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A Lindblad model for a spin chain coupled to heat baths

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Abstract

We study an XY model which consists of a spin chain coupled to heat baths. We give a repeated quantum interaction Hamiltonian describing this model. We compute the explicit form of the associated Lindblad generator in the case of the spin chain coupled to one, two and several heat baths. We further study the properties of the quantum master equation such as approach to equilibrium, local equilibrium states, entropy production and quantum detailed balance condition.

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1. Introduction

The object of the quantum theory of open systems is to study the interaction of a quantum system with very large orders. There are two different approaches which have usually been considered by physicists as well as mathematicians: the Hamiltonian and the Markovian approaches.

The Hamiltonian approach consists in studying the reversible evolution of a small system in interaction with an exterior system and its main tools are: modular theory, W^* -dynamical system, Liouvillean, etc.

The Markovian approach consists in studying the irreversible evolution of these systems in interaction picture. The interaction between the two systems is described by a quantum stochastic differential equation (quantum Langevin equation), a Lindblad generator (or Lindbladian) which is the generator of quantum Markovian semigroup, etc.

It is well known that any quantum Markovian semigroup dilates a quantum stochastic differential equation in the sense of Hudson–Parthasarathy (cf [HP]). Moreover, its Lindblad generator allows us to guess the quantum master equation, which is used for studying the physical properties of a quantum system in interaction with a quantum field: quantum decoherence, approach to equilibrium, quantum detailed balance condition, etc (cf [L, Dav, F], etc). In the literature, in order to explicit the form of a Lindblad generator, we use the weak

coupling limit which describes the passage from the Hamiltonian approach to the Markovian one.

Recently, in [AP] the authors considered the setup of a small system having repeated interactions, for a short duration h , with elements of a sequence of identical quantum systems. They prove that for a good choice of the repeated quantum interaction Hamiltonian, we get the explicit form for the associated Lindblad generator.

Here, we study an XY model which consists of a spin chain coupled to several heat baths. The heat bath is modeled by an infinite chain of identical spins. The full system is described by the means of a repeated quantum interaction Hamiltonian H defined on the Hilbert space $\mathcal{H}_S \otimes \eta$, where $\mathcal{H}_S = \otimes_{k=1}^N \mathbb{C}^2$ and $\eta = \mathbb{C}^2$. After computing the Lindblad generator, we study the properties of the associated master equation. We discuss the case of the spin chain coupled to heat baths at the same inverse temperature β and the case of distinct temperatures.

This paper is organized as follows. In section 2, we compute the Lindblad generator describing the spin chain coupled to one and two heat baths at inverse temperatures β and β' . In section 3, we study the Markovian properties of the spin chain coupled to two heat baths. We give the explicit form of the stationary state ρ^β of the associated master equation in the case of $\beta = \beta'$, this is proved in section 3.1. The property of approach to equilibrium is studied in section 3.2. The explicit form of the local equilibrium states is treated in section 3.3. In section 3.4, we compute the entropy production. If $\beta = \beta'$, we show that a quantum detailed balance condition is satisfied with respect to ρ^β , this is given in section 3.5. Finally, in section 4 we study the case of a spin chain coupled to r ($2 \leq r \leq N$) heat baths.

2. A Lindblad generator for a spin chain

In this section, we give a repeated quantum interaction model associated with a spin chain coupled to one and two heat baths. We model the heat bath by an infinite chain of spins. Further, we give the GNS representation associated with the spin chain coupled to one piece (spin) of the heat bath (cf [AJ]). Finally, from [AP] we obtain the associated Lindblad generator.

2.1. Repeated quantum interaction model

In this subsection, we present one of the main results of repeated quantum interaction models. We refer the interested reader to [AP] for more details.

Let us consider a small system \mathcal{H}_0 coupled with a piece of environment \mathcal{H} . The interaction between the two systems is described by a Hamiltonian H which is defined on $\mathcal{H}_0 \otimes \mathcal{H}$ and depends on time h . The associated unitary evolution during the interval $[0, h]$ of time is

$$\mathbb{L} = e^{-ihH}.$$

After the first interaction, we repeat this time coupling the same \mathcal{H}_0 with a new copy of \mathcal{H} . Hence, the sequence of the repeated quantum interactions is described by the space

$$\mathcal{H}_0 \otimes \bigotimes_{\mathbb{N}^*} \mathcal{H}.$$

The unitary evolution of the small system in interaction picture with the n th copy of \mathcal{H} , denoted by \mathcal{H}_n , is the operator \mathbb{L}_n which acts as \mathbb{L} on $\mathcal{H}_0 \otimes \mathcal{H}_n$ and acts as the identity on copy of \mathcal{H} different to \mathcal{H}_n . The discrete evolution equation describing this model is defined on $\mathcal{H}_0 \otimes \bigotimes_{\mathbb{N}^*} \mathcal{H}$ as follows:

$$\begin{cases} V_{n+1} = \mathbb{L}_{n+1} V_n \\ V_0 = I \end{cases} \quad (1)$$

Let $\{X_i\}_{i \in \Lambda \cup \{0\}}$ be an orthonormal basis of \mathcal{H} with $X_0 = \Omega$ and let us consider the coefficients $(\mathbb{L}_j^i)_{i,j \in \Lambda \cup \{0\}}$ which are operators on \mathcal{H}_0 of the matrix representation of \mathbb{L} with respect to the basis $\{X_i\}_{i \in \Lambda \cup \{0\}}$. Then, a natural basis of $\mathcal{B}(\mathcal{H})$ is given by the family of operators $\{a_j^i, i, j \in \Lambda \cup \{0\}\}$, where

$$a_j^i(X_k) = \delta_{ik}X_j, \quad \text{for all } i, j, k \in \Lambda \cup \{0\}.$$

It is useful to note that

$$\mathbb{L} = \sum_{i,j \in \Lambda \cup \{0\}} \mathbb{L}_j^i \otimes a_j^i.$$

Put $\Psi = \otimes_{\mathbb{N}^*} \Omega$. Then from [AP], we have

$$\langle \Psi, V_n^*(X \times I) V_n \rangle = L^n(X), \quad \text{for all } X \in \mathcal{B}(\mathcal{H}_0),$$

where $L(X) = \sum_{i \in \Lambda \cup \{0\}} \mathbb{L}_i^{0*} X \mathbb{L}_i^0$ is a completely positive map.

The following result is deduced from [AP].

Theorem 2.1. *Suppose that there exist operators $L_0^0, L_i^0, i \in \Lambda$, such that*

- (i) $\mathbb{L}_0^0 = I + hL_0^0 + o(h)$,
- (ii) $\mathbb{L}_i^0 = \sqrt{h}L_i^0 + o(\sqrt{h})$.

