Detailed balance and entanglement

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Abstract

We study a connection between quantum detailed balance, which is a concept of importance in statistical mechanics, and entanglement. We also explore how this connection fits into thermofield dynamics.

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1 Introduction

Entanglement is a central aspect of quantum physics. It is for example well established as a core concept in the broad field of quantum information [1]. It has also become clear that it has important applications in other areas of physics. One such area where much work has been done recently is statistical mechanics. See for example the book [2] and the reviews [3], as well as the papers [4] for various ideas that have been explored in this connection. It is therefore of interest to explore further general connections between entanglement and statistical mechanics. In particular in this paper we consider a connection to detailed balance.

Detailed balance is a form of microscopic reversibility and is intimately related to equilibrium. Quantum versions of detailed balance for open systems, which is what we are interested in this paper, have been studied for many years, one of the earliest papers being [5]. Other early work includes [6, 7]. This line of research continues in the present day as seen for example in [8], and includes studies of related aspects of dynamics, like mixing times, [9]. There are various approaches to quantum detailed balance with varying degrees of generality, as illustrated by the mentioned papers.

Connections between detailed balance and entangled states have in fact already been exploited in [10, 11, 12] with regards to entropy production for quantum Markov semigroups (also see [13] for related work). Here our goal is to study this connection itself more explicitly, in particular how it arises as well as one instance of how it fits into other parts of physics, specifically the area known as thermofield dynamics.

We only consider systems with finite dimensional Hilbert space in this paper. The relevant concepts regarding entanglement, in particular a convenient representation of purifications, are presented in Section 2. A heuristic motivation as to why one might in general expect a connection between detailed balance and entanglement is presented in Section 3. Two definitions of quantum detailed balance, one of which was also considered in [10, 11, 12], are discussed in Section 4. The characterization of these forms of detailed balance in terms of a certain entangled state is then described in Section 5, and proved in Section 6. In Section 7 we show how these results fit naturally into thermofield dynamics. Further general remarks are made in Section 8.

2 Entanglement

Here we set up a representation of the purification of a state, which will be convenient when we study the connection between detailed balance and entanglement in Section 5. At the same time we introduce some notation that will be used in the rest of the paper.

Consider a quantum system with $n \geq 2$ dimensional Hilbert space whose state is given by the density matrix ρ. The expectation value of an observable A of the system is therefore given by

$$\langle A \rangle = \mathrm{tr}(\rho A).$$

For mathematical convenience we define this functional $\langle \cdot \rangle$ on the whole of the algebra M_n of $n \times n$ complex matrices, rather than just on the self-adjoint matrices. Note that ρ can be recovered from $\langle \cdot \rangle$ so we may view $\langle \cdot \rangle$ as a representation of the system's state. Denoting the Hilbert-Schmidt inner product by $(\cdot|\cdot)$, we have

$$\langle A \rangle = \mathrm{tr}(r^\dagger A r) = (r|Ar)$$

for any $n \times n$ matrix r such that $\rho = rr^\dagger$. Note that such matrices r exist exactly because $\rho \geq 0$.

We introduce a faithful representation π of the tensor product $M_n \otimes M_n$ on the space M_n by

$$\pi(A \otimes B)X = AXB^\intercal \tag{1}$$

where $B^\intercal$ is the transpose of the matrix B, while X is any element of the representation space M_n. Note that this representation depends on the basis we are using, because of the transpose. Keep in mind that π is well defined on the whole of $M_n \otimes M_n$ because of the universal property of tensor products. We can view π as faithfully representing $M_n \otimes M_n$ on the Hilbert space M_n with the Hilbert-Schmidt norm, and in particular this Hilbert space can be taken as the Hilbert space of two copies of the system together, which we call the 2-system. So, if X in Eq. (1) is a normalized element of the Hilbert space M_n, then it represents a pure state of the 2-system. A way to see all this easily is to represent a pure state of the first system as a column vector ψ in the n dimensional Hilbert space, but to take the transpose of a pure state ϕ of the second system to get a row vector $\phi^\intercal$, in which case the elementary tensor $\psi \otimes \phi$ can be written as the matrix product

$$\psi\phi^\intercal = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_n \end{bmatrix} \begin{bmatrix} \phi_1 & \cdots & \phi_n \end{bmatrix},$$

since this is simply the Kronecker product of the two pure states (in terms of their components $\psi_1, ..., \psi_n$ and $\phi_1, ..., \phi_n$ respectively), represented as an $n \times n$ matrix. The general pure state X of the 2-system is simply a linear combination of such elementary tensors. In this representation it is clear that when $A \otimes B$ acts on $\psi \otimes \phi$, i.e. when A acts on ψ and B on ϕ, then it is represented by

$$(A\psi)(B\phi)^\intercal = A\psi\phi^\intercal B^\intercal$$

which extends linearly to Eq. (1) for general pure states X of the 2-system.

Using this representation and viewing r above as a pure state of the 2-system, we define the corresponding expectation functional ω on $M_n \otimes M_n$ by

$$\omega_r(A \otimes B) = (r|\pi[A \otimes B]r) = \mathrm{tr}(r^\dagger A r B^\intercal). \tag{2}$$

We use the notation ω_r rather than, say, $\langle\cdot\rangle_r$, to distinguish it more clearly from $\langle\cdot\rangle$, especially later on when we drop the subscript r. We can therefore view ω_r as a pure state of the 2-system (represented as an expectation functional), and since in terms of the $n \times n$ identity matrix I we clearly have

$$\omega_r(A \otimes I) = \langle A \rangle$$

where the left hand side corresponds to taking a partial trace, we see that ω_r is a purification of $\langle\cdot\rangle$, i.e. the state r in the Hilbert space M_n is a purification of ρ. (At this stage we have not assumed that ρ is necessarily mixed, but we will do so later.) This construction of ω_r is closely related to constructions used in [14], but the specific representation Eq. (1) is different, and in the mentioned references the tensor product of two slightly different algebras are taken instead of two copies of the same algebra M_n as in our case.

