Entropy production in quantum is different

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Currently ‘time’ does not play any essential role in quantum information theory. In this sense quantum information theory is underdeveloped similar to how quantum physics was before Erwin Schrödinger introduces his equation for the evolution of a quantum wave function. In this review article, we cope with the problem of time for one of the central quantities in quantum information theory, entropy. Recently a replica trick formalism, the so-called ‘multiple parallel world’, has been proposed that revolutionizes entropy evaluation for quantum systems. This formalism in one of the first attempts to introduce ‘time’ in quantum information theory. With the total entropy being conserved in a closed system, entropy can flow internally between subsystems, however we show that this flow is not limited only to physical correlations as the literature suggest. The nonlinear dependence on density matrix introduces new types of correlations with no analogue in physical quantities. Evolving a number of replicas simultaneously makes it possible that they exchange particles between different replicas. We will summarize some of the recent news about entropy in some example quantum devices. Moreover, we take a quick look at a new correspondence that was recently proposed that provides an interesting link between quantum information theory and quantum physics. The mere existence of such a correspondence allows exploring new physical phenomena as the result of controlling entanglement in a quantum device.

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I. INTRODUCTION

Entropy is one of the central quantities in thermodynamics and without its precise evaluation, one cannot predict what new phenomena are to be expected in the thermodynamics of a device. In quantum theory, entropy is defined a nonlinear function of density matrix, i.e. $S = -\text{Tr}\hat{\rho}\ln\hat{\rho}$, in the units of the Boltzmann constant. The mere nonlinearity indicates that entropy is not a physical quantity because by definition physical quantities are linear in density matrix. Let us further describe this statement. Here we do not assume that density matrix is a physical quantity. The reason is that identifying the elements of a density matrix
requires many repetition and reinitialization in the experiment, and at each iteration the
elements of density matrix cannot be measured precisely because measurement collapses or
modifies quantum states. A physical quantity, such as energy and charge, can be measured
in the lab in real time and can be defined in quantum theory to be linearly depending on
density matrix. Entropy by definition is not so and therefore we cannot assume it is a
physical quantity that is directly measurable in the lab.

In fact, the precise time evolution of entropy is still an open problem and has not been
properly addressed in the literature [1–3]. A consistent theory for quantum thermodynamics
can be achieved after finding nontrivial relations between the quantum of information and
physics. In recent years, exquisite mesoscopic scale control over quantum states has led
technology to the quantum realm. This has motivated exploring new phenomena such as
exponential speed up in computation as well as power extract from quantum coherence
[4, 5]. Recently there have been attempts to implement quantum versions of heat engines
using superconducting qubits [6]. However recent developments in realizing quantum heat
engines such as in References [7–9] rely on semiclassical stochastic entropy production after
discretizing energy. A long-lasting question is how the superposition of state transfers heat
and how much entropy is produced as the result of such a transfer.

A quantum heat engine (QHE) is a system with several discrete quantum states and,
similar to a common heat engine, is connected to several environments kept at different
temperature. In fact, in these engines a number of large heat baths share some degrees of
freedom quantum mechanically. Such a system is supposed to transfer heat according to the
laws of quantum mechanics. The motivation for research in QHE comes from differences they
may controllably make on the efficiency and output powers. Let us consider the example of
two heat baths A and B, both coupled through a quantum system q that contains discrete
energies and allows for the superposition of states with long coherence time. [42] This
quantum system that is coupled to two large system is in fact a physical quantum system
that is energetically- coupled to the reservoirs and allows for stationary flow of heat as well
as thermodynamic entropy from one reservoir to another one. We will see in the next section
that similar to physical quantities such as energy and change, the total entropy of a closed
system is a conserved quantity and does not change in time. However internally entropy
can flow from one subsystem to another, therefore sub-entropies may change in time and
this change may indicate a change in the energy transfer. Some important questions one
may ask are: *Does quantum superposition produce or reduce entropy?* This is one of the questions that we will address in this almost pedagogical review paper and describe how the information content in entropy can be meaningful in physics.

In a typical engine made of reservoirs $A$ and $B$ and intermediate quantum system $q$ with discrete energy levels, the change of entropy in one of the reservoirs, say $B$, between the time $t$ and 0 is

$$S_B(t) - S_B(0) = -\text{Tr} \left\{ \rho(t) \ln \rho_B(t) \right\} - \text{Tr}_B \left\{ \rho_B^{eq} \ln \rho_B^{eq} \right\},$$

where in the first term we have safely replaced one of the two partial density matrices with total density matrix, and accordingly the partial trace with total one. The conservation of entropy tells us that total entropy maintains its initial value at the separable compound state $\rho(0) = \rho_q(0) \rho_A^{eq} \rho_B^{eq}$, i.e. $-\text{Tr} \left\{ \rho(t) \ln \rho(t) \right\} = -\text{Tr}_q \left\{ \rho_q(0) \ln \rho_q(0) \right\} - \sum_{i=A,B} \text{Tr}_i \left\{ \rho_i^{eq} \ln \rho_i^{eq} \right\}$. After a few lines of algebra one can find the change of entropy at the reservoir is

$$S_B(t) - S_B(0) = S_B(\rho(t)||\rho_B^{eq} \rho_B(t) \rho_q(0)) + \sum_{i=q,A} \text{Tr}_i \left\{ (\rho_i(t) - \rho_i(0)) \ln \rho_i(0) \right\},$$

with relative entropy being $S(\rho||\rho') \equiv \text{Tr} \left\{ \rho \ln \rho \right\} - \text{Tr} \left\{ \rho \ln \rho' \right\}$. Since relative entropy is a positive number [10] and equals to zero only for identical density matrices $\rho = \rho'$, the first part of the entropy flow is positive and irreversible. This satisfies the classical laws of thermodynamics. We will show that in contrast to what has been so far presented in the literature [11], the second term in the entropy flow is *not* heat transfer —the average change of energy at the two times $Q_B \equiv \langle H(0) \rangle_B - \langle H(t) \rangle_B$. Instead it is the difference of incoherent and coherent heat transfers [12], i.e. $(Q_{B,\text{inhoc}}(t) - Q_{B,\text{coh}}(t)) - (Q_{B,\text{inhoc}}(0) - Q_{B,\text{coh}}(0))$. This is the new result that heavily modifies the flow of entropy in some quantum heat engines and lead to some recent new physics [13–16].