Then, there exists a self-adjoint operator H_0 on \mathcal{H}_0 such that

$$\lim_{h \rightarrow 0} \frac{L(X) - X}{h} = \mathcal{L}(X), \quad \forall X \in \mathcal{B}(\mathcal{H}_0),$$

with

$$\mathcal{L}(X) = i[H_0, X] + \frac{1}{2} \sum_{i \in \Lambda} (2L_i^{0*} X L_i^0 - X L_i^{0*} L_i^0 - L_i^{0*} L_i^0 X).$$

Proof. Let $X \in \mathcal{B}(\mathcal{H}_0)$. Then, we have

$$\begin{aligned} L(X) &= \sum_{i \in \Lambda \cup \{0\}} U_i^{0*} X U_i^0 \\ &= X + h \left(L_0^{0*} X + X L_0^0 + \sum_{i \in \Lambda} L_i^{0*} X L_i^0 \right) + o(h). \end{aligned} \tag{2}$$

Note that the operator \mathbb{L} is unitary. This gives

$$\mathbb{L}_0^{0*} \mathbb{L}_0^0 + \sum_{i \in \Lambda} \mathbb{L}_i^{0*} \mathbb{L}_i^0 = I.$$

This implies that

$$I + h \left(L_0^{0*} + L_0^0 + \sum_{i \in \Lambda} L_i^{0*} L_i^0 \right) + o(h) = I.$$

Hence, we obtain

$$L_0^{0*} + L_0^0 = - \sum_{i \in \Lambda} L_i^{0*} L_i^0 + o(1).$$

It follows that

$$L_0^0 + \frac{1}{2} \sum_{i \in \Lambda} L_i^{0*} L_i^0 = - \left(L_0^0 + \frac{1}{2} \sum_{i \in \Lambda} L_i^{0*} L_i^0 \right)^* + o(1).$$

Then, there exists a self-adjoint operator H_0 on \mathcal{H}_0 such that

$$L_0^0 + \frac{1}{2} \sum_{i \in \Lambda} L_i^{0*} L_i^0 = -iH_0 + o(1). \tag{3}$$

Thus, if we replace (3) with (2), then the operator L is written as

$$L(X) = X + h \left\{ i[H_0, X] + \frac{1}{2} \sum_{i \in \Lambda} (2L_i^{0*} X L_i^0 - X L_i^{0*} L_i^0 - L_i^{0*} L_i^0 X) \right\} + o(h). \tag{4}$$

This proves the above theorem. \square

2.2. Spin chains coupled to one heat bath

The system (S) we consider here consists of N spins, each of them is described by the two-dimensional Hilbert space $\eta = \mathbb{C}^2$. The Hilbert space of the system (spin chain) is $\mathcal{H}_S = \otimes_{k=1}^N \mathbb{C}^2$ and its Hamiltonian is given by

$$H_S = B \sum_{k=1}^N \sigma_z^{(k)} + \sum_{k=1}^{N-1} (J_x \sigma_x^{(k)} \otimes \sigma_x^{(k+1)} + J_y \sigma_y^{(k)} \otimes \sigma_y^{(k+1)}),$$

where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and B is a real number describing the influence of an external magnetic field in the z -direction, while the interaction between nearest neighbors is described by $J_x, J_y \in \mathbb{R}$.

Let $\mathcal{B} = \{\Omega, X\}$ be the orthonormal basis of \mathbb{C}^2 equipped with its canonical scalar product, where

$$\Omega = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad X = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The heat bath is modeled by a sequence of independent photons, where each of which is described by a two-level atom \mathbb{C}^2 . Then, the Hilbert space of the heat bath is described by $\otimes_{\mathbb{N}^*} \mathbb{C}^2$, where the infinite tensor product is defined with respect to the stabilizing sequence $(\Omega)_n$. Therefore, the system (S) interacts with the photons one after another for the same short time. For more details on the physical motivation of this approach, we refer the interested reader to [EM].

The repeated quantum interaction Hamiltonian of the system coupled to the heat bath at the first spin is written as

$$H = H_S \otimes I + I \otimes H_R + H_I(h),$$

where $H_R = B\sigma_z$ is the Hamiltonian of the i th copy of the infinite chain $\otimes_{\mathbb{N}^*} \mathbb{C}^2$ and

$$H_I(h) = \frac{1}{\sqrt{h}} (\sigma_x^{(1)} \otimes \sigma_x + \sigma_y^{(1)} \otimes \sigma_y)$$

is the interaction Hamiltonian between the first spin and one piece \mathbb{C}^2 .

Put

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad n_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad n_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

In the following, we assume that $J_x = J_y = 1$ and without loss of generality we suppose that $B = 1$. Note that with respect to the basis \mathcal{B} , we have

$$H = \begin{pmatrix} H_S + I & \frac{2}{\sqrt{h}} \sigma_-^{(1)} \\ \frac{2}{\sqrt{h}} \sigma_+^{(1)} & H_S - I \end{pmatrix}$$

and the unitary evolution during the interval $[0, h]$ of times is given by

$$\mathbb{L} = \begin{pmatrix} I - ihI - ihH_S - 2h\sigma_-^{(1)}\sigma_+^{(1)} + o(h^2) & -2i\sqrt{h}\sigma_-^{(1)} + o(h^{3/2}) \\ -2i\sqrt{h}\sigma_+^{(1)} + o(h^{3/2}) & I + ihI - ihH_S - 2h\sigma_+^{(1)}\sigma_-^{(1)} + o(h^2) \end{pmatrix}.$$

Let us define the scalar product on $M_2(\mathbb{C})$ by

$$\langle A, B \rangle_\beta = \text{Tr}(\rho_\beta A^* B), \quad \forall A, B \in M_2(\mathbb{C}),$$

with

$$\rho_\beta = \frac{e^{-\beta\sigma_z}}{\text{Tr}(e^{-\beta\sigma_z})} = \begin{pmatrix} \beta_0 & 0 \\ 0 & \beta_1 \end{pmatrix}$$

being the equilibrium state at inverse temperature β of a single spin.

Put

$$X_0 = I, \quad X_1 = \frac{1}{\sqrt{\beta_0}} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad X_2 = \frac{1}{\sqrt{\beta_1}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad X_3 = \frac{1}{\sqrt{\beta_0\beta_1}} \begin{pmatrix} \beta_1 & 0 \\ 0 & -\beta_0 \end{pmatrix}.$$

It is clear that $\{X_0, X_1, X_2, X_3\}$ form an orthonormal basis of $M_2(\mathbb{C})$ equipped with the scalar product $\langle \cdot, \cdot \rangle_\beta$.

The GNS representation of $(\mathbb{C}^2, \rho_\beta)$ is the triple $(\pi, \tilde{\mathcal{H}}, \Omega_R)$, where

- $\Omega_R = I$,
- $\tilde{\mathcal{H}} = M_2(\mathbb{C})$,
- $\pi : M_2(\mathbb{C}) \rightarrow \mathcal{B}(\tilde{\mathcal{H}})$, such that $\pi(M)A = MA, \forall M, A \in M_2(\mathbb{C})$.

Actually, we prove the following.

