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Effective Hamiltonian Description of Nonequilibrium Spin Systems

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We present a method to study the existence of effective Hamiltonians for lattice, Ising-type model systems with competing dynamics, and find explicit expressions for some relevant nonequilibrium situations. We also define dynamical versions of the random-field and spin-glass models.

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The study of far-from-equilibrium phenomena such as the so-called nonequilibrium phase transitions and critical phenomena is hampered nowadays by the lack of a global consistent theory, e.g., one which is comparable to the powerful Gibbs ensemble theory designed to deal with equilibrium phenomena in macroscopic systems with a well-defined Hamiltonian. Consequently, most basic questions in that field, such as the existence and/or significance of steady states, fluctuations, universality classes, etc., still need some clarification. This (and some other facts) motivated a series of recent studies[1-19] concerning specific spin lattice, say, Ising-type systems which are characterized by some more or less complex dynamics, e.g., dynamics governed by the action of some external agent besides the usual thermal bath,[1] by several locally competing thermal baths,[13] by competing microscopic mechanisms[7] such as Glauber spin flips[20] and Kawasaki spin exchanges,[21] etc. Those studies have revealed that the system is forced in general to present far-from-equilibrium steady states usually deserving practical (in addition to theoretical) interest. Also, many properties of those states have been clarified in several cases. So far, however, general results remain scarce,[11,18,19] mainly because those studies are based on specific methods of solution which, excluding a few exact treatments in certain limiting conditions,[2,3,7,13] also have an approximate nature.

It thus seems interesting to investigate now all of those nonequilibrium Ising-type systems at hand looking for general features of nonequilibrium phenomena. We present here some results in that direction. Namely, we state sufficient conditions for a nonequilibrium spin system to present "Gibbs states" with respect to some effective, short-ranged Hamiltonian and conclude explicit expressions for the latter in a number of interesting cases. Even though we shall avoid here any general statement about stability or uniqueness of steady states, a problem which is better investigated at present by considering specific cases (cf. Refs. 1-12), this follows among other consequences the existence of a large class of nonequilibrium systems which can be analyzed, in principle, by using the standard methods of equilibrium theory. Those systems have a time-independent distribution $P(\mathbf{s}) \propto \exp[-\tilde{H}(\mathbf{s})]$ for the spin configuration $\mathbf{s}$, and we find that some effective Hamiltonians [the functions $\tilde{H}(\mathbf{s})$] have the familiar nearest-neighbor (NN) Ising structure, i.e., they only involve sums over NN pairs of lattice sites, while others may also contain sums over more complex clusters of lattice sites.

Consider any infinite lattice Ω whose associated spin configurations $\mathbf{s} \equiv \{s_\mathbf{x} = \pm 1,\ \mathbf{x} \in \Omega\}$ have energy $H(\mathbf{s})$, e.g.,

$$H = -K \sum_{|\mathbf{x}-\mathbf{y}|=1} s_\mathbf{x} s_\mathbf{y}\,, \tag{1}$$

where the sum is over NN pairs of lattice sites. The model systems of interest are such that the probability of $\mathbf{s}$ at time t, $P(\mathbf{s};t)$, evolves in time according to a Markovian master equation which describes the competition between $n+m$ different stochastic processes:

$$\frac{dP(\mathbf{s};t)}{dt}=\left[\sum_{i=1}^{n}L_i^G+\sum_{j=1}^{m}L_j^K\right]P(\mathbf{s};t)\,. \tag{2}$$

Here L_i^G represent generators for "Glauber processes,"[20] i.e., they cause stochastic spin flips at site $\mathbf{x}$ generating new configurations $\mathbf{s}^{\mathbf{x}}$ from $\mathbf{s}$ with a rate $w_i(\mathbf{s};\mathbf{x})$, and L_j^K are generators for "Kawasaki processes"[21] in which unequal spins at NN sites $\mathbf{x}$ and $\mathbf{y}$, $|\mathbf{x}-\mathbf{y}|=1$, exchange stochastically, thus producing $\mathbf{s}^{\mathbf{x},\mathbf{y}}$ from $\mathbf{s}$, with a rate $w_j(\mathbf{s};\mathbf{x},\mathbf{y})$. We shall assume in the following that $w_i,w_j>0$ for any i, j, and $\mathbf{s}$. Both generators may be written as $L^{G,K}=\sum_{\mathbf{x}}C^{G,K}(\mathbf{s};\mathbf{x})$ which defines the local operators $c(\mathbf{s};\mathbf{x})$. Moreover, each rate in Eq. (2) satisfies a detailed balance property, i.e.,