As already mentioned, ω_r depends on the basis in which are working, but the fact that we allow any r such that $\rho = rr^\dagger$, in effect compensates for this, as we now explain. If we were to change the basis we are working in by a unitary transformation V, i.e. A, B and ρ are replaced by $V^\dagger AV$, $V^\dagger BV$ and $V^\dagger \rho V$ respectively, so in particular we would use r such that $rr^\dagger = V^\dagger \rho V$, then the definition of ω_r would change to

$$\omega_r(A \otimes B) = \mathrm{tr}[r^\dagger V^\dagger AVr(V^\dagger BV)^\intercal] = \mathrm{tr}(r_V^\dagger A r_V B^\intercal)$$

where $r_V = V r V^\intercal$ which clearly satisfies $r_V r_V^\dagger = \rho$, so we are back to the original definition, expressed in the original basis, by making a different choice of r, namely r_V.

Without loss of generality we can therefore assume that in Eq. (2) we are working in a basis in which ρ is diagonal, which is indeed what we do in the rest of the paper. Furthermore, it is easily shown that the most general form for such r is $r = \rho^{1/2} W$ where W is any $n \times n$ unitary matrix.

In the rest of this paper we focus on the choice $r = \rho^{1/2}$ in which case we denote ω_r simply by ω, i.e.

$$\omega(A \otimes B) = \mathrm{tr}(\rho^{1/2} A \rho^{1/2} B^\intercal) \tag{3}$$

with ρ diagonal. The reason for this is that it ensures that

$$\omega(I \otimes B) = \langle B \rangle \, ,$$

i.e. both copies of the system are in the same state ρ. More generally this can be ensured by requiring not only $rr^\dagger = \rho$, but also $r^\dagger r = \rho$, since $\rho^\intercal = \rho$, however $r = \rho^{1/2}$ is the simplest option.

To summarize, ω is a pure state of the 2-system whose reduced states to both systems are given by $\langle \cdot \rangle$, i.e. by ρ, and since in statistical mechanics we are particularly interested in cases where ρ is not pure, it follows then that ω is an entangled state.

Throughout the rest of the paper we in fact assume that ρ is invertible, i.e. all its eigenvalues are strictly positive. In particular ρ is not a pure state, and therefore the pure state ω is entangled.

3 Detailed balance and correlated states

Next we present a somewhat heuristic discussion of why a connection between quantum detailed balance and entanglement can be expected. In order to do this we start with detailed balance for a classical Markov chain and show how it can be expressed in terms of a correlated state of two copies of the system in question, where both of its marginals are the original state of the system.

Recall that if we have a probability distribution $p_1, ..., p_n$ over a finite set F of n elements, then a Markov chain satisfying detailed balance is described by transition probabilities γ_{jk} satisfying

$$p_j \gamma_{jk} = p_k \gamma_{kj}$$

for all $j, k = 1, ..., n$, which simply says that the probability to make a transition from one pure state to another is the same as the opposite transition. Denoting the observable algebra of functions on the n-point set F by

$K = \mathbb{C}^n$, we can express the probability distribution $p_1, ..., p_n$ by a normalized positive linear functional (a *state*) μ on K given by

$$\mu(f) = pf$$

where $f \in K$ is viewed as a column matrix and $p = [\ p_1 \quad \cdots \quad p_n\ ]$ is a row matrix. Now we consider two copies of the algebra K, namely the tensor product algebra $K \otimes K$ and define a state φ on it by

$$\varphi = \mu \circ \delta$$

where $\delta : K \otimes K \to K$ is given by componentwise multiplication, i.e. $\delta(f \otimes g) = fg$ where fg is the product in the algebra K, defined to have the components $f_j g_j$ if f and g have components f_j and g_j respectively. Note that δ is well-defined because of the universal property of the tensor product. It is clear that φ corresponds to the probability distribution $p_1, ..., p_n$ over the "diagonal" of the set $F \times F$ and is therefore a correlated state unless all but one of the probabilities are zero. Note that analogous to the entangled state ω from the previous section, the marginals of φ are simply the state μ of the single system we started with, namely

$$\varphi(f \otimes 1) = \mu(f) \quad \text{and} \quad \varphi(1 \otimes g) = \mu(g)$$

where the 1 here denotes the function which is identically 1 on F, i.e. the column consisting only of 1's.

Denoting the transition matrix by $\Gamma = (\gamma_{jk})$, the time-evolution on K is given by $f \mapsto \Gamma f$, and using the detailed balance condition above it follows that

$$\varphi((\Gamma f) \otimes g) = \sum_{j=1}^{n} \sum_{k=1}^{n} p_j \gamma_{jk} f_k g_j = \sum_{j=1}^{n} \sum_{k=1}^{n} p_k \gamma_{kj} f_k g_j = \varphi(f \otimes (\Gamma g))$$

and conversely, if

$$\varphi[(\Gamma f) \otimes g] = \varphi[f \otimes (\Gamma g)] \tag{4}$$

holds for all $f, g \in K$, then the detailed balance condition $p_j \gamma_{jk} = p_k \gamma_{kj}$ follows easily. So the detailed balance condition of a system, which says that a transition and its opposite are equally likely, can be reinterpreted in terms of two copies of the system by saying that in the correlated state φ time-evolution of only the first copy of the system is equivalent to time-evolution of only the second copy of the system, i.e. the two systems' time-evolutions are "balanced" in this sense. It is clear from the derivation of Eq. (4) from detailed balance that the fact that the transition probability $p_j \gamma_{jk}$ is equal to the opposite transition's probability $p_k \gamma_{kj}$ in the first system, is translated directly to time-evolution of the second system. A potentially useful way of thinking about this may be that the first system is going back in time relative to the second, in the right hand side of Eq. (4).

The above discussion makes it plausible that also in the quantum case detailed balance of a system should be related to a correlated state of two copies of the system. Our next step is to explore this in more detail to motivate the connection between detailed balance and entanglement. More precisely, if we attempt to express quantum detailed balance in the form of Eq. (4), the question is which state of two copies of the quantum system should be used in place of φ.

