Entropy-based characterizations of the observable dependence of the fluctuation-dissipation temperature

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The definition of a nonequilibrium temperature through generalized fluctuation-dissipation relations relies on the independence of the fluctuation-dissipation temperature from the observable considered. We argue that this observable independence is deeply related to the uniformity of the phase-space probability distribution on the hypersurfaces of constant energy. This property is shown explicitly on three different stochastic models, where observable dependence of the fluctuation-dissipation temperature arises only when the uniformity of the phase-space distribution is broken. The first model is an energy transport model on a ring, with biased local transfer rules. In the second model, defined on a fully connected geometry, energy is exchanged with two heat baths at different temperatures, breaking the uniformity of the phase-space distribution. Finally, in the last model, the system is connected to a zero temperature reservoir, and preserves the uniformity of the phase-space distribution in the relaxation regime, leading to an observable-independent temperature.

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I. INTRODUCTION

The definition of macroscopic quantities that can characterize nonequilibrium systems is a challenging and active field in statistical physics. Several approaches have been proposed in the literature, by generalizing thermodynamic [1] or statistical physics approaches [2–6]. One of these approaches is based on the possible generalization to nonequilibrium situations of intensive thermodynamic parameters (chemical potential, compactivity, etc.) conjugated to conserved quantities [7–9]. Such parameters are then defined as the logarithmic derivative of a generalized partition function with respect to the corresponding conserved quantity. Yet, energy is in general not conserved in nonequilibrium systems, and other approaches are necessary in order to define a nonequilibrium temperature. Along this line, the introduction of effective temperatures in nonequilibrium systems through generalized fluctuation-dissipation relations (FDR) has played a major role [3,10].

In equilibrium the FDR turns out to be a powerful tool to describe the relaxation of slightly perturbed systems toward their equilibrium states. The fluctuation-dissipation theorem relies on the principle that the response of a system in thermodynamic equilibrium to a small perturbation is the same as its response to a spontaneous fluctuation. Accordingly, there is a direct relation between the fluctuation characteristics of the thermodynamic system for a given observable and its linear response. This is a very strong property, because it is valid for all systems in equilibrium, independent of the details of the microscopic dynamics and the observable considered. Hence the relation gives rise to a universal proportionality factor, precisely given by the equilibrium temperature.

However, in a nonequilibrium system this relation is a priori not valid. The theoretical investigation of the breaking of the fluctuation-dissipation theorem in spin-glass systems [10,11] and in turbulence [12] has stimulated a wide range of experimental and numerical studies aiming to define an effective temperature in many different systems, ranging from granular materials [13–16] to glasses [17–22], spin-glasses [23,24], gels and colloidal suspensions [25–27], liquid crystals [28], or turbulent flows [29]. Despite the large body of theoretical work devoted to nonequilibrium generalizations of the FDR [10,30–48], the question of the observable dependence of the effective temperature defined from the FDR has mainly been studied case by case in specific models [13,21,22,49–54], and no clear rationale has been proposed to interpret the observable dependence.

In this paper we study, following our recent letter [55], how the characteristics of a nonequilibrium distribution of the microstates influence the possibility to define an observable-independent temperature in the system. We relate the observable dependence of the FDR temperature to the "lack of entropy," defined as the entropy difference between the nonequilibrium distribution and the equilibrium distribution with the same energy. We also observe that the entropy production, which is a natural characterization of nonequilibrium systems [30,56,57], seems to bear no systematic relation to the dependence of the temperature on the choice of observable. Our study is however restricted to systems that remain close to an equilibrium state, and where correlation functions decay to zero on a single time scale. Most aging systems [58] are thus excluded from our analysis.

The paper is organized as follows. In Sec. II we present the general framework, introducing a generalized fluctuation-dissipation relation and the notion of lack of entropy. We also relate quantitatively the observable dependence of the effective temperature to the lack of entropy. In Sec. III, this relation is quantitatively illustrated on three different stochastic models. First, an exactly solvable energy transport model on a ring in contact to a reservoir is studied (Sec. III A). In this model, the internal flux results from the

bulk dynamics rather than from an external drive. In the second example, an external drive is introduced (Sec. III B). More specifically, we consider a fully connected model in contact with two heat baths at slightly different temperatures, resulting in a nonequilibrium steady state [55]. As a last example, we discuss a variant of the latter model, in which the system is connected to a single heat bath at zero temperature (Sec. III C). This dynamics leads to a slow relaxation toward the ground state, during which the nonstationary distribution can be computed. Finally, Sec. IV summarizes and briefly discusses the obtained results.

II. GENERAL FRAMEWORK

A. Evaluation of the response function

We first introduce the form of the generalized fluctuation-dissipation relation that we use to define the out-of-equilibrium effective temperatures. We shall consider a generic system that is described by a set of N variables x_i, $i=1,\ldots,N$. Since we are interested in the observable dependence of the effective temperatures we introduce a family of observables B_p indexed by an integer p. In analogy to the equilibrium response theory, we are interested in the dynamics of the observables due to the application of a perturbation to a system that is in a nonequilibrium steady state, or relaxing to equilibrium. This response will then be related to the fluctuations in the system in the absence of perturbation. In order to perturb the system a probe field can be applied. For nonequilibrium systems that can be described by an Hamiltonian, the system can be perturbed by applying a small external field h, conjugated to an observable M, leading to an additional term in the Hamiltonian. But note that for stochastic systems defined through transition rates, like for example out-of-equilibrium lattice spin systems, the appropriate perturbation is introduced by modifying the transition rates [59–61]. However, we shall consider in this work the Hamiltonian case.

The following protocol for the applied perturbation allows for the definition of the linear response of the observable B_p to the external probe field. The field h takes a constant and small nonzero value until time t_s, and it is then suddenly switched off. The subsequent evolution of the observable B_p then provides the linear response to the probe field. More precisely, the two-time linear response $\chi_p(t,t_s)$ is defined, for $t>t_s$, as

$$\chi_p(t,t_s) = \left.\frac{\partial}{\partial h}\right|_{h=0} \langle\langle B_p(t,t_s)\rangle\rangle, \tag{1}$$

where $\langle\langle\cdots\rangle\rangle$ denotes an average over the dynamics corresponding to the field protocol described above.

The basic idea of the FDR is to relate the linear response function $\chi_p(t,t_s)$ to the correlation function (computed in the absence of field)

$$C_p(t,t_s) = \langle [B_p(t) - \langle B_p(t)\rangle][M(t_s) - \langle M(t_s)\rangle]\rangle. \tag{2}$$

In general, such a relation is not necessarily linear. However, in cases when it is linear, a FDR is said to hold, namely,

$$\chi_p(t,t_s) = \frac{1}{T_p(t_s)} C_p(t,t_s), \quad t>t_s. \tag{3}$$

The proportionality factor is the inverse of the effective temperature T_p. In equilibrium, T_p depends neither on time nor on the observable, it is simply the bath temperature. In contrast, out of equilibrium, T_p can be time dependent, and it can a priori depend on p, that is, on the observable. In the specific case of nonequilibrium steady state, the above FDR simplifies to, setting $t_s=0$,

$$\chi_p(t) = \frac{1}{T_p} C_p(t), \tag{4}$$

where T_p becomes time independent.

In the following we will consider situations such that a fluctuation-dissipation relation as given in Eq. (3) or (4) exists, and we shall focus on the possible dependence of T_p on the choice of the observable B_p. We shall mainly consider steady-state systems, but we will also briefly study a nonstationary model (Sec. III C), so that we keep a time-dependent formalism. The response of an observable to the perturbation can be formally rewritten using the distribution $\mathcal{P}(\{x_i\},h,t_s)$ of the microstate $\{x_i\}\equiv\{x_i, i=1,\ldots,N\}$ in the presence of the field h. To this aim we express $\langle\langle B_p(t,t_s)\rangle\rangle$ as

$$\langle\langle B_p(t,t_s)\rangle\rangle = \int \prod_{i=1}^{N} dx_i dx_i' B_p(\{x_i\}) \times G^0_{t,t_s}(\{x_i\}|\{x_i'\})\mathcal{P}(\{x_i'\},h,t_s), \tag{5}$$

where $G^0_{t,t_s}(\{x_i\}|\{x_i'\})$ is the zero-field propagator, that is the conditional probability to be in a microstate $\{x_i\}$ at time t given that the system was in a microstate $\{x_i'\}$ at time t_s, in the absence of the probe field. Taking the derivative of Eq. (5) with respect to h at $h=0$, and using the relation $\partial\mathcal{P}/\partial h = \mathcal{P}\partial \ln \mathcal{P}/\partial h$, we get

$$\chi_p(t,t_s) = \left\langle B_p(t) \frac{\partial \ln \mathcal{P}}{\partial h}(\{x_i(t_s)\},0,t_s) \right\rangle, \tag{6}$$

the average being computed at zero field. Similar forms of this expression of the response function can be found in the literature [46–48,62]. In the case of a steady-state system, with a distribution $\mathcal{P}(\{x_i\},h)$, the result does not depend on t_s, so that we set $t_s=0$, yielding

$$\chi_p(t) = \left\langle B_p(t) \frac{\partial \ln \mathcal{P}}{\partial h}(\{x_i(0)\},0) \right\rangle. \tag{7}$$

B. Properties of the phase-space distribution

1. Uniform distribution on energy shells

In order to go beyond the formal expression (6) of the response function, we need to choose a specific form of the distribution $\mathcal{P}(\{x_i\},h,t_s)$. We first consider the case when the distribution only depends on the total energy E_h, namely, $\mathcal{P}(\{x_i\},h,t_s)=Z(t_s)^{-1}\exp[-\theta(E_h,t_s)]$, with $Z(t_s)$ being the normalization factor. The distribution $\mathcal{P}(\{x_i\},h,t_s)$ is thus uniform over constant energy surfaces in phase space for all

times. A linear time-independent $\theta(E,t_s)=\beta E+\theta_0$ corresponds to the equilibrium canonical ensemble. However, we consider here the more general case of a regular function $\theta(E,t_s)$ monotonically increasing with the total energy. It is easy to check that for $h=0$, $\partial \ln Z/\partial h=\langle M\theta'\rangle=0$, so that $\partial \ln \mathcal{P}/\partial h=M\theta'$, where θ' is the derivative of θ with respect to the total energy. For a macroscopic system, the average in Eq. (6) is dominated by the most probable energy level $E^*(t_s)$. From a saddle-point evaluation, we obtain

$$\chi_p(t,t_s)=\frac{\partial\theta}{\partial E}(E^*(t_s),t_s)C_p(t,t_s). \tag{8}$$

Hence a fluctuation-dissipation temperature

$$T_{\mathrm{FD}}(t_s)=\left\{\frac{\partial\theta}{\partial E}(E^*(t_s),t_s)\right\}^{-1}, \tag{9}$$

independent of the observable, can be defined. As the value $E^*(t_s)$ maximizes the energy distribution $\rho(E,t_s)\propto\exp(S(E)-\theta(E,t_s))$, where $S(E)$ is the microcanonical entropy, it turns out that $\partial\theta/\partial E(E^*(t_s),t_s)=S'(E^*(t_s))$, so that the standard definition of temperature is recovered.

