangle^{1/2} \langle |L_\Lambda^2 f|^2 \rangle^{1/2}$ for all $\Lambda \in \Gamma$.

Hence there exists a unique self-adjoint, negative definite extension (Friedrich's extension), again denoted by L, of $\hat{L}$.[7] Therefore

$$\gamma_t = \exp tL, \qquad t \geqslant 0 \tag{7}$$

is a well-defined strongly continuous semigroup of self-adjoint contractions on $\mathscr{H}_\omega$ leaving invariant the unit function $\mathbb{1}$.

The semigroup (7) yields a dynamics of the system satisfying the detailed balance property with respect to a probability measure ω.

Now we are interested in the behavior of what is called the autocorrelation functions. This becomes in our framework the following functions of time t: for each $\psi \in \mathcal{H}_\omega$ such that $(\psi, \mathbb{1}) = 0$ we study the function

$$t \in \mathbb{R}_+ \to f_\psi(t) = \frac{(\psi, \gamma_t \psi)}{(\psi, \psi)} \tag{8}$$

Let $\{E(\lambda) \mid \lambda \in \mathbb{R}^+\}$ be the spectral resolution of $-L$; then

$$f_\psi(t) = \int_0^\infty e^{-\lambda t}\, dm_\psi(\lambda) \tag{9}$$

where

$$dm_\psi(\lambda) = d\,\frac{(\psi, E(\lambda)\,\psi)}{(\psi, \psi)}$$

As usual the mean relaxation time τ_ψ is defined by

$$\tau_\psi = \int_0^\infty dt\, f_\psi(t) = \int_0^\infty \frac{1}{\lambda}\, dm_\psi(\lambda) \tag{10}$$

and the mean relaxation constant v_ψ by

$$v_\psi = -\left.\frac{df}{dt}\right|_{t=0} = \int_0^\infty \lambda\, dm_\psi(\lambda) \tag{11}$$

By convexity of the exponential one gets from Jenssen's inequality

$$\begin{aligned} f_\psi(t) &= \int_0^\infty e^{-\lambda t}\, dm_\psi(\lambda) \\ &\geqslant \exp\left[-\int_0^\infty \lambda\, dm_\psi(\lambda)\, t\right] = \exp(-v_\psi t) \end{aligned} \tag{12}$$

Therefore

$$\tau_\psi \geqslant \frac{1}{v_\psi}$$

In the following we relate for an observable its mean relaxation constant with its fluctuation.

3. CRITICAL SLOWING DOWN

We consider a particular class of observables: let ϕ be a map from the finite subsets of S into $\bigcup_\Lambda C(K_\Lambda)$, i.e., $X \to \phi(X)$, then for each subset Δ of S we construct the observable

$$\Phi_\Delta = \sum_{X \subset \Delta} \phi(X) \tag{13}$$

Lemma 3.1. Let ω be a state of $C(K_S)$ and L a detailed balance generator with respect to ω [see (7)] satisfying the condition

$$\sup_{j \in S} \sum_{k \in S} \sum_{\substack{\Lambda \in \Gamma \\ j,k \in \Lambda}} \|L_\Lambda\| \leqslant M < \infty \tag{14}$$

then for each observable Φ_Δ (13), satisfying

$$\sup_{j \in S} \sum_{k \in S} \sum_{\substack{X \subset S \\ j,k \in X}} \|\phi(X)\| = Q < \infty \tag{15}$$

one has

$$0 \leqslant -(\Phi_\Delta, L\Phi_\Delta) \leqslant MQ^2 \, |\Delta|$$

where $|\Delta|$ is the number of elements of Δ.

