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On the Entropy Production for the Davies Model of Heat Conduction

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The formula for the entropy production in open quantum systems is examined for the Davies model of heat conduction.

KEY WORDS: Master equation; entropy production; nonequilibrium thermodynamics; heat conduction.

1. INTRODUCTION

The theory of open quantum systems provides a rigorous description of irreversible processes and therefore provides a natural base for phenomenological nonequilibrium thermodynamics. In particular, the well-known balance equation for the entropy[(1)]

$$dS/dt = \int_v \sigma \, dv + \int_\Omega \mathbf{J}^S \, d\Omega \tag{1.1}$$

where S is the entropy of the open system, $\sigma \geqslant 0$ is the local entropy production, and $\mathbf{J}^S$ is the entropy flow through the surface of the system, should be explained by this theory. We consider the open quantum system $\mathscr{S}$, the dynamics of which is a one-parameter family $\{\Lambda_t; t \geqslant 0\}$ of linear trace-preserving maps and with completely positive dual maps $\{\Lambda_t^*, t \geqslant 0\}$ (see Refs. 2 and 3 for details).

The entropy of $\mathscr{S}$ in the state ρ is given by

$$S(\rho) = -\mathrm{tr}(\rho \ln \rho) \tag{1.2}$$

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One can introduce the relative entropy for the pair of states ρ, σ

$$S(\rho|\sigma) = -\mathrm{tr}(\rho \ln \rho - \rho \ln \sigma) \tag{1.3}$$

whenever this formula is well-defined.

If the system $\mathscr{S}$ possesses a stationary state $\rho_0 = \Lambda_t \rho_0$, $t \geqslant 0$, then the entropy production can be defined by

$$\sigma(t) =: \frac{d}{dt} S(\rho(t)|\rho_0) \tag{1.4}$$

whenever the derivative exists.

Following from the results of Lindblad,$^{(4)}$ $\sigma(t) \geqslant 0$. Taking into account (1.2) and (1.3), we obtain the total entropy flow

$$J^S = -\mathrm{tr}\left[\frac{d\rho(t)}{dt} \ln \rho_0\right] \tag{1.5}$$

Formulas (1.4) and (1.5) were suggested in Refs. 5 and 6 for the case of a dynamical semigroup and were independently studied in Refs. 7–9.

However, the above definitions (1.4) and (1.5) reproduce the formulas of nonequilibrium phenomenological thermodynamics only if ρ_0 is an equilibrium state.

In the case of an open system weakly interacting with N independent reservoirs one can define the entropy production in a slightly different way. The dynamics of such a system is governed by the following master equation:

$$\frac{d\rho}{dt} = \frac{1}{i}[H, \rho] + \sum_{k=1}^{N} L_k \rho \tag{1.6}$$

where L_k is a generator arising from the coupling of $\mathscr{S}$ to the kth reservoir.

We assume that for every $k = 1, 2, \ldots, N$ there exists a state $\rho_0(k) > 0$ such that

$$L_k \rho_0(k) = 0 \tag{1.7}$$

To avoid mathematical difficulties with unbounded operators we assume the Hilbert space of $\mathscr{S}$ to be finite-dimensional ($\dim \mathscr{H} < \infty$).

Then one can define the entropy production $\sigma(\rho)$ and the entropy flow $J^S(\rho)$ by

$$\sigma(\rho) = -\mathrm{tr} \sum_{k=1}^{N} \{L_k \rho(\ln \rho - \ln \rho_0(k))\} \tag{1.8}$$

$$J^S(\rho) = -\sum_{k=1}^{N} \mathrm{tr}\{(L_k \rho) \ln \rho_0(k)\} \tag{1.9}$$

Formulas (1.8) and (1.9) were studied in Refs. 8 and 9 for the special case of thermal reservoirs.

For further applications we prefer the more general forms (1.8) and (1.9) introduced independently but later in Ref. 10. If for certain models the stationary states $\rho_0(k)$ are not unique, then the entropy production (1.8) may not be uniquely defined.

However, we shall show in Section 3 that for the Davies model of heat conduction no ambiguity occurs in the form of the entropy production. The importance of the Davies model lies in the fact that it is simple enough but possesses a nontrivial thermodynamic local structure.

2. THE DAVIES MODEL OF HEAT CONDUCTION

In Ref. 11 Davies considers a finite, one-dimensional chain of quantum mechanical atoms with nearest neighbor interaction of a special type coupled at the ends to two infinite, quasifree reservoirs at different temperatures. A more general model of such a system consists of N subsystems $\{\mathscr{S}_k\}_{k=1}^N$ fixed in space. The M subsystems $\{\mathscr{S}_1, \mathscr{S}_2, ..., \mathscr{S}_M\}$ form the "surface" of the total open system and each of them weakly interacts with the thermal reservoir R_k, $k = 1, 2, ..., M$, at the inverse temperature β_k. Moreover, every subsystem $\mathscr{S}_k$ interacts with its neighbors via intermediate reservoirs $\{W(k|n)\}$. To avoid mathematical difficulties we assume the Hilbert spaces $\{\mathscr{H}_k\}$ of the subsystems $\{\mathscr{S}_k\}$ to be *finite-dimensional.*