2. Beyond uniformity: the lack of entropy

In a more general situation, the distribution $\mathcal{P}(\{x_i\},h,t_s)$ is not uniform over the shells of constant energy, and the above simplification does not occur, leading generically to an observable dependence of the fluctuation-dissipation temperature [65]. The above remarks suggest that this dependence on the observable could be related to a macroscopic quantity, namely, the Shannon entropy difference between the stationary state and the equilibrium state with the same average energy. When the distribution is uniform over the most probable energy shell, the entropy is maximal, so that a nonuniform state necessarily corresponds to a lower entropy. The entropy difference may thus be interpreted as a measure of the deviation from equilibrium.

In the rest of this section, we focus on steady-state distributions in order to simplify the notations, but our argument can straightforwardly be extended to situations where the distribution $\mathcal{P}(\{x_i\},h,t_s)$ depends on time. As a general framework, we consider in the following a class of stochastic Markovian models, where an energy $E=\Sigma_{i=1}^N\varepsilon_h(x_i)$ is exchanged in a random way between the internal degrees of freedom. Either the internal dynamics, or in more realistic scenarios additional external sinks and sources, drive the system into a nonequilibrium steady state. The resulting drive can be encompassed by a dimensionless parameter γ, like a normalized temperature difference or external force. Note that in some cases the parameter γ may be the square of the physical driving force, as we define γ as the order of magnitude of the leading correction to the equilibrium distribution (see below). In the absence of driving ($\gamma=0$), detailed balance is satisfied and the system is described by an equilibrium distribution

$$\mathcal{P}_{\mathrm{eq}}(\{x_i\},h)=Z_N^{-1}\exp\left(-\beta\sum_{i=1}^N\varepsilon_h(x_i)\right), \tag{10}$$

where $\beta=1/T$ is the inverse temperature of the thermal bath, and Z_N is the canonical partition function.

As a simplification, we assume that the N-body steady-state distribution $\mathcal{P}(\{x_i\},h)$ can be factorized according to $\mathcal{P}(\{x_i\},h)=\Pi_{i=1}^N p(x_i,h)$, meaning that the degrees of freedom are statistically independent. The system can thus be fully described by means of the single-variable probability distribution $p(x,h)$. We now consider the small driving limit $|\gamma|\ll 1$, and expand $p(x,h)$ around the equilibrium distribution $p_{\mathrm{eq}}(x,h)=Z_1^{-1}\exp[-\beta\varepsilon_h(x)]$ as

$$p(x,h)=p_{\mathrm{eq}}(x,h)\{1+\gamma F(\varepsilon_h(x))+\mathcal{O}(\gamma^2)\}. \tag{11}$$

Such a perturbation is consistent with some recent generic results on nonequilibrium distributions [63]. The constraints of normalization of $p(x,h)$ and $p_{\mathrm{eq}}(x,h)$ imply that $\langle F(\varepsilon)\rangle_{\mathrm{eq}}=0$, where ε is a shorthand notation for $\varepsilon_h(x)$ and $\langle\cdots\rangle_{\mathrm{eq}}$ denotes the equilibrium average. If $p(x,h)$ follows Eq. (11), the factorized N-body distribution $\mathcal{P}(\{x_i\},h)$ is generically not a function of the total energy $E=\Sigma_{i=1}^N\varepsilon_h(x_i)$, so that $\mathcal{P}(\{x_i\},h)$ is not uniform over the shells of constant energy. It follows that the nonequilibrium Shannon entropy is lower than the entropy of the reference equilibrium state having the same energy. Accordingly, the entropy difference between the equilibrium and nonequilibrium states with the same average energy provides a characterization of the deviation from equilibrium. To determine the entropy difference, we compute the average energy $E(\beta,\gamma)$ of the out-of-equilibrium system, and we evaluate the temperature β^* for which $E(\beta,\gamma)=E_{\mathrm{eq}}(\beta^*)$, where $E_{\mathrm{eq}}(\beta^*)$ is the equilibrium energy at temperature β^*. As the distribution $\mathcal{P}(\{x_i\},h)$ is factorized, the Shannon entropy of the whole system is simply computed as the sum of the entropies associated to each variables x_i. Hence only the Shannon entropy associated to a single degree of freedom,

$$S=-\int dx p(x,h)\ln p(x,h), \tag{12}$$

needs to be computed. We denote by $S_{\mathrm{eq}}(\beta)$ the equilibrium entropy at temperature β, and by $S(\beta,\gamma)$ the entropy in the nonequilibrium steady-state characterized by β and γ. We then define the entropy difference ΔS per degree of freedom through the relation

$$\Delta S=S_{\mathrm{eq}}(\beta^*)-S(\beta,\gamma). \tag{13}$$

A rather straightforward calculation yields (see Appendix A for details),

$$\Delta S=\frac{\gamma^2}{2}\left(\langle F(\varepsilon)^2\rangle_{\mathrm{eq}}-\frac{\langle\varepsilon F(\varepsilon)\rangle_{\mathrm{eq}}^2}{\langle\varepsilon^2\rangle_{\mathrm{eq}}-\langle\varepsilon\rangle_{\mathrm{eq}}^2}\right). \tag{14}$$

We have checked that $\Delta S\geq 0$ as expected (see Appendix A), even though this property does not appear explicitly in Eq. (14). In the case of a linear $F(\varepsilon)$, one finds $\Delta S=0$, which can be understood from the fact that the distribution $p(x,h)$ can be recast into an effective equilibrium form—see Eq. (11).

Considering now a generic function $F(\varepsilon)$, we parameterize it as

$$F(\varepsilon) = a + b\varepsilon + \eta f(\varepsilon), \tag{15}$$

where η characterizes the amplitude of the nonlinearity. The normalization condition $\langle F(\varepsilon)\rangle_{\rm eq}=0$ fixes the value of the parameter a. We then obtain the generic result

$$\Delta S = \gamma^2 \eta^2 \omega, \tag{16}$$

where ω is a constant which depends on the detailed expression of the functions $f(\varepsilon)$ and $\varepsilon_h(x)$. As an example, considering a nonlinearity of the form $f(\varepsilon)=\varepsilon^2$ and a zero-field local energy $\varepsilon_0(x)=\frac{1}{2}x^2$, one finds

$$\Delta S = \frac{3\gamma^2\eta^2}{4\beta^4}. \tag{17}$$

C. Fluctuation-dissipation relation and effective temperatures

We now proceed to derive the FDR associated to the variable B_p, and to analyze the dependence of the effective temperature on p. To this aim, we further restrict the class of models considered by making an additional simplification. Namely, we assume that each time a variable x_i is modified by a dynamical event, its new value is decorrelated from the previous one. Examples of models satisfying this assumption are given below (see also [33]). Qualitatively, such an assumption can be interpreted as a coarse graining of the dynamics on a time scale of the order of the correlation time of the system. Note that we focus here on systems with a single relaxation time scale, so that the present approach does not necessarily apply to systems with a more complex dynamics involving different time scales, such as glassy systems. This assumption of local decorrelation implies that the correlation function $C_p(t)$ is proportional to the persistence probability $\Phi(t)$ [33], defined as

$$\Phi(t) = \left\langle \frac{1}{N}\sum_{i=1}^{N} \phi_i(t) \right\rangle, \tag{18}$$

where the history-dependent local random variables $\phi_i(t)$ are equal to 1 if no redistribution involving site i occurred between $t=0$ and t, and are equal to 0 otherwise. As a consequence we can express the different averages involved in expressions (2) and (7) in terms of $\Phi(t)$.

We expand the local energy $\varepsilon_h(x)$ for small field h, namely, $\varepsilon_h(x)=\varepsilon_0(x)-h\psi(x)+\mathcal{O}(h^2)$, assuming $\psi(x)$ to be an odd function. It follows that the observable M, conjugated to the field h, is defined as

$$M = \sum_{i=1}^{N} \psi(x_i). \tag{19}$$

For the family of observables B_p, we choose the following definition:

$$B_p = \sum_{i=1}^{N} x_i^{2p+1} \tag{20}$$

with $p \geq 0$ an integer number. In this way, B_p has a zero mean value in the absence of the field, which slightly simplifies the calculations.