In this review paper, we look at some of the simplest and most important quantum heat engines. Depending on the external drive or internal degeneracy, the exact evaluation of entropy is indeed very different from what has been so far presented in the literature. We will describe how to precisely evaluate entropy and its flow by using a replica trick that properly allows for the mathematically involved nonlinearity. We introduce a new class of correlations that allow information transfers and are different from physical correlations. For equilibrium system, these informational correlations satisfy a generalized form of Kubo-Martin-Schwinger (KMS) relation [17]. This part of the analysis will be presented in a self-contained fashion after reviewing some of the classical and quantum definitions of entropy and introducing our replica trick for evaluating the time evolution of generalizing Keldysh contours. We describe a short protocol for evaluating Keldysh diagrams and in
some examples perform the evaluation of some diagrams. We present results of example quantum devices such as a two-level quantum heat engine, a photocell, as well as a resonator, each one mediating heat transfer between two large heat baths. Finally, we briefly report the new correspondence that makes entropy flow directly measurable in the lab by monitoring physical quantities, i.e. the statistics of energy transfer.

II. CLASSICAL SYSTEMS

A. Classical Entropy

Many systems in classical physics carry entropy. Some of the most studied systems are: charged transport at a point contact [18, 19], energy transport in heat engines [20], and a gravitational hypersurface falling into a black hole [21]. For simplicity of discussion let us review classical entropy the example of charge transport through a point contact. Consider two large conductor plates connected at a point, the so-called a ‘point contact system’. This classical point contact either transmits a charged particle with the probability $p$ or blocks the transmission with the probability $1 - p$. Let us consider $N$ attempts take place. For $N \gg 1$ it is most likely that in $pN$ out of $N$ times the particles are successfully transferred and in $(1 - p) N$ out of $N$ times, not. For unmarked particles the order of events does not matter, therefore the number of possibilities with $pN$ transfers out of $N$ attempts is

$$\mathcal{N} = \binom{N}{pN} \approx \frac{N^N}{(pN)^pN \left[(1 - p) N\right]^{(1-p)N}} = \frac{1}{p^{pN} (1 - p)^{(1 - p) N}}$$

This number rapidly grows with $N$. In order to keep the number small its logarithm defines the so-called Shannon entropy, i.e. $S = \log_2 \mathcal{N} = -N \left[p \log_2 p + (1 - p) \log_2 (1 - p)\right]$.

The linear dependence of the Shannon entropy to the number of attempts $N$ indicates its additivity. The definition of entropy can be generalized to account for extended geometries such as a $k+1$-path terminal that connect any reservoir to $k$ others. In this case $k$ probabilities contribute to understand the possibility of transmission from a reservoir to any one of the other $k$ reservoirs, thus entropy is generalized to $S = -N \sum_{n=1}^{k} p_n \log_2 p_n$. This entropy may vary in time. One possible reason for such variation could be due to time-dependent probabilities $p_n(t)$. Another possibility for time evolution of entropy could be the presence of some bias in controlling the system. For example consider that after one successful transfer
the transmission is reduced or closed for a rather long time before it opens again to another
transfer attempt. The entropy of such a system depends on whether or not a success transfer
has taken place in the past.

In fact this paper what we call entropy production refers to the time variation of partial
entropy associated to a part of a closed system. Moreover, as stated in the introduction, in
this paper we are only interested to the time variation of in thermodynamic system such as
heat baths, therefore our focus is only on thermodynamic entropies and its time evolution,
namely ‘entropy production’. Let us be more precise. In this subsection although we discuss
Shannon entropy, but we have to distinguish between the Shannon entropy, which can be
measured as a number of bits, and the thermodynamic entropy, which is all we mean by
entropy in this paper and can be measured in the unit Joule per Kelvin. The Shannon
entropy and the thermodynamic entropy are related by the Boltzmann constant $k_B$. Given
that we discussed such important difference, in this paper without the loss of generality we
use the convention that any constant cofactor of thermodynamic entropies are unit, thus
$k_B = 1$.

B. Renyi entropy

Alfred Renyi introduced the generalization of Shannon entropy that maintain additivity
[22]. For a finite set of $k$ probabilities $p_i$ with $i = 1, \cdots, k$ the Renyi entropy of degree $M$ is
defined as

$$S_M = -\log \sum_i (p_i)^M$$

with positive entropy order $M > 0$. [3] Shannon entropy can be reproduced after tak-
ing derivative of Renyi entropy at the limit of $M \to 1$. In fact given that $dx^M/dM =
d \exp (M \ln x)/dM = x^M \ln x$ one can write

$$\lim_{M \to 1} \frac{dS_M}{dM} = -\lim_{M \to 1} \frac{\sum_i (p_i)^M \ln p_i}{\sum_i (p_i)^M} = -\sum_i p_i \ln p_i = S_{\text{Shannon}}$$

In a point contact, given that Renyi entropy is additive for independent attempts, the
total Renyi entropy after $N$ uncorrelated attempts will be $S_M = -N \log (p^M + (1-p)^M)$. In
a classical heat reservoirs the Renyi entropy is more closely related to free energy. Consider
a bath at temperature $T$ with a large number of energy states $\epsilon_i$ with the Gibbs probability
\[ p_i = \exp(-\epsilon_i T) / Z(T) \] and \[ Z(T) \equiv \sum_i p_i \] being the partition function. The Renyi entropy of the heat bath is \[ S_M = -\ln \left( \sum_i \exp(-Ma_iT) \right) + M \ln Z(T) \]. Free energy will be \[ F(T) = -T \ln Z(T) \], which is related to the Renyi entropy as \[ S_M = (M/T) (F(T) - F(T/M)) \], i.e. the free energy difference at temperatures \( T \) and \( T/M \).

