Fluctuation-dissipation relation for stochastic dynamics without detailed balance

Mário J. de Oliveira
Instituto de Física, Universidade de São Paulo, Caixa Postal 66318, 05315-970 São Paulo, São Paulo, Brazil
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We show that the fluctuation-dissipation relation can be established for a class of stochastic dynamics that lack detailed balance. This class comprises lattice spin models whose time evolution is governed by a master equation with a one-spin-flip transition rate having the up-down symmetry. The relation is obtained by the introduction of a multiplicative perturbation of the transition rate, which reduces to the usual perturbation when detailed balance is fulfilled. As a part of the derivation we set up an equivalent two-spin-flip stochastic dynamics that conserves the magnetization.

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INTRODUCTION

The fluctuation-dissipation relation as introduced by Kubo [1] deals with the response of a system in thermodynamic equilibrium to a small perturbation. The system is described by a Hamiltonian to which a perturbation term is added in the form of a small field coupled to a dynamic variable and the relation is understood as a connection between the response function induced by the perturbation and the time correlation function. Kubo [1] arrived at the fluctuation-dissipation relation by the use of a response theory grounded on the deterministic and reversible dynamics described by the Liouville equation. But stochastic dynamics having microscopic reversibility in the steady state can also be used to deduce the fluctuation-dissipation relation [2,3]. By microscopic reversibility we mean that detailed balance is fulfilled in which case it is possible to define *a priori* a Hamiltonian and the associated equilibrium Gibbs probability distribution.

Although the fluctuation-dissipation relation was conceived to be applied to systems having microscopic reversibility it is natural to ask whether the relation could be extended to systems described by stochastic dynamics that lack detailed balance, that is, systems that are microscopically irreversible in the steady state. In fact, it has been found [4–9] that a generalized form of the fluctuation-dissipation relation can be obtained for such systems. However, this generalized relation has an extra term, distinguishing it from the usual fluctuation-dissipation relation, that vanishes only when detailed balance is fulfilled [6]. A possible connection between the lack of detailed balance and the violation of the fluctuation-dissipation relation has also been raised [10,11].

Our main purpose here is to show that it is actually possible to establish the usual fluctuation-dissipation relation for a class of stochastic models that lack detailed balance. To be specific we focus on the class of lattice spin models with continuous time stochastic Markovian dynamics governed by a master equation with a one-spin-flip transition rate having up-down symmetry. This is a large class that includes all the one-spin-flip algorithms used to simulate Ising models such as the heat bath algorithm and the stochastic dynamics introduced by Glauber [12] to describe the time evolution of the one-dimensional Ising model. It also includes, of course, models that do not obey detailed balance [13–20]. The models of this class, with up-down symmetry, with or without detailed balance, have generally the same critical behavior defining thus a universality class [21].

The models we consider here are defined on a regular lattice with N sites where a spin variable $\sigma_i = \pm 1$ is attached to each site i of the lattice. The total lattice configuration is denoted by $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_i, \ldots, \sigma_N)$. The one-spin-flip stochastic dynamics is defined by the spin-flip transition rate $w_i(\sigma)$, related to the ith spin of the lattice, which usually depends on the configuration of spins in a small neighborhood of the site i. The master equation, which governs the time evolution of the probability $P(\sigma,t)$ of state σ at time t, reads

$$\frac{d}{dt}P(\sigma,t) = \sum_i \{w_i(\sigma^i)P(\sigma^i,t) - w_i(\sigma)P(\sigma,t)\}, \tag{1}$$

where σ^i is the configuration obtained from σ by changing σ_i to $-\sigma_i$, that is, $\sigma^i = (\sigma_1, \sigma_2, \ldots, -\sigma_i, \ldots, \sigma_N)$.