Using the fact that the random variables x_i and x_j are independent for $i \neq j$, and that $\langle B_p\rangle=\langle M\rangle=0$, one can simplify the expression (2) for the correlation function, leading to

$$C_p(t) = N\langle x(t)^{2p+1}\psi(x(0))\rangle. \tag{21}$$

Further using the assumption of decorrelation by the local dynamical events, we get

$$C_p(t) = N\langle x^{2p+1}\psi(x)\rangle\Phi(t). \tag{22}$$

The average in the last expression is performed on the steady-state distribution. From Eq. (7), the response function can also be evaluated using the decorrelation assumption, yielding

$$\chi_p(t) = N[\beta\langle x^{2p+1}\psi(x)\rangle - \gamma\langle x^{2p+1}\psi(x)F'(\varepsilon_0)\rangle]\Phi(t), \tag{23}$$

where ε_0 is a simplified notation for $\varepsilon_0(x)$. The average in the second term can be replaced by the equilibrium average, neglecting higher order terms in γ. One can then express $\Phi(t)$ as a function of $C_p(t)$ from Eq. (22), which leads to a FDR of the form Eq. (4). The corresponding temperature $\beta_p=T_p^{-1}$ is given by

$$\beta_p = \beta - \gamma\frac{\langle x^{2p+1}\psi(x)F'(\varepsilon_0)\rangle_{\rm eq}}{\langle x^{2p+1}\psi(x)\rangle_{\rm eq}}. \tag{24}$$

As anticipated, the p dependence in Eq. (24) does not cancel in general, so that the temperature T_p generically depends on the observable. A notable exception is the case of a linear $F(\varepsilon)$, namely, $F(\varepsilon)=a+b\varepsilon$, where the effective temperature $\beta_p=\beta-\gamma b$ is observable independent.

When $F(\varepsilon)$ has a nonlinear contribution, parameterized as $F(\varepsilon)=a+b\varepsilon+\eta f(\varepsilon)$, the temperature difference between two distinct observables is proportional to the amplitude η of the nonlinearity. More precisely, one finds from Eq. (24) that

$$\beta_p - \beta_0 = \gamma\eta\left[\frac{\langle x\psi(x)f'(\varepsilon_0)\rangle_{\rm eq}}{\langle x\psi(x)\rangle_{\rm eq}} - \frac{\langle x^{2p+1}\psi(x)f'(\varepsilon_0)\rangle_{\rm eq}}{\langle x^{2p+1}\psi(x)\rangle_{\rm eq}}\right]. \tag{25}$$

On the other hand, we have seen in Eq. (16) that the lack of entropy ΔS is also a measure of the nonlinearity amplitude η. Hence it is natural to try to obtain a quantitative relation between $\beta_p-\beta_0$ and ΔS. Starting from Eqs. (16) and (25), we get a relation of the form

$$\frac{|\beta_p - \beta_0|}{\beta} = \kappa_p\sqrt{\Delta S}, \tag{26}$$

where we have introduced a dimensionless and positive constant κ_p. This constant a priori depends on p, as well as on the functional forms of $f(\varepsilon)$ and of the local energy $\varepsilon_h(x)$. Note however that κ_p does not depend on γ and η. In the

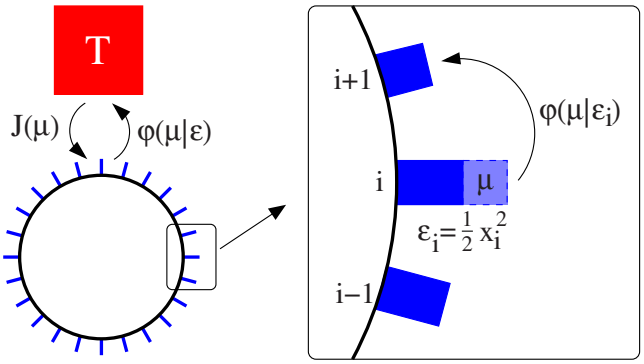

FIG. 1. (Color online) Left: scheme of the energy transport model on a ring in contact with a bath at temperature T. Energy is injected from the bath to the ring with rate $J(\mu)$ and dissipated from the ring to the bath with rate $\varphi(\mu|\varepsilon)$. Right: internal dynamics of the ring. A fraction μ of the local energy $\varepsilon_i=x_i^2/2$ is transported from site i to site $i+1$ on the ring according to the transport rate $\varphi(\mu|\varepsilon_i)$.

following section, we give two examples of models for which κ_p can be determined exactly.

From the above analysis, it turns out that the dependence of the fluctuation-dissipation temperature on the choice of observable is a direct measure of the deviation from equilibrium. As already mentioned, the above argument can be generalized to time-dependent probability distributions. In this case, β_p, κ_p, and $\sqrt{\Delta S}$ may all depend on time. Let us however emphasize again that the main assumptions made, namely, that the distribution remains close to some equilibrium state, and that local decorrelation occurs in a single step, may not apply to glassy systems.

III. ILLUSTRATION ON SIMPLE MODELS

A. Simple energy transfer model on a ring

1. Model and steady-state solution

To illustrate the above results let us consider as a first example an energy transfer model on a ring geometry that is connected to a bath with temperature T (see Fig. 1). The model is defined on a one-dimensional lattice with periodic boundary conditions. To every site i, $i=1\ldots N$, is attached a real quantity x_i, associated to a local energy $\varepsilon_i=\frac{1}{2}x_i^2$. A fraction μ of the local energy ε_i is transferred from site i to site $i+1$, according to the site independent rate

$$\varphi(\mu|\varepsilon_i)=v(\mu)\frac{g(\varepsilon_i-\mu)}{g(\varepsilon_i)},\quad g(\rho)=\rho^{\delta-1}, \tag{27}$$

with $\delta>0$, and $v(\mu)$ an arbitrary positive function. After the transport, the new variables denoted as x_i' and x_{i+1}' take the values

$$x_i'=\pm\sqrt{x_i^2-2\mu},\quad x_{i+1}'=\pm\sqrt{x_{i+1}^2+2\mu}, \tag{28}$$

with equiprobable and uncorrelated random signs. We consider a continuous time dynamics, where sites are updated in an asynchronous way. As can be easily checked, these transport rules locally conserve the energy. The choice of the function $g(\rho)$ entering the transport rates also ensures that the system remains homogeneous (no condensation occurs) [64].

In addition, each site i of the system is also connected to an external heat bath at temperature T, according to the following dynamics. An amount of energy μ is injected from the bath with a probability rate $J(\mu)$ given by

$$J(\mu)=v(\mu)e^{-\mu/T}. \tag{29}$$

Energy is transferred back to the bath with the same energy transport rate $\varphi(\mu|\varepsilon_i)$ as for the internal transport.

Given this dynamics, the steady-state probability distribution for a microscopic state $\{x_i\}$ takes the factorized form

$$\mathcal{P}_0(\{x_i\})=\frac{1}{Z_N}\prod_{i=1}^{N}\left\{|x_i|g\left(\frac{x_i^2}{2}\right)\right\}e^{-\Sigma_i x_i^2/2T}, \tag{30}$$

with Z_N the normalization factor of the distribution, and where the index 0 indicates a zero-field dynamics.

In the following, we show that the temperature defined from the FDR does not necessarily coincide with the bath temperature, consistently with Sec. II and with the results obtained in a similar model [33]. The two temperature definitions become equivalent only for the special choice $\delta=1/2$ in the transport rates in Eq. (27), when the probability distribution has an equilibrium form.

2. Fluctuation-dissipation relations

To relate the spontaneous fluctuations present in this stochastic system to the response of an observable to a small perturbation, let us introduce an external field $h(t)$ perturbing the system. A natural way to couple the field to the system is to add to the energy a linear term proportional to the external field,

$$E_h=\sum_{i=1}^{N}\frac{1}{2}x_i^2-h\sum_{i=1}^{N}x_i+\frac{Nh^2}{2}=\sum_{i=1}^{N}\frac{1}{2}(x_i-h)^2, \tag{31}$$

where we included for convenience an additional shift to the energy $Nh^2/2$ which is only changing the reference of the energy scale without loss of generality. Note that Eq. (31) implies $\psi(x)=x$ and $M=\Sigma_{i=1}^N x_i$. Introducing the new variables $v_i=x_i-h$ we ask that they obey the same dynamics as the former variables x_i, that is given in Eqs. (27) and (28). Further we assume the same protocol for the externally applied perturbation as described in the previous section: the field $h(t)$ is nonzero at times $t<0$, but small in comparison to the mean value $\langle x\rangle$ of the variables. We assume that the nonequilibrium steady state is established for $t<0$. At time $t=0$ the field is switched off in order to analyze the response of an observable $B_p(t)$ to this variation in the field.

Following Sec. II, we consider the observables B_p defined as $B_p=\Sigma_{i=1}^N x_i^{2p+1}$, with p a positive integer number. Given that the distribution in Eq. (30) is factorized, the results of Sec. II can be applied, and the steady-state correlation function $C_p(t)=\langle B_p(t)M(0)\rangle$ (we recall that $\langle B_p\rangle=\langle M\rangle=0$) is given by

$$C_p(t) = N\langle x(t)^{2p+1}x(0)\rangle. \tag{32}$$

To obtain the general formulation of the response function we use expression (7) with $\mathcal{P}(\{x_i(0)\},h)$ being the distribution for the nonequilibrium steady state in the presence of the field h. This distribution is given by Eq. (30) with respect to the new variables $v_i=x_i-h$, namely, $\mathcal{P}(\{x_i(0)\},h)=\mathcal{P}_0(\{v_i(0)\})$, meaning that the dynamics of the variables $\{x_i\}$ in the presence of the field h can be effectively described as a zero-field dynamics, once expressed in terms of the variables $\{v_i\}$.

For arbitrary values of the integer $p\geq 0$, we obtain the following relation between the response and the correlation in the system for the observable $B_p(t)$ (details are given in Appendix B),

$$\chi_p(t) = \frac{2p+1}{2(p+\delta)}\frac{1}{T}C_p(t). \tag{33}$$

The temperature defined by the fluctuation-dissipation relation generically depends on p and therefore on the observable chosen

$$T_p = \frac{2(p+\delta)}{(2p+1)}T. \tag{34}$$

Only for $\delta=1/2$, when the energy distribution [Eq. (30)] is uniform, the temperature takes independently of the observable the value $T_p=T$. But for nonuniform energy distributions, the temperature determined from the slope of the FDR depends on the observable and is therefore not well defined.