$$w_\alpha(\mathbf{s})/w_\alpha(\mathbf{s}')=\exp\{-[H_\alpha(\mathbf{s}')-H_\alpha(\mathbf{s})]\}\,,\quad \alpha=i,j\,, \tag{3}$$

where $\mathbf{s}'$ refers either to $\mathbf{s}^{\mathbf{x},\mathbf{y}}$ or to $\mathbf{s}^{\mathbf{x}}$, and $H_i(\mathbf{s})$ may be of type (1) or else.

The familiar kinetic Ising model, with conserved[20] (nonconserved[21]) magnetization evolving as $t\to\infty$ towards the equilibrium state determined by $H(\mathbf{s})$, follows from above when $L_i^G\equiv 0$ for all i and $m=1$ ($L_j^K=0$ for all j and $n=1$) assuming the sufficient condition of detailed balance (3) with respect to $H(\mathbf{s})$. Otherwise, it is known that the system may evolve asymptotically towards a nonequilibrium steady state with a nontrivial dependence in general on the choices for the transition rates w_i and w_j; cf. Refs. 5, 7, 10, and 12, for instance. Our results for those nonequilibrium situations may be summarized as follows:

Definition.—Consider the object

$$\tilde{H}(\mathbf{s})=\sum_{k=1}^{\infty}\sum_{\mathbf{y}_1\cdots\mathbf{y}_k}^{*}J^{(k)}_{\mathbf{y}_1\cdots\mathbf{y}_k}\prod_{i=1}^{k}s_{\mathbf{y}_i}\,. \tag{4}$$

where $\sum^*$ sums over every k different lattice sites, defined as the solution of

$$\left[\sum c_i^G(\mathbf{s};\mathbf{x})+\sum c_j^K(\mathbf{s};\mathbf{x})\right]\exp[-\tilde{H}(\mathbf{s})]=0\,.$$

When $\tilde{H}(\mathbf{s})$ exists with either the strong property,

$$J^{(k)}_{\mathbf{y}_1\cdots\mathbf{y}_k}=0\quad\text{for } k>k_0\,, \tag{5a}$$

or else the weaker one,

$$\lim_{r\to\infty}|J^{(r)}_{\mathbf{z}_i\cdots\mathbf{z}_r}/J^{(r-1)}_{\mathbf{z}_1\cdots\mathbf{z}_{r-1}}|=0\,, \tag{5b}$$

$\tilde{H}(\mathbf{s})$ will be called the system *effective Hamiltonian* (EH).

Theorem 1.—For a dynamics consisting only of Glauber (spin flip) processes, i.e., $L_j^K\equiv 0$ for all j, $\tilde{H}(\mathbf{s})$ exists with

$$J^{(k)}_{\mathbf{y}_1\cdots\mathbf{y}_k}=2^{-N-1}\sum_{\mathbf{s}}s_{\mathbf{y}_1}\cdots s_{\mathbf{y}_k}\ln\left[\sum_{i=1}^{n}w_i(\mathbf{s};\mathbf{y}_k)\Big/\sum_{i=1}^{n}w_i(\mathbf{s}^{\mathbf{y}_k};\mathbf{y}_k)\right] \tag{6}$$

when the following holds

$$\sum_{\mathbf{s}}s_{\mathbf{y}_1}\cdots s_{\mathbf{y}_k}\ln\left[\frac{w(\mathbf{s};\mathbf{y}_\alpha)w(\mathbf{s}^{\mathbf{y}_\beta};\mathbf{y}_\beta)}{w(\mathbf{s}^{\mathbf{y}_\alpha};\mathbf{y}_\alpha)w(\mathbf{s};\mathbf{y}_\beta)}\right]=0\,,\quad w\equiv\sum_i w_i \tag{7}$$

for all $\mathbf{y}_\alpha$ and $\mathbf{y}_\beta$, $\alpha\neq\beta=1,\ldots,k$. The condition (7) implies a necessary symmetry for the coefficients (6).