The rather artificial interaction between the subsystems via the intermediate reservoirs has the effect of destroying phase relationships between the subsystems but conserves the total energy of the open system. This is a simple caricature of real nonlinear energy transfer processes (for example, collisions of phonons in solids). Omitting the derivations, which are given in Refs. 11 and 12, we write down the equation of motion for such a system in the Markovian approximation:

$$\frac{d\rho}{dt} = \frac{1}{i}[H, \rho] + \sum_{k=1}^{M} L_k\rho + \sum_{\{m-n\}} K_{mn}\rho \tag{2.1}$$

Here, the generator L_k acts on the Banach space $L^1(\mathscr{H}_k)$, and K_{mn} acts on $L^1(\mathscr{H}_m \otimes \mathscr{H}_n)$. The sum $\sum_{\{m-n\}}$ is taken over all pairs of neighbors $\{\mathscr{S}_n, \mathscr{S}_m\}$

The stationary state of the "surface" generator L_k has the form

$$\rho_0(k) = Z^{-1}(k)e^{-\beta_k H_k} \otimes \gamma, \qquad k = 1, 2, ..., M \tag{2.2}$$

where H_k is a free Hamiltonian of the subsystem $\mathscr{S}_k$ and γ is an arbitrary state on $\otimes_{n \neq k} \mathscr{H}_n$.

Under some natural assumptions concerning the coupling of $\mathscr{S}_k$ to the thermal reservoir R_k,⁽⁹⁾ the ambiguity of the arbitrary stationary state for L_k is related to γ only. The generator K_{mn} has the form

$$K_{mn}\rho = -\tfrac{1}{2}[A_{mn}, [A_{mn}, \rho]] \tag{2.3}$$

where $A_{mn} = A_{mn}^{\dagger}$ acts on the Hilbert space $\mathscr{H}_m \otimes \mathscr{H}_n$ and commutes with $H_m + H_n$.

Directly from (2.3) we have the following result:

Corollary 1. The stationary states of the generator (2.3) are the positive matrix with unit trace contained in the subalgebra $\mathscr{A}_{mn}$,

$$\mathscr{A}_{mn} = \mathscr{L}in\left\{B \otimes C;\ B \in \mathscr{B}(\mathscr{H}_m \otimes \mathscr{H}_n);\ [B, A_{mn}] = 0;\ C \in \mathscr{B}\left(\bigotimes_{l \neq m,n} \mathscr{H}_l\right)\right\}$$

Moreover, K_{mn} is self-dual, $K_{mn} = K_{mn}^{\dagger}$, and its kernel on the space $\mathscr{B}(\otimes_{l=1}^{N} \mathscr{H}_l)$ is equal to $\mathscr{A}_{mn}$.

3. THE ENTROPY BALANCE FOR THE DAVIES MODEL

Lemma 1. The component $\sigma_{mn}(\rho)$ $[J_{mn}^{S}(\rho)]$ of the entropy production [flow] related to the generator K_{mn} is equal to

$$\sigma_{mn}(\rho) = -\operatorname{tr}\{(K_{mn}\rho) \ln \rho\} \tag{3.1}$$

$$[J_{mn}^{S}(\rho) = 0] \tag{3.2}$$

for the arbitrary stationary state $\rho_0(mn)$.

Proof. Let us consider the term $\operatorname{tr}[K_{mn}\rho \ln \rho_0(mn)]$ [see (1.8), (1.9)]. Because $\rho_0(mn) \in \mathscr{A}_{mn}$, and $\mathscr{A}_{mn}$ is a subalgebra, then $\ln \rho_0(mn) \in \mathscr{A}_{mn}$; therefore, taking into account Corollary 1,

$$\operatorname{tr}\{(K_{mn}\,\rho) \ln \rho_0(mn)\} = \operatorname{tr}\{\rho(K_{mn} \ln \rho_0(mn))\} = 0 \tag{3.3}$$

Using (1.8), (1.9), (3.1), and (3.2), we obtain the following uniquely defined formulas for the entropy production and the entropy flow:

$$\sigma(\rho) = \sum_{k=1}^{M} -\operatorname{tr}[(L_k\rho)(\ln \rho + \beta_k H_k)] + \sum_{\{m-n\}} -\operatorname{tr}[(K_{mn}\rho) \ln \rho] \tag{3.4}$$

$$J^{S}(\rho) = \sum_{k=1}^{M} \beta_k \operatorname{tr}[(L_k\rho)H_k] \tag{3.5}$$

Formula (3.4) corresponds to the volume term in (1.1) and (3.5) to the surface term in (1.1).

4. A SIMPLE EXAMPLE

The entropy production in an arbitrary state (3.4) contains an enormous number of contributions related to the microscopic quantum processes in the system.

