On A Local Carnot Engine

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Abstract

Starting from a master equation in a quantum Hamilton form we study analytically a nonequilibrium system which is coupled locally to two heat bathes at different temperatures. Based on a lattice gas description an evolution equation for the averaged density in the presence of a temperature gradient is derived. Firstly, the case is analysed where a particle is removed from a heat bath at a fixed temperature and is traced back to the bath at another temperature. The stationary solution and the relaxation time is discussed. Secondly, a collective hopping process between different heat bathes is studied leading to an evolution equation which offers a bilinear coupling between density and temperature gradient contrary to the conventional approach. Whereas in case of a linear decreasing static temperature field the relaxation time offers a continuous spectrum it results a discrete spectrum for a quadratically decreasing temperature profile.

05.50.+q, 05.70.Ln, 82.20Mj, 44.90.+c
I. INTRODUCTION

Within the classical equilibrium thermodynamics the Carnot cycle had been considered as the standard example for studying the efficiency of heat devices acting between two heat bathes. The analysis is restricted to reservoirs with fixed temperatures and furthermore to the reversible limit. Consequently Carnot’s engine works only with a fixed rate of heat provided from the reservoirs. Recently, Velasco et al. studied a finite time Carnot refrigerator to get an upper bound for the coefficient of performance of endoreversible refrigerators. They found an upper bound for the mentioned coefficient depending on the ratio between the temperature of the cold and the hot reservoir.

There is a general interest in nonequilibrium systems with two temperatures. The analysis is motivated by searching for some generic features of nonequilibrium steady states. In particular, the question appears for a universal behavior under nonequilibrium conditions. As an example, a two-temperature, kinetic Ising model is investigated extended to a diffusive kinetic system. The authors found a bicritical point where two nonequilibrium critical lines meet. The analysis is strongly supported by Monte Carlo simulations in two dimensions. Recently, a similar simulation has been performed studying a two-temperature lattice gas model with repulsive interactions. A complete different approach is used where a thermally driven ratchet is studied under periodic, dichotomous temperature changes. The behavior of the engine is significant different from a quasistatically working one. In the author used a local heat conduction operator to study the corresponding thermal processes observed in complex fluids. Another approach consists of the analysis of a cyclic working thermodynamic devise driven by an external applied steady flow. A nonlinear oscillator coupled to various heat bathes had been considered as a simple toy model.

Here we are interested in a ‘local Carnot engine’ on a lattice gas, i.e. each point of a lattice will be contacted with two heat bathes at local different temperatures. A particle taken away from a reservoir is created at a lattice point where the creation rate depends on the local temperature related to this lattice point. In the same way a particle is annihilated from the neighboring point. This particle is removed to a reservoir on a different temperature. As the result we consider the hopping of particles from a lattice point to its neighboring one whereas both points are in contact to heat bathes on different temperatures. Alternatively, a model is studied where a particle at a certain lattice point is able to change its state, may be from spin up to spin down, however this flip process is organized by coupling to local bathes. As before the up and down states are also coupled to reservoirs at different temperatures. As a useful method to study such situations we apply the quantum formalism for nonequilibrium processes based upon spin variables.

II. QUANTUM APPROACH TO NONEQUILIBRIUM

The analysis is based on a master equation

\[ \partial_t P(\vec{n}, t) = L'P(\vec{n}, t) \]  

where \( P(\vec{n}, t) \) is the probability that a certain configuration characterized by a state vector \( \vec{n} = (n_1, n_2 \ldots n_N) \) is realized at time \( t \). In a lattice gas description each point is either
empty or single occupied \( n_i = 0, 1 \). These numbers can be considered as the eigenvalues of the particle number operator. The dynamics is determined completely by the form of the evolution operator \( L' \), specified below, and the commutation relations of the Pauli-operators. Thus, the problem is to formulate the dynamics in such a way that this restrictions in the occupation number are taken into account explicitly. The situation in mind can be analyzed in a seemingly compact form using the master equation in a quantum Hamilton formalism\([1,3]\), for a recent review see\([4,5]\). Within that approach\([4]\) the probability distribution \( P(\vec{n}, t) \) is related to a state vector \( | F(t) \rangle \) in a Fock-space according to \( P(\vec{n}, t) = \langle \vec{n} | F(t) \rangle \). The basic vectors \( | \vec{n} \rangle \) are composed of Pauli-operators. Using the relation

