The quantum open system as a model of the heat engine

1979 J. Phys. A: Math. Gen. 12 L103

(http://iopscience.iop.org/0305-4470/12/5/007)

J. Phys. A: Math. Gen., Vol. 12, No. 5, 1979. Printed in Great Britain

LETTER TO THE EDITOR

The quantum open system as a model of the heat engine†

Robert Alicki
Institute of Physics, Gdańsk University, 80-952 Gdańsk, Poland

Received 9 January 1979

Abstract. The quantum open system weakly coupled to thermal reservoirs at different temperatures and under the influence of slowly varying external conditions is studied. The famous Carnot inequality for the efficiency of any heat engine is obtained.

1. Introduction

Recent studies on the entropy balance in quantum open systems (Alicki 1976, McAdory and Schieve 1977, Spohn 1978, Spohn and Lebowitz 1979, Alicki 1979a) give in some cases a rigorous and elegant explanation of the fundamental laws of phenomenological non-equilibrium thermodynamics.

In order to further these studies we modify the model of an open system by introducing the influence of varying external conditions.

We investigate the quantum open system $\mathscr{S}$ weakly interacting with N independent thermal reservoirs, the initial states of which are KMS states at inverse temperatures $\{\beta_k\}$. We may also assume a weak interaction with 'conservative' reservoirs without exchange of the energy which describes the dissipation processes in an open system, such as, for example, heat conduction (Davies 1978).

We denote by H_0 the free Hamiltonian of the open system, and in order to avoid the difficulties with unbounded operators we assume the Hilbert space $\mathscr{H}$ of $\mathscr{S}$ to be finite-dimensional. Under certain technical conditions the dynamics of the system in the weak-coupling limit exists and is Markovian (Davies 1974, 1976). Then for the open system weakly interacting with the reservoirs—or equivalently if the relaxation times of the reservoirs are much shorter than the relaxation time of an open system—we can approximate the exact dynamics by the completely positive dynamical semigroup (Gorini and Kossakowski 1976, Lindblad 1976, Davies 1976) governed by the following master equation in the Schrödinger picture:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathrm{i}^{-1}[H, \rho] + \sum_{k=1}^{N} L_k\rho + K\rho. \tag{1.1}$$

Here

$$H = H_0 + \sum_n \Delta H_n, \qquad [H_0, \Delta H_n] = 0, \tag{1.2}$$

$\sum_n \Delta H_n$ describes the energy shift due to the interaction with the reservoirs, and $L_k(K)$

† This work is supported by the Polish Ministry of Higher Education, Science and Technology, project MRI7.

0305-4470/79/050103+05$01.00

is a dissipative generator arising from the interaction of $\mathcal{S}$ with a (conservative) heat reservoir.

The general forms of ΔH_n and L_k are given in the literature (e.g. Davies 1974, Kossakowski *et al* 1977, Spohn 1978), and K is studied by Davies (1978) (see also Alicki 1979b).

We present here only some relevant properties of L_k and K.

(i) The generators L_k and K depend functionally on H_0.

(ii) $L_k\rho_{\beta_k} = 0$, $k = 1, 2, \ldots, N$, where $\rho_{\beta_k} = Z^{-1}\exp(-\beta_k H_0)$.

(*iii*) K is self-dual, i.e.

$$\mathrm{tr}\{(K\rho)A\} = \mathrm{tr}\{\rho(KA)\}$$

for all $\rho \in L^1(\mathcal{H})$, $A \in \mathcal{B}(\mathcal{H})$.

(iv) $K\mathcal{A}(H_0) = 0$, where $\mathcal{A}(H_0)$ is an abelian subalgebra of $\mathcal{B}(\mathcal{H})$ generated by the Hamiltonian H_0.

To describe the possibility of such an open system performing mechanical work we introduce the family of self-adjoint operators $\{h_t;\, t \geqslant 0\}$ acting on $\mathcal{H}$. This represents a change in the external conditions, e.g. switching on some external fields or moving the walls confining the space accessible to the system (Pusz and Woronowicz 1978). We assume that these external conditions change very slowly in comparison with the relaxation time of the reservoir, τ_{R}. Therefore in every time interval $\Delta t \simeq t_1 - t$, $\Delta t \geqslant \tau_{\mathrm{R}}$ such that $h_{t'}$ is almost constant ($t' \in [t, t_1]$), the arguments used in the derivation of the Markovian master equaton (1.1) are valid, and we obtain

$$\rho(t+\Delta t) = \exp\left[\left(\mathrm{i}^{-1}[H_0 + h_t, \cdot\,] + \sum_{k=1}^{N} L_k^t + K^t\right)\Delta t\right]\rho(t) \tag{1.3}$$

where L_k^t and K^t are calculated by the substitution of $H_0 + h_t$ for the free Hamiltonian H_0 (see property (i)). For simplicity we also include in L_k^t and K the Hamiltonian parts $\mathrm{i}^{-1}[\Delta H_n^t, \cdot\,]$. This does not change the properties (i)–(iv).