To study the weakly nonequilibrium regime, we consider values of δ close to the equilibrium value $\delta=1/2$, namely, $\delta=1/2+\gamma$ with $|\gamma|\ll 1$. We find for the linear correction $F(\varepsilon)$ to the probability distribution $p(x,h)$, as defined in Eq. (11), the following expression:

$$F(\varepsilon) = \ln\varepsilon + C_\beta, \tag{35}$$

where $C_\beta=\ln\beta-\psi_0(\frac{1}{2})$, and ψ_0 denotes the digamma function, defined as the logarithmic derivative of the Euler gamma function [numerically, $\psi_0(\frac{1}{2})\approx -1.963$]. Knowing $F(\varepsilon)$ then allows for the determination of all important quantities, necessary for the establishment of the crucial relation (26). Thus we end up with a quantitative expression of the observable dependence of the FDR temperature in terms of the lack of entropy. From Eq. (24), the observable dependence can be expressed through

$$\frac{|\beta_p-\beta_0|}{\beta} = |\gamma|\frac{4p}{2p+1}. \tag{36}$$

Besides, the entropy difference can be evaluated from Eq. (14), yielding

$$\Delta S = \frac{\gamma^2}{2}[\langle(\ln\varepsilon+C_\beta)^2\rangle - 2\beta^2\langle\varepsilon(\ln\varepsilon+C_\beta)\rangle^2]$$
$$= \frac{\gamma^2}{2}\left[\psi_0'\left(\frac{1}{2}\right)-2\right], \tag{37}$$

where ψ_0' is the derivative of ψ_0. Numerically, we find $\Delta S/\gamma^2\approx 1.467$. From the relation (26), we then get

$$\kappa_p = \frac{4p}{2p+1}\left[\frac{2}{\psi_0'\left(\frac{1}{2}\right)-2}\right]^{1/2}, \tag{38}$$

which is, as expected, independent of the physical parameters of the system, like the driving γ and the temperature β.

3. Discussion of the transport model results

We learn from the study of this exactly solvable transport model several interesting facts. First, this model illustrates explicitly how a probability distribution that is not uniform on energy shells (namely, $\delta\neq 1/2$) leads to a FDR temperature which depends on the observable. The result (38) depends uniquely on the form of the probability distribution and not on the energy flux in the system. We chose the rules of the dynamics such that the transport of energy is totally biased. But it is known that the symmetric case, where energy is transported with the same probability to the left or to the right, leads to exactly the same probability distribution for the microstates [64]. More precisely, the distribution only depends on the transport rates, but the direction of the transport, that defines the total flux, is not of any influence.

Further, it is interesting to compare the characterization in terms of ΔS with that in terms of entropy production. On general grounds, the entropy production σ_s can be defined from a balance equation involving the rate of entropy change, and the entropy fluxes with the reservoirs to which the system is connected,

$$\frac{dS}{dt} = \sum_{i=1}^{n}\frac{\mathcal{J}_i}{T_i} + \sigma_s, \tag{39}$$

where $\mathcal{J}_i$ is the energy flux exchanged with the ith bath at temperature T_i. In the present model, the steady state implies $dS/dt=0$. The system is in contact with a single bath, and the energy flux $\mathcal{J}$ is zero. Thus the entropy production is also equal to zero. This means that in the framework of this model the entropy production cannot give any information about the observable dependence of the effective temperature in the system. In the next section we present a different situation, where the nonequilibrium character no longer results from an artificial bulk dynamics, but rather from an external drive.

B. Fully connected model driven by two heat baths

1. Model and evolution equation

In general we would expect that the nonuniformity of the probability distribution results from the fact that the system is externally driven into a nonequilibrium steady state, for example by two reservoirs at different temperatures [55]. In the following we consider a model with N fully connected sites, associated to variables x_i, such that the local energy $\varepsilon_i=\frac{1}{2}(x_i-h)^2$ can be transferred between any pair of sites and with two different thermal baths. A sketch of the model is shown on Fig. 2. Energy transfers correspond to the dynamical rules in Eq. (28) in terms of variables x_i. An amount of energy μ is transferred from an arbitrary site i, with energy ε_i, to any other site j with a rate

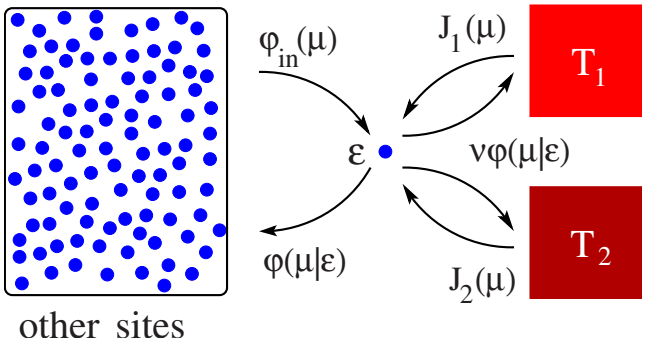

FIG. 2. (Color online) Scheme of the fully connected model considered in Sec. III B. A single site contains an amount of energy ε. It is in contact with two baths at different temperatures $T_1=\beta_1^{-1}$ and $T_2=\beta_2^{-1}$ and with the other sites.

$$\varphi(\mu|\varepsilon_i)=\frac{g(\varepsilon_i-\mu)}{g(\varepsilon_i)},\quad g(\rho)=\rho^{-1/2}. \tag{40}$$

Such a rate is similar to the rate in Eq. (27) for $\delta=\frac{1}{2}$ and $v(\mu)=1$. The value $\delta=\frac{1}{2}$ is chosen such that equilibrium is recovered when the two baths have the same temperature. Energy is transferred to the baths with the same rate as in the bulk, given in Eq. (40), but weighted with a factor ν characterizing the coupling strength between the baths and the system. The injection from the bath is defined as the transfer, with a rate $\nu\varphi(\mu|\varepsilon)$, from an equilibrated site having a distribution $P_{\rm eq}(\varepsilon,\beta_\alpha)$ at inverse temperature β_α, leading to

$$J_\alpha(\mu)=\nu\int_\mu^\infty d\varepsilon\varphi(\mu|\varepsilon)P_{\rm eq}(\varepsilon,\beta_\alpha). \tag{41}$$

A straightforward calculation then yields

$$J_\alpha(\mu)=\nu e^{-\beta_\alpha\mu}. \tag{42}$$

At this stage, it is convenient to describe the dynamics in terms of the local energy ε_i rather than with the variables x_i. In the thermodynamic limit $N\to\infty$, the master equation governing the N-body distribution can be recast into a nonlinear evolution equation for the one-site probability distribution $P(\varepsilon)$, namely,

$$\begin{aligned}\frac{\partial P(\varepsilon,t)}{\partial t}&=\int_0^\varepsilon d\mu[J_1(\mu)+J_2(\mu)]P(\varepsilon-\mu,t)\\&-\int_0^\infty d\mu[J_1(\mu)+J_2(\mu)]P(\varepsilon,t)\\&+(2\nu+1)\int_0^\infty d\mu\varphi(\mu|\varepsilon+\mu)P(\varepsilon+\mu,t)\\&-(2\nu+1)\int_0^\varepsilon d\mu\varphi(\mu|\varepsilon)P(\varepsilon,t)\\&+\int_0^\varepsilon d\mu\varphi_{\rm in}(\mu,t)P(\varepsilon-\mu,t)\end{aligned}$$

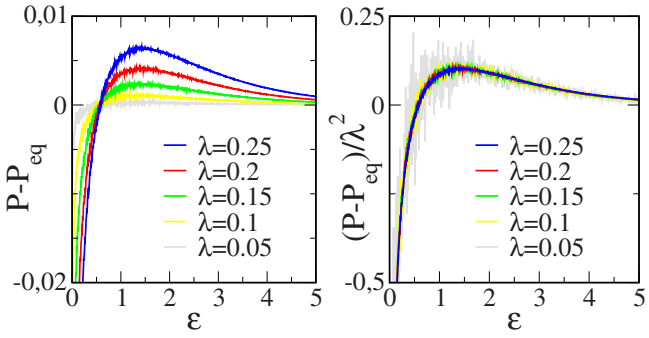

FIG. 3. (Color online) Test of the analyticity of $P(\varepsilon)$. Numerical simulations of the fully connected model show that the curves for $[P(\varepsilon)-P_{\rm eq}(\varepsilon)]/\lambda^2$ match to a very good accuracy for small values of λ, justifying the assumption of analyticity of the λ expansion made in Eq. (46). Parameter values: $\nu=1$, $\beta=1$, $T_{\rm max}=10^8$.

$$-\int_0^\infty d\mu\varphi_{\rm in}(\mu,t)P(\varepsilon,t). \tag{43}$$

The distribution $\varphi_{\rm in}(\mu,t)$ accounts for the energy transfer coming from all the other sites, given by the averaged transport rate $\varphi(\mu|\varepsilon)$,

$$\varphi_{\rm in}(\mu,t)=\int_\mu^\infty d\varepsilon\varphi(\mu|\varepsilon)P(\varepsilon,t). \tag{44}$$

The local energy distribution $P(\varepsilon,t)$ is related to the distribution $p(x,h,t)$ through

$$p(x,h,t)=\frac{1}{2}P(\varepsilon,t)\left|\frac{d\varepsilon_h}{dx}\right| \tag{45}$$

where $\varepsilon=\varepsilon_h(x)=\frac{1}{2}(x-h)^2$.