Theorem 2.—For a dynamics consisting only of Kawasaki (spin exchange) processes, i.e., $L_i^G\equiv 0$ for all i, $\tilde{H}(\mathbf{s})$ exists with

$$J^{(k)}_{\mathbf{z}_i\cdots\mathbf{z}_{k-1},\mathbf{x}}-J^{(k)}_{\mathbf{z}_1\cdots\mathbf{z}_{k-1},\mathbf{y}}=2^{-N-1}\sum_{\mathbf{s}}s_{\mathbf{z}_1}\cdots s_{\mathbf{z}_{k-1}}(s_{\mathbf{y}}-s_{\mathbf{x}})\ln\left[\sum_{j=1}^{m}w_j(\mathbf{s}^{\mathbf{x},\mathbf{y}};\mathbf{x},\mathbf{y})\Big/\sum_{j=1}^{m}w_j(\mathbf{s};\mathbf{x},\mathbf{y})\right]\,, \tag{8}$$

$\mathbf{z}_i\neq\mathbf{x},\mathbf{y}$ for all i when this series of equations has a solution.

Theorem 3.—For a dynamics actually combining Glauber and Kawasaki processes as in Eq. (2), with the Glauber rate satisfying (7), $\tilde{H}(\mathbf{s})$ exists given by Eqs. (4) and (5) when

$$\frac{w(\mathbf{s};\mathbf{x},\mathbf{y})}{w(\mathbf{s}^{\mathbf{x},\mathbf{y}};\mathbf{x},\mathbf{y})}=\frac{w(\mathbf{s}^{\mathbf{x}};\mathbf{x})w(\mathbf{s}^{\mathbf{y}};\mathbf{y})}{w(\mathbf{s};\mathbf{x})w(\mathbf{s};\mathbf{y})}\,, \tag{9}$$

where $w(\mathbf{s};\mathbf{x},\mathbf{y})\equiv\sum_j w_j(\mathbf{s};\mathbf{x},\mathbf{y})$. This corresponds to the case where $\tilde{H}(\mathbf{s})$ is simultaneously a solution of both $\sum_i c_i^G(\mathbf{s};\mathbf{x})\exp[-\tilde{H}(\mathbf{s})]=0$ and $\sum_j c_j^K(\mathbf{s};\mathbf{x})\exp[-\tilde{H}(\mathbf{s})]=0$.

Remark.—The proof of Theorems 1–3 stating the existence of $\tilde{H}(\mathbf{s})$ under a relatively broad range of conditions, is simply a matter of algebra.

Theorem 4.—A sufficient condition for an existing $\tilde{H}(\mathbf{s})$ to represent an effective Hamiltonian (EH) is that any involved transition probability w only affects a finite number of spins.

Remarks.—Theorem 4 essentially reduces the search for an EH to that for $\tilde{H}(\mathbf{s})$: The condition stated there happens to hold in most familiar cases and, otherwise, one would also need to compute $\tilde{H}(\mathbf{s})$ before checking conditions (5).

Theorem 5.—The cases in which Theorem 1 holds always have an EH with the original NN Ising structure when any involved transition probability $w(\mathbf{s};\mathbf{x})$ has the following (familiar) properties: (1) they only depend on

$s_{\mathbf{x}}$ and $s_{\mathbf{y}}$ where $\mathbf{y}=\mathbf{x}\pm\hat{\mathbf{i}}$, $i=1,\ldots,d$ represent the NN sites of site $\mathbf{x}$, and (2) the following symmetry property holds:

$$w(\mathbf{s};\mathbf{x})=w(\mathbf{s}^{\mathbf{y},\mathbf{z}};\mathbf{x}),\quad \mathbf{y}=\mathbf{x}-\hat{\mathbf{i}},\quad \mathbf{z}=\mathbf{x}+\hat{\mathbf{i}}. \qquad (10)$$

Remark.—Arguments to prove Theorems 4 and 5 may simply be worked out from (5).