It follows that for slowly varying external conditions we can use the following master equation:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \mathrm{i}^{-1}[H_0 + h_t, \rho] + \sum_{k=1}^{N} L_k^t\rho + K^t\rho \equiv \mathcal{L}(t)\rho. \tag{1.4}$$

Because for every $t \geqslant 0$, $\mathcal{L}(t)$ is a generator of a completely positive dynamical semigroup, the time evolution described by (1.4) is given by the family $\{\Lambda_{t,s},\, t \geqslant s \geqslant 0\}$ of linear, trace-preserving maps on $L^1(\mathcal{H})$ with the completely positive dual maps $\{\Lambda_{t,s}^*,\, t \geqslant s \geqslant 0\}$. We have explicitly

$$\Lambda_{t,s} = T\exp\left(\int_s^t \mathcal{L}(t')\,\mathrm{d}t'\right), \tag{1.5}$$

where T stands for the time ordering, and therefore

$$\rho(t) = \Lambda_{t,s}\rho(s) \tag{1.6}$$

$$\Lambda_{t,s}\Lambda_{s,\sigma} = \Lambda_{t,\sigma}, \qquad \Lambda_{t,t} = \mathbb{I} \tag{1.7}$$

2. The principles of thermodynamics

Thermodynamics is based on two fundamental laws—the first law of thermodynamics or the law of conservation of energy, and the second law or entropy law (de Groot and Mazur 1969).

The first principle has the following form

$$dE = dW + dQ \tag{2.1}$$

where E is the energy of the system, W is the work done by external forces, and Q is the heat supplied to the system by its surroundings.

The microscopic scheme for the description of this law is as follows. One can define

$$E(t) =: \operatorname{tr}\{\rho(t)(H_0 + h_t)\} \tag{2.2}$$

$$Q(t) =: \int_0^t \operatorname{tr}\left\{\frac{d\rho(\tau)}{d\tau}(H_0 + h_\tau)\right\} d\tau \tag{2.3}$$

$$W(t) =: \int_0^t \operatorname{tr}\left\{\rho(\tau)\frac{dh_\tau}{d\tau}\right\} d\tau \tag{2.4}$$

and hence (2.1) is obviously fulfilled. Formula (2.4) was introduced by Pusz and Woronowicz (1978) in general C^*-algebraic context.

For the system defined in § 1 the heat $Q(t)$ can be represented as a sum of heat portions supplied by individual reservoirs:

$$Q(t) = \sum_{k=1}^{N} Q_k(t) \tag{2.5}$$

$$Q_k(t) = \int_0^t \operatorname{tr}\{L_k^\tau \rho(H_0 + h_\tau)\} d\tau. \tag{2.6}$$

According to the principles of thermodynamics one can introduce for any open system a state function S, the entropy of the system.

The variation of the entropy dS may be written as the sum of two terms

$$dS = d_eS + d_iS \tag{2.7}$$

where d_eS is the entropy supplied to the system by its surroundings, and d_iS is the entropy produced inside the system.

The second law of thermodynamics states that

$$d_iS \geqslant 0. \tag{2.8}$$

One can explain this principle on microscopic grounds in some special cases of open systems (Alicki 1976, McAdory and Schieve 1977, Spohn 1978, Spohn and Lebowitz 1979, Frigerio and Spohn 1979, Alicki 1979a) using the Gibbs–von Neumann form of entropy

$$S(\rho) = -\operatorname{tr}\{\rho \ln \rho\} \tag{2.9}$$

and the results of Lindblad (1975).

For the case of the system defined in § 1 we start with the definition of the entropy flow per unit time interval:

$$J^S = \sum_{k=1}^{N} J_k^S \tag{2.10}$$

$$J_k^S = \beta_k \, dQ_k(t)/dt = \beta_k \operatorname{tr}\{L_k^t \rho(H_0 + h_t)\}. \tag{2.11}$$