\[
| F(t) \rangle = \sum_{n_i} P(\vec{n}, t) | \vec{n} \rangle
\]

the master Eq. (1) can be transformed into an equivalent one in a Fock-space

\[
\partial_t | F(t) \rangle = L | F(t) \rangle
\]

where the operator \( L' \) in (1) is mapped onto the operator \( L \) in Eq.(3). It should be emphasized that the procedure is up to now independent on the realization of the basic vectors. Originally, the method had been applied for the Bose case\([2,3]\). Recently, an extension to restricted occupation numbers (two discrete orientations) was proposed\([4,5]\). Further extensions to p–fold occupation numbers\([6,7]\) as well as to models with kinetic constraints are possible\([8]\).

As shown by Doi\([10]\) the average of an arbitrary physical quantity \( B(\vec{n}) \) can be calculated by the average of the corresponding operator \( B(t) \)

\[
\langle B(t) \rangle = \sum_{n} P(\vec{n}, t) B(\vec{n}) = \langle s | B | F(t) \rangle
\]

with the state function \( \langle s | = \sum \langle \vec{n} |. \) The evolution equation for an operator \( B(t) \) reads now

\[
\partial_t \langle B \rangle = \langle s | [B(t), L] | F(t) \rangle
\]

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 either by spin-flip or by exchange processes, respectively.

### III. COUPLING TO HEAT BATHES

The evolution operator for a local flip–process reads\([2]\)

\[
L_i = \lambda (d_i^\dagger - d_i d_i^\dagger) + \gamma (d_i - d_i^\dagger d_i)
\]

where \( \lambda \) and \( \gamma \) are independent flip–rates.

The occupation number operator \( n_i = d_i^\dagger d_i \) is related to the spin due to the relation \( S_i = 1 - 2n_i. \)
A generalization to processes under the influence of a heat bath with a fixed temperature $T$ is discussed in [24]. As demonstrated in [24], the evolution operator has to be replaced by

$$L = \nu \sum_i \left[ (1 - d_i) \exp(-\beta H/2) d_i \exp(\beta H/2) \right]$$

$$+ \left[ (1 - d_i^\dagger) \exp(-\beta H/2) d_i \exp(\beta H/2) \right]$$

where $\nu$ is the flip-rate defined on a microscopic time scale; $\beta = T^{-1}$ is the inverse temperature of the heat bath and $H$ is the Hamiltonian responsible for the static interaction.

A. Flip-dynamics

Whereas by Eq.(7) the coupling to a global heat bath is realized we discuss now a further generalization by introducing two local heat bathes with different temperatures $T$ and $T'$, respectively. The two reservoirs are coupled directly to each lattice point. This situation can be described by an evolution operators

$$L(f) = \nu \sum_i \left( (1 - d_i^\dagger) e^{-\mu n_i/2T'} d_i e^{\mu n_i/2T} + (1 - d_i) e^{-\mu n_i/2T'} d_i^\dagger e^{\mu n_i/2T} \right)$$

Here $\mu$ is a characteristic energy which is necessary to remove a particle from the heat bath or to give it back to the bath. The approach reminds of using a grand canonical ensemble in equilibrium statistics. Therefore, the quantity $\mu$ plays the role of the chemical potential assumed to be identically for both processes under consideration. The potential $\mu$ can be positive or negative. Taking into account that the occupation operator $n_i$ has the eigenvalues 0 or 1 we get

$$e^{-\mu n_i/2T'} d_i e^{\mu n_i/2T} = d_i e^{\mu/2T} e^{-\mu n_i/2T'}$$

$$e^{-\mu n_i/2T'} d_i^\dagger e^{\mu n_i/2T} = d_i^\dagger e^{-\mu/2T'}$$

Thus, the operator $d_i$ annihilates a particles at the temperature $T$ independently on the temperature $T'$ of the other bath. Contrary, the operator $d_i^\dagger$ creates a particles at the temperature $T'$. The evolution operator $L(f)$ describes the process of annihilation and creation of particles within the system at different temperatures. Using the Eq.(5) and the algebraic properties of Pauli–operators, the evolution equation for the averaged density reads