We consider now some physically relevant *examples.* The one-dimensional Ising model with several locally competing *spin-flip* mechanisms, each satisfying a condition (3) with respect to $H_i(\mathbf{s})=-K_i\sum_{\mathrm{NN}}s_{\mathbf{x}}s_{\mathbf{y}}$, is characterized by Eq. (2) with $w_i(\mathbf{s};\mathbf{x})=f_i(\mathbf{s})[1+s_{\mathbf{x}}\tanh(h_i)]$ where $-h_i(\mathbf{s})\equiv\frac{1}{2}s_{\mathbf{x}}[H_i(\mathbf{s}^{\mathbf{x}})-H_i(\mathbf{s})]$ and f_i represents a function of $\mathbf{s}$ which is arbitrary except that $f_i(\mathbf{s})=f_i(\mathbf{s}^{\mathbf{x}})$. Theorems 1 and 5 then imply the existence of an EH having the Ising structure, namely, $\tilde{H}=-\tilde{K}\sum_x s_x s_{x+1}$, with

$$\tilde{K}=\tfrac{1}{4}\ln\left[\sum_i b_i(1+\tau_i)\Big/\sum_i b_i(1-\tau_i)\right]$$

(notice by the way that $\tilde{K}$ may be either positive or negative defined), when $f(\mathbf{s})$ only depends on the NN of site $\mathbf{x}$, it satisfies (10), and

$$\sum_i(a_i+c_i)\tau_i\Big/\sum_i(a_i+c_i)=\sum_i b_i\tau_i\Big/\sum_i b_i$$

[condition (7)]; we wrote here $f_i(\mathbf{s})=a_i+b_is+c_is^2$, i.e., a_i, b_i, and c_i, are independent of $\mathbf{s}$, $s\equiv\frac{1}{2}(s_{x-1}+s_{x+1})$, and $\tau_i\equiv\tanh(2K_i)$.

The rates introduced originally by Glauber[20] correspond to $f_i(\mathbf{s})=a_i=\text{const}\ (>0)$ above; one has then that

$$\tilde{K}=\tfrac{1}{4}\ln\left[\sum_i a_i(1+\tau_i)\Big/\sum_i a_i(1-\tau_i)\right].$$

Consider the interesting case of a system whose dynamics is a competition between two mechanisms; e.g., one acts with a probability p as if the spin interactions were ferromagnetic of strength K_1 $(=J_1/k_BT>0)$, and the other acts with probability $1-p$ as if the interactions were antiferromagnetic of strength K_2 $(=J_2/k_BT<0)$, $a_1=a_2=a$. It follows immediately that the EH is necessarily zero (as for the infinite temperature or zero-coupling limits) when $p\tanh(2K_1)=(1-p)\tan(2K_2)$, e.g., when $K_1=|K_2|$ for $p=\frac{1}{2}$. It also follows that $\tilde{K}=\pm\infty$ when $K_i=\pm\infty$, respectively, for all i; i.e., one may have an effective zero temperature when all the mechanisms are either ferromagnetic or antiferromagnetic, while the combination described before does not allow one to reach the region $\tilde{K}>\frac{1}{4}\ln[p/(1-p)]$, a fact revealing a kind of *dynamic frustration.*