## III. QUANTUM

### A. von Neumann and Renyi entropy

Let us now consider a tripartite system made of two large systems A and B individually coupled to an intermediate quantum system q. This can be thought of as two large systems A and B share some degrees of freedom via q. The quantum system q exchanges energy with A and B independently. The quantumness indicates that q carries a discrete energy spectrum and can be found in long time superposed states. Let \( \rho \) be the density matrix of the compound system. Considering that there is no direct interaction between A and B, the reduced partial density matrix of the system A is \( \rho_A = \text{Tr}_B \text{Tr}_q \rho \). The von Neumann entropy is defined as

\[ S^{(A)} = -\text{Tr}_A \rho_A \ln \rho_A \] (4)

The generalization of entropy in quantum mechanics will naturally gives rise to defining the following quantum Renyi entropies:

\[ S^{(A)}_M = -\ln \text{Tr}_A (\rho_A)^M \] (5)

Let us consider the density matrix of a closed (isolated) system that evolves from the time \( t' \) to \( t \) with the help of a unitary transformation that depends on the time difference, i.e. \( U(t-t') \). The Renyi entropy at time \( t \) is then

\[
\text{Tr} \rho(t)^M = \text{Tr} \left\{ (U(t-t') \rho(t') U^\dagger(t-t'))^M \right\} = \text{Tr} \left\{ U(t-t') \rho(t')^M U^\dagger(t-t') \right\} = \text{Tr} \rho(t')^M
\]

The Renyi entropy at time \( t \) is equal to that at time \( t' \), which proves that in closed systems the Renyi entropy, similar to physical quantities such as energy and charge, is a conserved measure of information content:

\[ \frac{dS_M}{dt} = 0 \] (6)
For noninteracting subsystems $A$ and $B$ they together make up the entire isolated system, therefore the entropies of subsystems $A$ and $B$ are equal as they do not interact, i.e. $S^{(A)} = S^{(B)}$. This shows that for non-interacting subsystems not only total Renyi entropy but also partial entropies are conserved:

$$\frac{dS^{(A)}_M}{dt} = \frac{dS^{(B)}_M}{dt} = 0$$  \hspace{1cm} (7)

Interesting physical systems carry interactions, therefore interacting subsystems $A$ and $B$ if and only if interact with each other and not anybody else, they make a compound system with total conserved informational and physical quantities. However partial quantities behave differently. Consider the total Hamiltonian $H = H_A + H_B + H_{AB}$. The evolution of a part of the system takes place by a non-unitary operator one expects non-vanishing partial flows $\frac{dS^{(A)}_M}{dt}$ and $\frac{dS^{(A)}_M}{dt}$. Only for very weak interacting system, i.e. $H_{AB} \ll H_A, H_B$, the Renyi (von Neumann) entropy of total system is approximately equal to the sum of two partial Renyi (von Neumann) entropies, therefore only for this case one can expect $\frac{dS^{(A)}_M}{dt} + \frac{dS^{(B)}_M}{dt} \approx 0$, Outside of the validity of weak coupling approximation we must expect that although for the total isolated system $dS_M/dt = 0$, its interacting parts take on different flows not only in sign but also in value

$$\frac{dS^{(A)}_M}{dt} \neq -\frac{dS^{(B)}_M}{dt}$$  \hspace{1cm} (8)

This makes the Renyi entropy conservation to be different from the conservation of physical quantities. One can track down the root for such difference in the nonlinear dependence of entropy in density matrix [24].

\section*{B. Replica trick}

Calculating the full reduced density matrix for a general system is the subject of active research. Here we use a different method that is reminiscent of the ‘replica trick’ in disorder system. The trick has been introduced in the context of quantum field theory by Wilczek [25] and Cardy [26] and later in the context of quantum transport by Nazarov [24]. The key point is that if we can evaluate $\text{Tr} \rho^M$ for any $M \geq 1$, we are able to evaluate von Neumann entropy using the following relation:

$$S^{(A)} = \lim_{M \to 1} \frac{d}{dM} S^{(A)}_M = \lim_{M \to 1} \frac{d}{dM} \text{Tr}_A (\rho_A)^M$$  \hspace{1cm} (9)
One can see there is no need for taking logarithm from $\text{Tr}_A (\rho_A)^M$. This is only a mathematical simplicity in the vicinity of $M \to 1$, i.e. when we want to reproduce von Neumann entropy by analytically continuing the derivative of Renyi entropy. Otherwise the presence of logarithm is essential for the definition of Renyi entropy. \[44\]

However, calculating $\text{Tr}_A (\rho_A)^M$ for real or complex number $M$ is hopeless task. The ‘replica trick’ does the following: compute $\text{Tr}_A (\rho_A)^M$ only for integer $M$ and then analytically continue it to a general real or even complex number.