A most direct adaptation of the state φ to the quantum case from the previous section is to consider the following density matrix for two copies of the quantum system, where as for the classical case above we assign the probabilities only to pairs consisting of two copies of the same pure state (i.e. a probability distribution over a "diagonal" of 2-system pure states):

$$\rho^{(2)} = \sum_{j=1}^{n} \rho_j \left| e_j \otimes e_j \right\rangle \left\langle e_j \otimes e_j \right|$$

where we are working in a basis in which ρ from the previous section is diagonal, say

$$\rho = \begin{bmatrix} \rho_1 & & \\ & \ddots & \\ & & \rho_n \end{bmatrix}, \tag{5}$$

and with e_j the column matrix with 1 in the j 'th position and 0 elsewhere for $j = 1, ..., n$, to give the pairs of states $e_j \otimes e_j$ referred to above. Then it is easily verified that if we define a state θ on $M_n \otimes M_n$ by

$$\theta(C) = \operatorname{tr}(\rho^{(2)} C)$$

for all $C \in M_n \otimes M_n$, then $\theta(A \otimes I) = \langle A \rangle$ and $\theta(I \otimes B) = \langle B \rangle$ as required to correspond to the classical case above, and it is also clear that θ is a correlated state (as long as more than one of the ρ_j are non-zero) although it contains no entanglement, i.e. the correlations in θ are purely classical. One could now try to define quantum detailed balance, for some time-evolution of the system, in terms of θ by using a similar condition as in Eq. (4).

However the question is whether θ is sufficiently correlated to produce a good analogue of the classical case. So let us heuristically compare θ with φ in terms of how correlated they are. Let us assume that $\rho_j \neq 0$ for all j, since this is the case that we are interested later on, and correspondingly we assume that $p_j \neq 0$ for all j. A very simple way to check that the state φ is indeed quite correlated, is to note that $\varphi(f \otimes f) > 0$ for any non-zero observable $f \in K$, by which we mean f is self-adjoint in K, i.e. f is real-valued. But it is easily seen that θ does not satisfy the corresponding condition in the quantum case, namely if $A \in M_n$ is an observable (i.e. it is self-adjoint) but all its diagonal entries are zero, then $\theta(A \otimes A) = 0$ even if A is non-zero. This is despite the fact that we do have $\theta(A \otimes A) \geq 0$ for all observables A. In this sense θ is heuristically speaking not as correlated for the two copies of the quantum system as φ is for the two copies of the classical system.

Heuristically, in order to have a quantum version of Eq. (4) which is a good analogue of the classical situation, we need to require the 2-system state in the quantum situation to be correlated in the above sense for all observables, as is the case in the classical situation, rather than just for some observables (namely for observables with non-zero diagonal entries). But this then means that θ is not good enough.

Exactly here entanglement comes to the rescue. Firstly, it is easily verified that for the entangled state ω as defined in the previous section we have $\omega(A\otimes A^T) \geq 0$ for all observables A. Note that this is not true for $\omega(A\otimes A)$, so this form is not suitable for looking for correlations in the above sense. For θ we have $\theta(A \otimes A^T) = \theta(A \otimes A)$ so the two forms are equivalent in the case of θ. The form $\omega(A\otimes A^T)$ is the appropriate one to use in the case of ω, and note that indeed $\omega(A \otimes A^T) > 0$ for any non-zero observable $A \in M_n$, in perfect analogy to the classical case. This suggests that it would be more natural to use the entangled state ω in place of φ, rather than the non-entangled state θ, if we attempt to express quantum detailed balance in the form of Eq. (4) in terms of a state which has a similar degree of correlations for the quantum observables that φ has for classical observables.

Below we use two definitions of quantum detailed balance appearing in the literature to illustrate this connection with entanglement explicitly.

4 Definitions of quantum detailed balance

We now describe two definitions of quantum detailed balance for which the connection to the entangled state ω from Section 2 can be made in a particularly clear way.

For a simple and clear discussion of how one can rewrite the classical definition of detailed balance in a form that suggests the basic form of the definitions of quantum detailed balance presented below, please refer to [10, 15]. This gives some intuition regarding the origins of these definitions. Also see [16, 5, 6] for some of the early literature on detailed balance, as well as [17]. More specific references will be given as we proceed.

As before we consider a system with n dimensional Hilbert space. We allow the system to interact with its environment, i.e. it is an open system. A standard approach to this situation is to model the time-evolution of the system in the Heisenberg picture as a quantum Markov semigroup (QMS) τ_t on the algebra M_n, where we take the time variable to be either continuous, i.e. $t \geq 0$, or discrete, i.e. $t = 0, 1, 2, 3, \dots$. This means that for each t the corresponding τ_t is a completely positive linear map from M_n to itself which is also unital, i.e. $\tau_t(I) = I$, and furthermore the semigroup property

$\tau_s \tau_t = \tau_{s+t}$ is satisfied. Extensive discussions as to when a QMS is a good approximation to the physical time-evolution is given for example in the books [18] and [19], but also see [20] for one of the original papers.

It turns out that for the framework presented in this section and the results discussed in the next, the semigroup property is not needed, so this assumption can in fact be dropped, which may be relevant when studying non-Markovian dynamics. We do however keep the rest of the above mentioned assumptions regarding τ_t, in which case we simply refer to τ_t as *dynamics*. The literature on detailed balance related to our approach typically assumes the semigroup property.

The first definition of quantum detailed balance we consider is from [21], and is called detailed balance II. In [21] the dynamics is only assumed to be positive, rather than completely positive, and they only consider the case of discrete time. We therefore adapt their approach to completely positive maps and also to include continuous time. Our results in the next section in fact still hold when working with positivity instead of complete positivity, but as is well known [22] there are convincing physical reasons to assume complete positivity, and this also happens to be mathematically convenient in many cases. In this regard also see again the books [18] and [19]. The above mentioned extension from discrete to continuous time on the other hand is a minor mathematical issue in our setup in this section. All our arguments in this section, as well as Sections 5 and 6, work for both the case of continuous time and the case of discrete time.

We are going to define detailed balance of the dynamics τ_t of the system relative to a given fixed density matrix ρ of the system. The key mathematical idea to define and study detailed balance is to consider certain duals or adjoints of τ_t. In particular for detailed balance II we need the following.

With $\langle \cdot \rangle$ the expectation functional given by ρ as in Section 2, we can define the *dual* (relative to ρ) of any linear map $\alpha : M_n \to M_n$ as the linear map $\alpha' : M_n \to M_n$ such that

$$\left\langle \alpha'(A) B \right\rangle = \langle A \alpha(B) \rangle$$

for all $n \times n$ matrices A and B. Note that since ρ is invertible, such an α' necessarily exists and is unique, since it can be obtained from the Hermitian adjoint of α with respect to the inner product $(A, B)_\rho := \mathrm{tr}(\rho A^\dagger B) = \left\langle A^\dagger B \right\rangle$. Indeed, denoting this Hermitian adjoint by α^ρ, it is easy to check that $\alpha'(A) = \alpha^\rho(A^\dagger)^\dagger$.