In contrast, the phenomenological formulas⁽¹⁾ are simple because they represent only the processes with a long time scale in comparison with the microscopic relaxation times.

In order to obtain the more familiar expressions for the entropy production we introduce simplifying assumptions concerning the model and especially the state. We consider a finite, one-dimensional chain of N identical atoms with nearest neighbor interaction.⁽¹¹⁾ The dimensionality of the lattice is fixed only in order to simplify the notation. The state of this system is supposed to have the following form:

$$\tilde{\rho} = \bigotimes_{k=1}^{N} Z_k^{-1} \exp\left\{ -\beta(k) H_k - \sum_{\alpha=1}^{Q} \lambda_\alpha(k) X_\alpha(k) \right\} \tag{4.1}$$

where $X_\alpha(k) = X_\alpha^\dagger(k)$ acts on $\mathscr{H}_k$ and moreover

$$[X_\alpha(k), H_k] = 0, \qquad [X_\alpha(k), X_\beta(k)] = 0 \tag{4.2}$$

Although this form of the density matrix is not preserved during the time evolution, it is instructive to calculate the entropy production with such an Anzatz.

We define the local thermodynamic fluxes $J_\alpha(k)$, $k = 0, 1, 2,..., N$, related to $X_\alpha(k)$, $\alpha = 0, 1,..., Q$, $X_0(k) \equiv H_k$:

$$J_\alpha(0) = \operatorname{tr}\{(L_1\tilde{\rho}) X_\alpha(1)\}, \qquad J_\alpha(N) = -\operatorname{tr}\{(L_N\tilde{\rho}) X_\alpha(N)\} \tag{4.3}$$

where L_1 and L_N are "surface generators"; we have

$$J_\alpha(k) = -\tfrac{1}{2} \operatorname{tr}\{(K_{k(k+1)}\tilde{\rho})\, \nabla X_\alpha(k)\} \tag{4.4}$$

$k = 1, 2,..., N - 1$, where

$$\nabla X_\alpha(k) =: X_\alpha(k+1) - X_\alpha(k) \tag{4.5}$$

For every Hilbert space $\mathscr{H}_n \otimes \mathscr{H}_{n+1}$ we define the interchange operator π_n acting on $\mathscr{B}(\mathscr{H}_n \otimes \mathscr{H}_{n+1})$

$$\pi_n(Q(n) \otimes R(n+1)) =: R(n) \otimes Q(n+1) \tag{4.6}$$

where, for example, $R(n)$ is a fixed operator R acting on the Hilbert space $\mathscr{H}_n$. The natural symmetry of a one-dimensional lattice implies [see (2.3)]

$$\pi_k A_{k(k+1)} = A_{k(k+1)} \tag{4.7}$$

Corollary 2. Suppose that (4.1)–(4.7) hold. Then the entropy production (3.4) is given by

$$\sigma(\tilde{\rho}) = -\sum_{k=0}^{N} \sum_{\alpha=0}^{Q} J_\alpha(k)\, \nabla\lambda_\alpha(k) \tag{4.8}$$

where

$$\nabla\lambda_\alpha(k) =: \lambda_\alpha(k+1) - \lambda_\alpha(k) \tag{4.9}$$

$\lambda_0(0) =: \beta_1$ is the inverse temperature of the left reservoir and $\lambda_0(N+1) =: \beta_2$ is the inverse temperature of the right reservoir; for $\alpha \geqslant 1$, $\lambda_\alpha(0) = \lambda_\alpha(N+1) = 0$.

Proof. Formula (4.8) can be obtained by simple calculations using (3.4) and (4.2) if one notices that following (4.7) and the condition

$$[A_{k(k+1)}, H_k + H_{k+1}] = 0$$

we have

$$[A_{k(k+1)}, B_k] = [A, \tfrac{1}{2}(B_k - \pi_k B_k)] \tag{4.10}$$

for $B_k = B_k^+$ acting on $\mathscr{H}_k \otimes \mathscr{H}_{k+1}$ and commuting with $H_k + H_{k+1}$.

Corollary 3. If the gradients $\nabla\lambda_\alpha(k)$ are small, then in linear approximation we obtain the Onsager relations in a local form

$$J_\alpha(k) \approx -\sum_\beta L_{\alpha\beta}(k)\, \nabla\lambda_\beta(k) \tag{4.11}$$

where

$$L_{\alpha\beta}(k) = L_{\beta\alpha}(k) \tag{4.12}$$

$$[L_{\alpha\beta}(k)] \geqslant 0 \tag{4.13}$$

Comment. This is a special case of the general derivation of Onsager relations for open systems given in Refs. 5 and 6, where the explicit form of $L_{\alpha\beta}(k)$ can be found. The above example is even much simpler because of the commutativity of $\{X_\alpha(k)\}$. The conditions (4.12) and (4.13) are closely related to the local detail balance property of the dynamics of open system (see Refs. 6, 10, and 13 for details).

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