C. Time evolution of entropy

Let us mention that we limit our analysis here only to weak coupling. In this regime the dynamics of quantum system is reversible and can be formulated in terms of density matrix evolution using the time-dependent Hamiltonian $H(t) = H_A + H_B + H_{AB}$ as follows:

$$\frac{d\rho}{dt} = i [H(t), \rho(t)]$$

(10)

The noninteracting part of the Hamiltonian can define the unitary transformation operator $U(t) = \exp \left[-i (H_A + H_B) t \right]$. This non-interacting operator transforms density matrix as follows $R(t) = U(t) \rho(t) U^\dagger(t)$. This transformation does not change the entropy, neither in parts nor in total. Transforming both sides of Eq. (10) into the new basis the interacting time evolution of density matrix will be governed by the following equation

$$\frac{dR}{dt} = i \left[U^\dagger(t) H_{AB}(t) U(t), R(t)\right]$$

(11)

Let us rename the transformed interaction hamiltonian $H_I$ and defining it as $H_I \equiv U^\dagger(t) H_{AB}(t) U(t)$, the solution to the time evolution equation (11) can be written as

$$R(t) = R_0 + R^{(1)}$$

$$R_0 \equiv R(0) \quad \text{non-interacting}$$

$$R^{(1)} \equiv i \int_0^t ds [H_I(s), R(s)] \quad \text{1st order}$$

(12)

This solution can be inserted back in the right side of Eq. (11), which declares its cycle
of internal interaction and we truncate the series at the second order:

\[
\frac{dR(t)}{dt} = \Delta^{(1)} + \Delta^{(2)}
\]

\[
\Delta^{(1)} \equiv i \left[ H_I(t), R_0 \right] \quad \text{1st order}
\]

\[
\Delta^{(2)} \equiv - \int_0^t ds \left[ H_I(t), [H_I(s), R(s)] \right] \quad \text{2nd order}
\]

(13)

In order to find the time evolution of Renyi and von Neumann entropies, we first notice that the unitary transformation made of the noninteracting Hamiltonian can transform any power of the density matrix too, i.e. \((R(t))^M = U(t)(\rho(t))^M U(t)\). Now all we need to do is to generalize the evolution of density matrix to that of nonlinear terms in the density matrix \((R(t))^M\). We follow the terminology of Nazarov in [24] and name each replica \(R(t)\) in the matrix \((R(t))^M\) a ‘world’, thus \((R(t))^M\) is the generalized density matrix of \(M\) worlds.

\[
\frac{d}{dt} (R(t))^M = \left[ \frac{d}{dt} R(t) \right] (R(t))^{M-1} + R(t) \left[ \frac{d}{dt} R(t) \right] (R(t))^{M-2}
\]

\[
+ \cdots + (R(t))^{M-2} \left[ \frac{d}{dt} R(t) \right] R(t) + (R(t))^{M-1} \left[ \frac{d}{dt} R(t) \right]
\]

By substituting the solutions (13) and limiting it to the second order we find the time evolution of \(M\) world density matrix:

\[
\frac{d}{dt} (R(t))^M = \Delta^{(2)} R_0^{M-1} + R_0 \Delta^{(2)} R_0^{M-2} + \cdots + R_0^{M-1} \Delta^{(2)}
\]

\[
+ \Delta^{(1)} \left\{ R^{(1)} R_0^{M-2} + R_0 R^{(1)} R_0^{M-3} + \cdots + R_0^{M-2} R^{(1)} \right\}
\]

\[
+ R_0 \Delta^{(1)} \left\{ R^{(1)} R_0^{M-3} + R_0 R^{(1)} R_0^{M-4} + \cdots + R_0^{M-3} R^{(1)} \right\}
\]

\[
+ R_0^2 \Delta^{(1)} \left\{ R^{(1)} R_0^{M-4} + R_0 R^{(1)} R_0^{M-5} + \cdots + R_0^{M-4} R^{(1)} \right\}
\]

\[
+ \cdots
\]

\[
+ \left\{ R^{(1)} R_0^{M-2} + R_0 R^{(1)} R_0^{M-3} + \cdots + R_0^{M-2} R^{(1)} \right\} \Delta^{(1)}
\]

(14)

This is how the \(M\) world density matrix evolves in time before taking partial traces over its parts. The first line in Eq. (14) denotes the case where 2nd order perturbation takes place in one world while the \(M - 1\) other worlds remain non-interacting. The remaining terms all have one thing in common: there are no 2nd order terms in one world any more. Instead, there are two 1st order interactions each acting in a separate world, combining to a 2nd order perturbation term. These new terms have been recently found in [27].

If you decide to consider higher perturbative orders, say \(k\)-th order with \(k \leq M\), in the expansion there will be terms like \(R_0^{M-1} \Delta^{(k)}\) —with \(k\) interactions taking place in one
replica and noninteracting $M - 1$ replicas—as well as all-first-order configurations such as $R_0^{M-k} (\delta^{(1)})^k$. In the case $k > M$ obviously some of the lowest-order interactions will become excluded from the summations.

Let us show the time evolution pictorially using the following diagrams, in which the evolution of $(R(t))^M$ is shown by $M$ parallel lines, each one denoting the time evolution of one world starting in the past at bottom and arriving at present time on the top. In the following diagrams, we show five time-slices by horizontal dashed lines. Blue dots denote interaction $H_I(t)$ and our diagrams are limited to the 2nd order only. Curly photon-like lines connect the two interactions and represent the correlation function.

The first line of Eq. (14) contains all terms which have two interactions in single world. Such an interaction within the same world are called ‘self-replica interaction’. They can be illustrated pictorially by the following diagrams from left to the right:

![Diagram of self-replica interaction](image)

**FIG. 1:** Diagrammatic representation of terms in first line in Eq. (14).

The following diagram illustrates the typical term $(R_0)^2 \Delta^{(1)} R_0 R_0 (R_0)^{M-4}$ from Eq. (14) and pictorially shows the contribution of two first order interactions at two different worlds that get together and evolve the generalized density matrix of $M$ worlds in the second order.