Definition 4.1. We say that τ_t as given above satisfies *detailed balance II with respect to* ρ if τ_t' is a completely positive unital linear map for every t.

As a general remark, note that if τ_t has the semigroup property, then τ_t' automatically has it as well, since

$$\left\langle \tau_{s+t}'(A) B \right\rangle = \langle A \tau_{s+t}(B) \rangle = \langle A \tau_s[\tau_t(B)] \rangle = \left\langle \tau_t'[\tau_s'(A)] B \right\rangle .$$

Note that roughly speaking detailed balance II boils down to requiring that the dual τ_t' is a sensible physical time-evolution.

Next we consider a type of standard quantum detailed balance (see[23], and also [24] for related work). The particular form of standard quantum detailed balance considered below was studied in [8, 11]. It will immediately be seen that it is defined in a form directly related to the entangled state ω, a point we come back to in the next section. It is defined in terms of a *reversing operation* $\Theta : M_n \to M_n$, meaning that Θ is a $*$-anti-automorphism, i.e. it is linear, $\Theta(A^\dagger) = \Theta(A)^\dagger$ and $\Theta(AB) = \Theta(B)\Theta(A)$, and we furthermore assume that Θ^2 is the identity map on M_n. Note that some form of time reversal plays a central role in a number of approaches to detailed balance; see for example [5, 25], and also the discussion in [21].

For any linear $\alpha : M_n \to M_n$ we define its *KMS-dual* $\alpha^{(1/2)} : M_n \to M_n$ (relative to ρ) by

$$\mathrm{tr}(\rho^{1/2}\alpha^{(1/2)}(A)\rho^{1/2}B) = \mathrm{tr}(\rho^{1/2}A\rho^{1/2}\alpha(B))$$

for all $n \times n$ matrices A and B. We note that $\alpha^{(1/2)}$ exists and is uniquely determined. In fact it is easily seen to be given by

$$\alpha^{(1/2)}(A) = \rho^{-1/2}\alpha^\dagger(\rho^{1/2}A^\dagger\rho^{1/2})^\dagger\rho^{-1/2}$$

where $\alpha^\dagger$ is the Hermitian adjoint of α with respect to the Hilbert-Schmidt inner product. From this formula it also follows that $\alpha^{(1/2)}$ is positive if α is, and completely positive if α is. Furthermore, if τ_t is a QMS, it can be seen that $\tau_t^{(1/2)}$ is as well. However, the semigroup property will again not be essential for our work.

Definition 4.2. We say that τ_t on M_n satisfies *standard quantum detailed balance w.r.t. the reversing operation* Θ *and the density matrix* ρ, abbreviated as Θ-*sqdb w.r.t.* ρ, if

$$\tau_t^{(1/2)} = \Theta \circ \tau_t \circ \Theta.$$

As the references above and in the introduction shows, there are also a number of other definitions of quantum detailed balance in the literature. For remarks comparing some of these definitions, we refer the reader to [8, 21] in particular.

5 Detailed balance and entanglement

In this section we turn to our main goal, namely to characterize quantum detailed balance in terms of the entangled state ω introduced in Section 2. Here we only present the results along with some discussion, while the technical details regarding their derivations are given in the next section.

As mentioned in Section 2, ρ is an invertible density matrix throughout and we have chosen some fixed basis in which ρ is diagonal to define the transposition. Furthermore, the term *dynamics* is as defined in the previous section.

The central tool towards our goal is the modular operator Δ defined by

$$\Delta(A) = \rho A \rho^{-1}$$

for all $n \times n$ matrices A. This operator is part of a very general theory, namely modular theory or Tomita-Takesaki theory, which is discussed for example in [26], but since we work in finite dimensions we don't need to delve into the general theory.

We start with the following characterization of detailed balance II in terms of the modular operator.

Theorem 5.1. *The dynamics τ_t satisfies detailed balance II w.r.t. ρ if and only if it commutes with the modular operator, i.e.*

$$\tau_t \Delta = \Delta \tau_t, \tag{6}$$

and it leaves the state ρ invariant in the sense that

$$\langle \tau_t(A) \rangle = \langle A \rangle \tag{7}$$

for all $n \times n$ matrices A.

One direction of this theorem is given in [21], namely that Eq. (6) and (7) follow from detailed balance, but the converse is not, though it is closely related to Theorem 6 of [21]. This characterization of detailed balance II is one of the ingredients in deriving the characterization of detailed balance II in terms of the entangled state ω presented below.

For any linear map $\alpha : M_n \to M_n$ we can define another linear map $\hat{\alpha} : M_n \to M_n$ by

$$\hat{\alpha}(A) = \alpha'(A^\intercal)^\intercal$$

where α' is as defined in Section 4. In order to formulate the characterization of detailed balance II in terms of ω, we apply this to the dynamics τ_t, i.e. we consider $\hat{\tau}_t$ given by

$$\hat{\tau}_t(A) = \tau_t'(A^\intercal)^\intercal \tag{8}$$

for all $n \times n$ matrices A and every t. Keep in mind that τ_t' and therefore $\hat{\tau}_t$ are mathematically well-defined operators for every t. However, it is only under the condition of detailed balance II that τ_t' becomes dynamics, i.e. that it is unital and completely positive. When this is the case, $\hat{\tau}_t$ similarly becomes dynamics (see Section 6). In certain examples, similar to those in [27], but in arbitrary finite dimensions, one can show using Theorem 5.1 and Choi matrices [28] that the dynamics $\hat{\tau}_t$ is just the original dynamics τ_t, as opposed to τ_t' which in such examples turns out to be in effect a time-reversal of τ_t. This cannot be expected to be true in general though. Note that since the transpose appears in Eq. (8), the definition of $\hat{\tau}_t$ is basis dependent, so we have made a specific choice to fit in with our choice of ω from Section 2. When using the more general construction ω_r, one could in principle explore a corresponding generalization of Eq. (8), but here we deal exclusively with Eq. (8).