The rates introduced by Metropolis *et al.*[22] are for $f=1+\frac{1}{2}[\exp(-4|K|)-1]s^2$; this follows the same EH as before with

$$\tilde{K}=\tfrac{1}{4}\ln\left\{\left[r+\sum_{i=r+1}^{n}\exp(4K_i)\right]\Big/\left[n-r+\sum_{i=1}^{r}\exp(-4K_i)\right]\right\}$$

for the interesting (one-dimensional) case of $K_i>0$ when $i=1,\ldots,r$ and $K_i\le 0$ when $i=r+1,\ldots,n$. The EH becomes zero now either when every mechanism acts as if the temperature were infinite or when, in the presence of only two different values for K_i as before, it is

$$(1-p)/p=[1-\exp(-4K_1)]/[1-\exp(-4|K_2|)];$$

i.e., there is only a quantitative difference with the Glauber case $f_i=a$. Two rates considered before in various one-dimensional problems, which are characterized, respectively, by $f=1-(1-2s^2)\tanh^2K$ (Ref. 7) and by $f=1+s^2[\cosh(2K)-1]$,[2] also have an associated EH when used to implement the above model with competing spin-flip mechanisms, e.g., the latter one has an EH with the Ising structure and

$$\tilde{K}=\tfrac{1}{4}\ln\left[\sum_i\exp(2K_i)\Big/\sum_i\exp(-2K_i)\right].$$

Also interesting is the model in Ref. 13 where the dynamics consists of spin flips performed with probability p as if the selected spin was in contact with a heat bath at temperature T_1 and with probability $1-p$ as if the temperature of the heat bath was T_2; define $K_i=J/k_BT_i$, $i=1,2$. Assuming that model in the case of a one-dimensional lattice, Glauber rates, and *spin interchanges* (instead of spin flips), as it may be of some relevance to study special phase-segregation processes, it follows from Theorem 2 that an EH has the Ising structure with

$$\tanh(2\tilde{K})=p\tanh(2K_1)+(1-p)\tanh(2K_2).$$

The same result follows when the dynamical processes are spin flips.

Our method is also useful to study a class of model systems[16,17] whose definition does not involve any Hamiltonian but only a certain dynamical process. As an illustration, consider the *voter model*[16] in a d-dimensional space where the configuration $\mathbf{s}$ evolves via a spin-flip process with rate

$$w(\mathbf{s};\mathbf{x})=\tfrac{1}{2}-\tfrac{1}{4}d(1-l)s_{\mathbf{x}}\sum_{\mathbf{y}}s_{\mathbf{y}}+\tfrac{1}{2}l(1-2p)s_{\mathbf{x}},$$

where the sum is over $\mathbf{y}$ such that $|\mathbf{x}-\mathbf{y}=1$, $0\le l\le 1$, and $0\le p\le 1$. When $d=1$, Theorems 1 and 5 only apply for $l=1$ or $p=\frac{1}{2}$; the EH for $p=\frac{1}{2}$ is $\tilde{H}(\mathbf{s})=\frac{1}{4}\ln[l/(1-l)]\sum_x s_x s_{x+1}$. When $d>1$, there is only an EH, $\tilde{H}(\mathbf{s})=\text{const}$, for $l=1$.

Concerning Theorem 3, the following holds: When, for all i and j, $w_i(\mathbf{s};\mathbf{x})$ and $w_j(\mathbf{s};\mathbf{x},\mathbf{y})$ satisfy the detailed balance condition (3) with respect to the same Hamiltonian, say, $H(\mathbf{s})=H_i(\mathbf{s})=H_j(\mathbf{s})$, then $\tilde{H}(\mathbf{s})=H(\mathbf{s})$. Further examples satisfying Eq. (9) may be worked out.

As a final example, we define a kind of *dynamical random-field model*, namely, $\mathbf{s}$ evolves now as a consequence of competing spin flips with rates $w_i(\mathbf{s};\mathbf{x})$ depending on $H_i(\mathbf{s}^{\mathbf{x}})-H_i(\mathbf{s})$ where, for $d=1$, $H_i(\mathbf{s}) = -K\sum_x s_x s_{x+1} - h_i \sum_x s_x$. (Notice that one may assume instead a given distribution for the coupling constants, $K_i = J_i/k_B T$: This follows a dynamical version of the so-called spin-glass Ising model.) Considering the simplest case of rates such that $f_i = a =$const and a symmetric continuous distribution for the fields, $g(h)=g(-h)$, this follows the existence of an EH with the Ising structure which, in the limit $K \rightarrow 0$, is $\tilde{H}(\mathbf{s}) = -2KI\sum_x s_x s_{x+1}$ to first order in K with $I=\int_0^\infty dh\, g(h)[\cosh(h)]^{-2}$. We shall soon report more facts about these models.