Then the entropy production can be defined by

$$\sigma(t) = \mathrm{d}S(\rho)/\mathrm{d}t - J^S. \tag{2.12}$$

Theorem 1 The entropy production $\sigma(t)$ can be written in the form

$$\sigma(t) = \sum_{k=1}^{N} \operatorname{tr}\{(L_k^t\rho)[\ln\rho + \beta_k(H_0 + h_t)]\} + \operatorname{tr}\{(K^t\rho)\ln\rho\} \tag{2.13}$$

and moreover

$$\sigma(t) \geqslant 0, \qquad \forall\rho(t), t \geqslant 0. \tag{2.14}$$

Proof The formulae (2.13) and (2.14) can be easily obtained using (1.4), the equality

$$\mathrm{d}S(\rho)/\mathrm{d}t = -\operatorname{tr}\{(\mathrm{d}\rho/\mathrm{d}t)\ln\rho\} \tag{2.15}$$

and the inequality

$$-\operatorname{tr}\{(\mathscr{L}\rho)(\ln\rho - \ln\rho_0)\} \geqslant 0 \tag{2.16}$$

where $\mathscr{L}$ is the generator of a completely positive semigroup, and moreover $\mathscr{L}\rho_0 = 0$, $\rho_0 > 0$ (see Spohn 1978, Spohn and Lebowitz 1979, Frigerio and Spohn 1979, Alicki 1979a).

3. The heat engine model

We consider the model described in § 1 with two thermal reservoirs at the temperatures $T_1 \geqslant T_2$. We assume that the external conditions are changed in such a way that this open system becomes a heat engine working periodically with period t_0, i.e. we must assume the following conditions of macroscopic periodicity:

$$h_0 = h_{t_0} = 0 \tag{3.1}$$

$$\operatorname{tr}\{\rho(0)H_0\} = \operatorname{tr}\{\rho(t_0)H_0\} \tag{3.2}$$

$$S\{\rho(0)\} = S\{\rho(t_0)\}. \tag{3.3}$$

Following (2.4), (1.4), (2.3) and (3.1), (3.2) the mechanical work performed by an open system per cycle is equal to

$$-W(t_0) = -\int_0^{t_0} \operatorname{tr}\left\{\rho(t)\frac{\mathrm{d}h_t}{\mathrm{d}t}\right\}\mathrm{d}t = \int_0^{t_0} \operatorname{tr}\left(\frac{\mathrm{d}\rho}{\mathrm{d}t}\cdot H_0 + h_t\right)\mathrm{d}t = Q_1(t_0) + Q_2(t_0). \tag{3.4}$$

Taking into account (3.3), (2.12), (2.14) and (2.11) we have

$$0 = \int_0^{t_0} \frac{\mathrm{d}S(\rho)}{\mathrm{d}t}\mathrm{d}t = \int_0^{t_0} \sigma(t)\,\mathrm{d}t + \beta_1 Q_1(t_0) + \beta_2 Q_2(t_0) \tag{3.5}$$

and therefore

$$\beta_1 Q_1(t_0) + \beta_2 Q_2(t_0) \leqslant 0. \tag{3.6}$$

The formulae (3.4) and (3.5) are well known in phenomenological thermodynamics and for instance lead to the famous Carnot inequality for the efficiency η of any heat engine:

$$\eta = -W(t_0)/Q_1(t_0) \leqslant (T_1 - T_2)/T_1. \tag{3.7}$$

The similar result for two non-interacting systems in KMS states was obtained by Pusz and Woronowicz (1978) without introducing the intermediate open system but using only the changing external conditions $\{h_t\}$.

The model studied in the present Letter seems to be closer to physical reality.

References

Alicki R 1976 *Rep. Math. Phys* **10** 249
—— 1979a to be published
—— 1979b *J. Stat. Phys.* to be published
Davies E B 1974 *Commun. Math. Phys.* **39** 91
—— 1976 *Quantum Theory of Open Systems* (London: Academic)
—— 1978 *J. Stat. Phys.* **18** 161
Frigerio A and Spohn H 1979 *Proc. Mathematical Problems in the Theory of Quantum Irresversible Processes* ed Accardi, to be published
Gorini V and Kossakowski A 1976 *J. Math. Phys.* **17** 1298
de Groot S R and Mazur P 1969 *Non-Equilibrium Thermodynamics* (Amsterdam: North-Holland)
Kossakowski A, Frigerio A, Gorini V and Verri M 1977 *Commun. Math. Phys.* **57** 97
Lindblad G 1975 *Commun. Math. Phys.* **40** 147
—— 1976 *Commun. Math. Phys.* **48** 119
McAdory R T and Schieve W C 1977 *J. Chem. Phys.* **67** 1899
Pusz W and Woronowicz S L 1978 *Commun. Math. Phys.* **58** 273
Spohn H 1978 *J. Math. Phys.* **19** 1227
Spohn H and Lebowitz J L 1979 *Adv. Phys. Chem.* to be published