Quantum entropy production as a measure of irreversibility

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Abstract

We consider conservative quantum evolutions possibly interrupted by macroscopic measurements. When started in a nonequilibrium state, the resulting path-space measure is not time-reversal invariant and the weight of time-reversal breaking equals the exponential of the entropy production. The mean entropy production can then be expressed via a relative entropy on the level of histories. This gives a partial extension of the result for classical systems, that the entropy production is given by the source term of time-reversal breaking in the path-space measure.

Key words: quantum systems, entropy production, time-reversal
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1 Quantum entropy

In bridging the gap between classical mechanics and thermal phenomena, the founding fathers of statistical mechanics realized that a statistical characterization of macrostates in terms of microstates is essential for understanding the typical time evolution of thermodynamic systems. But statistical reasoning requires proper counting, starting from a set of *a priori* equivalent microstates. That is different in quantum statistics from what is done in classical statistics. Nevertheless the same concepts can be put in place. In this paper, we show for the quantum case what has been proven useful in the classical case: that entropy production measures the breaking of time-reversal invariance. More exactly, we show that the logarithmic ratio of the probability of a trajectory and its time-reversal coincides with the physical entropy production.

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We continue with an introduction about entropy, both classical and quantum, to specify what we mean by entropy production. The main message is contained in Sections 2 and 3 where the relation between entropy production and time-reversal is demonstrated. Section 2 deals with a unitary evolution (one initial preparation and one final measurement) and can be considered as a special case of Section 3 where the unitary evolution is further interrupted with measurements of the macrostate. The paper is based on elementary mathematical manipulations and the emphasis is on the conceptual framework.

1.1 Classical set-up

Suppose a classical closed and isolated system of N particles. A complete description consists in specifying its microstate, that is a point x in its phase space, $x = (q_1, \ldots, q_N, p_1, \ldots, p_N)$ of positions and momenta. The dynamics is Hamiltonian and energy is conserved. Each microstate x determines a macrostate $M(x)$ corresponding to a much coarser division of phase space. To be specific, we consider the surface Γ of constant energy and we suppose that the macrostates induce a finite partition $\hat{\Gamma}$ of Γ. The different macroscopic values thus specify a (finite) number of regions in phase space. We emphasize that this reduced description is in terms of macroscopic variables (in contrast with the partitions as used e.g in constructions of dynamical entropies), such as position or velocity profiles and we denote by $|M|$ the corresponding phase space volume.
The Boltzmann entropy (also called Boltzmann-Planck-Einstein or microcanonical or configurational entropy) is, up to multiplicative and additive constants, defined by

$$S_B(x) \equiv \log |M(x)| \tag{1.1}$$

When the microstate belongs to the region of phase space of unconstrained equilibrium, then, at least in the thermodynamic limit, $S_B(x)$ equals the thermodynamic entropy defined operationally by Clausius. But also out of equilibrium, say when a constraint is lifted and the system is free to evolve, the Boltzmann entropy remains relevant as it will typically increase towards equilibrium. It gives in fact the microscopic foundation of the second law of thermodynamics.
There is another entropy that generalizes (1.1). Suppose we only specify a distribution of macrovalues. This means that we do not know the exact macrostate, perhaps not even initially. The statistics of macroscopic values is then given by a probability distribution $\hat{\nu}(M), M \in \hat{\Gamma}$; e.g. our best guess about the position and velocity profile. In the absence of any further information, there is a natural probability density, written $\rho_{\hat{\nu}}$, on Γ which gives equal

probability to each microstate compatible with a macrostate M:

$$\rho_{\hat\nu}(x) = \frac{\hat\nu(M(x))}{|M(x)|}$$

The functional

$$S_G(\hat\nu) = -\int_\Gamma dx\, \rho_{\hat\nu}(x) \ln \rho_{\hat\nu}(x)$$

is appropriately called Gibbs entropy as it is, since Gibbs, the usual statistical mechanical entropy for constrained equilibrium [2]. Put differently, by Gibbs' variational principle,

$$S_G(\hat\nu) = \sup_{p(\mu)=\hat\nu} -\int_\Gamma dx\, \mu(x) \ln \mu(x) \tag{1.2}$$