Proof. Let

$$a_{jk} = \sum_{\substack{X \subset S \\ j,k \in X}} \|\phi(X)\|$$

$$b_{jk} = \sum_{\substack{\Lambda \in \Gamma \\ j,k \in \Lambda}} \|L_\Lambda\|$$

$$c_{jk} = \frac{1}{|\Delta|} \chi_\Delta(j)\, \chi_\Delta(k)$$

where

$$\chi_\Delta(j) = \begin{cases} 1 & \text{if } j \in \Delta \\ 0 & \text{if } j \notin \Delta \end{cases}$$

By definition $c = (c_{jk})$ is a one-dimensional projection operator on $l^2(S)$

and by (14) and (15), $b=(b_{jk})$ and $a=(a_{jk})$ are bounded operators on $l^2(S)$, indeed

$$\|a\| \leqslant \sup_{j\in S} \sum_{k\in S} |a_{jk}| = Q < \infty$$

$$\|b\| \leqslant \sup_{j\in S} \sum_{k\in S} |b_{jk}| \leqslant M < \infty$$

Now

$$\begin{aligned} |(\Phi_\Delta, L\Phi_\Delta)| &\leqslant \sum_{\Lambda\in\Gamma} \sum_{\substack{X\subset S\\ X\cap\Lambda\neq\phi\\ X\cap\Delta\neq\phi}} \sum_{\substack{Y\subset S\\ Y\cap\Lambda\neq\phi\\ Y\cap\Delta\neq\phi}} \|\phi(X)\|\,\|\phi(Y)\|\,\|L_\Lambda\| \\ &\leqslant \sum_{\Lambda\in\Gamma} \Big(\sum_{\substack{j\in\Lambda\\ k\in\Delta}} a_{jk}\Big)\Big(\sum_{\substack{j'\in\Lambda\\ k'\in\Delta}} a_{j'k'}\Big)\|L_\Lambda\| \\ &= |\Delta| \sum_{j,k,j',k'\in S} a_{jk}a_{j'k'} \sum_{\substack{\Lambda\in\Gamma\\ j,j'\in\Lambda}} \|L_\Lambda\| \frac{1}{|\Delta|}\chi_\Delta(k)\,\chi_\Delta(k') \\ &= |\Delta| \operatorname{tr} acab \leqslant |\Delta|\,\|a\|^2\,\|b\| \leqslant Q^2 M\,|\Delta| \end{aligned}$$

This proves the lemma. ▌

Theorem 3.2. Let ω be a measure on K_S and γ_t a detailed balance evolution with respect to ω [see (7)], then for each finite subset Δ of S one has

$$\frac{(\Phi_\Delta, \gamma_t\Phi_\Delta) - \langle\Phi_\Delta\rangle^2}{\langle(\Phi_\Delta - \langle\Phi_\Delta\rangle)^2\rangle} \geqslant \exp\left[-\frac{MQ^2\,|\Delta|\,t}{\langle(\Phi_\Delta - \langle\Phi_\Delta\rangle)^2\rangle}\right]$$

where Φ_Δ is as in (13), M as in condition (14) Section 2, and ϕ is as in (15).

Proof. Using formula (12) with $\psi = \Phi_\Delta - \langle\Phi_\Delta\rangle$ one gets

$$\frac{(\Phi_\Delta, \gamma_t\Phi_\Delta) - \langle\Phi_\Delta\rangle^2}{\langle(\Phi_\Delta - \langle\Phi_\Delta\rangle)^2\rangle} \geqslant \exp\frac{(\Phi_\Delta, L\Phi_\Delta)}{\langle(\Phi_\Delta - \langle\Phi_\Delta\rangle)^2\rangle}$$

The theorem follows by Lemma 3.1. ▌

Next we specialize to ω being an equilibrium measure ω_β at some inverse temperature $\beta = 1/kT$.

Suppose L is a generator of a dynamical semigroup given by a sum of local ones as in (5). If L is supposed to satisfy the detailed balance condition with respect to ω_β, then L will depend on β, we denote it by L_β.