Theorem 2.2. *The Lindblad generator of the repeated quantum interaction model associated with the spin chain coupled to one heat bath at positive temperature β^{-1} is given by*

$$\mathcal{L}_1(X) = i[H_S, X] + 2\beta_0[2\sigma_-^{(1)}X\sigma_+^{(1)} - \{n_-^{(1)}, X\}] + 2\beta_1[2\sigma_+^{(1)}X\sigma_-^{(1)} - \{n_+^{(1)}, X\}],$$

for all $X \in \mathcal{B}(\mathcal{H}_S)$.

Proof. Set $\tilde{\mathbb{L}} = \pi(\mathbb{L})$. With respect to the basis $\{X_0, X_1, X_2, X_3\}$, we have

$$\begin{aligned} \tilde{\mathbb{L}}_0^0 &= I - ihH_S + ih(\beta_1 - \beta_0)I - 2h\beta_0\sigma_-^{(1)}\sigma_+^{(1)} - 2h\beta_1\sigma_+^{(1)}\sigma_-^{(1)} + o(h^2), \\ \tilde{\mathbb{L}}_1^0 &= -2i\sqrt{\beta_0}\sqrt{h}\sigma_+^{(1)} + o(h^{3/2}), \\ \tilde{\mathbb{L}}_2^0 &= -2i\sqrt{\beta_1}\sqrt{h}\sigma_-^{(1)} + o(h^{3/2}), \\ \tilde{\mathbb{L}}_3^0 &= o(h). \end{aligned}$$

Set

$$\begin{aligned} H_0 &= H_S + (\beta_0 - \beta_1)I, \\ L_0^0 &= -iH_0 - 2\beta_0\sigma_+^{(1)}\sigma_-^{(1)} - 2\beta_1\sigma_-^{(1)}\sigma_+^{(1)}, \\ L_1^0 &= -2i\sqrt{\beta_0}\sigma_-^{(1)}, \\ L_2^0 &= -2i\sqrt{\beta_1}\sigma_+^{(1)}. \end{aligned}$$

Then, it is clear that

$$L_0^0 = -iH_0 - \frac{1}{2} \sum_{i=1}^2 L_i^0 L_i^{0*}.$$

Hence, by using theorem 2.1, the result of the above theorem holds. □

Remark. Note that if $N = 1$, then the Lindblad generator is written as

$$\mathcal{L}_1(X) = i[H_S, X] + 2\beta_0[2\sigma_- X \sigma_+ - \{n_-, X\}] + 2\beta_1[2\sigma_+ X \sigma_- - \{n_+, X\}],$$

for all $X \in M_2(\mathbb{C})$. This Lindbladian describes a two-level atom in interaction with a heat bath. It is easy to show that the associated master equation has the properties of approach to equilibrium and the quantum detailed balance condition with respect to thermodynamical state of the spin at inverse temperature β is satisfied. We refer the interested reader to [D] for more details. Moreover at zero temperature, that is $\beta = \infty$, we can prove in the same way at [D] that the associated quantum dynamical semigroup converges towards the equilibrium.

2.3. Spin chains coupled to two heat baths

Here, we suppose that the spin chain is coupled to two heat baths respectively at the first and the n th spin. Moreover, the two heat baths are supposed to be respectively at inverse temperatures β and β' . The associated repeated quantum interaction Hamiltonian is

$$H = H_S \otimes I + I \otimes H_R + H_I(h),$$

where

$$H_I(h) = \frac{1}{\sqrt{\hbar}} (\sigma_x^{(1)} \otimes \sigma_x^{(L)} + \sigma_y^{(1)} \otimes \sigma_y^{(L)} + \sigma_x^{(N)} \otimes \sigma_x^{(R)} + \sigma_y^{(N)} \otimes \sigma_y^{(R)}),$$

which describes the the left heat bath in interaction with the first spin and the right heat bath in interaction with the n th spin.

The proof of the following theorem is similar as the one of theorem 2.2.

Theorem 2.3. *The Lindblad generator associated with the spin chain coupled to two heat baths at inverse temperatures β and β' is given by*

$$\begin{aligned} \mathcal{L}(X) = & i[H_S, X] + 2\beta_0[2\sigma_-^{(1)} X \sigma_+^{(1)} - \{n_-^{(1)}, X\}] + 2\beta_1[2\sigma_+^{(1)} X \sigma_-^{(1)} - \{n_+^{(1)}, X\}] \\ & + 2\beta'_0[2\sigma_-^{(N)} X \sigma_+^{(N)} - \{n_-^{(N)}, X\}] + 2\beta'_1[2\sigma_+^{(N)} X \sigma_-^{(N)} - \{n_+^{(N)}, X\}], \end{aligned}$$

for all $X \in \mathcal{B}(\mathcal{H}_S)$.

3. Markovian properties of a spin chain coupled to two heat baths

In this section, we describe the Markovian properties of the spin chain coupled to two heat baths at inverse temperatures β and β' . We start by giving the associated quantum master equation. Moreover, we study the property of approach to equilibrium and we compute the local states. Finally for $\beta = \beta'$, we compute the entropy production and we study the quantum detailed balance condition.

Note that, in order to study the two last physical properties, we need to know explicitly the stationary state which is complicated to compute in the case where $\beta \neq \beta'$.

3.1. Quantum master equation

For all density matrix $\rho \in \mathcal{B}(\mathcal{H}_S)$, the quantum master equation of the spin chain coupled to two heat baths at inverse temperatures β and β' is defined as

$$\begin{aligned} \mathcal{L}^*(\rho) = & -i[H_S, \rho] + 2\beta_0[2\sigma_+^{(1)} \rho \sigma_-^{(1)} - \{n_-^{(1)}, \rho\}] + 2\beta_1[2\sigma_-^{(1)} \rho \sigma_+^{(1)} - \{n_+^{(1)}, \rho\}] \\ & + 2\beta'_0[2\sigma_+^{(N)} \rho \sigma_-^{(N)} - \{n_-^{(N)}, \rho\}] + 2\beta'_1[2\sigma_-^{(N)} \rho \sigma_+^{(N)} - \{n_+^{(N)}, \rho\}]. \end{aligned}$$

Note that $\dim \mathcal{H}_S < \infty$. Then, there exists a stationary state for the above master equation. Hence, in order to prove the uniqueness of the equilibrium state we need the following theorem (cf [F]).

Theorem 3.1. *Let $(\Theta_t)_t$ be a norm continuous quantum dynamical semigroup on $\mathcal{B}(\mathcal{K})$ for some separable Hilbert space \mathcal{K} whose generator L is given by*

$$L(A) = \sum_j V_j^* A V_j + K A + A K^*, \tag{5}$$

where $V_j \in \mathcal{B}(\mathcal{H})$ and $K = iH - \frac{1}{2} \sum_j V_j^* V_j$, $H = H^* \in \mathcal{B}(\mathcal{K}) (L(I) = 0)$. Suppose that $(\Theta_t^*)_t$ has a stationary faithful state ρ . Then, ρ is the unique stationary state for $(\Theta_t^*)_t$ if and only if

$$\{H, V_j^*, V_j\}' = \mathbb{C}I.$$

Put

$$\rho^\beta = \rho_\beta \otimes \dots \otimes \rho_\beta = \otimes_{i=1}^N \rho_\beta.$$

Now, we prove the following.

