

Master equation and two heat reservoirs

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A simple spin-flip process is analyzed under the presence of two heat reservoirs. While one flip process is triggered by a bath at temperature T , the inverse process is activated by a bath at a different temperature T' . The situation can be described by using a master equation approach in a second quantized Hamiltonian formulation. The stationary solution leads to a generalized Fermi-Dirac distribution with an effective temperature T_e . Likewise the relaxation time is given in terms of T_e . Introducing a spin representation we perform a Landau expansion for the averaged spin $\langle\sigma\rangle$ as order parameter and consequently, a free energy functional can be derived. Owing to the two reservoirs the model is invariant with respect to a simultaneous change $\sigma\leftrightarrow-\sigma$ and $T\leftrightarrow T'$. This symmetry generates a third order term in the free energy which gives rise a dynamically induced first order transition.

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I. INTRODUCTION

Whereas equilibrium statistical mechanics has based on a secure theoretical foundation, this is far from being the case in nonequilibrium. The feature of equilibrium phenomena is the existence of a probability distribution describing the statistical properties of these systems. In general this distribution depends on the interaction among the particles and the temperature of a single external source called a heat bath. In nonequilibrium the situation is different and consequently also the methods, attacking the problems are different. A variety of processes are described by Markovian models, where the dynamical process depends only on the present configuration of the system. The master equation is one important tool for describing different stochastic processes on a complex energy landscape [1]. The inputs, required for the master equation [2], are a set of states and a set of transition rates between those states, for a very recent approach see [3]. Often the transition rates are determined according to the principle of detailed balance, in particular in case the system is coupled to a single heat bath with a certain but fixed temperature. Thus for stochastic jump processes the rates are assumed to follow an Arrhenius ansatz with an activation energy in terms of the temperature of the underlying heat bath. Otherwise, there is no necessity for having only one bath. Therefore we consider here a simple model with two separate heat baths at different temperatures. To be specific let us study an annihilation and creation process of particles or an equivalent spin-flip process, however, both processes should be activated by different heat reservoirs. While the spin-flip up-down is triggered by a bath at the temperature T , the reversed down-up-flip is activated by the heat bath at the different temperature T' . Apparently both flip rates are likewise determined by different temperatures. One could speculate about a generalization by introducing as many heat baths as energy levels exist, i.e., each state is related to its own bath and maybe there is a flow between the baths which established a typical nonequilibrium situation.

In the present paper we are interested in a two-level model which can be visualized in terms of a spin variable or alternatively by lattice gas variables. The flip process will be organized by a coupling to two local reservoirs. An appropriate method to study such a situation is given by the master equation approach formulated in terms of second quantized operators [4–10]. In that approach the flip-processes are described by creation and annihilation operators, whereas the temperate dependence of the rates are incorporated in the approach by using a Heisenberg-like picture [11–13]. The approach is generalized in such a manner which enables us to consider two different heat baths.

The analysis can be grouped into the current interest in studying systems with different heat reservoirs [14–33]. The analysis is motivated by searching for some generic features of nonequilibrium steady states. In particular, the question arises for a universal behavior under nonequilibrium conditions. In one of the first papers on this topic [14] the stationary nonequilibrium states in the Ising model with locally competing temperatures had been studied. The system reveals a variety of stationary states and phase transitions. A two-temperature, kinetic Ising model is investigated in [16] and extended to a diffusive kinetic system in [18]. The authors found a bicritical point, where two nonequilibrium critical lines meet. The analysis is strongly supported by Monte Carlo simulations in two dimensions. A similar simulation has been performed studying a two-temperature lattice gas model with repulsive interactions [20]. The two-dimensional nonequilibrium Ising model with competing dynamics induced by two heat baths had been studied in [15,17,21]. Despite the two reservoirs the critical exponents belong to the same universality class as the corresponding equilibrium model. In [15] the authors found a change of the phase transition from second to first order. Alternatively a two temperature lattice gas model with repulsive interactions is studied [20,27]. Hereby, the nonequilibrium transition remains continuous unlike in our approach. Another field of interest is the Carnot engine, Carnot refrigerator [22,30] including a thermally driven ratchet under periodic dichotomous temperature change [16], which can be likewise characterized by two reservoirs. General aspects of a thermodynamic cycle with open flow had been considered in

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[25] and a rectification of the Clausius inequality is recently discussed in [33]. Totally different physical situations occur, when the flow of complex fluids had been analyzed under different heat sources [19], or in case of a nonlinear oscillator coupled to various heat baths [24]. As pointed out in [26] magnetic systems with annealed degrees of freedom are predestined to offer some features of two-temperature systems. An interesting physical explanation for a two reservoir system is discussed recently [29], where the fast and the slow variables of a Hamiltonian system are related to different heat baths. In [29] it is demonstrated that the Onsager relations do not apply if the two baths are not too close. Apparently transport properties are determined by the heat sources. In [31] the occurrence of anomalous heat conductivity in a one-dimensional non-Markov process is studied, whereas in [32] a hidden heat transfer is observed, when the nonequilibrium steady states are maintained by two heat reservoirs. Very recently in a series of papers [34] the phase space probability density for steady heat flow is discussed. In that case the two baths are mutually connected leading to a flow.