Furthermore we are particularly interested in systems showing a phase transition at a certain temperature β_c, called critical temperature. Moreover we assume that the phase transition manifests itself by the occurrence of abnormal fluctuations when $\beta \to \beta_c$, i.e., there exists at least one observable of the type as given in (13) such that the fluctuation

$$\lim_{\Delta \to S} \frac{\langle (\Phi_\Delta - \langle \Phi_\Delta \rangle)^2 \rangle}{|\Delta|} \equiv g(\beta) \tag{16}$$

exists for all β in an interval U containing β_c and $\beta \neq \beta_c$, and such that $g(\beta)$ diverges at $\beta = \beta_c$.

Moreover, we consider generators $L_{\beta,\Lambda}$, $\Lambda \in \Gamma$ such that the bound M in (14) is uniform for all $\beta \in U$.

Corollary 3.3. (Critical slowing down). Let ω_β be an equilibrium state of the system showing a phase transition at β_c of the type described above. Take $\beta \in U$, an interval containing β_c, and let $\gamma_t^\beta = e^{tL_\beta}$ be a detailed balance evolution with respect to ω_β; then

$$\lim_{\Delta \to S} \inf \frac{(\Phi_\Delta, \gamma_t^\beta \Phi_\Delta) - \langle \Phi_\Delta \rangle^2}{\langle (\Phi_\Delta - \langle \Phi_\Delta \rangle)^2 \rangle} \geqslant \exp\left[-\frac{MQ^2 t}{g(\beta)} \right]$$

where $g(\beta)$ is the fluctuation of Φ given by (16). In particular

$$0 \leqslant \operatorname{Inf} \{ -\sigma \mid \sigma \in \operatorname{Spectr} L_\beta,\ \sigma \neq 0 \} \leqslant \frac{MQ^2}{g(\beta)}$$

or the spectral gap of L_β is bounded by the inverse of the fluctuation of Φ. Hence if $\beta \to \beta_c$ we observe the critical slowing down of the autocorrelation function.

Proof. The corollary is an immediate consequence of the theorem and the assumptions. ∎

In the usual theories on critical slowing down one assumes the existence of the critical exponents

$$\gamma_\pm = \lim_{T - T_c \to 0_\pm} -\frac{\log g(\beta)}{\log |T - T_c|}$$

Using definition (11)

$$\nu_{\Phi_\Delta - \langle \Phi_\Delta \rangle} = -\frac{(\Phi_\Delta, L_\beta \Phi_\Delta)}{\langle (\Phi_\Delta - \langle \Phi_\Delta \rangle)^2 \rangle}$$

Assume that there exists $\varepsilon > 0$ such that

$$l_\beta = \lim_{\Delta \to S} -\frac{(\Phi_\Delta, L_\beta \Phi_\Delta)}{|\Delta|} > \varepsilon \tag{17}$$

then using (16)

$$v_\beta = \lim_{\Delta \to S} v_{\Phi_\Delta - \langle \Phi_\Delta \rangle} = l_\beta / g(\beta)$$

By Lemma 3.1, l_β is uniformly bounded and hence

$$\lim_{T - T_c \to 0_\pm} \frac{\log v_\beta}{\log |T - T_c|} = - \lim_{T - T_c \to 0_\pm} \frac{\log g(\beta)}{\log |T - T_c|} = -\gamma_\pm \tag{18}$$

yielding a rigorous proof of what is called the conventional theory of critical slowing down.[3,4]

We close the paper with some illustrations. Let $S = \mathbb{Z}^\nu$ the cubic lattice in ν dimensions and $K = \{0, 1\}$, i.e., we have a lattice gas or a lattice occupied by spin-1/2 particles. Consider an interaction Hamiltonian of the type

$$H_\Lambda = \sum_{i,j \in \Lambda} J(|i - j|)\, \sigma_i \sigma_j + b \sum_{i \in \Lambda} \sigma_i$$

where the σ_i are the spin variables and where the coupling constants satisfy

$$\sum_{j \in \mathbb{Z}^\nu} |J(j)| < \infty \tag{19}$$

Consider

$$\Gamma = \mathbb{Z}^\nu \qquad \text{and} \qquad \tau_k (k \in \mathbb{Z}^\nu)$$

the spin-flip transformation at the lattice site $k \in \mathbb{Z}^\nu$:

$$\begin{aligned} \tau_k \sigma_i &= \sigma_i \qquad && \text{if} \quad i \neq k \\ &= -\sigma_k && \text{if} \quad i = k \end{aligned}$$