Theorem 3.2. *If $\beta = \beta'$, then ρ^β is the unique faithful stationary state for the quantum dynamical semigroup $(e^{t\mathcal{L}^*})_{t \geq 0}$.*

Proof. Note that it is straightforward to show that

$$[\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y, \rho_\beta \otimes \rho_\beta] = 0.$$

Hence, we get $[H_S, \rho^\beta] = 0$. Moreover, if we note by \mathcal{L}_d^* the dissipative part of \mathcal{L}^* , then it is easy to show that $\mathcal{L}_d^*(\rho^\beta) = 0$. Therefore, we have $\mathcal{L}^*(\rho^\beta) = 0$. Thus, ρ^β is a stationary state for the above master equation.

Consider an operator A such that

$$A \in \{H_S, \sigma_+^{(1)}, \sigma_-^{(1)}, \sigma_-^{(N)}, \sigma_+^{(N)}\}'.$$

In particular, we have

$$A \in \{\sigma_+^{(1)}, \sigma_-^{(1)}, \sigma_-^{(N)}, \sigma_+^{(N)}\}'.$$

This gives

$$A = I^{(1)} \otimes A_1 \otimes I^{(N)},$$

where A_1 is an operator defined on $\otimes_{k=2}^{N-1} \mathbb{C}^2$. On the other hand, we have A that commutes with H_S . Hence, we get

$$\begin{aligned} & \sigma_x^{(1)} \otimes [A_1, \sigma_x^{(2)}] \otimes I^{(N)} + \sigma_y^{(1)} \otimes [A_1, \sigma_y^{(2)}] \otimes I^{(N)} \\ & + I^{(1)} \otimes [A_1, \sigma_x^{(N-1)}] \otimes \sigma_x^{(N)} + I^{(1)} \otimes [A_1, \sigma_y^{(N-1)}] \otimes \sigma_y^{(N)} \\ & + I^{(1)} \otimes \left[A_1, \sum_{k=2}^{N-1} \sigma_z^{(k)} + \sum_{k=2}^{N-2} (\sigma_x^{(k)} \otimes \sigma_x^{(k+1)} + \sigma_y^{(k)} \otimes \sigma_y^{(k+1)}) \right] \otimes I^{(N)} = 0. \end{aligned}$$

Hence, we obtain the following:

$$[A_1, \sigma_x^{(2)}] = [A_1, \sigma_y^{(2)}] = [A_1, \sigma_x^{(N-1)}] = [A_1, \sigma_y^{(N-1)}] = 0.$$

This implies that

$$A_1 = I^{(2)} \otimes A_2 \otimes I^{(N-1)},$$

where A_2 is an operator on $\otimes_{k=3}^{N-2} \mathbb{C}^2$.

Repeating this argument until one arrives at $A = \lambda I$. Thus, we obtain

$$\{H_S, \sigma_+^{(1)}, \sigma_-^{(1)}, \sigma_+^{(N)}, \sigma_-^{(N)}\}' = \mathbb{C}I.$$

Finally, by theorem 3.1 we can conclude. □

3.2. Approach to equilibrium

The aim of this section is to prove that the quantum dynamical semigroup associated with the spin chain coupled to two heat baths has the property of approach to equilibrium.

The following theorem is introduced in [B].

Theorem 3.3. *Let L be a generator of a norm continuous quantum dynamical semigroup $(\Theta_t)_t$ on $\mathcal{B}(\mathcal{K})$ which has the form given in (3.1) and where the number of induces j is finite. Assume that the following hypothesis holds:*

- (i) *There exists a stationary state ρ for the quantum dynamical semigroup $(\Theta_t^*)_t$,*
- (ii) *The linear span of all V_j is self-adjoint,*
- (iii) *If $A \in \mathcal{B}(\mathcal{K})$ such that $\Theta_t(A^*A) = (\Theta_t A^*)(\Theta_t A)$, for all $t \geq 0$, then $A = \mathbb{C}I$.*

Then, the state ρ is faithful and the quantum dynamical semigroup $(\Theta_t^)_t$ has the property of approach to equilibrium, that is*

$$\lim_{t \rightarrow \infty} \text{Tr}(\Theta_t^* \xi A) = \text{Tr}(\rho A), \quad \text{for all normal state } \xi \text{ and for all } A \in \mathcal{B}(\mathcal{K}).$$

Under the hypothesis of the above theorem, ρ is the unique stationary state for the quantum dynamical semigroup $(\Theta_t^*)_t$. In fact, let us consider an element A in $\mathcal{B}(\mathcal{K})$ such that $[H, A] = [V_j, A] = [V_j^*, A] = 0$ for all j . Thus, from hypothesis (ii), $[V_j, A] = 0$ implies that $[V_j^*, A] = 0$. Hence, we obtain

$$L(A) = L(A^*) = L(A^*A) = 0.$$

It follows that $\Theta_t A^* = A^*$, $\Theta_t A = A$ and $\Theta_t(A^*A) = A^*A$ for all $t \geq 0$. Then, we get $\Theta_t(A^*A) = (\Theta_t A^*)(\Theta_t A)$, for all $t \geq 0$. Finally, from hypothesis (iii), we have $A = \lambda I$. Note that ρ is a faithful state. Therefore, by theorem 3.1 we can conclude.

As a corollary of theorem 3.3, we prove the following.

Theorem 3.4. *The quantum dynamical semigroup $\{T_t^* = e^{t\mathcal{L}^*}, t \in \mathbb{R}_+\}$ associated with the spin chain coupled to two heat baths at inverse temperatures β and β' has the property of approach to equilibrium to a unique stationary faithful state $\rho^{\beta, \beta'}$.*

Proof. Note that $\dim \mathcal{H}_S < \infty$. Then, there exists a stationary state for the quantum dynamical semigroup $(T_t^*)_t$. This implies that assumption (i) of the above theorem is satisfied. Moreover, it is clear that the linear span $\{\sigma_-^{(1)}, \sigma_+^{(1)}, \sigma_-^{(N)}, \sigma_+^{(N)}\}$ is self-adjoint.

Let $A \in \mathcal{B}(\mathcal{H}_S)$ such that

$$T_t(A^*A) = (T_t A^*)(T_t A), \quad \forall t \geq 0. \tag{6}$$

By using the properties of semigroup we deduce that for all $s \geq 0$,

$$\begin{aligned} T_s((T_t A)^*(T_t A)) &= T_s((T_t A^*)(T_t A)) \\ &= T_s(T_t(A^*A)) \\ &= T_{s+t}(A^*A) \\ &= (T_{s+t} A^*)(T_{s+t} A) \\ &= (T_s(T_t A)^*)(T_s(T_t A)). \end{aligned}$$

Hence, for all $t \geq 0$ the operator $T_t A$ satisfies relation (6).