As mentioned above we study a spin-flip process under the influence of two heat reservoirs. Because this process is on a mesoscopic description related to model A in the classification of Hohenberg and Halperin [35] we also analyze the critical dynamics under a two-temperature reservoir.

II. QUANTUM APPROACH TO NONEQUILIBRIUM

The further analysis is based on a master equation which is written in the form

$$\partial_t P(\vec{n}, t) = \mathcal{L}P(\vec{n}, t). \quad (1)$$

Here $P(\vec{n}, t)$ is the joint probability density that a certain configuration, characterized by a state vector $\vec{n} = (n_1, n_2, \dots, n_N)$, is realized at time t . In a lattice gas description each point is either empty or single occupied leading to $n_i = 0, 1$. Since these numbers can be considered as the eigenvalues of the particle number operator and because of the similarity of the evolution equation (1) to the Schrödinger equation one can introduce a quantum formulation of the master equation. This is firstly done by Doi [4] for a Bose-like system and later by other authors for spin operators [5–7], for reviews compare [8–10]. The dynamics of the system is determined completely by the the evolution operator \mathcal{L} and the commutation relations of the underlying operators. In case of using Pauli-operators the restrictions for the occupation numbers to empty and single occupied states is guaranteed, see Eq. (7). To transform the basic equation (1) in a second quantized form one has to relate the probability distribution $P(\vec{n}, t)$ to a state vector $|F(t)\rangle$ in a Fock-space according to $P(\vec{n}, t) = \langle \vec{n} | F(t) \rangle$. If the state vectors $|\vec{n}\rangle$ are a complete set then the last relation implies the expansion

$$|F(t)\rangle = \sum_{n_i} P(\vec{n}, t) |\vec{n}\rangle. \quad (2)$$

Under this transformation Eq. (1) can be rewritten as an equivalent equation in a Fock-space

$$\partial_t |F(t)\rangle = L|F(t)\rangle, \quad (3)$$

where the operator L is determined in such a manner that its matrix elements correspond to \mathcal{L} . It should be emphasized that the procedure is up to now independent on the realization of the basic vectors. As shown by Doi [4] the average of an arbitrary physical quantity $\mathcal{B}(\vec{n})$ can be calculated by the average of the corresponding operator $B(t)$

$$\langle B(t) \rangle = \sum_{n_i} P(\vec{n}, t) \mathcal{B}(\vec{n}) = \langle s | B | F(t) \rangle \quad (4)$$

with the state function $\langle s | = \sum \langle \vec{n} |$. Defining the density operator

$$\rho = |F(t)\rangle \langle s|, \quad (5)$$

the mean value can be even expressed in the conventional manner as follows:

$$\langle B(t) \rangle = \text{Tr}(\rho B(t)).$$

The evolution equation for an operator $B(t)$ reads now

$$\partial_t \langle B \rangle = \langle s | [B(t), L]_- | F(t) \rangle. \quad (6)$$

As the result of the procedure, all the dynamical equations governing the classical problem are determined by the structure of the evolution operator L and the commutation rules of the operators. In our case the dynamics will be realized by spin-flip processes.

III. COUPLING TO HEAT BATHS

Introducing Pauli-operators satisfying the commutation relation

$$[d_i, d_j^\dagger] = \delta_{ij}(1 - 2d_i d_i^\dagger), \quad (7)$$

the evolution operator of a flip-process at lattice site i reads [11], compare also [10],

$$L_i = \lambda(d_i^\dagger - d_i d_i^\dagger) + \gamma(d_i - d_i^\dagger d_i). \quad (8)$$

Here the flip-rates λ and γ are parameters which are temperature dependent in case the system is coupled to a heat bath. As demonstrated in [11–13] such a coupling can be directly incorporated into the quantum formulation by replacing the operator in Eq. (8) through

$$L = \nu \sum_i [(1 - d_i^\dagger) \exp(-\beta H/2) d_i \exp(\beta H/2) + (1 - d_i) \exp(-\beta H/2) d_i^\dagger \exp(\beta H/2)]. \quad (9)$$