![Diagram with two first order interactions](image)

**FIG. 2:** A typical diagram with two first order interactions acting on two different worlds.

A typical higher order diagram limited to two-correlation interactions can diagrammatical be shown as below
D. Extended Keldysh diagrams

In all the above diagrams quantum states have been represented as labels on the contours. By definition, we know that density matrix contains both ket and bra states. The second order interactions can, in fact, only take place either between two kets, or between two bras, or between a ket and a bra. This internal degree of freedom makes it necessary to add more details to our diagrams and represent each replica with the well-known Keldysh contour diagrams [28]. The Keldysh technique permits a natural formulation of density matrix dynamics in terms of path integrals, which is a generalization of the Feynman–Vernon formalism.

Considering that the time evolution of a quantum system takes place by the Hamiltonian $H$, ket states evolve as $|\psi(t)\rangle = \exp(iHt)|\psi(0)\rangle$ and bra evolves with the opposite phase: $\langle\psi(t)| = \langle\psi(0)|\exp(iHt)$. Based on this simple observation, in the Keldysh contour bra (ket) states evolve in the opposite (same) direction of time. Therefore in the process of evolving density matrix $R$ from present time to the initial time, diagrammatically one can start the evolution from the present bra state and go down to its past, pass through initial
density matrix, and finally move upward from the initial ket state to the present ket state. If
we are interested in the evolution of the trace of density matrix this diagrammatically takes
place by closing contours at present time which means that we return from the present ket
state back to the present bra state. Of course, this is a bit too awkward to take the trace
of total density matrix because it is identical to 1 at any time, however taking trace from
partial density matrices is meaningful for more than one system.

For two interacting A and B systems, a double-contour is required. We assume separa-
bility of A and B at the initial time:
\[ R(0) = R_A(0) R_B(0) \]
Interaction makes an energy
exchange, which we represent by a cross between the two contours, somewhere between ini-
tial and present times, i.e. \( 0 < t' < t \). In the case we are interested in the evolution of one
of the subsystem, say B, the partial trace over contour A should be taken, which can be
shown by connecting the present bra and ket states of system A, see right diagram in Fig.
[4]. Further details about this Keldysh representation of quantum dynamics can be found
in [13].

In order to evaluate the time evolution of von Neumann and Renyi entropies, we need
extended Keldysh contours on multiple parallel worlds (replicas). For this purpose all, we
consider multiple copies of the Keldysh diagrams with the initial state of each world being
independently assigned. Partial trace will get the contours of different worlds connected.

Let us consider the flow of Renyi entropy at system B, which by definition is
\[ \frac{d}{dt} S^{(B)}_M = - \left( \frac{1}{S^{(B)}_M} \right) d \text{Tr}_B (R_B)^M / dt. \]
Using up to the second order time evolution of partial density
matrix \( R_B(t) = R_B(0) + R_B^{(1)} + R_B^{(2)} + O(3) \) and its flow \( dR_B(t) dt = \Delta_B^{(1)} + \Delta_B^{(2)} + O(3) \),
one can show

\[
\frac{d}{dt} S^{(B)}_M = - \left( \frac{1}{S^{(B)}_M} \right) \text{Tr}_B \left\{ \Delta_B^{(2)} R_B(0)^{M-1} + R_0 \Delta_B^{(2)} R_B(0)^{M-2} + \ldots + R_B(0)^{M-1} \Delta_B^{(2)} \right\}
- \left( \frac{1}{S^{(B)}_M} \right) \text{Tr}_B \left\{ \Delta_B^{(1)} \left[ R_B^{(1)} R_B(0)^{M-2} + \ldots + R_B(0)^{M-2} R_B^{(1)} \right] + R_B(0) \Delta_B^{(1)} \left[ R_B^{(1)} R_B(0)^{M-3} + \ldots + R_B(0)^{M-3} R_B^{(1)} \right] + \ldots \right.
\left. + R_B(0) \Delta_B^{(1)} \left[ R_B^{(1)} R_B(0)^{M-21} + \ldots + R_B(0)^{M-21} R_B^{(1)} \right] \right\} \Delta_B^{(1)}
\]

(15)

The first line contains terms with second-order interactions taking place in only one world.
A typical such diagram for \( M = 3 \) has been shown in Fig. [5].
FIG. 5: A diagram with two energy exchanges in one replica and no interaction in others.

The rest of the lines other than the first line in Eq. (15) denote maximally no more than first-order interaction in a replica. The diagram in Fig. 6 shows a typical such term.

FIG. 6: A diagram with two replicas taking over 1st order interactions and others remain intact.

E. Calculating the diagrams

The main reason why the time evolution of entropy in Eq. (15) has been diagrammatically represented is that due to the multiplicity in time ordering interactions, these extended Keldysh diagrams can help to correctly determine all possible symmetries that may simplify the problem. We need to express all ‘single-worlds’ interactions that carry the highest order perturbation as well as all ‘cross-world’ terms with lower orders of perturbation.

We assume the interaction Hamiltonian does not implicitly depend on time through its parameters, instead, the time dependence is globally assigned in the rotating frame and state evolutions. Explicit formulation of quantum dynamics and keeping track of symmetries between different diagrams have summarized the following rules for diagrams evaluations:

1. With each system having its own contours in each world, label each separate segment of these contours, according to the state of the associated bra or ket of that segment.
The state of the bras and kets change after an interaction, at the initial time and at the final time.

2. Starting from the present time in any world, say the leftmost world, we encompass all contours in their direction. The following operators and changes must be written from left to right as we encompass the contours:

   (a) Every interaction on ket contour will be \((i) H_I(t')\) and on a bra \((-i) H_I(t')\),

   (b) After passing an interaction the states must change on the follow up segment of the contour. The new state remains on the segment of the contour up to either another interaction, or we reach the initial ket and bra states.