Now we can characterize detailed balance II in terms of entanglement.

Theorem 5.2. *The dynamics τ_t satisfies detailed balance II w.r.t. ρ if and only if*

$$\omega[A \otimes \hat{\tau}_t(B)] = \omega[\tau_t(A) \otimes B] \tag{9}$$

for all $n \times n$ matrices A and B, and

$$\hat{\tau}_t(I) = I, \tag{10}$$

for every t. Alternatively Eq. (9) can be expressed as

$$\omega \circ (\mathrm{id}_{M_n} \otimes \hat{\tau}_t) = \omega \circ (\tau_t \otimes \mathrm{id}_{M_n}), \tag{11}$$

i.e. evolving the 2-system by $\mathrm{id}_{M_n} \otimes \hat{\tau}_t$ has the same effect on the entangled pure state ω as $\tau_t \otimes \mathrm{id}_{M_n}$, where id_{M_n} denotes the identity map on the algebra M_n.

Next we consider a similar characterization of Θ-sqdb. The definition of Θ-sqdb is indeed already in a form that is aligned with ω. We simply define $\alpha^\Theta : M_n \to M_n$ by

$$\alpha^\Theta(A) = (\Theta \circ \alpha \circ \Theta(A^\intercal))^\intercal$$

for any linear $\alpha : M_n \to M_n$. Then one can immediately reformulate the definition of Θ-sqdb to obtain the following characterization which is inherent to the work in [10, 11, 12]:

Proposition 5.3. *The dynamics τ_t satisfies Θ-sqdb w.r.t. ρ if and only if*

$$\omega[A \otimes \tau_t^\Theta(B)] = \omega[\tau_t(A) \otimes B]$$

for all $n \times n$ matrices A and B and every t.

A typical choice of Θ is $\Theta(A) = A^\intercal$. In this case $\tau_t^\Theta = \tau_t$ and the above condition simplifies to

$$\omega[A \otimes \tau_t(B)] = \omega[\tau_t(A) \otimes B]$$

so this choice of Θ seems to fit in naturally with our choice of ω.

It is straightforward to construct examples of Θ-sqdb in M_2 where τ_t does not commute with Δ, unlike the case of detailed balance II. This aspect of standard quantum detailed balance was emphasized in for example [8].

On the other hand, should we assume that τ_t does commute with Δ, one can show that Θ-sqdb implies detailed balance II.

Lastly we mention that all of the results in this section still hold if we work in terms of positivity instead of complete positivity, as discussed in the previous section.

6 Proofs

Here we prove the results presented in Section 5. We begin by discussing a number of mathematical facts which will be of use in the proofs.

Given any linear map $\alpha : M_n \to M_n$ we define the linear map $\alpha^\ddagger : M_n \to M_n$ by

$$\mathrm{tr}[\alpha^\ddagger(A)B] = \mathrm{tr}[A\alpha(B)].$$

Notice that it is a version of the dual α', but w.r.t. the trace instead of $\langle\cdot\rangle$. Similar to α', $\alpha^\ddagger$ can be obtained from the usual Hermitian adjoint $\alpha^\dagger$ of the operator α with respect to the Hilbert-Schmidt inner product by the formula

$$\alpha^\ddagger(A) = \alpha^\dagger(A^\dagger)^\dagger$$

where the last $\dagger$ refers to the Hermitian adjoint of the $n \times n$ matrix $\alpha^\dagger(A^\dagger)$. Note that $\alpha(I) = I$ if and only if $\mathrm{tr} \circ \alpha^\ddagger = \mathrm{tr}$. It is similarly easy to see that $\langle\alpha(A)\rangle = \langle A\rangle$ for all A if and only if $\alpha^\ddagger(\rho) = \rho$. In the case that α is a Hermitian map, i.e. it satisfies $\alpha(A^\dagger) = \alpha(A)^\dagger$, we see that $\alpha^\dagger$ is also Hermitian, since

$$\begin{aligned}
\mathrm{tr}\left[\alpha^\dagger(A^\dagger)B\right] &= \mathrm{tr}\left[A^\dagger\alpha(B)\right] = \{\mathrm{tr}[\alpha(B^\dagger)A]\}^* = \{\mathrm{tr}[B^\dagger\alpha^\dagger(A)]\}^* \\
&= \mathrm{tr}\left[\alpha^\dagger(A)^\dagger B\right].
\end{aligned}$$

Therefore

$$\alpha^\ddagger = \alpha^\dagger$$

if α is Hermitian. So in our physical context we in fact only need to work with $\alpha^\dagger$, since positive maps are Hermitian. Mathematically it will however be convenient to consider $\alpha^\ddagger$ as well.

From the definition $\Delta(A) = \rho A\rho^{-1}$ of the modular operator Δ, it is easily verified that $\Delta^\dagger = \Delta$, where again the Hermitian adjoint $\Delta^\dagger$ is taken with respect to the Hilbert-Schmidt inner product. I.e. Δ is self-adjoint, and similarly $\Delta^{1/2} = \rho^{1/2}(\cdot)\rho^{-1/2}$ is self-adjoint. The latter means that $\Delta = \Delta^{1/2}\Delta^{1/2} \geq 0$. Furthermore, $\Delta^{-1} = \rho^{-1}(\cdot)\rho$ exists so all of the eigenvalues of Δ are strictly positive, so in fact

$$\Delta > 0$$

as an operator on the Hilbert space M_n with the Hilbert-Schmidt norm. This means that Δ^{-iz} is well-defined for all $z \in \mathbb{C}$. We consider Δ^{-iz} rather than Δ^z as a convention, since then in the case of a Gibbs state and real z it follows that Δ^{-iz} is essentially a scaled version of the system's isolated dynamics; see Eq. (13) below.

A convenient and standard representation of a linear map $\alpha : M_n \to M_n$, for example Δ above, is to arrange the columns of an $n \times n$ matrix in order below one another in an n^2 dimensional column, in which case α can be written as an $n^2 \times n^2$ matrix. This is just a choice of basis, and is essentially an explicit case of the GNS construction with respect to the trace (see for example [26] for the general GNS construction). In this representation $\alpha^\dagger$ is then easily seen to be represented by the Hermitian adjoint of the $n^2 \times n^2$ matrix (i.e. transpose and complex conjugation).