2. Stationary distribution for a small bath temperature difference

In order to determine the steady-state distribution of the model, we consider the case of a small temperature difference $|\beta_1-\beta_2|\ll(\beta_1+\beta_2)/2$, and parameterize the bath temperatures as $\beta_1=\beta(1-\lambda)$ and $\beta_2=\beta(1+\lambda)$, with $\lambda\ll1$. We then assume that the stationary distribution $P(\varepsilon)$ has an analytical expansion as a function of λ. The linear term in λ is excluded by a simple symmetry argument: exchanging the two bath temperatures changes λ into $-\lambda$, but should not modify the distribution $P(\varepsilon)$ since the two heat baths play a symmetric role. The leading correction should thus behave as λ^2, so that $P(\varepsilon)$ can be written as

$$P(\varepsilon)=P_{\rm eq}(\varepsilon)[1+\lambda^2F(\varepsilon)+\mathcal{O}(\lambda^4)], \tag{46}$$

in analogy to expression (11) with $\gamma=\lambda^2$. The distribution

$$P_{\rm eq}(\varepsilon)=\sqrt{\frac{\beta}{\pi}}\varepsilon^{-1/2}e^{-\beta\varepsilon} \tag{47}$$

is the known equilibrium distribution, namely, the stationary solution of the Eq. (43) for $\beta_1=\beta_2=\beta$. The scaling form in Eq. (46) is validated by numerical simulations, as shown on Fig. 3. The function $F(\varepsilon)$ determined from numerical data is

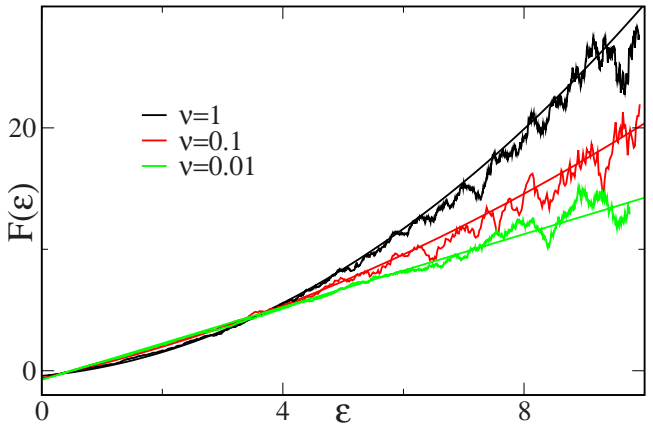

FIG. 4. (Color online) The function $F(\varepsilon)$ obtained by simulations (noisy lines) in comparison with the analytically obtained results for $F^{(2)}(\varepsilon)$ (solid lines) for different values of ν ($\lambda=0.2$, $\beta=1$, $T_{\max}=10^7$).

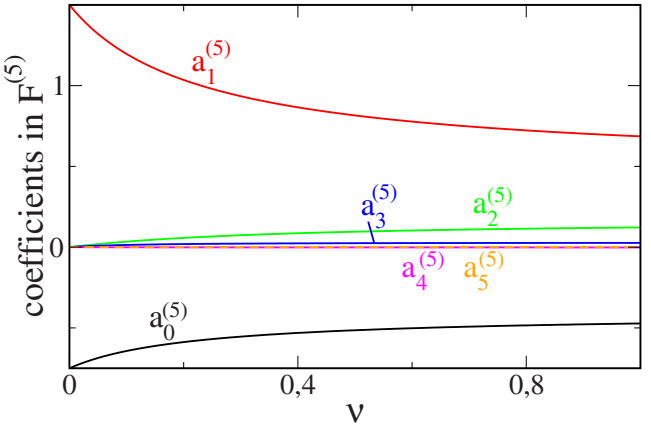

FIG. 5. (Color online) ν dependence of the coefficients in $F^{(5)}(\varepsilon)$ (see text).

also shown in Fig. 4 for different values of the coupling strength ν. The numerical results were obtained by directly simulating the stochastic dynamics, on a system of size $N=102$. Such a relatively small size allows for long time averaging, over a time $T_{\max}$ of the order of 10^7 or 10^8, in order to reach a sufficient statistics. Note that the time unit is defined in such a way that all sites have typically experienced about one redistribution event in a unit of time.

It can be checked that Eq. (43) has no exact solution involving a finite polynomial function $F(\varepsilon)$. To find the best polynomial approximation $F^{(L)}(\varepsilon)$ at a given order L we use a variational procedure, as detailed in Appendix C. We approximate the function $F(\varepsilon)$ by a polynomial of order L, $F^{(L)}(\varepsilon)=\Sigma_{n=0}^{L}a_n^{(L)}\beta^n\varepsilon^n$. The best approximation is then obtained analytically by minimizing the error, under the constraints of normalization and zero net flux with the baths, in the evolution Eq. (43) linearized with respect to the parameter $\gamma=\lambda^2$. The error is defined as the equilibrium average of the square of the rhs in the linearized equation.

If we use for example $F^{(2)}(\varepsilon)$ to approximate $F(\varepsilon)$, the normalization constraint and the constraint of zero net flux in the system yields for the coefficients $a_0^{(2)}$ and $a_1^{(2)}$ (see Appendix C),

$$a_0^{(2)}=-\frac{3}{4}+\frac{5}{4}a_2^{(2)},\quad a_1^{(2)}=\frac{3}{2}-4a_2^{(2)}. \tag{48}$$

Hence the only remaining free parameter is $a_2^{(2)}$. Minimizing the error with respect to $a_2^{(2)}$ yields an analytic expression for the coefficient $a_2^{(2)}$ as a function of the coupling strength ν (see Appendix C),

$$a_2^{(2)}(\nu)=\frac{3\nu(7+37\nu)}{13+136\nu+358\nu^2}. \tag{49}$$

Note that in the limit of small ν this expression vanishes linearly in ν, whereas the coefficients $a_0^{(2)}$ and $a_1^{(2)}$ take the finite values $-\frac{3}{4}$ and $\frac{3}{2}$, respectively.

Similarly, one can find analytically higher order approximations for $F(\varepsilon)$. Through this procedure we find that for approximations with $L>2$ the coefficients $a_k^{(L)}$, $k>2$, in the expansion are numerically small, as illustrated in Fig. 5. A second-order polynomial is thus already a good approximation of $F(\varepsilon)$ for $\nu\lesssim 1$ [see Fig. 4]. Taking into account higher order terms in $F(\varepsilon)$, we find that the relation (26) between the observable dependence and the entropy difference is satisfied to a good accuracy, as seen in Fig. 6. We have also checked for $L\leq 5$ that in the limit $\nu\to 0$, the coefficients $a_k^{(L)}$, $k>1$ vanish while $a_0^{(L)}\to-\frac{3}{4}$ and $a_1^{(L)}\to\frac{3}{2}$.

3. Observable dependence and its relation to the lack of entropy

In terms of the variable x, the stationary one-body distribution $p(x,h)$ reads, to second order in λ

$$p(x,h)=\sqrt{\frac{\beta}{2\pi}}e^{-\beta(x-h)^2/2}\left[1+\lambda^2F\left(\frac{1}{2}(x-h)^2\right)\right]. \tag{50}$$

Following our standard procedure, we introduce the response $\chi_p(t)$ of the observable B_p to a small perturbing field h. From

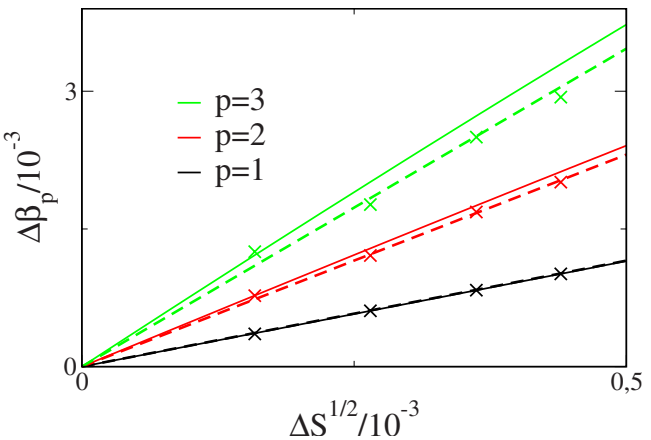

FIG. 6. (Color online) Parametric plot in ν of $\Delta\beta_p=|\beta_p-\beta_0|/\beta$ versus $\sqrt{\Delta S}$ obtained using $F^{(5)}(\varepsilon)$, either fitted to numerical data ($\times$) or calculated in the analytical approximation (solid lines). Dashed lines: Eq. (26) with $\kappa_p=4p/\sqrt{3}$. Simulation parameters: $\lambda=0.05$, $T_{\max}=10^7$.

Sec. II we know how to obtain the FDR temperature and the entropy difference using the correction $F(\varepsilon)$. As shown above $F(\varepsilon)$ can be well approximated by a quadratic function $F^{(2)}(\varepsilon)=a_0^{(2)}+a_1^{(2)}\beta\varepsilon+a_2^{(2)}\beta^2\varepsilon^2$. Consequently we obtain for the observable-dependent inverse temperature, using Eq. (24) with $\psi(x)=x$

$$\beta_p = \beta - \lambda^2 \frac{\langle \varepsilon^{p+1}(a_1^{(2)}\beta + 2a_2^{(2)}\beta^2\varepsilon)\rangle_{\rm eq}}{\langle \varepsilon^{p+1}\rangle_{\rm eq}} \tag{51}$$

leading to

$$\frac{|\beta_p - \beta_0|}{\beta} = 2p\lambda^2 |a_2^{(2)}|. \tag{52}$$

The calculation of ΔS using Eq. (14) with $F^{(2)}(\varepsilon)$ is also simple, involving averages of different powers of the energy, and the result takes the form

$$\Delta S = \frac{3}{4}\lambda^4 (a_2^{(2)})^2. \tag{53}$$

Thus we obtain for the relation between the entropy difference ΔS and observable dependence of the temperature

$$\frac{|\beta_p - \beta_0|}{\beta} = \frac{4p}{\sqrt{3}}\sqrt{\Delta S} \tag{54}$$

in agreement with the general results presented in Sec. II—see Eq. (26).

4. Discussion of the fully connected model

The study of this model shows that observable dependence occurs as soon as the dynamics results in nonuniform probability distributions for the microstates. Further it is again possible to use the proposed general approach to characterize this nonuniformity by the entropy difference ΔS. For small driving we find a direct relation between this entropy difference and the observable dependence given in Eq. (54). The proportionality factor turns out to be independent of the coupling strength and the driving parameter. However, in the zero coupling limit, where $F(\varepsilon)$ becomes linear, both ΔS and $|\beta_p - \beta_0|/\beta$ vanish, meaning that for small coupling we expect no observable dependence.