   (c) A contour arriving at the initial time will capture the initial density matrix in the interaction picture \(R_0\).

3. In general the result should be integrated over individual interaction times, i.e. \(\int_0^\infty \int_0^\infty dt_1 dt_2\) subject to time order between them. This is much simpler for a small quantum system coupled to a large reservoir kept at a temperature, because the correlation function for absorption and decay of particles only depend on the time difference between two interaction [29]. In this case, the integrations can be simplified to the time difference between two interactions, i.e. \(\int_0^\infty d\tau\).

F. Quantum entropy production

Let us consider two large heat reservoirs A and B, each one containing many degrees of freedom and kept at a temperature, are coupled to one another via only a few numbers of shared degrees of freedom. The Hamiltonian can be written as \(H = H_A + H_B + H_{AB}\) with \(H_{AB}\) representing the coupled degrees of freedom.

In order to compute the flow of a quantity between A and B, that quantity should be conserved in the combined system A+B. As we discussed in the first section of this paper Renyi entropy is a conserved quantity in a closed system, therefore \(d \ln S_M^{(A+B)}/dt = 0\). However, one should notice that there is a difference between the conservation of physical quantities such as energy and the conservation of entropy. Because physical quantities linearly depend on density matrix, when it is conserved for a closed system, internally it
can flow from a subsystem to another one such that its production in a subsystem is exactly equal to the negative sign of its removal from the other subsystem. However, entropy is not so. In fact, due to nonlinear dependence of entropy to density matrix, when it is conserved for a bipartite closed system, it is not equally added and subtracted from the subsystem due to the non-equality in Eq. (8).

Below we will present some example systems with rather general Hamiltonians and using the diagram rules we evaluated all entropy production diagrams.

1. Example 1: Entropy in two-level quantum heat engine

In Ref. [12] we used the extended Keldysh technique and evaluated entropy flow for the simplest quantum heat engine in which a two-level system quantum heat engine is coupled two two heat baths kept at different temperature. After taking all physical and informational correlations into account we found that the exact evaluation in the second order is much different from what physical correlations predict. Here we reproduce the exact result by giving a pedagogical used of diagram evaluation described above.

Let us consider two heat baths that are kept at different temperatures weakly interact by exchanging the quantum energy $\omega_o$. Such a quantum system can be thought of as a two-level system that couples the two heat baths through shared excitations and de-excitation. The Hilbert space of the two-level system contains the states $|0\rangle$ and $|1\rangle$. The free Hamiltonian contains heat bath energy levels $E_{A}^{(A)}\alpha$s and $E_{B}^{(B)}\beta$s and quantum system energies $E_n$ with $n = 0, 1$, i.e. $H_0 = \sum_{\alpha} E_{A}^{(A)}\alpha |\alpha\rangle\langle\alpha| + \sum_{\beta} E_{B}^{(B)}\beta |\beta\rangle\langle\beta| + \sum_{n=0,1} E_n|n\rangle\langle n|.$

![FIG. 7: A two level system quantum hat bath.](image)

We assume the so-called ‘transversal’ interaction is taken into account between A/B and the two-level system q. This means that they interact via exchanging the quantum of energy $\omega_o$. Of course, we can generalize the discussion to longitudinal interactions in which no energy is exchanged, however since such interactions are not of the immediate interest for heat transfer in quantum heat devices we ignore them.
This interaction we assume for the heat bath has the following general form: \( H_{\text{int}} = \sum_{n,m=0,1} |n\rangle \langle m| \left[ \hat{X}^{(A)}_{nm}(\omega_0) + \hat{X}^{(B)}_{nm}(\omega_0) \right] \) subject to \( E_m \neq E_n \) and \( \hat{X}_{nm} \) representing energy absorption/decay in heat baths. The summation in \( H_{\text{int}} \) can be generalized to arbitrary number of heat bath interacting at shared degrees of freedom.

Moreover, the entire system including the two levels system is externally driven. The classical heat baths are naturally not influenced effectively by the driving field, however, the driving can pump in and out energy to the two-level system by the following Hamiltonian \( H_{dr} = \Omega \cos(\omega_{dr} t) (|0\rangle \langle 1| + |1\rangle \langle 0|) \).

For simplicity we take the Hamiltonian into the rotating frame that makes excitation/relaxation with the frequency \( \omega_{dr} \). In this frame the excited and ground states are transformed as follows: \( |1\rangle_R = \exp(i\omega_{dr} t) |1\rangle \) and \( |0\rangle_R = |0\rangle \). This will introduce the unitary transformation \( U_R = \exp(i\omega_{dr} t) \langle 1| \rangle |1\rangle \) on the Hamiltonian, i.e. \( H_R = U_R H U_R^\dagger + i (\partial U_R/\partial t) U_R^\dagger \). A few lines of simplification will result in the following Hamiltonian in the rotating frame:

\[
\begin{align*}
H_R &\equiv H_0 + V_{qA} + V_{qB} + V_{AB} + V_{dr}, \\
H_0 &= E_0 |0\rangle \langle 0| + (E_1 - \omega_{dr}) |1\rangle \langle 1| + \sum_\alpha E^{(A)}_\alpha |\alpha\rangle \langle \alpha| + \sum_\alpha E^{(B)}_\alpha |\alpha\rangle \langle \alpha|, \\
V_{qA} &= |0\rangle \langle 1| \hat{X}^{(A)}_{01}(t) e^{i\omega_{dr} t} + |1\rangle \langle 0| \hat{X}^{(A)}_{10}(t) e^{-i\omega_{dr} t} = \sum_{n,m=0,1(n\neq m)} |n\rangle \langle m| \hat{X}^{(A)}_{nm}(t) e^{i\omega_{dr} t} \eta_{nm}, \\
V_{qB} &= |0\rangle \langle 1| \hat{X}^{(B)}_{01}(t) e^{i\omega_{dr} t} + |1\rangle \langle 0| \hat{X}^{(B)}_{10}(t) e^{-i\omega_{dr} t} = \sum_{n,m=0,1(n\neq m)} |n\rangle \langle m| \hat{X}^{(B)}_{nm}(t) e^{i\omega_{dr} t} \eta_{nm}, \\
V_{AB} &= 0, \quad V_{dr} = \frac{\Omega}{2} (|0\rangle \langle 1| + |1\rangle \langle 0|),
\end{align*}
\]