PERTURBATION

To establish the fluctuation-dissipation for microscopically irreversible systems one has to know first how to introduce a perturbation since now the models are described by a transition rate and not by a Hamiltonian to which a perturbation term could be added. The appropriate perturbation is introduced by modifying the flipping rate, which now reads

$$w_i^*(\sigma) = w_i(\sigma)e^{-h\sigma_i}, \tag{2}$$

where h is the time-dependent disturbance coupled to the dynamic variable σ_i. With the perturbation given by Eq. (2), the following fluctuation-dissipation relation will be shown to hold

$$R(t,t') = -\frac{\partial}{\partial t}C(t,t'), \tag{3}$$

where $C(t,t') = \langle M(t)M(t')\rangle$ is the correlation function of a dynamical variable M between the times t and t', and $R(t,t') = \lim_{h\to 0} \delta\langle M(t)\rangle / \delta h(t')$ is the response function. In the present case the dynamical variable M is the total magnetization $M = \sum_i \sigma_i$.

Another version of the fluctuation-dissipation relation connects the susceptibility related to the total magnetization M to its variance

$$\frac{d}{dh}\langle M\rangle = \langle M^2\rangle - \langle M\rangle^2, \tag{4}$$

where here h is a static, i.e., time-independent disturbance introduced by the prescription given by Eq. (2).

When the model is microscopically reversible, that is, when the unperturbed system described by the transition rate w_i obeys detailed balance the steady state is an equilibrium state described by a Gibbs probability distribution associated to a Hamiltonian $\mathcal{H}$. In this case it is straightforward to show that the perturbed system described by the transition rate w_i^* given by Eq. (2) also obeys detailed balance and is described by the Hamiltonian $\mathcal{H}^* = \mathcal{H} - B\Sigma_i\sigma_i$ where the field B is related to the disturbance h by $h=\beta B$ with β proportional to the inverse of temperature. Therefore, for systems that obey detailed balance, the perturbation introduced by Eq. (2) is indeed appropriate. When detailed balance is not fulfilled, we will show that the rate given by Eq. (2) is also suited in the sense that it leads to the usual fluctuation-dissipation relation.

MODELS

Most of the models mentioned above are invariant under the up-down symmetry operation meaning that the corresponding spin-flip rate is invariant under the transformation $\sigma\to-\sigma$. However, we will consider a more general unperturbed transition rate $w_i(\sigma)$ of the form

$$w_i(\sigma) = w_i^0(\sigma)e^{-H\sigma_i}, \tag{5}$$

where $w_i^0(\sigma)$ is invariant under the up-down symmetry operation, that is, $w_i^0(-\sigma)=w_i^0(\sigma)$ and H is a parameter that breaks the up-down symmetry and which need not be small.

For convenience we write the rate $w_i^0(\sigma)$ as the sum

$$w_i^0(\sigma) = w_i^+(\sigma) + w_i^-(\sigma), \tag{6}$$

with $w_i^\pm(\sigma)=(1/2)(1\pm\sigma_i)\omega^\pm(\sigma)$ where $\omega^\pm(\sigma)$ do not depend on σ_i. Given the rate w_i^0 it is always possible to univocally find ω^+ and ω^-. These quantities are simply the values of w_i^0 when $\sigma_i=+1$ and $\sigma_i=-1$, respectively. The one-spin-flip rate $w_i(\sigma)$ can then be written as

$$w_i(\sigma) = w_i^+(\sigma)e^{-H} + w_i^-(\sigma)e^{H}. \tag{7}$$

The steady state probability distribution $P(\sigma)$ of the system described by the transition rate $w_i(\sigma)$ obeys the balance equation

$$\sum_i \{w_i(\sigma^i)P(\sigma^i) - w_i(\sigma)P(\sigma)\} = 0, \tag{8}$$

which is equivalent to the equation

$$\sum_\sigma \sum_{i\in A} [f_A(\sigma^i) - f_A(\sigma)]w_i(\sigma)P(\sigma) = 0, \tag{9}$$

where A is any arbitrary and finite set of sites of the lattice and $f_A(\sigma)=\Pi_{j\in A}\sigma_j$.