Denote by

$$h(\tau_k) = \lim_{\Lambda \to \mathbb{Z}^\nu} \tau_k H_\Lambda - H_\Lambda$$

the relative Hamiltonian for the spin flip τ_k. It is well defined because of condition (19). Take

$$L = \sum_{j \in \mathbb{Z}^\nu} L_j \tag{20}$$

where

$$L_k = e^{-(\beta/2)h(\tau_k)}(\tau_k - 1)$$

then L defines the usual Glauber dynamics. On the other hand consider the set of all pairs (i, j), $(i \neq j)$ of elements in $\mathbb{Z}^\nu$ and τ_{ij} the permutation transformation

$$\tau_{ij}\sigma_j = \sigma_i, \qquad \tau_{ij}\sigma_i = \sigma_j, \qquad \tau_{ij}\sigma_k = \sigma_k \qquad \text{if} \quad k \neq i, j$$

Again let

$$h(\tau_{ij}) = \lim_{\Lambda \to \mathbb{Z}^\nu} \tau_{ij} H_\Lambda - H_\Lambda$$

be the relative Hamiltonian for the transformation τ_{ij} and put

$$L = \sum_{i \in \mathbb{Z}^\nu} \sum_{\substack{j \in \mathbb{Z}^\nu \\ j \neq i}} L_{i,i+j} \tag{21}$$

where

$$L_{i,j} = \lambda_{j-i} e^{-(\beta/2)h(\tau_{ij})}(\tau_{ij} - 1)$$

with $\lambda_j \geqslant 0$ such that $\sum_{j \in \mathbb{Z}^\nu} \lambda_j < \infty$.

This example of L describes a generalized hopping process.

Clearly the generators in the examples (20) and (21) and their sums satisfy the conditions (1), (2), (3), (4) and condition (14).

Finally we give two physically relevant examples of observables satisfying condition (15). First choose in formula (13):

$$\begin{aligned} \phi(X) &= \sigma_i \qquad && \text{if} \quad X = \{i\} \\ &= 0 && \text{otherwise} \end{aligned}$$

then Φ_Δ is the (local) magnetization in the volume Δ.

Secondly choose in formula (13)

$$\begin{aligned} \phi(X) &= b\sigma_i \qquad && \text{if} \quad X = \{i\};\ b \in \mathbb{R} \\ &= J(|i-j|)\,\sigma_i\sigma_j && \text{if} \quad X = \{i, j\};\ i \neq j \\ &= 0 && \text{otherwise} \end{aligned}$$

then Φ_Δ is the (local) energy in the volume Δ. Obviously these two observables satisfy condition (15).

For the example (20) of the generator L_β and for the observable of the magnetization, by a straightforward computation one observes the validity of the condition (17). Therefore the result (18) on the critical exponents is valid in this case. The same holds for the generator L being a sum of (20) and (21) while the spectrum of (21) alone has no gap at zero.

REFERENCES

1. R. J. Glauber, *J. Math. Phys.* **4**:294 (1963).
2. R. A. Holley and D. W. Stroock, *Commun. Math. Phys.* **55**:37 (1977).
3. L. Van Hove, *Phys. Rev.* **95**:1374 (1954).
4. T. Schneider, *Phys. Rev. B* **9**:3819 (1974).
5. W. G. Sullivan, *Markov Processes for Random Fields*, Comm. DIAS No. 23.
6. H. O. Georgii, *Canonical Gibbs Measures*, Lectures Notes in Mathematics No. 760 (Springer, New York, 1979).
7. M. Reed and B. Simon, *Methods of Modern Mathematical Physics*, Vol. II, (Academic Press, New York, 1975).