with \( \eta_{01} = -\eta_{10} = 1 \) and \( \eta_{00} = \eta_{11} = 0 \). Given the fact that there is no direct exchange of energy between A and B, the density matrix can be represented as \( R = R_{qA} \otimes R_B + R_A \otimes R_{qB} \) in interaction picture, thus determining entropy flow in the heat bath B will depends on the quantum system and the heat bath B, although indirectly the heat bath A will influence the quantum system. In general \( d(R_B)^M/dt = Tr_q \left\{ d(R_{qB})^M/dt \right\} \). Let us recall that this quantity determines the flow of von Neumann entropy and using Eq. \( [9] \) it can be simplified to \( dS^{(B)}/dt = \lim_{M \to 1} d \left( Tr_B Tr_q \left\{ (dR_{qB}/dt) (R_{qB})^{M-1} + \cdots + (R_{qB})^{M-1} (dR_{qB}/dt) \right\} \right)/dM \). Each term in the sum is evaluated in the interaction picture using \( d/dt = (-i) [V, R] \). One can show that the external driving will cause density matrix to evolve as \( dR_{nm}/dt = \)
(i\Omega/2) (R_{n0}\delta_{m1} + R_{n1}\delta_{m0} - \delta_{n0}R_{1m} - \delta_{n1}R_{0m}).

The interaction Hamiltonian evolves quantum states and below we evaluate the entropy flow in the \( M = 3 \) example to the second order perturbation theory. As discussed above there are in general two types of diagrams in the second order: 1) ‘self-interacting’ diagrams with second order interaction taking place in one replica, and 2) cross-world-interacting terms in which two different replicas take on each 1st order interaction. The self-interacting diagrams for two level system are listed in Fig. (8).

**FIG. 8:** Self-interacting diagrams for interaction between a quantum system and a heat bath.

These diagrams correspond to the following flows, respectively.

\[
(a) : \quad \left( -1 \right) \int_{0}^{\infty} d\tau \text{Tr}_{B} \left\{ \sum_{m,k=0,1} (m \neq k) \hat{X}_{mk}^{(B)}(t')\hat{X}_{km}^{(B)}(t' - \tau) \hat{R}_{B}\hat{R}_{mm}e^{-i\omega_{dr}\eta_{km}\tau}e^{i\omega_{dr}(\eta_{mk}+\eta_{km})t'}\hat{R}_{B}^{2} \right\} \\
(b) : \quad \left( +1 \right) \int_{0}^{\infty} d\tau \text{Tr}_{B} \left\{ \sum_{m,k=0,1} (m \neq k) \hat{X}_{mk}^{(B)}(t')\hat{R}_{B}\hat{R}_{kk}\hat{X}_{km}^{(B)}(t' - \tau) e^{-i\omega_{dr}\eta_{mk}\tau}e^{i\omega_{dr}(\eta_{mk}+\eta_{km})t'}\hat{R}_{B}^{2} \right\} \\
(c) : \quad \left( +1 \right) \int_{0}^{\infty} d\tau \text{Tr}_{B} \left\{ \sum_{m,k=0,1} (m \neq k) \hat{R}_{B}\hat{R}_{mm}\hat{X}_{mk}^{(B)}(t')\hat{X}_{km}^{(B)}(t' - \tau) e^{-i\omega_{dr}\eta_{km}\tau}e^{i\omega_{dr}(\eta_{mk}+\eta_{km})t'}\hat{R}_{B}^{2} \right\} \\
(d) : \quad \left( -1 \right) \int_{0}^{\infty} d\tau \text{Tr}_{B} \left\{ \sum_{m,k=0,1} (m \neq k) \hat{R}_{B}\hat{R}_{mm}\hat{X}_{mk}^{(B)}(t' - \tau)\hat{X}_{km}^{(B)}(t') e^{-i\omega_{dr}\eta_{mk}\tau}e^{i\omega_{dr}(\eta_{mk}+\eta_{km})t'}\hat{R}_{B}^{2} \right\} \\
\text{Tr}_{B} \left( \hat{R}_{B}^{3} \right)
\]