CONSERVATIVE ENSEMBLE

Next we introduce a stochastic process that defines a conservative ensemble, which will be shown to be equivalent, in the thermodynamic limit, to the ensemble defined by the rate (5). This will be accomplished by an approach used before [22–24]. We start by introducing a process described by a two-spin-flip rate $w_{ij}(\sigma)$ defined by

$$w_{ij}(\sigma) = \frac{1}{N}w_i^+(\sigma)w_j^-(\sigma), \tag{10}$$

for any pair of sites of the lattice. The process defined by this transition rate conserves the magnetization M because w_{ij} is nonzero only when $\sigma_i+\sigma_j=0$. The steady state probability $P_M(\sigma)$, corresponding to a given magnetization M, obeys the equation

$$\sum_{ij} \{w_{ij}(\sigma^{ij})P_M(\sigma^{ij}) - w_{ij}(\sigma)P_M(\sigma)\} = 0, \tag{11}$$

which is equivalent to the equation

$$\sum_\sigma \sum_{ij} [f_A(\sigma^{ij}) - f_A(\sigma)]w_{ij}(\sigma)P_M(\sigma) = 0. \tag{12}$$

It is straightforward to show that this equation is equivalent to

$$\frac{1}{N}\sum_\sigma \sum_{i\in A}\sum_{j\notin A} [f_A(\sigma^i) - f_A(\sigma)][w_i^+(\sigma)w_j^-(\sigma) + w_j^+(\sigma)w_i^-(\sigma)]P_M(\sigma) = 0. \tag{13}$$

Now, for sufficiently large N,

$$\frac{1}{N}\sum_{j\notin A} w_j^\pm(\sigma) \to \langle w_j^\pm(\sigma)\rangle_M, \tag{14}$$

a result that follows from the law of large numbers where we have taken into account that the number of sites outside A is of the order N because the set A is finite. The notation $\langle\ldots\rangle_M$ stands for an average over the distribution $P_M(\sigma)$.

Inserting result (14) into Eq. (13), and result (7) into Eq. (9), we see that Eq. (13) is equivalent to Eq. (9) as long as H is chosen such that

$$\frac{e^H}{e^{-H}} = \frac{\langle w_j^+(\sigma)\rangle_M}{\langle w_j^-(\sigma)\rangle_M}. \tag{15}$$

This establishes the equivalence between the constant-M ensemble defined by the rate w_{ij} and the constant-H ensemble defined by the rate w_i, a result valid in the thermodynamic limit.

STATIC FLUCTUATION-DISSIPATION

The probability distribution Q_M of the magnetization M related to the system described by $w_i(\sigma)$ is given by

$$Q_M = \sum_\sigma \delta\left(M - \sum_j \sigma_j\right)P(\sigma), \tag{16}$$

whereas the conditional probability of σ given M is defined by

$$P(\sigma|M) = \delta\left(M - \sum_j \sigma_j\right)\frac{P(\sigma)}{Q_M}. \tag{17}$$

From the balance equation (8) it is straightforward to show that Q_M obeys the equation

$$A^{+}_{M+2}e^{-H}Q_{M+2} - A^{-}_{M}e^{H}Q_M + A^{-}_{M-2}e^{H}Q_{M-2} - A^{+}_{M}e^{-H}Q_M = 0, \tag{18}$$

where

$$A^{\pm}_M = \sum_\sigma w^{\pm}_i(\sigma)P(\sigma|M). \tag{19}$$

Due to the equivalence of ensembles we may replace $P(\sigma|M)$ by $P_M(\sigma)$ and, since this last probability distribution does not depend on H, the quantity $A^{\pm}_M$ will not depend on H.