Note that by taking the derivative in (6) with respect to t , we have

$$\mathcal{L}T_t(A^*A) = (\mathcal{L}T_t A^*)(T_t A) + (T_t A^*)(\mathcal{L}T_t A).$$

But we have $T_t A^* = (T_t A)^*$. Thus, we get

$$\mathcal{L}((T_t A^*)(T_t A)) = (\mathcal{L}(T_t A^*)(T_t A)) + (T_t A^*)(\mathcal{L}T_t A), \quad \forall t \geq 0. \tag{7}$$

In particular, for $t = 0$ we have

$$\mathcal{L}(A^* A) = (\mathcal{L}A^*)A + A^*(\mathcal{L}A). \tag{8}$$

On the other hand we have the following:

$$\begin{aligned} \mathcal{L}(A^* A) - (\mathcal{L}A^*)A - A^*(\mathcal{L}A) &= 4\beta_0[\sigma_+^{(1)}, A]^*[\sigma_+^{(1)}, A] + 4\beta_1[\sigma_-^{(1)}, A]^*[\sigma_-^{(1)}, A] \\ &+ 4\beta'_0[\sigma_+^{(N)}, A]^*[\sigma_+^{(N)}, A] + 4\beta'_1[\sigma_-^{(N)}, A]^*[\sigma_-^{(N)}, A]. \end{aligned}$$

Hence, if A satisfies relation (6), then the operator A satisfies

$$A \in \{\sigma_-^{(1)}, \sigma_+^{(1)}, \sigma_-^{(N)}, \sigma_+^{(N)}\}'.$$

This gives

$$A = I^{(1)} \otimes \tilde{A} \otimes I^{(N)},$$

where \tilde{A} is an operator on $\otimes_{k=2}^{N-1} \mathbb{C}^2$. Besides, from relation (7), the operator $T_t^* A$ also satisfies also (8). Therefore, $T_t A$ has to be of the same form as A , that is

$$T_t A = I^{(1)} \otimes \tilde{S}_t \otimes I^{(N)},$$

with \tilde{S}_t being an operator on $\otimes_{k=2}^{N-1} \mathbb{C}^2$. Furthermore, by taking the derivative of $T_t A$ with respect to t at $t = 0$ we obtain

$$\begin{aligned} \mathcal{L}(A) = i[H_S, A] &= i\sigma_x^{(1)} \otimes [\sigma_x^{(2)}, \tilde{A}] \otimes I^{(N)} + i\sigma_y^{(1)} \otimes [\sigma_y^{(2)}, \tilde{A}] \otimes I^{(N)} \\ &+ iI^{(1)} \otimes \left[\sum_{k=2}^{N-2} (\sigma_x^{(k)} \otimes \sigma_x^{(k+1)} + \sigma_y^{(k)} \otimes \sigma_y^{(k+1)}), \tilde{A} \right] \otimes I^{(N)} \\ &+ iI^{(1)} \otimes [\sigma_x^{(N-1)}, \tilde{A}] \otimes \sigma_x^{(N)} + iI^{(1)} \otimes [\sigma_y^{(N-1)}, \tilde{A}] \otimes \sigma_y^{(N)} \\ &= I^{(1)} \otimes \tilde{B} \otimes I^{(N)}, \end{aligned} \tag{9}$$

where $\tilde{B} = \frac{d}{dt} \tilde{S}_t|_{t=0}$. Then, from equality (9) we have

$$[\sigma_x^{(2)}, \tilde{A}] = [\sigma_y^{(2)}, \tilde{A}] = [\sigma_x^{(N-1)}, \tilde{A}] = [\sigma_y^{(N-1)}, \tilde{A}] = 0.$$

This implies that

$$\tilde{A} = I^{(2)} \otimes \tilde{A}_1 \otimes I^{(N-1)}$$

and

$$A = I^{(1)} \otimes I^{(2)} \otimes \tilde{A}_1 \otimes I^{(N-1)} \otimes I^{(N)}.$$

Note that $T_t A$ satisfies relation (6) for all $t \geq 0$. Hence, by the same argument as before, $T_t A$ is written as

$$T_t A = I^{(1)} \otimes I^{(2)} \otimes \tilde{R}_t \otimes I^{(N-1)} \otimes I^{(N)},$$

where \tilde{R}_t is an operator on $\otimes_{k=3}^{N-2} \mathbb{C}^2$. This reasoning is repeated until obtaining the result that is only possible if A is a multiple of the identity. This ends the proof. \square

3.3. Local equilibrium states

Here we suppose that the spin chain is coupled to two heat baths at inverse temperatures β and β' . Let us recall that there exists a unique stationary state $\rho^{\beta, \beta'}$ of the associated quantum dynamical semigroup. For $i \in \{1, \dots, N\}$, we denote by $\rho^{(i)}$ the local state associated with the i th spin which is given by

$$\text{Tr}(\rho^{(i)} A^{(i)}) = \text{Tr}(\rho^{\beta, \beta'} (I \otimes A^{(i)} \otimes I)), \quad (10)$$

where $A^{(i)}$ is an operator acting on the i th copy of \mathbb{C}^2 in the chain $\otimes_{k=1}^N \mathbb{C}^2$ ($\mathbb{C}_{(i)}^2$). On the other hand, $\rho^{(i)}$ can be obtained by computing the trace on the other copies than $\mathbb{C}_{(i)}^2$.

In this section, we treat the cases of the spin chain when it is made up of 2, 3 and 4 spins.

(i) For $N = 2$, we have

$$\begin{aligned} \rho^{\beta, \beta'} &= \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) - \frac{1}{8} (\beta_0 - \beta'_0)^2 \sigma_z \otimes \sigma_z \\ &\quad + \frac{(\beta_0 - \beta'_0)}{4} [n_+ \otimes n_- - n_- \otimes n_+] + i \frac{(\beta_0 - \beta'_0)}{4} [\sigma_+ \otimes \sigma_- - \sigma_- \otimes \sigma_+]. \end{aligned}$$

Hence, from (10) the local states are given by

$$\begin{aligned} \rho^{(1)} &= \langle \Omega^{(2)}, \rho_{\beta, \beta'} \Omega^{(2)} \rangle_{\mathbb{C}_{(2)}^2} + \langle X^{(2)}, \rho^{\beta, \beta'} X^{(2)} \rangle_{\mathbb{C}_{(2)}^2} \\ &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right), \\ \rho^{(2)} &= \langle \Omega^{(1)}, \rho_{\beta, \beta'} \Omega^{(1)} \rangle_{\mathbb{C}_{(1)}^2} + \langle X^{(1)}, \rho^{\beta, \beta'} X^{(1)} \rangle_{\mathbb{C}_{(1)}^2} \\ &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_{\beta'} - \rho_\beta}{2} \right), \end{aligned}$$

where $\{\Omega^{(i)} = \Omega, X^{(i)} = X\}$ is the orthonormal basis of the i th copy $\mathbb{C}_{(i)}^2$ of \mathbb{C}^2 in the atom chain $\otimes_{N^*} \mathbb{C}^2$.