To compare these results with the information given by the entropy production σ_s we calculate the total energy fluxes caused by the contact to the different baths. We denote as $\mathcal{J}_{\rm out}$ the total energy flux transferred from the systems to both heat baths, and by $\mathcal{J}_{\rm in}$ the total flux injected by the baths. In steady state, one has $|\mathcal{J}_{\rm out}|=|\mathcal{J}_{\rm in}|$. The flux $\mathcal{J}_{\rm in}$ is computed as

$$\mathcal{J}_{\rm in} = \int_0^\infty d\mu [J_1(\mu) + J_2(\mu)]\mu. \tag{55}$$

Expanding the above integral to second order in λ, we obtain

$$\mathcal{J}_{\rm in} = \frac{\nu}{\beta^2}[2 + 6\lambda^2 + \mathcal{O}(\lambda^4)]. \tag{56}$$

A similar calculation yields for the net energy fluxes $\mathcal{J}_\alpha$ exchanged by the bath α with the system

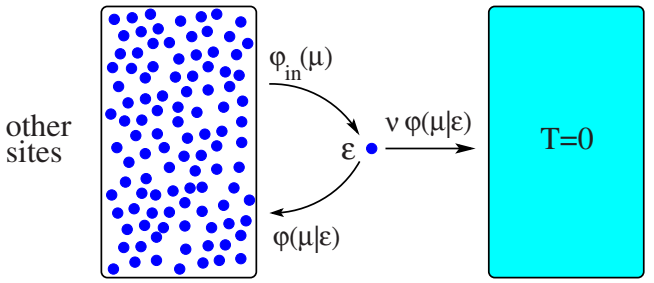

FIG. 7. (Color online) Scheme of the fully connected model in contact with a bath at zero temperature.

$$\mathcal{J}_1 = \int_0^\infty d\mu J_1(\mu)\mu - \frac{1}{2}|\mathcal{J}_{\rm out}| = 2\frac{\lambda\nu}{\beta^2} + \mathcal{O}(\lambda^3), \tag{57}$$

$$\mathcal{J}_2 = \int_0^\infty d\mu J_2(\mu)\mu - \frac{1}{2}|\mathcal{J}_{\rm out}| = -2\frac{\lambda\nu}{\beta^2} + \mathcal{O}(\lambda^3). \tag{58}$$

These results lead to an entropy production

$$\sigma_s = -(\beta_1\mathcal{J}_1 + \beta_2\mathcal{J}_2) = \frac{4\nu\lambda^2}{\beta}. \tag{59}$$

Hence we can relate $|\beta_p - \beta_0|$ to the entropy production as follows:

$$\frac{|\beta_p - \beta_0|}{\beta} = \zeta(\nu)\frac{p\beta}{2}\sigma_s, \tag{60}$$

with $\zeta(\nu)=|a_2^{(2)}(\nu)|/\nu$, the coefficient $a_2^{(2)}(\nu)$ being given in Eq. (49). Consequently in the framework of this model it is possible to relate the dependence of the temperature on the observable to the entropy production.

The quantity $|\beta_p - \beta_0|/\beta$ results linear in σ_s in contrast with the characterization through the entropy difference—see Eq. (54). Similarly to Eq. (54) the proportionality factor does not depend on the bath temperature difference λ. But contrary to the characterization via the lack of entropy, the coupling strength ν now enters into relation (60). Hence the entropy difference ΔS seems to be more directly related to $|\beta_p - \beta_0|$ than the entropy production σ_s. Note however that in the small coupling limit $\zeta(\nu)$ becomes a constant, so that the dependence upon the coupling constant disappears in this limit.

C. Slow relaxation model

1. Model and time-dependent probability distribution

The former results seem to indicate that in the case of driven systems the observable dependence is a direct result of the nonuniformity of the phase space distribution. In Sec. II, we argued that such results also hold in the time-dependent case. In the following we will investigate a similar fully connected model as in the above example, but put into contact with a single heat bath at zero temperature (see Fig. 7). Interestingly this model can be solved exactly in the nonstationary regime. In this case the evolution equation for the probability distribution of the microstates in the thermodynamic limit reads

$$\frac{\partial P(\varepsilon,t)}{\partial t} = (\nu+1)\int_0^\infty d\mu\varphi(\mu|\varepsilon+\mu)P(\varepsilon+\mu,t) - (\nu+1)\int_0^\varepsilon d\mu\varphi(\mu|\varepsilon)P(\varepsilon,t) + \int_0^\varepsilon d\mu\varphi_{\rm in}(\mu,t)P(\varepsilon-\mu,t) - \int_0^\infty d\mu\varphi_{\rm in}(\mu,t)P(\varepsilon,t), \quad (61)$$

with $\varphi_{\rm in}(\mu,t)$ given in Eq. (44). Using as an ansatz the time-dependent Gibbs distribution $P(\varepsilon,t)=\sqrt{\beta(t)/\pi\varepsilon}e^{-\beta(t)\varepsilon}$ in Eq. (61), we find the following differential equation, which should be valid for all $\varepsilon>0$:

$$\frac{1}{2}\frac{\dot\beta}{\beta} - \dot\beta\varepsilon = \frac{\nu}{\beta} - 2\nu\varepsilon, \quad (62)$$

where $\dot\beta$ denotes the time derivative of $\beta(t)$. One can easily check that the above equation implies $\dot\beta=2\nu$. Hence, starting at $t=0$ from an equilibrium distribution at temperature $T(0)=\beta_{\rm init}^{-1}$, the probability distribution is for $t>0$ a Gibbs-like distribution at temperature $T(t)=\beta(t)^{-1}$ given by

$$T(t) = \frac{1}{\beta_{\rm init}+2\nu t}. \quad (63)$$

Once expressed in terms of the variable x, the distribution reads

$$p(x,h,t) = \frac{1}{\sqrt{2\pi T(t)}}\exp\left[-\frac{(x-h)^2}{2T(t)}\right]. \quad (64)$$

The entropy difference ΔS is thus equal to zero for all times.

2. Fluctuation dissipation relation

From Eq. (6), and taking into account the factorization property, the response $\chi_p(t,t_s)$ of the observable B_p is given for $t>t_s$ by

$$\chi_p(t,t_s) = N\left\langle x(t)^{2p+1}\frac{\partial \ln p}{\partial h}(x(t_s),0,t_s)\right\rangle, \quad (65)$$

the average being computed at zero field. Therefore, we obtain the following result for the fluctuation-dissipation relation, using the probability density $p(x,h,t_s)$ given by Eq. (64)

$$\chi_p(t,t_s) = N\beta(t_s)\langle x(t)^{2p+1}x(t_s)\rangle = \beta(t_s)C(t,t_s), \quad (66)$$

where $C(t,t_s)=N\langle x(t)^{2p+1}x(t_s)\rangle$ denotes the two-time correlation function for the relaxation dynamics without field. Thus the FDR defines an effective temperature that is independent of the observable. This result is consistent with the generic relation (26) we obtained between the entropy difference and the observable dependence of the FDR (although κ_p does not have here a well-defined value).

3. Discussion of the relaxation model

We could show within this model that even for relaxation dynamics, the generic relation (26) that we derived for the observable dependence of the fluctuation-dissipation temperature still holds. We find that the probability distribution has a Gibbs form for all times, which results in zero entropy difference and no observable dependence of the fluctuation-dissipation temperature.

Can we have similar predictions using the entropy production, as was the case in the former model? The definition of the entropy production [Eq. (39)] is not valid for a zero temperature bath. Such a situation is however a theoretical idealization. The entropy production can be evaluated for an arbitrarily small bath temperature. In this limit the entropy production becomes arbitrarily large, in contrast to the entropy difference which is zero. Thus again, like in the example of the ring model, the entropy production cannot be considered as a relevant characterization of the observable dependence of the fluctuation-dissipation temperature.

IV. DISCUSSION AND CONCLUSION

In this work we were aiming for some general statements regarding the issue of observable-dependent temperatures defined from fluctuation-dissipation relations. We studied two stochastic models with nonuniform probability distributions and another stochastic model in a relaxation regime, that exhibits a time-dependent distribution of Gibbs form. These studies, complemented by the more general arguments developed in Sec. II, support the view that the observable dependence of fluctuation-dissipation temperatures in driven systems results from the nonuniformity of the phase space distribution.

In order to find a characterization of the observable dependence we related the nonuniformity of microstate distribution on a given energy shell to a quantity we call "lack of entropy" or "entropy difference" ΔS, namely, the Shannon entropy difference of the nonequilibrium system with respect to the equilibrium state with the same average energy. We generically found that the difference between the temperatures associated to two different observables is proportional to the square root of ΔS. This relation has been confirmed in the three explicit examples studied. In contrast, another quantity deeply rooted in nonequilibrium theory, namely, the entropy production, does not seem to provide a systematic characterization of the dependence of the effective temperature upon the observable. A summary of the results is presented in Table I.

It would be interesting to further test the present approach in experiments or numerical simulations of realistic models. One possibility would be to measure on the one hand the FDR temperature for different observables and different driving intensities, and on the other hand the correction $F(\varepsilon)$ to the equilibrium distribution, from which ΔS could be evaluated. This independent determination of β_p and of ΔS would then allow for a test of the relation (26) between these two quantities. Alternatively, assuming the validity of Eq. (26), one could estimate the order of magnitude of the observable dependence of the FDR temperature from the knowledge of

TABLE I. Summary of the results obtained for the three different models used as illustration, recalling the values of the entropy difference ΔS and of the entropy production σ_s, together with the observable dependence of the FDR temperature.

One-dimensional model on a ring	Fully connected model, two reservoirs	Fully connected model, one bath at $T=0$
$\Delta S^{1/2} \propto \frac{\lvert\beta_p-\beta_0\rvert}{\beta}$	$\Delta S^{1/2} \propto \frac{\lvert\beta_p-\beta_0\rvert}{\beta}$	$\Delta S=0,\ \beta_p=\beta_0$
$\sigma_s=0$	$\sigma_s \propto \zeta(\nu)\frac{\lvert\beta_p'-\beta_0\rvert}{\beta}$	$\sigma_s \to \infty$
Observable dependence	Observable dependence	No observable dependence

ΔS (assuming that κ_p is of order unity) or, in the opposite way, assess ΔS from measurements of the temperatures associated to different observables.