The remaining parameter ν is determined by the microscopic time scale given by the duration of a single spin flip. The quantity $\beta = T^{-1}$ is the inverse temperature (in units of k_B) of the heat bath and H describes the static interaction. For further motivation of this approach and the relation to the Glauber model see also see [13]. Now let us generalize the model by including two heat baths with different temperatures T and T' . A possible extension of Eq. (9) is given by

$$L = \nu \sum_i [(1 - d_i^\dagger) e^{-H_i/2T'} d_i e^{H_i/2T} + (1 - d_i) e^{-H_i/2T} d_i^\dagger e^{H_i/2T}]. \quad (10)$$

The two reservoirs are coupled directly to each lattice point i , therefore the Hamiltonian is not the global one but a local energy functional. To illustrate the approach let us discuss the simplest case where the Hamiltonian is given by

$$H_i = (\varepsilon_i - \mu) d_i^\dagger d_i. \quad (11)$$

Here ε is a characteristic energy and μ is the chemical potential. Using the algebraic properties of the Pauli operators we get

$$L = \nu \sum_i [(1 - d_i^\dagger) d_i \exp((\varepsilon_i - \mu)/2T) + (1 - d_i) d_i^\dagger \exp(-(\varepsilon_i - \mu)/2T)]. \quad (12)$$

Instead of the lattice gas variable $n_i = d_i^\dagger d_i$ with the eigenvalues 0, 1 we can introduce a spin variable by $\sigma_i = 1 - 2n_i$. Thus the empty state $|0\rangle$ corresponds to the spin-up state $|\uparrow\rangle$ and the occupied state $|1\rangle$ is related to the spin-down state $|\downarrow\rangle$. With regard to Eq. (11) we find the nonzero terms of the evolution operator (10)

$$\exp(-H_i/2T') d_i \exp(H_i/2T) |1\rangle = \exp(\varepsilon_i - \mu)/2T |0\rangle,$$

$$\exp(-H_i/2T') d_i^\dagger \exp(H_i/2T) |0\rangle = \exp(-(\varepsilon_i - \mu)/2T') |1\rangle. \quad (13)$$

The flip process $|\downarrow\rangle \rightarrow |\uparrow\rangle$ is triggered by the heat bath at temperature T whereas the inverse process $|\uparrow\rangle \rightarrow |\downarrow\rangle$ is activated by the bath at T' . Here we have assumed that the activation energy ε is the same for both baths. However, a generalization to different activation energy and bath baths consequently different chemical potential is possible. We remark that there is no further restriction for the chemical potential μ . Using Eq. (6) and the algebraic properties of Pauli operators, the evolution equation for the averaged density reads

$$\nu^{-1} \partial_t \langle n_i \rangle = \exp(-(\varepsilon_i - \mu)/2T') (1 - n_i) - \exp((\varepsilon_i - \mu)/2T) \times \langle n_i \rangle. \quad (14)$$

This equation can be solved exactly and exhibits a stationary solution of the form

$$\langle n_i \rangle_s = \frac{1}{\exp((\varepsilon_i - \mu)/T_e) + 1} \quad \text{with} \quad \frac{1}{T_e} = \frac{1}{2} \left[\frac{1}{T} + \frac{1}{T'} \right]. \quad (15)$$

Obviously, the effective temperature is not the mixing temperature of both baths. Instead of that it is the harmonic average of T and T' . The result is the consequence that the inverse temperature is the integrating factor for the heat and thus the entropy, governing the steady states, is the sum of both reservoirs. Let us remark that according to Eq. (5) the nonequilibrium entropy could be defined usually by

$$S = -\text{Tr} \rho \ln \rho.$$

Due to the restriction to single flips the problem is to reduce this many particle entropy to a single particle entropy expected to be

$$S = - \sum_i [\langle n_i \rangle \ln \langle n_i \rangle + (1 - \langle n_i \rangle) \ln (1 - \langle n_i \rangle)].$$

Maximizing this expression under the constraints of a grand canonical example with two reservoirs one gets Eq. (15).