Since we are working in a basis in which ρ is diagonal, as mentioned in Section 2, namely Eq. (5), it follows that in the above mentioned representation,

$$\Delta = \begin{bmatrix} \begin{bmatrix} \rho_1\rho_1^{-1} & & \\ & \ddots & \\ & & \rho_n\rho_1^{-1} \end{bmatrix} & & \\ & \ddots & \\ & & \begin{bmatrix} \rho_1\rho_n^{-1} & & \\ & \ddots & \\ & & \rho_n\rho_n^{-1} \end{bmatrix} \end{bmatrix} \tag{12}$$

where we have indicated $n \times n$ blocks for clarity. From this we see that

$$\Delta^{-iz}(A) = \rho^{-iz} A \rho^{iz}. \tag{13}$$

Now we turn to the proofs of the results of the previous section. The first step is the following:

Assuming that the dynamics τ_t of our system satisfies detailed balance II w.r.t. ρ as described in Section 4, it follows that

$$\tau_t'(A) = \rho^{-1/2}\tau_t^\dagger(\rho^{1/2}A\rho^{1/2})\rho^{-1/2} \tag{14}$$

for all $n \times n$ matrices A, where $\tau_t^\dagger$ denotes the Hermitian adjoint of τ_t with respect to the Hilbert-Schmidt inner product.

The derivation of Eq. (14) is given in [21], but we provide it here for completeness in slightly more elementary form, which is possible since we are working in finite dimensions. We in fact prove something a bit more general than Eq. (14); see Eq. (18). Along the way we prove some general results which will be used in the subsequent proofs as well.

For any linear $\alpha : M_n \to M_n$ we have $\langle \alpha'(A)B \rangle = \langle A\alpha(B) \rangle = \mathrm{tr}[\alpha^\ddagger(\rho A)B] = \left\langle \rho^{-1}\alpha^\ddagger(\rho A)B \right\rangle$, therefore

$$\alpha'(A) = \rho^{-1}\alpha^\ddagger(\rho A) \tag{15}$$

Furthermore,

$$\begin{aligned}\langle A\alpha(B)\rangle &= \left\langle \alpha'(A)B\right\rangle = \mathrm{tr}[B\rho\alpha'(A)] = \mathrm{tr}[\alpha'^{\ddagger}(B\rho)A] = \mathrm{tr}[\rho A\alpha'^{\ddagger}(B\rho)\rho^{-1}] \\ &= \left\langle A\alpha'^{\ddagger}(B\rho)\rho^{-1}\right\rangle\end{aligned}$$

so $\alpha(B) = \alpha'^{\ddagger}(B\rho)\rho^{-1}$, i.e. $\alpha'^{\ddagger}(B\rho) = \alpha(B)\rho$. Assuming that α and α' are Hermitian, it follows that $\alpha^{\ddagger} = \alpha^{\dagger}$ and $\alpha'^{\ddagger} = \alpha'^{\dagger}$ are also Hermitian, therefore we also have $\alpha'^{\dagger}(\rho B) = \rho\alpha(B)$. Hence

$$\begin{aligned}\langle A\alpha(B)\rangle &= \mathrm{tr}[\rho A\rho^{-1}\alpha'^{\dagger}(\rho B)] = \mathrm{tr}[\alpha'(\rho A\rho^{-1})\rho B] = \left\langle \alpha'(\rho A\rho^{-1})\rho B\rho^{-1}\right\rangle \\ &= \left\langle A\rho^{-1}\alpha(\rho B\rho^{-1})\rho\right\rangle\end{aligned}$$

from which it follows that $\alpha(B) = \rho^{-1}\alpha(\rho B\rho^{-1})\rho$.

I.e. we have shown that

$$\alpha\Delta = \Delta\alpha \tag{16}$$

if both α and α' are Hermitian. But then it follows that $\alpha\Delta^{-iz} = \Delta^{-iz}\alpha$, thinking in terms of operators on the Hilbert space M_n, in other words

$$\alpha(\rho^{-iz}A\rho^{iz}) = \rho^{-iz}\alpha(A)\rho^{iz} \tag{17}$$

according to Eq. (13). This implies that

$$\begin{aligned}\mathrm{tr}[\alpha^{\dagger}(\rho^{iz}A\rho^{-iz})B] &= \mathrm{tr}[A\rho^{-iz}\alpha(B)\rho^{iz}] = \mathrm{tr}[A\alpha(\rho^{-iz}B\rho^{iz})] \\ &= \mathrm{tr}[\rho^{iz}\alpha^{\dagger}(A)\rho^{-iz}B]\end{aligned}$$

hence $\alpha^{\dagger}(\rho^{iz}A\rho^{-iz}) = \rho^{iz}\alpha^{\dagger}(A)\rho^{-iz}$. In particular $\rho^{1/2}\alpha^{\dagger}(A)\rho^{-1/2} = \alpha^{\dagger}(\rho^{1/2}A\rho^{-1/2})$ so $\rho^{1/2}\alpha^{\dagger}(\rho^{1/2}A\rho^{1/2})\rho^{-1/2} = \alpha^{\dagger}(\rho A) = \rho\alpha'(A)$, where in the last equality we used Eq. (15).

We have therefore shown that

$$\alpha'(A) = \rho^{-1/2}\alpha^{\dagger}(\rho^{1/2}A\rho^{1/2})\rho^{-1/2} \tag{18}$$

for any Hermitian linear $\alpha : M_n \to M_n$ for which α' is also Hermitian.

In particular this means that Eq. (14) holds when τ_t satisfies detailed balance w.r.t. ρ, since then τ_t and τ_t' are both positive, and therefore Hermitian.

Proof of Theorem 5.1. Assume that τ_t satisfies detailed balance II w.r.t. ρ. Then Eq. (6) follows from Eq. (16). Furthermore, Eq. (7) holds, since $\langle\tau_t(A)\rangle = \langle\tau_t'(I)A\rangle = \langle A\rangle$ directly from the definition of τ_t' and detailed balance II.