(ii) For $N = 3$, the equilibrium state $\rho^{\beta, \beta'}$ is given by

$$\begin{aligned} \rho^{\beta, \beta'} &= \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) - \frac{3}{4} \left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right) \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \\ &\quad \otimes \left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right) + \frac{3}{4} \left[\left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right) \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \right. \\ &\quad \left. \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) - \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \otimes \left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right) \right] \\ &\quad + \frac{\beta_0 - \beta'_0}{8} [(\rho_\beta \otimes n_- \otimes n_+ - \rho_\beta \otimes n_+ \otimes n_-) \\ &\quad + (n_- \otimes n_+ \otimes \rho_{\beta'} - n_+ \otimes n_- \otimes \rho_{\beta'})] \\ &\quad + i \frac{\beta_0 - \beta'_0}{8} \left[\sigma_+ \otimes \sigma_- \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) - \sigma_- \otimes \sigma_+ \otimes \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \right] \\ &\quad + i \frac{\beta_0 - \beta'_0}{8} \left[\left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \otimes \sigma_+ \otimes \sigma_- - \left(\frac{\rho_\beta + \rho_{\beta'}}{2} \right) \otimes \sigma_- \otimes \sigma_+ \right] \\ &\quad + i \frac{\beta_0 - \beta'_0}{8} [\rho_\beta \otimes \sigma_+ \otimes \sigma_- - \rho_\beta \otimes \sigma_- \otimes \sigma_+] \\ &\quad + i \frac{\beta_0 - \beta'_0}{8} [\sigma_+ \otimes \sigma_- \otimes \rho_{\beta'} - \sigma_- \otimes \sigma_+ \otimes \rho_{\beta'}] \\ &\quad - \frac{(\beta_0 - \beta'_0)^2}{16} [\sigma_+ \otimes I \otimes \sigma_- + \sigma_- \otimes I \otimes \sigma_+]. \end{aligned}$$

In the same way as the case $N = 2$, we get

$$\begin{aligned}\rho^{(1)} &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right), \\ \rho^{(2)} &= \frac{\rho_\beta + \rho_{\beta'}}{2} = \frac{\rho^{(1)} + \rho^{(3)}}{2}, \\ \rho^{(3)} &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_{\beta'} - \rho_\beta}{2} \right).\end{aligned}$$

(iii) For $N = 4$, after computing the stationary state $\rho^{\beta, \beta'}$, we have obtained the following

$$\begin{aligned}\rho^{(1)} &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right), \\ \rho^{(2)} &= \rho^{(3)} = \frac{\rho_\beta + \rho_{\beta'}}{2} = \frac{\rho^{(1)} + \rho^{(4)}}{2}, \\ \rho^{(4)} &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_{\beta'} - \rho_\beta}{2} \right).\end{aligned}$$

Note that for $N \geq 5$, it is very hard to compute the stationary state $\rho^{\beta, \beta'}$. Moreover, from the computation done in the cases of the spin chain when it is made up of 2, 3 and 4 atoms, we see that when N increases, the number of the off-diagonal terms increases quickly in the explicit form of the matrix of the state $\rho^{\beta, \beta'}$ in the canonical basis of \mathcal{H}_S . Besides, the off-diagonal terms do not contribute to the calculation of the partial trace at any site. However, the form of the diagonal terms given in the cases $N = 2, 3$ and 4 are similar enough that we believe that the following conjecture is true: for $N \geq 5$, the local states are given by

$$\begin{aligned}\rho^{(1)} &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_\beta - \rho_{\beta'}}{2} \right), \\ \rho^{(2)} &= \dots = \rho^{(N-1)} = \frac{\rho_\beta + \rho_{\beta'}}{2} = \frac{\rho^{(1)} + \rho^{(N)}}{2}, \\ \rho^{(N)} &= \frac{\rho_\beta + \rho_{\beta'}}{2} + \frac{1}{2} \left(\frac{\rho_{\beta'} - \rho_\beta}{2} \right).\end{aligned}$$

3.4. Entropy production

In this section, we treat the case of the spin chain coupled to two heat baths at the same temperature β^{-1} . Let us recall that from theorem 3.2, there exists a unique stationary faithful state ρ^β for the associated quantum master equation in the case of the same temperature $\beta = \beta'$. The definition of entropy production, that we give here, is taken from [SL].

Let ρ be a state on \mathcal{H}_S and set $\rho(t) = e^{t\mathcal{L}^*}(\rho)$. Then the relative entropy of ρ with respect to ρ^β is defined by

$$S(\rho(t)|\rho^\beta) = \text{Tr}(\rho(t)(\log \rho^\beta - \log \rho(t))).$$

Hence, the entropy production is given by

$$\begin{aligned}\sigma(\rho) &= -\left. \frac{d}{dt} S(\rho(t)|\rho^\beta) \right|_{t=0} \\ &= \text{Tr}(\mathcal{L}^*(\rho)(\log \rho^\beta - \log \rho)),\end{aligned}$$

where $\text{Tr}(\mathcal{L}^*(\rho) \log \rho)$ is given as

$$\begin{aligned} \text{Tr}(\mathcal{L}^*(\rho) \log \rho) &= \sum_j \langle \Psi_j, \mathcal{L}^*(\rho) \Psi_j \rangle \log \rho_j, \\ \langle \Psi_j, \mathcal{L}^*(\rho) \Psi_j \rangle \log \rho_j &= \begin{cases} -\infty & \text{if } \langle \Psi_j, \mathcal{L}^*(\rho) \Psi_j \rangle \neq 0 \text{ and } \rho_j = 0 \\ 0 & \text{if } \langle \Psi_j, \mathcal{L}^*(\rho) \Psi_j \rangle = 0. \end{cases} \end{aligned}$$

Theorem 3.5. *The entropy production associated with the spin chain coupled to two heat baths at the same inverse temperature β is written as*

$$\sigma(\rho) = 4\beta_0 \left[\sum_{j,k} [|\langle \Psi_k, \sigma_+^{(1)} \Psi_j \rangle|^2 + |\langle \Psi_k, \sigma_+^{(N)} \Psi_j \rangle|^2] (e^{2\beta} \rho_k - \rho_j) (\log \rho_k - \log \rho_j + 2\beta) \right],$$

where $\rho = \sum_j \rho_j |\Psi_j\rangle \langle \Psi_j|$ is the spectral decomposition of ρ .