To illustrate the approach let us consider the spin representation leading to

$$\langle \sigma_i \rangle_s = \frac{e^{(\varepsilon_i - \mu)/2T} - e^{-(\varepsilon_i - \mu)/2T'}}{e^{(\varepsilon_i - \mu)/2T} + e^{-(\varepsilon_i - \mu)/2T'}}. \quad (16)$$

In the special case $T = T'$ the stationary solution coincides with the conventional equilibrium solution

$$\langle \sigma_i \rangle_s = \tanh \frac{\varepsilon_i - \mu}{2T}. \quad (17)$$

If the temperature of one of the heat baths tends to infinity (for instance $T' \rightarrow \infty$) the stationary solution is

$$\langle \sigma \rangle_s = \tanh \frac{\varepsilon_i - \mu}{4T}.$$

When both temperatures T and T' are infinitesimally [14] different from each other $T' = T + \Delta T$ the averaged spin is

$$\langle \sigma \rangle_s = \tanh \frac{\varepsilon_i - \mu}{2T} \left[1 - \frac{\Delta T (\varepsilon_i - \mu)}{2T^2 \sinh(\varepsilon_i - \mu)/T} \right]. \quad (18)$$

The relaxation time t_r related to the Eq. (14) is simply given by

$$(\nu t_{\text{rel}})^{-1} = \exp\left(\frac{\varepsilon_i - \mu}{2T}\right) + \exp\left(-\frac{\varepsilon_i - \mu}{2T'}\right). \quad (19)$$

The relaxation time for $T' \neq T$ is either enhanced for $T' < T$ or diminished in the opposite case. In particular this behavior can be observed for small difference between both baths resulting in

$$(\nu t_{\text{rel}})^{-1} = 2 \cosh\left(\frac{\varepsilon_i - \mu}{2T}\right) + \frac{\Delta T \varepsilon_i}{2T^2} e^{-(\varepsilon_i - \mu)/2T}.$$

IV. PHASE TRANSITION

Now let us study Eq. (14) for a magnetic system, where the energy ε_i at the lattice site i depends on the surrounding spin configuration. The chemical potential in that case is zero and the interaction is assumed to follow the Ising type. In the simplest mean field approximation the energy is given by

$$\varepsilon_i = 2 \left[h_i + \sum_j J_{ij} \langle \sigma_j \rangle \right], \quad (20)$$

where h_i is an external field and J_{ij} is the interaction between the z nearest neighbors. First the homogeneous case in zero field is discussed. Thus, we have

$$\varepsilon = 2Jz\langle\sigma\rangle \equiv 2T_0\langle\sigma\rangle, \quad (21)$$

whereby T_0 plays the role of the critical temperature for the conventional case with only one heat bath. Inserting Eq. (21) in Eq. (14) we get

$$\begin{aligned} \nu^{-1}\partial_t\langle\sigma\rangle &= \exp\frac{T_0\langle\sigma\rangle}{T} - \exp\left(-\frac{T_0\langle\sigma\rangle}{T'}\right) \\ &- \langle\sigma\rangle\left[\exp\frac{T_0\langle\sigma\rangle}{T} + \exp\left(-\frac{T_0\langle\sigma\rangle}{T'}\right)\right]. \end{aligned} \quad (22)$$

According to the flip rules defined in Eq. (13), this equation is invariant against the simultaneous symmetry transformation $\sigma \leftrightarrow -\sigma$ and $T \leftrightarrow T'$. Thus, making an expansion with respect to $\langle\sigma\rangle$ we find

$$\begin{aligned} \nu^{-1}\partial_t\langle\sigma\rangle &= -r\langle\sigma\rangle + b\langle\sigma\rangle^2 - u\langle\sigma\rangle^3, \\ \text{with } r &= 2T_0\left[\frac{1}{T_e} - \frac{1}{T_0}\right], \quad b = T_0^2\left[\frac{1}{T} - \frac{1}{T'}\right]\left[\frac{1}{T_e} - \frac{1}{T_0}\right], \\ u &= \frac{T_0^2}{2}\left[\frac{1}{T^2} + \frac{1}{T'^2}\right] - \frac{T_0^3}{6}\left[\frac{1}{T^3} - \frac{1}{T'^3}\right]. \end{aligned} \quad (23)$$

One can easily check that for $T=T'$ the conventional Landau expansion results. Otherwise for two different heat baths with $b \neq 0$ the extended symmetry allows a quadratic term in $\langle\sigma\rangle$. Thus one concludes that a first order transition is dynamically induced. Such a situation had been discussed already in [14,15,21] applying a different approach. To illustrate the situation in more detail let us derive directly from Eq. (23) an analog of the free energy for a two bath system:

$$\begin{aligned} \nu^{-1}\frac{\partial\langle\sigma\rangle}{\partial t} &= -\frac{\partial F}{\partial\langle\sigma\rangle} \text{ with} \\ F &= F_0 + \frac{r}{2}\langle\sigma\rangle^2 - \frac{b}{3}\langle\sigma\rangle^3 + \frac{u}{4}\langle\sigma\rangle^4. \end{aligned} \quad (24)$$

From here we find another peculiarity of the two bath system, namely the stationary solution is different from the minimum of the free energy. The stationary solution follows from Eq. (16) with Eq. (21) to be

$$\langle\sigma\rangle_s = \tanh\frac{T_0\langle\sigma\rangle_s}{T_e}. \quad (25)$$

Apparently this solution is totally different from the minimum of the free energy, which follows from Eq. (23) by setting $\partial_t\langle\sigma\rangle=0$.