Now for the converse. First note that for a linear map $\alpha : M_n \to M_n$ we have that α is completely positive if and only if $\alpha^{\dagger}$ is completely positive. This follows immediately from the definition of $\alpha^{\dagger}$ and the fact [22, 29] that a linear map $\varphi : M_n \to M_n$ is completely positive if and only if it can be written in the form

$$\varphi(A) = \sum_{j=1}^{n^2} V_j A V_j^\dagger$$

for all A, for some set of matrices $V_j \in M_n$. (It can also be shown by a slightly longer argument that α is positive if and only if $\alpha^\dagger$ is positive.)

Assuming Eq. (6) and Eq. (7), we define $\varphi_t : M_n \to M_n$ by

$$\varphi_t(A) = \rho^{-1/2}\tau_t^\dagger(\rho^{1/2}A\rho^{1/2})\rho^{-1/2},$$

from which follows that

$$\begin{aligned}\langle \varphi_t(A)B\rangle &= \mathrm{tr}[\rho\rho^{-1/2}\tau_t^\dagger(\rho^{1/2}A\rho^{1/2})\rho^{-1/2}B] = \mathrm{tr}[\rho^{1/2}A\rho^{1/2}\tau_t(\rho^{-1/2}B\rho^{1/2})] \\ &= \left\langle A\rho^{1/2}\tau_t(\rho^{-1/2}B\rho^{1/2})\rho^{-1/2}\right\rangle = \langle A\tau_t(B)\rangle\end{aligned}$$

where in the last step we applied $\tau_t(\rho^{iz}A\rho^{-iz}) = \rho^{iz}\tau_t(A)\rho^{-iz}$ which follows from Eq. (6) just like Eq. (17) followed from Eq. (16). This shows that $\tau_t' = \varphi_t$, i.e.

$$\tau_t'(A) = \rho^{-1/2}\tau_t^\dagger(\rho^{1/2}A\rho^{1/2})\rho^{-1/2}, \tag{19}$$

from which we conclude that τ_t' is completely positive, since τ_t and therefore $\tau_t^\dagger$ are. (Similarly, τ_t' is positive if we only assume that τ_t is positive.) Furthermore

$$\left\langle \tau_t'(I)A\right\rangle = \langle \tau_t(A)\rangle = \langle A\rangle,$$

implying that τ_t' is unital. This shows that τ_t satisfies detailed balance II w.r.t. ρ as required.

Proof of Theorem 5.2. Assume that τ_t satisfies detailed balance II w.r.t. ρ. Then Eq. (14) holds as already shown above, so by also using Eq. (3) and Eq. (8) it follows that

$$\begin{aligned}\omega[A\otimes\hat{\tau}_t(B)] &= \mathrm{tr}[\rho^{1/2}A\rho^{1/2}\tau_t'(B^\intercal)] \\ &= \mathrm{tr}[\rho^{1/2}A\rho^{1/2}\rho^{-1/2}\tau_t^\dagger(\rho^{1/2}B^\intercal\rho^{1/2})\rho^{-1/2}] \\ &= \mathrm{tr}[\tau_t(A)\rho^{1/2}B^\intercal\rho^{1/2}] = \omega[\tau_t(A)\otimes B],\end{aligned}$$

i.e. Eq. (9) holds. Since $\tau_t'(I) = I$ because of detailed balance II, we also have Eq. (10) by Eq. (8).

Conversely, assuming Eqs. (9) and (10), we are going to use Theorem 5.1 to show that τ_t satisfies detailed balance II w.r.t. ρ. Since

$$\omega(A\otimes B) = \mathrm{tr}(\rho B^\intercal\rho^{1/2}A\rho^{-1/2}) = \left\langle B^\intercal\Delta^{1/2}(A)\right\rangle,$$

we have by our assumption Eq. (9) that

$$\left\langle B^{\intercal}\tau_t[\Delta^{1/2}(A)]\right\rangle = \left\langle \tau'_t(B^{\intercal})\Delta^{1/2}(A)\right\rangle = \omega[A\otimes\tau'_t(B^{\intercal})^{\intercal}] = \omega[A\otimes\hat{\tau}_t(B)]$$
$$= \omega[\tau_t(A)\otimes B] = \left\langle B^{\intercal}\Delta^{1/2}[\tau_t(A)]\right\rangle$$

which means that $\tau_t\Delta^{1/2} = \Delta^{1/2}\tau_t$, hence $\tau_t\Delta = \Delta\tau_t$. Furthermore,

$$\langle\tau_t(A)\rangle = \omega[\tau_t(A)\otimes I] = \omega[A\otimes\hat{\tau}_t(I)] = \langle A\rangle\,,$$

since we assumed that $\hat{\tau}_t(I) = I$. The conditions in Theorem 5.1 are therefore satisfied, implying that τ_t satisfies detailed balance II w.r.t. ρ, completing the proof of Theorem 5.2.

Remarks regarding $\hat{\tau}_t$ as dynamics. Note that for a linear map $\alpha : M_n \to M_n$ we have that α is completely positive if and only if $\bar{\alpha}$ is completely positive, where $\bar{\alpha}$ is defined by $\bar{\alpha}(A) = \alpha(A^{\intercal})^{\intercal}$ in terms of the transposition in our chosen basis as discussed in Section 2. This again follows from the representation of completely positive maps used in the proof of Theorem 5.1. In particular it then follows from $\hat{\tau}_t(A) = \tau'_t(A^{\intercal})^{\intercal}$ that $\hat{\tau}_t$ is completely positive if τ'_t is. (Since transposition is a positive map, the corresponding results in terms of positivity instead of complete positivity also hold.) Clearly $\hat{\tau}_t$ is unital if τ'_t is. Should we work with the case where τ_t has the semigroup property, then τ'_t has the semigroup property as well, as explained in Section 4, from which it is easily seen that $\hat{\tau}_t$ also has the semigroup property.

7 Thermofield dynamics

The characterization of detailed balance in terms of the entangled state ω turns out to fit naturally into the framework of thermofield dynamics and in this section our goal is to show this. Our first step is to briefly outline some of the basic elements of thermofield dynamics in a finite dimensional set-up.

Thermofield dynamics was developed in [30], although a number of the key ideas already appeared in [31, 32]. A very useful discussion of thermofield dynamics can be found in [33]. The formulation in terms of operator algebras was presented in [34], and reviewed in [35]. Our exposition is largely based on the latter two sources, but adapted to our setting.