We argued that in out-of-equilibrium systems, the effective temperature generically depends on the observable. Our derivation relies on some rather strong assumptions (statistical independence of the degrees of freedom, and local decorrelation by each dynamical event), but there is no reason to imagine that the observable independence of the FDR temperature would be restored when such assumptions are not fulfilled. We also believe that our arguments qualitatively extend beyond the perturbative regime obtained for weak driving forces, in the sense that we expect the nonuniformity of the phase-space distribution on energy shells to yield, in a generic way, an observable dependence of the FDR temperature [even though Eq. (26) may not be valid in a strong forcing regime]. Hence the notion of effective temperature defined from fluctuation-dissipation relations in nonequilibrium systems seems to have a limited range of applicability. Recently, other types of generalization have been proposed, not relying on a notion of temperature, but rather relating the response function to a suitable, and often more complicated, correlation function [27,34,45–47]. Such an approach is certainly promising as it allows the deviations from the equilibrium FDR to be understood in more details [45]. These deviations often appear in the form of an additive term [34,44], as can also be seen from Eqs. (22) and (23). In the framework of Langevin equations, such additive corrections have been interpreted in terms of dissipated energy flux [34]. In some case, for instance when a particle is trapped in a moving potential well, an equilibrium form of the FDR can be restored by moving from the standard Eulerian frame to the Lagrangian frame associated to the trap [27]. Finally, we note that it would be interesting to further clarify the link between the present work and the results of [30]. In the latter, an upper bound for the deviation from equilibrium FDR was reported in the context of Langevin equations. This upper bound is a function of the entropy production, and implies that there should be no deviation from the equilibrium FDR if the entropy production is zero. In the ring model presented in Sec. III A, we found a systematic deviation in the FDR, although the entropy production remains equal to zero. Although there is strictly speaking no contradiction with the results of [30] since the latter apply to Langevin systems, it would be interesting to understand through which mechanism the bound provided by [30] can be violated.

ACKNOWLEDGMENT

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APPENDIX A: CALCULATION OF ΔS

In order to calculate the entropy difference $\Delta S=S_{\mathrm{eq}}(\beta^*)-S(\beta,\gamma)$ to leading order in the driving γ, we need to include in the expansion [Eq. (11)] the second-order term in γ,

$$p(x,h)=p_{\mathrm{eq}}(x,h)\{1+\gamma F[\varepsilon_h(x)]+\gamma^2 G[\varepsilon_h(x)]+\mathcal{O}(\gamma^3)\}. \tag{A1}$$

To lighten the notation we shall omit the index and the variable dependence of $\varepsilon_h(x)$ in the following and simply write ε instead. Let us first concentrate on the entropy of the nonequilibrium steady state in the presence of the forcing γ. Expanding S to order γ^2, we get

$$S(\beta,\gamma)=S_{\mathrm{eq}}(\beta)+\gamma\beta\langle\varepsilon F(\varepsilon)\rangle_{\mathrm{eq}}+\gamma^2\left[\beta\langle\varepsilon G(\varepsilon)\rangle_{\mathrm{eq}}-\frac{1}{2}\langle F(\varepsilon)^2\rangle_{\mathrm{eq}}\right]+\mathcal{O}(\gamma^3), \tag{A2}$$

where we took into account that the equilibrium averages $\langle F(\varepsilon)\rangle_{\mathrm{eq}}$ and $\langle G(\varepsilon)\rangle_{\mathrm{eq}}$ are identically zero due to the normalization condition on $p(x,h)$. We denote as $\varepsilon_{\mathrm{eq}}(\beta)$ the equilibrium average energy per degree of freedom, $\langle\varepsilon\rangle_{\mathrm{eq}}$, at temperature β. The nonequilibrium average energy $\langle\varepsilon\rangle$ in the presence of a forcing γ is denoted as $\varepsilon(\beta,\gamma)$. To calculate the equilibrium entropy at temperature β^*,

$$S_{\mathrm{eq}}(\beta^*)=\ln Z(\beta^*)+\beta^*\varepsilon_{\mathrm{eq}}(\beta^*), \tag{A3}$$

we write β^* as a second-order expansion in γ

$$\beta^*=\beta_0^*+\gamma\beta_1^*+\gamma^2\beta_2^*+\mathcal{O}(\gamma^3). \tag{A4}$$

Remember that the temperature β^* is defined implicitly by $\varepsilon_{\mathrm{eq}}(\beta^*)=\varepsilon(\beta,\gamma)$. Thus we can determine the coefficients in the above expression by comparing the expansion of $\varepsilon_{\mathrm{eq}}(\beta^*)$ with the expansion of $\varepsilon(\beta,\gamma)$. This yields $\beta_0^*=\beta$ and further

$$\varepsilon_{\mathrm{eq}}'(\beta)\beta_1^*=\langle\varepsilon F(\varepsilon)\rangle_{\mathrm{eq}}, \tag{A5}$$

$$\varepsilon_{\mathrm{eq}}'(\beta)\beta_2^*+\frac{1}{2}\varepsilon_{\mathrm{eq}}''(\beta)\beta_1^{*2}=\langle\varepsilon G(\varepsilon)\rangle_{\mathrm{eq}}, \tag{A6}$$

where $\varepsilon_{\mathrm{eq}}'(\beta)$ and $\varepsilon_{\mathrm{eq}}''(\beta)$ denote the first, respectively, the second, derivative of $\varepsilon_{\mathrm{eq}}(\beta)$. Note that here and below, the equilibrium average $\langle\cdots\rangle_{\mathrm{eq}}$ is evaluated at temperature β.

We now proceed to compute $S_{\mathrm{eq}}(\beta^*)$ from Eq. (A3). The expansion of $\ln Z(\beta^*)$ reads

$$\ln Z(\beta^*)=\ln Z(\beta)-\gamma\beta_1^*\langle\varepsilon\rangle_{\mathrm{eq}}-\gamma^2\left[\beta_2^*\langle\varepsilon\rangle_{\mathrm{eq}}+\frac{1}{2}\beta_1^*\langle\varepsilon F(\varepsilon)\rangle_{\mathrm{eq}}\right]+\mathcal{O}(\gamma^3). \tag{A7}$$

From the expansion of $\varepsilon(\beta,\gamma)$,

$$\varepsilon(\beta,\gamma) = \varepsilon_{\rm eq}(\beta) + \gamma\langle \varepsilon F(\varepsilon)\rangle_{\rm eq} + \gamma^2\langle \varepsilon G(\varepsilon)\rangle_{\rm eq} + \mathcal{O}(\gamma^3), \tag{A8}$$

and the expansion of β^*, we obtain

$$\begin{aligned}\beta^*\varepsilon_{\rm eq}(\beta^*) = \beta^*\varepsilon(\beta,\gamma) &= \beta\langle\varepsilon\rangle_{\rm eq} + \gamma[\beta_1^*\langle\varepsilon\rangle_{\rm eq} + \beta\langle\varepsilon F(\varepsilon)\rangle_{\rm eq}] \\ &+ \gamma^2[\beta_2^*\langle\varepsilon\rangle_{\rm eq} + \beta_1^*\langle\varepsilon F(\varepsilon)\rangle_{\rm eq} + \beta\langle\varepsilon G(\varepsilon)\rangle_{\rm eq}] \\ &+ \mathcal{O}(\gamma^3)\end{aligned} \tag{A9}$$

so that we finally get for the equilibrium entropy at β^*,

$$\begin{aligned}S_{\rm eq}(\beta^*) = S_{\rm eq}(\beta) &+ \gamma\beta\langle\varepsilon F(\varepsilon)\rangle_{\rm eq} \\ &+ \gamma^2\left[\beta\langle\varepsilon G(\varepsilon)\rangle_{\rm eq} + \frac{\beta_1^*}{2}\langle\varepsilon F(\varepsilon)\rangle_{\rm eq}\right].\end{aligned} \tag{A10}$$

Using this expression and the result [Eq. (A2)] yields for the entropy difference

$$\Delta S = \frac{\gamma^2}{2}\left[\langle F(\varepsilon)^2\rangle_{\rm eq} - \frac{\langle\varepsilon F(\varepsilon)\rangle_{\rm eq}^2}{\langle\varepsilon^2\rangle_{\rm eq} - \langle\varepsilon\rangle_{\rm eq}^2}\right], \tag{A11}$$

where we also took into account Eq. (A5) as well as the relation $\varepsilon'_{\rm eq}(\beta) = -(\langle\varepsilon^2\rangle_{\rm eq} - \langle\varepsilon\rangle_{\rm eq}^2)$.

Equation (A11) can be rewritten as

$$\Delta S = \frac{\gamma^2}{2\langle(\varepsilon - \langle\varepsilon\rangle)^2\rangle}[\langle(\varepsilon - \langle\varepsilon\rangle)^2\rangle\langle F(\varepsilon)^2\rangle - \langle(\varepsilon - \langle\varepsilon\rangle)F(\varepsilon)\rangle^2], \tag{A12}$$

where we omitted the index on the brackets, which all indicate averaging with respect to the equilibrium distribution. From this expression, one can deduce that $\Delta S \geq 0$, since the prefactor is strictly positive and the expression in the brackets is greater or equal to zero due to the Cauchy-Schwarz inequality.