where the supremum is taken over all phase space densities μ with the same macro-statistics as $\hat\nu$, i.e., the projection $p(\mu)$ of μ on $\hat\Gamma$ coincides with $\hat\nu$:

$$\mu(M) = \int_\Gamma dx\, \mu(x)\, \delta(M(x) - M) = \hat\nu(M)$$

and the supremum is reached for $\mu = \rho_{\hat\nu}$. Equivalently, by a simple calculation, the Gibbs entropy equals

$$S_G(\hat\nu) \equiv \sum_M \hat\nu(M) \log |M| - \sum_M \hat\nu(M) \log \hat\nu(M) \tag{1.3}$$

Obviously, if $\hat\nu$ concentrates on just one macrostate M, $\hat\nu(M') = \delta_{M,M'}$, then $S_G(\hat\nu) = \log |M|$ which is the Boltzmann entropy for that macrostate. More generally, the first term in (1.3) is the expected or estimated entropy, being unsure as we are about the exact macrostate. The second term in (1.3) is non-negative and is most often negligible, certainly upon dividing by the number of particles.

When we start the system from a microstate that is randomly drawn (according to the Liouville measure) from M with probability $\hat\nu(M)$ and we record the statistics $\hat\nu_t$ on the macrostates after time t, then, always,

$$S_G(\hat\nu_t) \geq S_G(\hat\nu) \tag{1.4}$$

This is not the second law (e.g. it does not imply that $S_G(\hat\nu_t)$ is non-decreasing in t, see [5] for more discussion). To bring it closer to the second law, one needs to explain under what conditions $S_G(\hat\nu_t)$ approximates the Boltzmann entropy $S_B(x_t)$ with x_t the time-evolved phase point. Looking back at the first term in (1.3), that implies understanding how and when the empirical distribution for

[2] Often, even without a specific physical context or meaning, $-\int_\Gamma dx\, \mu(x) \log \mu(x)$ is called the Gibbs entropy of μ. There is however another name for that functional: the Shannon entropy. A way out would be to call $S_G(\hat\nu)$ the Boltzmann-Gibbs-Shannon entropy as in [7] but that sounds overdone.

the macrovariables becomes peaked, as the number of particles increases, at a fixed macroscopic trajectory as described e.g. by hydrodynamic equations of irreversible thermodynamics.
In [5] we have discussed at length how these entropies relate to time-reversal. The main result there was that both for closed systems and for open systems, be it in the transient regime or in the steady state regime, the entropy production equals the source term of time-reversal breaking in the action functional for the distribution of the histories (on some thermodynamic scale) of the system. This representation gives the entropy production as a function of the trajectories and it allows simple manipulations for taking the average (to prove that it is positive) and for studying its fluctuations (to understand symmetries under time-reversal). In the present paper we begin explaining a similar reasoning for finite quantum systems.

1.2 Quantum set-up

We take the simplest mathematical set-up for describing a quantum system within conventional quantum mechanics. We denote by $\mathcal{H}$ the Hilbert space of the system, assumed finite dimensional. The system is described in terms of a wavefunction ψ, or perhaps better, a normalized vector in $\mathcal{H}$. The variables defining the macrostate are not different from that in the classical situation. For example, they specify (again to some appropriate accuracy) the particle number and the momentum profiles by associating numbers to a family of macroscopically small but microscopically large regions of the volume occupied by the system. Therefore, the macrostate is given in terms of the values of a set of macroscopic observables represented by commuting operators. The macroscopic partition in the classical case above is replaced by the orthogonal decomposition

$$\mathcal{H} = \bigoplus \mathcal{H}_\alpha \tag{1.5}$$

into linear subspaces. The macrovariables are represented by the projections P_α on the respective $\mathcal{H}_\alpha, P_\alpha P_\beta = \delta_{\alpha,\beta} P_\alpha, \sum_\alpha P_\alpha = \mathrm{id}$. We write d_α for the dimension of $\mathcal{H}_\alpha$; it is the analogue of the phase space volume $|M|$ in the classical case. We can think of the macrostates as labeled by the running index α. For a given macrostate α represented by the projection P_α above, we stretch the notation of (1.1) and write its Boltzmann entropy as

$$\widehat{S_B}(\alpha) \equiv \log d_\alpha \equiv \log d(P_\alpha) \tag{1.6}$$

So far, the above does not depart essentially from the classical set-up except for the important difference that (1.1) is defined on microstates and (1.6) is defined on macrostates. At this moment the treatment starts to differ. Following von Neumann, page 411 in his well-known book [6], as discussed e.g.