Now let us consider the case that $T'=T+\Delta T$. The coefficient, defined in Eq. (23), are for temperatures in the vicinity of T_0 ,

$$\begin{aligned} r &= 2\left[\tau + \frac{\Delta T}{2T_0}\right], \quad b = -\tau\frac{\Delta T}{T_0}, \quad u = \frac{2}{3}\left[1 - \frac{3\Delta T}{4T_0}\right] \\ \text{with } \tau &= \frac{T-T_0}{T_0}. \end{aligned} \quad (26)$$

When $\Delta T \ll T \approx T_0$ the coefficient b can be neglected leading to a stationary solution

$$\langle\sigma\rangle_s = \pm \sqrt{\frac{3}{T_0}\left[\left(T_0 - \frac{\Delta T}{2}\right) - T\right]}.$$

In that case a second order phase transition results where the critical temperature is shifted to $T_0 - \frac{\Delta T}{2}$.

In the case of an inhomogeneous field h_i we calculate the response function defined by

$$\chi_{ij} = \left.\frac{\partial\langle\sigma_i\rangle}{\partial h_j}\right|_{h_j=0}. \quad (27)$$

Inserting Eq. (20) into Eq. (14), then the response function fulfills after performing the Fourier transformation in the following equation:

$$\begin{aligned} \partial_t\chi(\vec{q}, t) &= -R(\vec{q})\left[\chi(\vec{q}, t) - \frac{\prod(T, T')}{R(\vec{q})}\right] \text{ with} \\ R(\vec{q}) &= \frac{e^{T_0\langle\sigma\rangle_s/T} + e^{-T_0\langle\sigma\rangle_s/T'} - J(\vec{q})\prod(T, T')}{\prod(T, T')}, \\ \prod(T, T') &= \frac{e^{T_0\langle\sigma\rangle_s/T}[1 - \langle\sigma\rangle_s]}{T} + \frac{e^{-T_0\langle\sigma\rangle_s/T'}[1 + \langle\sigma\rangle_s]}{T'}. \end{aligned} \quad (28)$$

Here $\langle\sigma\rangle(t)$ is replaced by the stationary magnetization $\langle\sigma\rangle_s$, which satisfies Eq. (25). In case of long wave excitations it is convenient to expand the interaction as follows:

$$J(\vec{q}) = J(0)(1 - c\vec{q}^2) \quad \text{with} \quad J(0) = Jz = T_0.$$

Inserting this expression into the solution of Eq. (28) we get in the limit $t \rightarrow \infty$ the stationary susceptibility of the form

$$\begin{aligned} \chi_s^{-1}(\vec{q}) &= cT_0\vec{q}^2 + r \\ \text{with } r &= \frac{T_e - T_0(1 - \sigma_s^2)}{1 - \sigma_s^2}. \end{aligned} \quad (29)$$

In the special case $T=T'$ it results $r = [T - T_0(1 - \sigma_s^2)]/(1 - \sigma_s^2) \approx T - T_0$ as expected.

V. CONCLUSIONS

We have considered spin-flip processes where the rates are conditioned by two different heat baths. The situation in mind can be analyzed in a seemingly compact form using the master equation in a quantum Hamilton formalism. Using this formalism we find an evolution equation for the averaged occupation number, where the stationary solution gives

rise to a generalized Fermi-Dirac distribution with an effective temperature. This temperature is not the mean value of both baths. In terms of equilibrium statistics such a distribution is obtained by coupling separate baths to each energy level. Instead of using a lattice gas variable we rewrite the evolution equation in terms of spin variables and end up with a Landau-like expansion for the order parameter. From here we conclude the existence of a free energy functional, where the coefficients depend on both temperatures. Owing to the two reservoirs the system allows a novel symmetry consisting of the invariance of the evolution equation against the

change of the spin orientation and simultaneously the interchange of the baths. Consequently, a first order phase transition is dynamically induced. In a further step both baths should be coupled leading to a temperature flow.

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