Proof. Note that

$$\mathcal{L}^* = \mathcal{L}_h^* + \mathcal{L}_d^*,$$

where \mathcal{L}_h^* is the Hamiltonian part of \mathcal{L}^* and $\mathcal{L}_d^* = \mathcal{L}_d^{*(1)} + \mathcal{L}_d^{*(N)}$ is its dissipative part with

$$\begin{aligned} \mathcal{L}_d^{*(1)}(\rho) &= 2\beta_0 [2\sigma_+^{(1)} \rho \sigma_-^{(1)} - \{n_-^{(1)}, \rho\}] + 2\beta_1 [2\sigma_-^{(1)} \rho \sigma_+^{(1)} - \{n_+^{(1)}, \rho\}], \\ \mathcal{L}_d^{*(N)}(\rho) &= 2\beta_0' [2\sigma_+^{(N)} \rho \sigma_-^{(N)} - \{n_-^{(N)}, \rho\}] + 2\beta_1' [2\sigma_-^{(N)} \rho \sigma_+^{(N)} - \{n_+^{(N)}, \rho\}]. \end{aligned}$$

Put

$$H^{(S)} = \sum_{k=1}^N \sigma_z^{(k)}.$$

It is easy to show that the equilibrium state ρ^β is given by

$$\rho^\beta = \frac{1}{Z} e^{-\beta H^{(S)}},$$

where $Z = \text{Tr}(e^{-\beta H^{(S)}})$. Thus, we obtain $\log \rho^\beta = -\beta H^{(S)} - \log Z$. On the other hand, a straightforward computation shows that

$$\text{Tr}([H_S, \rho] \log \rho) = \text{Tr}(H_S[\rho, \log \rho]) = 0$$

and

$$\text{Tr}([H_S, \rho] \log \rho^\beta) = -\beta \text{Tr}([H^{(S)}, H_S]\rho) = 0.$$

Hence, we get

$$\text{Tr}(\mathcal{L}_h^*(\rho(\log \rho^\beta - \log \rho))) = 0.$$

This gives

$$\sigma(\rho) = \sigma_1(\rho) + \sigma_N(\rho) = -\text{Tr}(\mathcal{L}_d^*(\rho) \log \rho) - \beta \text{Tr}(\mathcal{L}_d^*(\rho) H^{(S)}), \quad (11)$$

where $\sigma_i(\rho) = -\text{Tr}(\mathcal{L}_d^{*(i)}(\rho) \log \rho) - \beta \text{Tr}(\mathcal{L}_d^{*(i)}(\rho) H^{(S)})$ with $i = 1, N$.

Let us compute the terms of the second member in (11). We have

$$\begin{aligned} \text{Tr}(\mathcal{L}_d^{*(1)}(\rho) \log \rho) &= 4\beta_0 \left[\sum_{j,k} \langle \Psi_j, \sigma_-^{(1)} \Psi_k \rangle \langle \Psi_k, \sigma_+^{(1)} \Psi_j \rangle \rho_j \log \rho_k - \sum_j \langle \Psi_j, n_-^{(1)} \Psi_j \rangle \rho_j \log \rho_j \right] \\ &\quad + 4\beta_1 \left[\sum_{j,k} \langle \Psi_j, \sigma_+^{(1)} \Psi_k \rangle \langle \Psi_k, \sigma_-^{(1)} \Psi_j \rangle \rho_j \log \rho_k - \sum_j \langle \Psi_j, n_+^{(1)} \Psi_j \rangle \rho_j \log \rho_j \right], \\ \text{Tr}(\mathcal{L}_d^{*(1)}(\rho) H^{(S)}) &= 8\beta_0 \sum_j \langle \Psi_j, n_-^{(1)} \Psi_j \rangle \rho_j - 8\beta_1 \sum_j \langle \Psi_j, n_+^{(1)} \Psi_j \rangle \rho_j. \end{aligned}$$

Note that

$$\begin{aligned} \langle \Psi_j, n_+^{(1)} \Psi_j \rangle &= \|\sigma_+^{(1)} \Psi_j\|^2 = \sum_k |\langle \Psi_k, \sigma_+^{(1)} \Psi_j \rangle|^2, \\ \langle \Psi_j, n_-^{(1)} \Psi_j \rangle &= \|\sigma_-^{(1)} \Psi_j\|^2 = \sum_k |\langle \Psi_j, \sigma_+^{(1)} \Psi_k \rangle|^2. \end{aligned}$$

This gives

$$\begin{aligned} \sigma_1(\rho) &= 4\beta_0 \left[\sum_{j,k} |\langle \Psi_k, \sigma_+^{(1)} \Psi_j \rangle|^2 \rho_j (\log \rho_j - \log \rho_k - 2\beta) \right] \\ &\quad + 4\beta_1 \left[\sum_{j,k} |\langle \Psi_j, \sigma_+^{(1)} \Psi_k \rangle|^2 \rho_j (\log \rho_j - \log \rho_k + 2\beta) \right]. \end{aligned} \tag{12}$$

If we substitute β_1 by $e^{2\beta} \beta_0$ into (12), then we get

$$\sigma_1(\rho) = 4\beta_0 \left[\sum_{j,k} |\langle \Psi_k, \sigma_+^{(1)} \Psi_j \rangle|^2 (e^{2\beta} \rho_k - \rho_j) (\log \rho_k - \log \rho_j + 2\beta) \right].$$

In the same way, we prove that

$$\sigma_N(\rho) = 4\beta_0 \left[\sum_{j,k} |\langle \Psi_k, \sigma_+^{(N)} \Psi_j \rangle|^2 (e^{2\beta} \rho_k - \rho_j) (\log \rho_k - \log \rho_j + 2\beta) \right].$$

This ends the proof of the above theorem. □

Remark. Note that as a corollary of the above theorem, we have $\sigma(\rho) \geq 0$ for any density matrix ρ .

3.5. Quantum detailed balance condition

In this section, we suppose that the spin chain is coupled to two heat baths the at same inverse temperature β . Let us recall that

$$\rho^\beta = \otimes_{k=1}^N \rho_\beta$$

is the only stationary faithful state of the quantum dynamical semigroup $(T_t^*)_t$.

The following definition is introduced in [AL].

Definition 1. Let Θ be a generator of a quantum dynamical semigroup written as

$$\Theta = -i[H, \cdot] + \Theta_0,$$

where H is a self-adjoint operator. We say that Θ satisfies a quantum detailed balance condition with respect to a stationary state ρ if

- (i) $[H, \rho] = 0$,
- (ii) $\langle \Theta_0(A), B \rangle_\rho = \langle A, \Theta_0(B) \rangle_\rho$, for all $A, B \in D(\Theta_0)$,
- (iii) with $\langle A, B \rangle_\rho = \text{Tr}(\rho A^* B)$.

Now, we prove the following.

Theorem 3.6. The generator \mathcal{L}^* of the quantum dynamical semigroup of the spin chain coupled to two heat baths at the same inverse temperature β satisfies a quantum detailed balance condition with respect to the stationary state ρ^β .