in [3], the formula (1.1) is changed to

$$S_N(\psi) = \sum_\alpha (\psi, P_\alpha \psi) \log d_\alpha - \sum_\alpha (\psi, P_\alpha \psi) \log (\psi, P_\alpha \psi) \tag{1.7}$$

where $(\psi, P_\alpha \psi)$ is the probability of finding the system described via the wavefunction ψ in the macrostate α (values corresponding to $\mathcal{H}_\alpha$). Observe that (1.7) very much resembles (1.3), eventhough (1.7) is the quantum analogue of (1.1), both defined as they are for the microstate. The reason is of course quantum mechanics itself: the wavefunction can still correspond to different (mutually exclusive) macrostates. If not initially, still later in time, superpositions in terms of wavefunctions of different macrostates are possible. This in contrast with the classical set-up where a unique macrostate is associated to each microstate. Just as the second term in the classical (1.3) arises from additional uncertainty as to the exact macrostate, here, even when the microstate is given (in terms of ψ), we still have a distribution on the macrostates [3].

Instead of taking a pure state in (1.7), we may want to consider the system in a mixed state and described by a density matrix. In fact, as we are interested in the thermodynamic time-evolution, we construct a special class of density matrices by specifying the macroscopic statistics just as we did for (1.3). We thus start from a probability distribution $\hat{\mu}$ on the possible macrovalues and we randomize within. More precisely, we consider density matrices $\rho(\hat{\mu})$ defined by

$$\rho(\hat{\mu}) \equiv \sum_\alpha \frac{\hat{\mu}(\alpha)}{d_\alpha} P_\alpha \tag{1.8}$$

for given $\hat{\mu}(\alpha) \geq 0, \sum_\alpha \hat{\mu}(\alpha) = 1$. Then,

$$\hat{\mu}(\alpha) = \mathrm{Tr}[P_\alpha \, \rho(\hat{\mu})] \tag{1.9}$$

is the probability to find the system in macrostate α. For the choice $\hat{\mu}(\alpha) = d_\alpha / d$ where, for normalization, $d \equiv \sum_\alpha d_\alpha$ is the dimension of $\mathcal{H}$, $\rho(\hat{\mu}) = \mathrm{id}/d$. In the other direction, given a general density matrix ρ, we can take its projection $p(\rho)$ on the macroscopic states:

$$p(\rho)(\alpha) \equiv \mathrm{Tr}[P_\alpha \, \rho] \tag{1.10}$$

and of course, $p(\rho(\hat{\mu})) = \hat{\mu}$.

We now apply the same principle as in (1.2) to obtain the (Gibbs - von Neumann) quantum entropy

$$S(\hat{\mu}) \equiv \sup_{p(\rho)=\hat{\mu}} - \mathrm{Tr}[\rho \, \log \rho] \tag{1.11}$$

[3] One of us, C.M., likes to emphasize that all this does not exclude that the actual system is all the time in exactly one of the macrostates — but the wavefunction does not provide a complete description of the system.

with solution (reached at $\rho = \rho(\hat{\mu})$)

$$S(\hat{\mu}) = \sum_{\alpha} \hat{\mu}(\alpha) \log d_\alpha - \sum_{\alpha} \hat{\mu}(\alpha) \log \hat{\mu}(\alpha) \tag{1.12}$$

which looks exactly like (1.3). Again, $S(\hat{\mu})$ equals $\widehat{S_B}(\alpha)$ when $\hat{\mu}$ concentrates on the macrostate α and, up to some irrelevant constants, $S(\hat{\mu})$ equals the relative entropy of $\rho(\hat{\mu})$ with respect to the equilibrium density matrix id/d. More generally, we call

$$S(\rho) \equiv S(p(\rho)) = \sum_{\alpha} \mathrm{Tr}[P_\alpha \, \rho] \log d_\alpha - \sum_{\alpha} \mathrm{Tr}[P_\alpha \, \rho] \, \log \mathrm{Tr}[P_\alpha \, \rho] \tag{1.13}$$

the macroscopic quantum entropy of the (mixed) state ρ, reducing to (1.12) for the choice (1.8) and to (1.7) for a pure state.