The basic idea is to double the degrees of freedom of the system in the sense that for each element A of the system's observable algebra M_n we define an element $\tilde{A}$ of the commutant of M_n in a cyclic representation given by the GNS construction for the faithful state $\langle\cdot\rangle$ on M_n given by ρ. This element has to satisfy a basic identity of thermofield dynamics called the tilde substitution rule, namely

$$\Delta^{-1/2}(\tilde{A}\rho^{1/2}) = A^{\dagger}\rho^{1/2}$$

for all $A \in M_n$. We need to find $\tilde{A}$ explicitly in a convenient representation. There are different, though unitarily equivalent, ways of writing the cyclic representation. For our purposes in this section it is most convenient to first represent M_n by $M_n \otimes I$, as a subalgebra of $M_n \otimes M_n$, in which case its commutant is given by $I \otimes M_n$. Furthermore, using our faithful representation π of $M_n \otimes M_n$ from Section 2, we obtain the cyclic representation of M_n we are going to use, namely $A \mapsto \pi(A \otimes I)$, the cyclic vector being $\rho^{1/2}$ in the Hilbert space M_n with Hilbert-Schmidt norm. Note that $(\rho^{1/2}|\pi(A \otimes I)\rho^{1/2}) = \langle A \rangle$ as is required of a cyclic representation associated to $\langle \cdot \rangle$. It is then a simple matter to verify that the tilde substitution rule above is satisfied exactly when we set

$$\tilde{A} = \pi(I \otimes \bar{A})$$

for all $A \in M_n$, where $\bar{A}$ is the complex conjugate of A, i.e. each entry of A is replaced by its complex conjugate. Indeed, we then have

$$\Delta^{-1/2}(\tilde{A}\rho^{1/2}) = \rho^{-1/2}(\rho^{1/2}\bar{A}^{\intercal})\rho^{1/2} = A^{\dagger}\rho^{1/2}$$

as required.

It is also clear from the latter that the tilde substitution rule is in fact simply an alternative way to write the definition of the modular operator Δ. Moreover, as one might expect from the fact that $\tilde{A}$ lies in the commutant, it can alternatively be obtained from the modular conjugation of Tomita-Takesaki theory [34, 35]. Therefore thermofield dynamics is in a sense contained in Tomita-Takesaki theory.

From a more physical point of view one can keep in mind that the KMS condition can be written as

$$\langle A\Delta(B) \rangle = \langle BA \rangle$$

for all $A, B \in M_n$, and this is yet another way of writing the definition of Δ. So the tilde substitution rule is in effect simply a way to write the KMS condition, i.e. to express thermal equilibrium.

Another core aspect of thermofield dynamics is the fact that

$$\langle A \rangle = \omega(A \otimes I)$$

as in Section 2, i.e. expectation values for the mixed state $\langle \cdot \rangle$, that is to say ρ, can be expressed in terms of the pure state ω.

This summarizes the main points from thermofield dynamics that are relevant for us. Further background, motivation and applications can be found in the references mentioned above. We now proceed to study detailed balance in this framework. To do this, it is convenient to extend the definition in Section 2 of the expectation functional $\langle \cdot \rangle$ to the algebra

$\pi(M_n \otimes M_n)$ in the following way that fits in neatly with the thermofield dynamics framework:

$$\left\langle A\tilde{B} \right\rangle = (\rho^{1/2}|A\tilde{B}\rho^{1/2})$$

for all $A, B \in M_n$, where we have written A as shorthand for $\pi(A \otimes I)$, which is natural, since $\pi(A \otimes I)X = AX$ for any $X \in M_n$. The point of this is that it can also be rewritten as

$$\left\langle A\tilde{B} \right\rangle = \omega(A \otimes \bar{B})$$

which will allow us to write our entanglement characterizations of detailed balance from Section 5 easily in the framework of thermofield dynamics.

We now have the following:

Theorem 7.1. *Consider dynamics τ_t as described in Section 4.*

(a) The dynamics τ_t satisfies detailed balance II w.r.t. ρ if and only if

$$\left\langle \tau_t(A)\tilde{B} \right\rangle = \left\langle A\widetilde{\tau_t'(B)} \right\rangle \tag{20}$$

for all $A, B \in M_n$, and

$$\tau_t'(I) = I$$

for every t.

(b) The dynamics τ_t satisfies Θ-sqdb w.r.t. ρ if and only if

$$\left\langle \tau_t(A)\tilde{B} \right\rangle = \left\langle A[\Theta \circ \tau_t \circ \Theta(B)]^{\tilde{}} \right\rangle$$

for all $A, B \in M_n$, where $[\cdot]^{\tilde{}}$ means we apply the tilde to the contents of $[\cdot]$.

Proof. Note that Eq. (20) is equivalent to $\omega(\tau_t(A) \otimes \bar{B}) = \omega(A \otimes \overline{\tau_t'(B)})$. Taking the complex conjugate of this, we see that it is in turn equivalent to $\omega(\tau_t(A^\dagger) \otimes B^\intercal) = \omega(A^\dagger \otimes \tau_t'(B)^\intercal)$, since $\tau_t(A)^\dagger = \tau_t(A^\dagger)$. So we have shown that Eq. (20) is equivalent to Eq. (9). The rest of the proof of this theorem is now straightforward from the results of Section 5. $\square$

This theorem shows that the entanglement characterizations of detailed balance in Section 5 fit naturally into the framework of thermofield dynamics.

8 Discussion

One may ask what the most fruitful ways are to motivate formulations of quantum detailed balance on direct physical grounds. Possibly characterization of detailed balance in terms of an entangled state can provide an alternative quantum mechanical foundation for, and interpretation of, detailed balance in terms of entanglement.

This would be in line with recent work where foundational aspects of statistical mechanics are studied and motivated directly in terms of entanglement [4]. This approach to the foundations of statistical mechanics appears promising, so despite the more traditional arguments in favour of the various quantum formulations of detailed balance, attempting to motivate it from the perspective of entanglement may prove fruitful. Possibly it could also give a wider perspective on detailed balance, considering that here we only used a very specific entangled state, while in principle one could consider conditions as in Theorem 5.2 and Proposition 5.3 with respect to more general entangled states. We hope that the connection between detailed balance and entanglement considered in this paper can further such studies.

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