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

This equation can be solved easily. It results a stationary state at an effective temperature $T_e$

$$\langle n \rangle_s = \frac{1}{1 + \exp(\mu/T_e)}$$

with

$$\frac{1}{T_e} = \frac{1}{2} \left( \frac{1}{T} + \frac{1}{T'} \right)$$

In a spin representation we obtain

$$\langle S \rangle_s = \frac{e^{\mu/2T} - e^{-\mu/2T'}}{e^{\mu/2T} + e^{-\mu/2T'}}$$
In the special case that $T = T'$ the stationary solution coincides with the conventional equilibrium solution

$$\langle S \rangle_s = \tanh \frac{\mu}{2T} \quad \langle n \rangle_s = \frac{1}{e^{\mu/T} + 1} \quad (13)$$

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

$$\langle S \rangle_s = \tanh \frac{\mu}{4T}$$

When both temperatures $T$ and $T'$ are infinitesimal different from each other $T' = T + \Delta T$ the averaged occupation number is

$$\langle n \rangle_s = \frac{1}{e^{\mu/T} + 1} + \frac{\mu(T' - T)}{4T^2} \tanh \frac{\mu}{2T} \left[ \frac{1}{e^{\mu/T} + 1} + \frac{1}{e^{\mu/T} - 1} \right] \quad (14)$$

The Fermi–distribution as the equilibrium solution is modified in lowest order in $\Delta T$ by an additional term proportional to the Bose–distribution. The relaxation time $\tau$ related to the Eq.(10) is simply given by

$$(\nu \tau)^{-1} = \exp\left(\frac{\mu}{2T}\right) + \exp\left(-\frac{\mu}{2T'}\right) \quad (15)$$

The relaxation time for $T' \neq T$ is either enhanced for $T' < T$ or diminished in the opposite case.

**B. Exchange Process**

Up to now we have analysed the case of independent flip processes (annihilation-creation-processes) at different temperatures without an internal coupling between the active particles. In the following, we discuss the situation that the particles can exchange their mutual position; with other words hopping processes are allowed between neighbor sites under the influence of the coupling to local heat baths. The evolution operator reads

$$L_{ex} = \nu \sum_{ij} \left[ (1 - d_i d_j^\dagger) e^{-\frac{\mu}{2T_i} + \frac{\mu}{2T_j}} d_i^\dagger d_j e^{\frac{\mu}{2T_i} + \frac{\mu}{2T_j}} \right] \quad (16)$$

It describes the exchange process between two adjacent neighboring sites, where the lattice site $i$ is coupled to the bath at the temperature $T_i$ and the site $j$ is related to $T_j$, respectively. The evolution equation for the averaged density can be written in the form

$$\nu^{-1} \partial_t \langle n_r \rangle = \sum_{j(r)} \langle n_j \rangle \exp[-(\mu/2)(\frac{1}{T_r} - \frac{1}{T_j})] - \langle n_r \rangle \exp[-(\mu/2)(\frac{1}{T_j} - \frac{1}{T_r})] - 2\langle n_r n_j \rangle \sinh[(\mu/2)(\frac{1}{T_j} - \frac{1}{T_r})] \quad (17)$$

In the special case of fixed temperatures $T_j = T_r = T$ the last equation is reduced to the conventional diffusion equation in a discrete representation. Here, the case will be studied
assuming a small temperature gradient. Moreover, Eq. (17) is investigated in the continuous
limit leading to the evolution equation for the density $n(x,t) = \langle n_\nu(t) \rangle l^{-d}$ (we set the lattice
size $l = 1$)

$$
\nu^{-1} \partial_t n = \nabla^2 n + \mu n \nabla^2 \frac{1}{T} + \mu \left( \nabla n \cdot \nabla \left( \frac{1}{T} \right) \right)
$$

(18)

To derive this equation we have neglected the bilinear terms in Eq. (17) which give only rise
to higher order corrections in the density. Due to the conservation of the spins within the
exchange model the evolution equation can be rewritten as a continuous equation with the current $\vec{j}(x,t)$

$$
\vec{j} = -\nu \nabla n - \nu \mu n \nabla (1/T)
$$

(19)

In contrast to the conventional nonequilibrium thermodynamics a bilinear coupling between
the density and the temperature gradient is included in the current. Such a nonlinear
coupling may change the physical behavior.

Using natural boundary conditions the stationary solution is

$$
n(x) = n_0 \exp\left( -\frac{\mu}{T(x)} \right)
$$

(20)

That means, the local density is determined by the local temperature in accordance with
the local temperature attached to each lattice site.