2 Entropy production for a unitary evolution

The goal of this section is to show that the total change of entropy under a quantum conservative evolution, that is the entropy production, can be given in terms of a logarithmic ratio of probabilities.

We suppose a quantum dynamics generated via a real Hamiltonian H. This means that the Hamiltonian is time-reversal invariant, $H\pi = \pi H$ where π is an anti-linear involution (kinematical time-reversal) which would be just complex conjugation for wavefunctions. The unitary evolution $U(t) \equiv \exp[-itH]$ where t is time (and Planck's constant is set equal to one) then satisfies

$$\pi U(t) \pi = U(t)^\star = U(t)^{-1}$$

an expression of dynamic reversibility. We also assume that the macrostates are mapped into each other via the involution π, i.e.,

$$\pi P_\alpha \pi = P_{\alpha'} \equiv P_{\pi\alpha} \tag{2.1}$$

for some α', for each α and we write $\pi\alpha = \alpha'$.

Let the system be initially prepared with macro-statistics $\rho(\hat{\mu})$, see (1.8). We now leave the system alone, undergoing its quantum evolution. The probability to see the system at the initial time in macrostate α_0 and at time t in macrostate α_t is given by

$$\mathrm{Prob}_{\hat{\mu}}[\alpha_0, \alpha_t] = \mathrm{Tr} \, [U(t) P_{\alpha_0} \rho(\hat{\mu}) P_{\alpha_0} U(t)^\star P_{\alpha_t}] \tag{2.2}$$

Its marginal at time t is

$$\hat{\mu}_t(\alpha) \equiv \sum_{\alpha_0} \mathrm{Prob}_{\hat{\mu}}[\alpha_0, \alpha_t = \alpha] = \mathrm{Tr}\ [U(t)\rho(\hat{\mu})U(t)^\star P_\alpha] \tag{2.3}$$

We consider the logarithmic ratio of probabilities

$$R_{\hat{\mu}}(\alpha_0, \alpha_t) \equiv \log \frac{\mathrm{Prob}_{\hat{\mu}}[\alpha_0, \alpha_t]}{\mathrm{Prob}_{\hat{\mu}_t\pi}[\pi\alpha_t, \pi\alpha_0]} \tag{2.4}$$

where the denominator gives the probability of the time-reversed order of measurement results starting from $\rho(\hat{\mu}_t\pi)$ with $\hat{\mu}_t\pi(\alpha) \equiv \hat{\mu}_t(\pi\alpha)$.

We make two observations. First, when $\hat{\mu}(\alpha) = d_\alpha/d$, then also at later times $\hat{\mu}_t(\alpha) = d_\alpha/d$ and moreover

$$\mathrm{Prob}_{\hat{\mu}}[\alpha_0, \alpha_t] = \mathrm{Prob}_{\hat{\mu}_t}[\pi\alpha_t, \pi\alpha_0] \tag{2.5}$$

expressing the time-reversal invariance when started from the time-invariant macro-statistics that assigns to macrostates probabilities proportional to the exponential of their Boltzmann entropy, see (1.6).
Secondly, for other choices of the initial macro-statistics, the $R_{\hat{\mu}}$ of (2.4) reproduces the change of entropy:

$$R_{\hat{\mu}}(\alpha_0, \alpha_t) = \log d_{\alpha_t} - \log d_{\alpha_0} - \log \hat{\mu}_t(\alpha_t) + \log \hat{\mu}(\alpha_0) \tag{2.6}$$

where we recognize the change of Boltzmann entropies (1.6) in the first two terms. Upon taking the expectation