APPENDIX B: FDR FOR THE RING MODEL

We provide in this appendix further details on the derivation of the FDR for the ring model studied in Sec. III A. The derivation of the expression for the response function reduces to the calculation of the logarithmic derivative of the probability distribution with respect to h. Starting from

$$\mathcal{P}(\{x_i\},h) = \frac{1}{Z_N}\prod_{i=1}^{N}\frac{|x_i - h|^{2\delta-1}}{2^{\delta-1}}\exp\left(-\frac{(x_i-h)^2}{2T}\right), \tag{B1}$$

we get

$$\left.\frac{\partial \ln \mathcal{P}(\{x_i\},h)}{\partial h}\right|_{h=0} = -\left.\frac{\partial \ln Z_N}{\partial h}\right|_{h=0} + \sum_{i=1}^{N}\left(\frac{x_i}{T} - \frac{2\delta-1}{x_i}\right). \tag{B2}$$

The first term on the right-hand side is identically zero, since Z_N is independent of h, as can be seen by the simple change in variable $v_i = x_i - h$ in the integral defining Z_N.

Using these results in the expression for the response $\chi_p(t)$, given in Eq. (7), of the observable $B_p(t)$ yields

$$\chi_p(t) = \left\langle\left(\sum_{i=1}^{N}\left\{\frac{x_i(0)}{T} - \frac{2\delta-1}{x_i(0)}\right\}\right)\left(\sum_{i=1}^{N}x_i^{2p+1}(t)\right)\right\rangle. \tag{B3}$$

As the variables x_i and x_j are independent for $i \neq j$, we find

$$\chi_p(t) = \frac{N}{T}\langle x(0)x(t)^{2p+1}\rangle - N(2\delta-1)\left\langle\frac{x(t)^{2p+1}}{x(0)}\right\rangle. \tag{B4}$$

Due to the random sign change in the definition of the dynamics, each event decorrelates the involved variables x_i from their previous values. As a consequence we can express the different averages involved in expression (B3) in terms of the persistence probability $\Phi(t)$ as explained in Sec. II, which leads to

$$\langle x(0)^{-1}x(t)^{2p+1}\rangle = \langle x^{2p}\rangle\Phi(t). \tag{B5}$$

As for the correlation function $C_p(t)$, we find from Eq. (32)

$$C_p(t) = N\langle x^{2p+2}\rangle\Phi(t), \tag{B6}$$

where the expression for the correlation function [Eq. (B6)] is the same as in Eq. (22) with the special choice $\psi(x)=x$, given by the coupling to the field [Eq. (31)]. Using these relations in Eq. (B4) greatly simplifies the expression, yielding

$$\chi_p(t) = \left(\frac{1}{T} - \frac{(2\delta-1)\langle x^{2p}\rangle}{\langle x^{2p+2}\rangle}\right)C_p(t). \tag{B7}$$

To obtain the final result, we have to calculate the even moments of x, which can be easily done due to the complete factorization of the probability distribution. The zero-field one-site distribution $p_0(x)$ is given by

$$p_0(x) = \frac{|x|^{2\delta-1}}{(2T)^\delta\Gamma(\delta)}e^{-x^2/2T}, \tag{B8}$$

with $\Gamma(\delta) = \int_0^\infty dz z^{\delta-1}e^{-z}$ being the Euler Gamma function. Using these results we can calculate the moments as

$$\langle x^{2n}\rangle = (2T)^n\frac{\Gamma(\delta+n)}{\Gamma(\delta)}, \tag{B9}$$

for $n \geq 0$ integer, from which Eq. (33) follows, using Eq. (B7).

APPENDIX C: BEST POLYNOMIAL APPROXIMATION FOR $F(\varepsilon)$

In this appendix, we explain the approximation scheme allowing us to derive the best polynomial approximation for $F(\varepsilon)$. The basic idea is to linearize the evolution equation for $P(\varepsilon)$ in the parameter $\gamma = \lambda^2$. The approximation is then found through a variational method, by minimizing the error in the linearized evolution equation, under the constraint of normalization and zero net flux in the system.

As an illustration of the method, we use the simplest example of a second-order polynomial $F^{(2)}(\varepsilon) = a_0^{(2)} + a_1^{(2)}\beta\varepsilon + a_2^{(2)}(\beta\varepsilon)^2$. The method however applies to polynomials of arbitrary order. We have considered polynomial approxima-

tions up to order $L=5$. To lighten the expressions we set $\beta=1$, without loss of generality.

To satisfy the normalization constraint $\langle F^{(L)}(\varepsilon)\rangle_{\mathrm{eq}}=0$ for $F^{(2)}(\varepsilon)$, we obtain $a_0^{(2)}=-\frac{1}{2}a_1^{(2)}-\frac{3}{4}a_2^{(2)}$. The balance of fluxes implies that the average energy flowing out

$$|\mathcal{J}_{\mathrm{out}}| = 2\nu\int_0^\infty d\varepsilon P(\varepsilon)\int_0^\varepsilon d\mu\varphi(\mu|\varepsilon)\mu, \tag{C1}$$

and into the system

$$|\mathcal{J}_{\mathrm{in}}| = \int_0^\infty d\mu[J_1(\mu)+J_2(\mu)]\mu, \tag{C2}$$

should be equal in absolute value $|\mathcal{J}_{\mathrm{in}}|=|\mathcal{J}_{\mathrm{out}}|$. This condition yields $a_0^{(2)}=-\frac{3}{4}+\frac{5}{4}a_2^{(2)}$ and $a_1^{(2)}=\frac{3}{2}-4a_2^{(2)}$.

We first need to obtain the equation satisfied by $F(\varepsilon)$. To this aim, we linearize the evolution Eq. (43) for the probability distribution $P(\varepsilon,t)$ with respect to the parameter $\gamma=\lambda^2$. Denoting as $R(\varepsilon)$ the linearized rhs of Eq. (43), we find

$$\begin{aligned}
R(\varepsilon) = {} & \int_0^\varepsilon d\mu\mu^2 J_0(\mu)P_{\mathrm{eq}}(\varepsilon-\mu) + 2\int_0^\varepsilon d\mu J_0(\mu)P_{\mathrm{eq}}(\varepsilon-\mu)F(\varepsilon-\mu) - \int_0^\infty d\mu\mu^2 J_0(\mu)P_{\mathrm{eq}}(\varepsilon) - 2\int_0^\infty d\mu J_0(\mu)P_{\mathrm{eq}}(\varepsilon)F(\varepsilon) \\
& + (2\nu+1)\int_0^\infty d\mu\varphi(\mu|\varepsilon+\mu)P_{\mathrm{eq}}(\varepsilon+\mu)F(\varepsilon+\mu) - (2\nu+1)\int_0^\varepsilon d\mu\varphi(\mu|\varepsilon)P_{\mathrm{eq}}(\varepsilon)F(\varepsilon) \\
& + \int_0^\varepsilon d\mu P_{\mathrm{eq}}(\varepsilon-\mu)F(\varepsilon-\mu)\int_\mu^\infty d\varepsilon'\varphi(\mu|\varepsilon')P_{\mathrm{eq}}(\varepsilon') + \int_0^\varepsilon d\mu P_{\mathrm{eq}}(\varepsilon-\mu)\int_\mu^\infty d\varepsilon'\varphi(\mu|\varepsilon')P_{\mathrm{eq}}(\varepsilon')F(\varepsilon') \\
& - \int_0^\infty d\mu P_{\mathrm{eq}}(\varepsilon)F(\varepsilon)\int_\mu^\infty d\varepsilon'\varphi(\mu|\varepsilon')P_{\mathrm{eq}}(\varepsilon') - \int_0^\infty d\mu P_{\mathrm{eq}}(\varepsilon)\int_\mu^\infty d\varepsilon'\varphi(\mu|\varepsilon')P_{\mathrm{eq}}(\varepsilon')F(\varepsilon'),
\end{aligned}$$

with $J_0(\mu)=\nu e^{-\beta\mu}$. In the stationary state this expression should be equal to zero, yielding

$$\begin{aligned}
0 = {} & \frac{16}{15}\nu\varepsilon^3 + (2\nu+1)\varepsilon^{1/2}\int_0^\varepsilon d\mu\mu^{-1/2}F(\mu) - (2\nu+1)F(\varepsilon) + (2\nu+1)\int_0^\infty d\mu e^{-\mu}F(\varepsilon+\mu) - 2\nu - 2(2\nu+1)\varepsilon F(\varepsilon) \\
& + \left(\frac{\varepsilon}{\pi}\right)^{1/2}\int_0^\varepsilon d\mu(\varepsilon-\mu)^{-1/2}\int_0^\infty d\rho\rho^{-1/2}e^{-\rho}F(\rho+\mu) - \frac{2}{\sqrt{\pi}}\int_0^\infty d\mu\mu^{1/2}e^{-\mu}F(\mu)
\end{aligned}$$

As the exact solution for $F(\varepsilon)$ is hard to obtain, we replace $F(\varepsilon)$ by its approximation $F^{(2)}(\varepsilon)$ in the rhs of the last equation, yielding

$$\begin{aligned}
R^{(2)}(\varepsilon) = {} & -a_2^{(2)} + \nu - 4a_2^{(2)}\nu + (2a_2^{(2)} + 4a_2^{(2)}\nu)\varepsilon \\
& + \frac{4}{3}(a_2^{(2)} - 3\nu + 8a_2^{(2)}\nu)\varepsilon^2 - \frac{8}{15}(a_2^{(2)} - 2\nu + 6a_2^{(2)}\nu)\varepsilon^3,
\end{aligned} \tag{C3}$$

which is not equal to zero. In order to minimize the error, we use a variational procedure. We first define a norm for the function $R^{(2)}(\varepsilon)$ as

$$\|R^{(2)}\| \equiv \langle R^{(2)}(\varepsilon)^2\rangle_{\mathrm{eq}}^{1/2}. \tag{C4}$$

Then we look for the value of $a_2^{(2)}$ that minimizes the norm $\|R^{(2)}\|$, namely,

$$\frac{d}{da_2^{(2)}}\|R^{(2)}\| = 0. \tag{C5}$$

Solving this equation, we find as best approximation for the coefficient $a_2^{(2)}=a_2^{(2)}(\nu)$,

$$a_2^{(2)}(\nu) = \frac{3\nu(7+37\nu)}{13+136\nu+358\nu^2}. \tag{C6}$$

Higher-order approximations can be obtained through similar calculations.

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