To find the dependence of Q_M on H, we define Q^0_M as the probability distribution of the magnetization for the case $H=0$, which should obey the equation

$$A^{+}_{M+2}Q^0_{M+2} - A^{-}_{M}Q^0_M + A^{-}_{M-2}Q^0_{M-2} - A^{+}_{M}Q^0_M = 0. \tag{20}$$

Using the up-down symmetry property $A^{\mp}_{-M}=A^{\pm}_M$ and $Q^0_{-M}=Q^0_M$ it follows that

$$A^{+}_{M+2}Q^0_{M+2} - A^{-}_{M}Q^0_M = 0. \tag{21}$$

From this result it is straightforward to show by substitution that

$$Q_M = \frac{1}{Z}e^{HM}Q^0_M \tag{22}$$

is the solution of Eq. (18), where Z is a normalization factor. We remark that Q^0_M does not depend on H so that Eq. (22) gives indeed the dependence of Q_M on H. If we denote by $P^0(\sigma)$ the steady state probability distribution of the system described by $w^0_i(\sigma)$ then from Eqs. (22) and (17) it follows that

$$P(\sigma) = \frac{1}{Z}\exp\left\{H\sum_i \sigma_i\right\}P^0(\sigma), \tag{23}$$

where again we used $P_M(\sigma)$ in the place of $P(\sigma|M)$ bearing in mind that $P_M(\sigma)$ does not depend on H.

From Eqs. (22) or (23) one can easily show that

$$\frac{d}{dH}\langle M\rangle = \langle M^2\rangle - \langle M\rangle^2, \tag{24}$$

which is the static fluctuation-dissipation relation. To get this relation from Eq. (22) it suffices to remember that Q^0_M does not depend on H. In the case of equilibrium (detailed balance fulfilled) the distribution (23) is a Gibbs distribution from which follows immediately that $H=\beta B$.

RESPONSE FUNCTION

To set up a dynamic fluctuation-dissipation relation it is convenient to use a vector space spanned by the vectors $|\sigma\rangle=|\sigma_1,\sigma_2,\ldots,\sigma_i,\ldots,\sigma_N\rangle$. The probability vector $|\psi(t)\rangle$ is defined by

$$|\psi(t)\rangle = \sum_\sigma P(\sigma,t)|\sigma\rangle, \tag{25}$$

and the master equation (1) is written in the form

$$\frac{d}{dt}|\psi(t)\rangle = W|\psi(t)\rangle, \tag{26}$$

where $W=\Sigma_i W_i$ is the evolution operator with W_i given by

$$W_i = \sum_\sigma (|\sigma^i\rangle - |\sigma\rangle)w_i(\sigma)\langle\sigma|. \tag{27}$$

Given the solution $|\psi(t)\rangle$ of Eq. (26) we wish to find the solution $|\psi^*(t)\rangle$ of the master equation defined by the evolution operator

$$W^* = \sum_\sigma\sum_i (|\sigma^i\rangle - |\sigma\rangle)w^*_i(\sigma)\langle\sigma|, \tag{28}$$

for small values of the disturbance h. To this end we use a time-dependent perturbation theory. For small values of h we may write Eq. (2) as $w^*_i(\sigma)=w_i(\sigma)-h\sigma_i w_i(\sigma)$, which allows us to express the perturbed evolution operator as $W^*=W-hV$, where V is given by

$$V = \sum_\sigma\sum_i (|\sigma^i\rangle - \sigma\rangle)\sigma_i w_i(\sigma)\langle\sigma|. \tag{29}$$

Assuming that the disturbance begins to act at $t=0$, the time-dependent perturbation theory [1] gives

$$|\psi^*(t)\rangle = |\psi(t)\rangle - e^{tW}\int_0^t h(t')e^{-t'W}V|\psi(t')\rangle dt'. \tag{30}$$