Finally, it seems worthwhile to remark that once the EH is known, one may construct a class of transition probabilities driving the system to the same (nonequilibrium) steady state. Namely, the class $w(\mathbf{s};\mathbf{x}) = g_1(\mathbf{s})\exp(-\frac{1}{2}\delta H)$ when the order parameter is conserved or the class $w(\mathbf{s};\mathbf{x},\mathbf{y}) = g_2(\mathbf{s})\exp(-\frac{1}{2}\delta H)$ when it is nonconserved. Here $\delta H \equiv \tilde{H}(\mathbf{s}') - \tilde{H}(\mathbf{s})$ with $\mathbf{s}' = \mathbf{s}^{\mathbf{x}}$ or $\mathbf{s}^{\mathbf{x},\mathbf{y}}$, respectively, and g_1 and g_2 are arbitrary functions satisfying a global detailed balance property, i.e., $g_1(\mathbf{s}^{\mathbf{x}}) = g_1(\mathbf{s})$, $g_2(\mathbf{s}^{\mathbf{x},\mathbf{y}}) = g_2(\mathbf{s})$. This may be of interest, for instance, when looking for the most efficient dynamics in a Monte Carlo study of a nonequilibrium model with a competing dynamics such as the one defined in (2).

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[1]S. Katz, J. L. Lebowitz, and H. Spohn, J. Stat. Phys. **34**, 497 (1984).

[2]H. van Beijeren and L. S. Schulman, Phys. Rev. Lett. **53**, 806 (1984).

[3]J. Krug, J. L. Lebowitz, H. Spohn, and M. Q. Zhang, J. Stat. Phys. **44**, 535 (1986).

[4]J. L. Vallés and J. Marro, J. Stat. Phys. **49**, 89 (1987); **49**, 121 (1987).

[5]P. L. Garrido, J. Marro, and R. Dickman, "Nonequilibrium Stationary States and Phase Transitions in a Driven Diffusive Lattice Model System," 1989 (to be published).

[6]R. Dickman, Phys. Rev. A **38**, 2588 (1988).

[7]A. de Masi, P. A. Ferrari, and J. L. Lebowitz, Phys. Rev. Lett. **55**, 1947 (1985).

[8]J. L. Lebowitz, Physica (Amsterdam) **140A**, 232 (1986).

[9]R. Dickman, Phys. Lett. A **122**, 463 (1987).

[10]J. M. González-Miranda, P. L. Garrido, J. Marro, and J. L. Lebowitz, Phys. Rev. Lett. **59**, 1934 (1987).

[11]J. S. Wang and J. L. Lebowitz, J. Stat. Phys. **51**, 893 (1988).

[12]P. L. Garrido, J. Marro, and J. M. González-Miranda, "Reaction-Diffusion Ising Model Systems," 1989 (to be published).

[13]P. L. Garrido, A. Labarta, and J. Marro, J. Stat. Phys. **49**, 551 (1987).

[14]P. L. Garrido and J. Marro, Physica (Amsterdam) **144A**, 585 (1987).

[15]T. M. Ligget, in *Interacting Particle Systems* (Springer-Verlag, Berlin, 1985), and references therein.

[16]J. L. Lebowitz and H. Saleur, Physica (Amsterdam) **138A**, 194 (1986).

[17]A. R. Kerstein, J. Stat. Phys. **45**, 921 (1986).

[18]J. Marro, J. L. Vallés, and J. M. González-Miranda, Phys. Rev. B **35**, 3372 (1987).

[19]H. Künsch, Z. Wahrsch. Verw. Gebiete **66**, 407 (1984); G. Grinstein, C. Jayaprakash, and Yu He, Phys. Rev. Lett. **55**, 2527 (1985).

[20]R. J. Glauber, J. Math. Phys. (N.Y.) **4**, 294 (1963).

[21]K. Kawasaki, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 4.

[22]N. Metropolis, A. W. Rosenbluth, M. M. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).