$$\sum_{\alpha_0,\alpha_t} \mathrm{Prob}_{\hat{\mu}}[\alpha_0, \alpha_t]\, R_{\hat{\mu}}(\alpha_0, \alpha_t) = S(\hat{\mu}_t) - S(\hat{\mu}) \tag{2.7}$$

we recover the change in entropy (1.11). Note that $S(\hat{\mu}_t) = S(\rho_t), S(\hat{\mu}) = S(\rho)$ defined in (1.13) for $\rho = \rho(\hat{\mu})$, $\rho_t = U(t)\rho U(t)^\star$ so that the right-hand side of (2.7) is really the change of macroscopic quantum entropy under the unitary evolution. The left-hand side of (2.7) is a relative entropy, hence is non-negative.

3 Perturbations by measurement

In contrast with the classical evolution, the unitary evolution can be non-trivially interrupted by measurements that reduce the state. We follow here the theory of von Neumann (or, convential quantum mechanics) that adds a dynamic interpretation to the projections (1.10). We extend here the results of the previous section to include interactions with a measurement apparatus.

Suppose that we start the system described by a density matrix ρ at time 0 and that we measure the macroscopic value α at time $\tau > 0$. Then, the new density matrix is

$$\frac{P_\alpha U\,\rho\, U^\star P_\alpha}{\mathrm{Tr}[P_\alpha U\,\rho\, U^\star]}$$

where $U \equiv U(\tau) = \exp[-i\tau H]$. This reduction takes place with probability

$$p(U\rho U^\star)(\alpha) = \mathrm{Tr}[P_\alpha U\,\rho\, U^\star]$$

We can generalize this to a sequence of measurements.

3.1 Path-space measure

We consider a sequence of times $0, \tau, 2\tau, \ldots, n\tau = t$ (evenly spaced for convenience). A macroscopic trajectory ω assigns to each of these times a value for the macroscopic observables. In short, $\omega = (\omega_0, \ldots, \omega_n)$ with each ω_i being equal to some projection P_α on the linear subspace $\mathcal{H}_\alpha$ of (1.5). We consider the operator

$$G_\omega \equiv \omega_n U \omega_{n-1} \ldots \omega_1 U \omega_0 \tag{3.1}$$

and, for a given density matrix ρ on $\mathcal{H}$, the matrix

$$\mathcal{D}_\rho(\omega, \omega') \equiv \ \mathrm{Tr}[G_\omega\, \rho\, G^\star_{\omega'}] \tag{3.2}$$

This resembles the correlation matrix that is used in the definition of quantum dynamical entropy, see p. 189 in [2], but again, here our partitioning corresponds to macrostates.
It is easy to verify that $\mathcal{D}_\rho$ is non-negative and has trace one. We call it the path-space density matrix.
$\mathcal{D}_\rho$ depends on the initial density matrix ρ and it also gives the probability to find the system after time $t = n\tau$ of (measurement-)free evolution in the macrostate α:

$$\sum_{\omega,\omega' : \omega_n = \omega'_n = P_\alpha} \mathcal{D}_\rho(\omega, \omega') = \ \mathrm{Tr}[P_\alpha\ \rho_t] \tag{3.3}$$

where $\rho_t \equiv U^n \rho U^{-n}$.
More importantly, the probability to measure the trajectory ω, i.e., to see the system at the initial time in the macrostate represented by ω_0, at time τ in macrostate ω_1, and so on till time $n\tau = t$, is given by the diagonal element

$$\mathrm{Prob}_\rho[\omega] = \mathcal{D}_\rho(\omega, \omega) \tag{3.4}$$

Its marginal at time $t = n\tau$,

$$\hat{\mu}_t(\alpha) \equiv \sum_{\omega : \omega_n = P_\alpha} \mathrm{Prob}_\rho[\omega] \tag{3.5}$$

is the probability of macrostate α when the unitary evolution was interrupted by n measurements. It equals (2.3) in case $n = 1$.