Proof. Note that

$$\mathcal{L}^* = -i[H_S, \cdot] + \mathcal{L}_d^*,$$

where \mathcal{L}_d^* is the dissipative part. On the other hand, we have $[H_S, \rho^\beta] = 0$. This proves that assumption (i) of the above definition is satisfied. Furthermore, it is easy to show that \mathcal{L}_d^* is a self-adjoint operator with respect to the scalar product $\langle A, B \rangle_{\rho^\beta}$. Thus, the above theorem holds. \square

4. Spin chain coupled to several heat baths

Consider a spin chain (N spins) coupled to r heat baths at inverse temperatures $\beta^{(k_1)}, \beta^{(k_2)}, \dots, \beta^{(k_r)}$, where $2 \leq r \leq N$ for all $j = 1, \dots, r$ and k_j is the k_j th site of the chain $\otimes_{i=1}^N \mathbb{C}^2$. The quantum repeated interaction Hamiltonian is given by

$$H = H_S \otimes I + I \otimes H_R + \frac{1}{\sqrt{\hbar}} \sum_{j=1}^r (\sigma_x^{(k_j)} \otimes \sigma_x^{(k_j)} + \sigma_y^{(k_j)} \otimes \sigma_y^{(k_j)}).$$

In the same way as in section 2.2, we prove that the associated Lindblad generator has the form

$$\begin{aligned} \mathcal{L}(X) = & i[H_S, X] + 2\beta_0^{(k_1)} [2\sigma_-^{(k_1)} X \sigma_+^{(k_1)} - \{n_-^{(k_1)}, X\}] + 2\beta_1^{(k_1)} [2\sigma_+^{(k_1)} X \sigma_-^{(k_1)} - \{n_+^{(k_1)}, X\}] \\ & + 2\beta_0^{(k_2)} [2\sigma_-^{(k_2)} X \sigma_+^{(k_2)} - \{n_-^{(k_2)}, X\}] + 2\beta_1^{(k_2)} [2\sigma_+^{(k_2)} X \sigma_-^{(k_2)} - \{n_+^{(k_2)}, X\}] \\ & \dots \\ & + 2\beta_0^{(k_r)} [2\sigma_-^{(k_r)} X \sigma_+^{(k_r)} - \{n_-^{(k_r)}, X\}] + 2\beta_1^{(k_r)} [2\sigma_+^{(k_r)} X \sigma_-^{(k_r)} - \{n_+^{(k_r)}, X\}], \end{aligned}$$

for all $X \in \mathcal{B}(\mathcal{H}_S)$.

The following theorem can be proved in the same way as theorem 3.4.

Theorem 4.1. *The quantum dynamical semigroup $T_t^* = e^{t\mathcal{L}^*}$ associated with the spin chain coupled to r heat baths at inverse temperatures $\beta^{(k_1)}, \beta^{(k_2)}, \dots, \beta^{(k_r)}$ has the property of approach to equilibrium to a unique stationary state. Moreover, if $\beta^{(k_1)} = \beta^{(k_2)} = \dots = \beta^{(k_r)} = \beta$, this stationary state is given by $\rho^\beta = \otimes_{i=1}^N \rho_\beta$.*

Now, our purpose is to give the explicit form of the associated entropy production. Assume that $\beta^{(k_1)} = \beta^{(k_2)} = \dots = \beta^{(k_r)} = \beta$ and put

$$\sigma_{k_i}(\rho) = 4\beta_0 \left[\sum_{j,m} [|\langle \Psi_m, \sigma_+^{(k_i)} \Psi_j \rangle|^2 (e^{2\beta} \rho_m - \rho_j) (\log \rho_m - \log \rho_j + 2\beta)] \right].$$

From the proof of theorem 3.5, it is straightforward to show that $\sigma_i(\rho)$ is the entropy production of the spin chain coupled to the i th heat bath at the k_i th spin.

Theorem 4.2. *If $\beta^{(k_1)} = \beta^{(k_2)} = \dots = \beta^{(k_r)} = \beta$, then the entropy production of the spin chain coupled to r heat baths is given by*

$$\sigma(\rho) = \sum_{i=1}^r \sigma_{k_i}(\rho). \tag{13}$$

Proof. Put

$$\mathcal{L}_d^{*(k_i)}(\rho) = 2\beta_0^{(k_i)} [2\sigma_-^{(k_i)} X \sigma_+^{(k_i)} - \{n_-^{(k_i)}, X\}] + 2\beta_1^{(k_i)} [2\sigma_+^{(k_i)} X \sigma_-^{(k_i)} - \{n_+^{(k_i)}, X\}].$$

Then, in the same way as the proof of theorem 3.5, the entropy production of the spin chain coupled to r heat baths is given by

$$\begin{aligned}\sigma(\rho) &= -\text{Tr}(\mathcal{L}_d^*(\rho) \log \rho) - \beta \text{Tr}(\mathcal{L}_d^*(\rho) H^{(S)}) \\ &= \sum_{i=1}^r [-\text{Tr}(\mathcal{L}_d^{*(k_i)}(\rho) \log \rho) - \beta \text{Tr}(\mathcal{L}_d^{*(k_i)}(\rho) H^{(S)})] \\ &= \sum_{i=1}^r \sigma_{k_i}(\rho).\end{aligned}\quad \square$$

It is worthwhile to note that $\sigma(\rho) \geq 0$ for any density matrix ρ . Moreover, $\sigma(\rho) = 0$ if and only if $\sigma_{k_i}(\rho) = 0$ for all $i = 1, \dots, r$. Finally, for $\beta^{(k_1)} = \beta^{(k_2)} = \dots = \beta^{(k_r)} = \beta$, it is easy to show that the quantum dynamical semigroup of the spin chain coupled to r heat baths satisfies quantum detailed balance condition with respect to the stationary state ρ^β .

Remark. The master equations introduced in this paper have been proposed on different grounds in [MHWG]. The authors have studied the transport processes in open spin chains coupled to heat baths of different temperatures and they have employed the Monte Carlo wavefunction approach for the computation of the stationary state.

5. Conclusion

We have proposed a repeated quantum interaction model describing a finite spin chain $\otimes_{n=1}^N \mathbb{C}^2$ in interaction with one and r heat baths, where $2 \leq r \leq N$, at inverse temperatures $\beta^{(k_1)}, \dots, \beta^{(k_r)}$: the k_i th spin in the chain $\otimes_{n=1}^N \mathbb{C}^2$ is coupled to the k_i th heat bath. The Lindblad generator of this model is explicitly computed and the associated quantum master equation is given. Further, we have proved that the spin chain $\otimes_{n=1}^N \mathbb{C}^2$ relaxes to a unique faithful stationary state $\rho^{\beta^{(k_1)}, \dots, \beta^{(k_r)}}$. Moreover, for $N = 1, 2, 3, 4$, $r = 2$, $k_1 = 1$, $k_2 = N$, we have given the explicit form of $\rho^{\beta, \beta'}$ where $\beta' = \beta^{(N)}$ and we have computed the local states. A conjecture on the local states is stated for $N \geq 5$. Finally, for $\beta^{(k_1)} = \beta^{(k_2)} = \dots = \beta^{(k_r)} = \beta$, the entropy production is computed and we have proved that the quantum dynamical semigroup of the spin chain coupled to r heat baths satisfies the quantum detailed balance condition with respect to the unique stationary state $\rho^\beta = \otimes_{i=1}^N \rho_\beta$.

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