Let us consider the special case assuming that

$$
\nabla \left( \frac{1}{T} \right) = 2\vec{c}
$$

where $\vec{c}$ is a constant vector leading to a decreasing temperature profile

$$
T(x) = \frac{T_0}{2T_0(\vec{c} \cdot x) + 1}
$$

(21)

where $T_0$ is an arbitrary initial temperature. Eq.(18) can be solved making the ansatz

$n(x,t) = \Phi(x) \psi(x,t)$. Chosing

$$
\Phi = \Phi_0 \exp[-\mu(\vec{c} \cdot x)]
$$

$\psi(x,t)$ obeys

$$
\dot{\psi} = -[\nu \nabla^2 + \nu(\mu \vec{c})^2] \psi
$$

(22)

which is nothing else as the Schrödinger equation for a free particle. The relaxation time is
the inverse eigenvalue of the Hamiltonian $\hat{H} = -\nu \nabla^2 + \nu(\mu \vec{c})^2$ defined in Eq.(22):

$$
\tau_k = \frac{1}{\nu(k^2 + (\mu \vec{c})^2)} = \frac{1}{\nu(k^2 + \mu^2(\nabla (1/T))^2/4)}
$$

(23)

where $\vec{k}$ is the wave vector. There is a gap in the quasi-continuous relaxation spectrum for
$\vec{k} \to 0$. Moreover, the relaxation time depends on the temperature gradient. The solution
for the density is
\[ n(\vec{x}, t) = n_0 \exp \left[ (-\mu \vec{c} + i \vec{k}) \cdot \vec{x} - \frac{t}{\tau_k} \right] \] (24)

Let us consider the further solvable case

\[ \nabla \left( \frac{1}{T} \right) = 2b \vec{x} \]

which leads to a quadratically decreasing temperature profile, \( b \) is a constant.

\[ T(\vec{x}) = \frac{T_0}{T_0 b \vec{x}^2 + 1} \]

The same procedure as used before yields the Hamiltonian \( \hat{H} \) of the d-dimensional harmonic oscillator

\[ \hat{H} = -\nu \nabla^2 + \nu (\mu b)^2 \vec{x}^2 - \nu \mu bd \]

It results a discrete relaxation time spectrum where the ground state energy of the harmonic oscillator is cancelled due to the last term in \( \hat{H} \).

\[ \tau = \frac{1}{2\nu \mu b (m_1 + m_2 + \ldots + m_d)} \] (25)

where the \( m_i \) are integer numbers. Obviously, the analysis can be extended to other static temperature profiles such as an arbitrary radial symmetric one without changing the results substantially.

A temperature flow is allowed if the heat bathes are coupled. This process leads to an equalization of temperatures. Assuming that this process follows the conventional heat conduction equation

\[ T(\vec{x}, t) = \frac{1}{(4\pi \lambda t)^{d/2}} \exp \left( -\frac{\vec{x}^2}{4\lambda t} \right) \]

we conclude that Eq.(18) can also be transformed into a Schrödinger-like equation

\[ \partial_t \psi(\vec{x}, t) = -[\nu \nabla^2 + V(\vec{x}, t)] \psi(\vec{x}, t) \] (26)

where the potential \( V(\vec{x}, t) \) is known. The procedure yields a similar result for an arbitrary temperature distribution of the form \( T(\vec{x}, t) = t^{-\alpha} g(x^2/t) \).

\textbf{IV. CONCLUSIONS}

Here we have considered a generalization of the well known Carnot cycle with open flow. Each point of a lattice is related to a local heat bath hold on different temperatures. Introducing the conventional temperature means that the system is not too far from equilibrium. Consistently with this assumption is the consideration of small gradients in temperature leading to a heat transport. Such a temperature gradient is coupled to the creation and annihilation of particles or to an exchange process where a particle is created at a certain lattice point at a fixed temperature and annihilated at another point with another but fixed temperature. Using a quantum formalism for the master equation we can derive an
evolution equation for the density which offers already in a mean field like approximation a bilinear coupling between density and temperature gradients. This leads to a stationary state where the local density is related to a local temperature. The dynamics is studied for some special cases with a static temperature profile. The relaxation time spectrum offers a different behavior depending on the realization of the temperature field. Moreover, the relation time depends also on the temperature field.
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