3.2 Time-reversal

On trajectories, the time-reversal transformation Θ is

$$(\Theta\omega)_m \equiv \pi\omega_{n-m}\pi, \quad m = 0, 1, \ldots, n$$

Since the microscopic dynamics is time-reversal invariant, we immediately deduce that

$$G_{\Theta\omega} = \pi G^\star_\omega \pi$$

and it is easy to verify that for $\rho = \mathrm{id}/d$ in (3.2)

$$\mathcal{D}(\Theta\omega', \Theta\omega) = \mathcal{D}(\omega, \omega') \tag{3.6}$$

In particular, for (3.4) with $\rho = \mathrm{id}/d$, $\mathrm{Prob}[\omega] = \mathrm{Prob}[\Theta\omega]$. This identity has two related interpretations. First, it is the expression of (quantum) detailed balance or microscopic reversibility for the trajectories sampled from the time-invariant density matrix id/d corresponding to equilibrium. It is the generalization of (2.5). Secondly, it generalizes the observation of [1] that measurements do not introduce a time-asymmetric element (or, the reduction of the wave packet does not lead to irreversibility).
Yet, in general, the system could start in a nonequilibrium state and evolve towards equilibrium. This involves a change of entropy; that is, for closed and thermally isolated systems, its total entropy production.
The time-reversal of the density matrix $\mathcal{D}_\rho$, written $\mathcal{D}_\rho\Theta$, is defined as

$$\mathcal{D}_\rho\Theta(\omega, \omega') \equiv \mathcal{D}_\rho(\Theta\omega', \Theta\omega) \tag{3.7}$$

so that by (3.6), $\mathcal{D}\Theta = \mathcal{D}$. This last equality is broken for a general $\mathcal{D}_\rho$ and it seems natural to estimate this breaking via the relative entropy

$$S(\mathcal{D}_{\rho_1}|\mathcal{D}_{\rho_2}\Theta) \equiv \mathrm{Tr}[\mathcal{D}_{\rho_1}(\log \mathcal{D}_{\rho_1} - \log \mathcal{D}_{\rho_2}\Theta)] \tag{3.8}$$

In view of the classical results of [4,5], it is to be expected that this relative entropy is related to the entropy production for the appropriate choices of ρ_1 (as initial state) and of ρ_2 (as time-reversal of the final state).

3.3 Entropy production

We start again from $\hat{\mu}$ as initial probability distribution (i.e., $\rho(\hat{\mu})$ is the initial density matrix) and the final probability distribution $\hat{\mu}_t$ is defined in (3.5). The

main result is now readily obtained starting with the analogue of (2.4): the logarithmic ratio of probabilities (3.4) of a macroscopic trajectory, one started from $\hat{\mu}$ and the other started from $\hat{\mu}_t\pi$, is abbreviated as

$$R_{\hat{\mu}}(\omega) \equiv \log \frac{\mathrm{Prob}_{\hat{\mu}}[\omega]}{\mathrm{Prob}_{\hat{\mu}_t\pi}[\Theta\omega]} \tag{3.9}$$

This object will not always be well-defined for all ω. We can suppose however that the $\hat{\mu}(\alpha) \neq 0 \neq \hat{\mu}_t(\alpha)$ so that a little calculation of (3.9) yields

$$R_{\hat{\mu}}(\omega) = \log d(\omega_n) - \log d(\omega_0) - \log \hat{\mu}_t(\omega_n) + \log \hat{\mu}(\omega_0) \tag{3.10}$$

In the notation of (1.6), the first difference in the right-hand side of (3.10) equals the change of Boltzmann entropy $\widehat{S_B}(\alpha_t) - \widehat{S_B}(\alpha_0)$ for a trajectory that starts in macrostate α_0 and ends in macrostate α_t. If the system is initially prepared in essentially one macrostate, $\hat{\mu}(\alpha_0) \simeq 1$, and if the evolution on the level of macrostates is quasi-autonomous till time t in the sense that $\hat{\mu}_t(\alpha_t) \simeq 1$, then only that change in Boltzmann entropies survives.
Taking the expectation of (3.9), we get, similar as in (2.7),

$$\sum_{\omega} \mathrm{Prob}_{\hat{\mu}}[\omega]\, R_{\hat{\mu}}(\omega) = S(\hat{\mu}_t) - S(\hat{\mu}) \geq 0 \tag{3.11}$$