The average $\langle M(t)\rangle^*$ of the magnetization M at time t for the perturbed system is then given by

$$\langle M(t)\rangle^* = \langle M(t)\rangle - \int_0^t h(t')\langle\Omega|Se^{(t-t')W}V|\psi(t')\rangle dt', \tag{31}$$

where $\langle M(t)\rangle$ is the average of M at time t for the unperturbed system and $S=\Sigma_i S_i$, where S_i is the diagonal operator defined by $S_i|\sigma\rangle=\sigma_i|\sigma\rangle$ and $\langle\Omega|=\Sigma_\sigma\langle\sigma|$ is the projector operator. From this expression we get the response function in the form

$$R(t,t') = -\langle\Omega|Se^{(t-t')W}V|\psi(t')\rangle. \tag{32}$$

Since we are interested in the response of the system to a perturbation in the steady state regime we have

$$R(t,t') = -\langle\Omega|Se^{(t-t')W}V|\psi\rangle, \tag{33}$$

where $|\psi\rangle=\Sigma_\sigma P(\sigma)|\sigma\rangle$ is the stationary vector and we have assumed, for convenience, that the unperturbed system is already in the stationary regime at time t'.

DYNAMIC FLUCTUATION-DISSIPATION

Now, from its definition, we see that the operation V can be written as

$$V = \sum_i W_i S_i. \tag{34}$$

Next we use the following property:

$$WS - SW = \sum_i (W_i S_i - S_i W_i), \tag{35}$$

which can be proved by using the property that W_i and S_j commute with each other if $i \neq j$. Therefore the perturbation V can be written in the form

$$V = WS - SW + \sum_i S_i W_i. \tag{36}$$

Taking into account that $W|\psi\rangle = 0$ we get

$$V|\psi\rangle = WS|\psi\rangle + \sum_i S_i W_i|\psi\rangle. \tag{37}$$

If detailed balance is fulfilled then $W_i|\psi\rangle = 0$ for any i so that

$$V|\psi\rangle = WS|\psi\rangle. \tag{38}$$

When detailed balance is not fulfilled this relation even so still holds because, as we shall prove next, the last term in Eq. (37) vanishes.

We start by inserting Eqs. (5) and (23) into Eq. (8) to get the result

$$\sum_i e^{-H\sigma_i}\{w_i^0(\sigma^i)P^0(\sigma^i) - w_i^0(\sigma)P(\sigma)\} = 0. \tag{39}$$

Since this equation is valid for any value of H, its derivative with respect to H gives

$$\sum_i \sigma_i e^{-H\sigma_i}\{w_i^0(\sigma^i)P^0(\sigma^i) - w_i^0(\sigma)P(\sigma)\} = 0. \tag{40}$$

Now the projection of the last term in Eq. (37) is

$$\sum_i \langle\sigma|S_i W_i|\psi\rangle = \sum_i \sigma_i\{w_i(\sigma^i)P(\sigma^i) - w_i(\sigma)P(\sigma)\}. \tag{41}$$

Taking into account the results (5) and (23), the right hand side of this equation can be written as

$$e^{HM}\sum_i \sigma_i e^{-H\sigma_i}\{w_i^0(\sigma^i)P^0(\sigma^i) - w_i^0(\sigma)P^0(\sigma)\}. \tag{42}$$

But the summation vanishes due to the result (40) and we get $\Sigma_i\langle\sigma|S_i W_i|\psi\rangle = 0$ so that Eq. (38) is also valid for systems that lack detailed balance.

Inserting the result (38) into Eq. (33), the response function can finally be written as

$$R(t,t') = -\langle\Omega|Se^{(t-t')W}WS|\psi\rangle = -\frac{\partial}{\partial t}\langle M(t)M(t')\rangle, \tag{43}$$

where $\langle M(t)M(t')\rangle = \langle\Omega|Se^{(t-t')W}S|\psi\rangle$ is the correlation function.

In conclusion, we have shown that the fluctuation-dissipation relation can be established for a class of models that lack detailed balance. We remark that an exact calculation of the response function and the correlation function has actually been made for a specific model of this class, namely, the linear Glauber model [19,20], confirming the general result obtained here.

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