equal to the change of quantum entropy (1.11)–(1.12). The non-negativity follows from Jensen's inequality applied to the left-hand side of (3.11).
One can easily check that this expectation (the left-hand side of (3.11)) and hence, the change of quantum entropy (the right-hand side of (3.11)), also coincides with the relative entropy on the level of density matrices for trajectories

$$S(\mathcal{D}_{\hat{\mu}}|\mathcal{D}_{\hat{\mu}_t\pi}\Theta) = \mathrm{Tr}\ [\mathcal{D}_{\hat{\mu}}\,(\log \mathcal{D}_{\hat{\mu}} - \log \mathcal{D}_{\hat{\mu}_t\pi}\Theta)]$$

as announced in (3.8).

4 Conclusions and additional remarks

Entropy production, also for the quantum situation, has been under intense investigation in recent years. A list of related references, even restricted to the last 5 years would soon fill an extra couple of pages. In the classical case, there have been essentially two types of approaches, dynamical versus statistical. In the dynamical approach, entropy production is connected with the fractal or singular nature of a class of natural stationary measures. A key-notion is the phase space contraction rate and with some extrapolations, nonequilibrium statistical mechanics becomes a branch of the theory of smooth dynamical systems. It was partially motivated by numerical work and it has given wonderful insights, guiding towards a study of fluctuations of the entropy production, possibly generalizing close to equilibrium relations. The statistical

approach emphasizes the sharp contrast between the microscopic and macroscopic scales and stochasticity enters the dynamical evolutions because of the reduced description. On space-time the histories have a distribution that share the essential properties of Gibbs measures. The entropy production can then be identified with the source term of time-reversal breaking in the action (or space-time Lagrangian) of the space-time distribution; the Gibbs formalism reproduces and extends the results for the fluctuations of the entropy production obtained in the purely dynamical approach. The projections on equal time surfaces reproduce the time-evolved measure. In the quantum case, the modern dynamical approach does not seem to have a natural generalization. Instead, the old machinery of operator-algebra and spectral theory, directly applied on infinite volume systems, has been providing encouraging results for relaxation to equilibrium and the positivity of entropy production in driven quantum systems. Again however, the conceptual framework and the essential distinction between microstates and macro-statistics is, at least to our taste, most often blurred in non-intuitive dynamical assumptions and in the heavy mathematical formalism. The present paper offers an alternative and starts the statistical approach for quantum systems. The first step indeed is to be quite clear as to the relation between time-reversal and entropy production. As in the classical case, we consider this important for constructing nonequilibrium statistical mechanics. Specifically, we hope that the characterizations of (2.6) and (3.10) will prove useful for deriving general fluctuation and response identities going beyond close to equilibrium.
We add some general remarks.

1. For reversible systems the entropy production is a state function. It does not depend on the actual path but can be written as a difference of the same quantity evaluated at the initial and the final time, see (2.6) or (3.10). This can be different for driven or irreversible systems. A similar treatment for such systems in the classical regime can be found in [5]. One of the main consequences of the identities that correspond there to (2.6) or (3.10) is that certain symmetries in the fluctuations of the entropy production rate are easily established. The quantum case is in preparation.

2. Nothing of the previous mathematical identities depends on the assumption that the system is large, of macroscopic size, containing a huge number of particles. Of course, to meaningfully discuss macroscopic variables or macrostates and their trajectories one has in mind a clear separation between micro and macro scales but the results of Sections 2 and 3 are true without. Yet again, their interpretation as thermodynamic entropy production and the relation with the second law can only be made when dealing with macroscopic systems. See also Appendix A in [5] for these considerations in the classical case.

3. The use of the projections P_α in the construction of the path-space density matrix of Section 3 refers to the so called von Neumann measurements. One

can imagine more *fuzzy* measurements (and more rounded-off macrostates) and a corresponding decomposition of unity as

$$\sum_\alpha X_\alpha^\star X_\alpha = \text{ id}$$

The treatment above was restricted to the case $X_\alpha = P_\alpha U$. This extension is very much related to the dynamics of open systems, see e.g. [2]. The involvement of measurements interrupting the unitary evolution already points to the interaction with the outside world. The question of isolation, even as an idealization, of a quantum system is much more subtle than for a classical system.

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