In all these terms there is a time dependent factor \( e^{i\omega_{dr}(\eta_{mk}+\eta_{km})t'} \) which is identical to 1 because we always have the following relation valid: \( \eta_{mk} = -\eta_{km} \). We assume that heat bath are large and at equilibrium, therefore the correlation function is the same at all times \( t' \) and only depends on the time difference \( \tau \) between the creation and annihilation of a photon. In the heat bath B, the equilibrium correlation is defined as \( S_{mn,pq}^{(B)}(\tau) \equiv \)
Tr\(B \left( \hat{X}_{mn}^{(B)} (0) \hat{X}_{pq}^{(B)} (\tau) R_B \right) \). The Fourier transformation the correlation defines the following frequency-dependent correlation: \( S_{mn,pq}^{(B)} (\omega) = \int_{-\infty}^{\infty} d\tau Tr_B \left( \hat{X}_{mn}^{(B)} (0) \hat{X}_{pq}^{(B)} (\tau) R_B \right) \exp (i\omega\tau) \). Therefore in the case of \( M = 1 \) (i.e. the absence of the last term \( R_B^2 \)) the diagrams can be rewritten in terms of \( S_{mn,pq}^{(B)} (\omega) \). For example the diagram (a) for the case of \( M = 1 \) can be simplified to \(-\sum_{m,k=0,1(m\neq k)} \hat{R}_{mm} \int_{0}^{\infty} d\tau Tr_B \left\{ \hat{X}_{mk}^{(B)} (0) \hat{\chi}_{km}^{(B)} (\tau) \hat{R}_B e^{-i\omega_{dr,\eta_{km}\tau}} \right\} \) in which the integral is a half of domain in Fourier transformation and therefore it can be proved to simplify to \(-\sum_{m,k=0,1(m\neq k)} \hat{R}_{mm} \left( 1/2 \right) S_{mk,km}^{(B)} (\omega_{dr,\eta_{mk}}) + i\Pi_{mk,km} (\omega_{dr,\eta_{mk}}) \) with \( \Pi_{mn,pq} \equiv (i/2\pi) \int d\nu S_{mn,pq}^{(B)} (\nu) / (\omega - \nu) \). What is left to be determined is the frequency-dependent correlation function \( S_{mn,pq}^{(B)} (\omega) \), which turns out to become completely characterized by the set of reduced frequency-dependent susceptibilities defined as \( \hat{\chi}_{mn,pq}^{(B)} (\omega) \equiv \left( \chi_{mn,pq}^{(B)} (\omega) - \chi_{pq,mn}^{(B)} (-\omega) \right) / i \) with the dynamical susceptibility in the environment being \( \chi_{mn,pq}^{(B)} (\omega) \equiv (-i) \int_{-\infty}^{0} Tr_B \left\{ \left[ \hat{X}_{mn}^{(B)} (\tau), \hat{X}_{pq}^{(B)} (0) \right] R_B \right\} \exp (-i\omega\tau) \). The fluctuation-dissipation theorem provides a link between the equilibrium correlation and the reduced dynamical susceptibility in the classical thermal bath \( B \) at temperature \( T_B \). This relation is usually called Kubo-Martin-Schwinger (KMS) relation: \( S_{mn,pq}^{(B)} (\omega) = n_B (\omega/T_B) \chi_{mn,pq}^{(B)} (\omega) \) with \( n_B (\omega/T_B) = 1 / (\exp (\omega T_B) - 1) \) being the Bose distribution and \( k_B \) the Boltzmann constant.

**Generalized KMS**

In the presence of replicas, similarly the generalized correlations are defined. For the case there are \( M \) replica in total and between creation and annihilation there are \( N \) replica with \( 0 \leq N \leq M \), the generalized correlation function is defined as

\[
S_{mn,pq}^{N,M} (B) (\tau) \equiv \frac{Tr_B \left( \hat{X}_{mn}^{(B)} (0) \hat{R}_{B}^N \hat{X}_{pq}^{(B)} (\tau) \hat{R}_{B}^{M-N} \right)}{Tr_B \left( \hat{R}_{B}^M \right)}
\]

Similarly one can show that

\[
\int_{0}^{\infty} d\tau Tr_B \left\{ \hat{X}_{mn}^{(B)} (0) \hat{R}_{B}^N \hat{X}_{pq}^{(B)} (\tau) \hat{R}_{B}^{M-N} e^{i\omega\tau} \right\} = \frac{S_{mn,pq}^{N,M} (B) (\omega)}{2} + i\Pi_{mn,pq}^{N,M} (B) (\omega)
\]

with the definition \( \Pi_{mn,pq}^{N,M} (B) (\omega) \equiv (i/2\pi) \int d\nu S_{mn,pq}^{N,M} (B) (\nu) / (\omega - \nu) \). One can also check from definitions that for any heat bath the following identities: \( S_{mn,pq}^{N,M} (-\omega) = S_{pq,mn}^{M-N,M} (\omega) \), \( \Pi_{mn,pq}^{N,M} (-\omega) = -\Pi_{pq,mn}^{M-N,M} (\omega) \), and \( \hat{\chi}_{mn,pq}^{(B)} (-\omega) = -\hat{\chi}_{pq,mn}^{(B)} (\omega) \).

Fourier transformation of this generalized correlation will defined the frequency-dependent generalized correlation and following the same mathematics as above, one can...
show at equilibrium thermal bath of temperature $T_B$ all correlation functions can be determined through a generalized KMS relation,

$$S^{N,M}_{mn,pq}(\omega) = n_B \left( \frac{\omega}{T_B} \right) \tilde{\chi}^{(B)}_{mn,pq}(\omega) e^{N \frac{\omega}{k_B T_B}}$$

(19)

Further details can be found in [27].

Using these definitions as well as Eq. (19), the sum of diagrams (a)-(d) in Fig. (8) can be further simplified to

$$\sum_{m,k=0,1(m\neq k)} \hat{R}_{mm} \left\{ - \left( \frac{1}{2} S^{3,3}_{km,mk}(\omega_{dr} \eta_{mk}) + i \Pi^{3,3}_{km,mk}(\omega_{dr} \eta_{mk}) \right) \right. - \left( \frac{1}{2} S^{0,3}_{mk,km}(\omega_{dr} \eta_{km}) + i \Pi^{0,3}_{mk,km}(\omega_{dr} \eta_{km}) \right) \right\}$$

$$\sum_{m,k=0,1(m\neq k)} \hat{R}_{kk} \left\{ + \left( \frac{1}{2} S^{1,3}_{mk,km}(\omega_{dr} \eta_{km}) + i \Pi^{1,3}_{mk,km}(\omega_{dr} \eta_{km}) \right) \right. + \left. \left( \frac{1}{2} S^{2,3}_{km,mk}(\omega_{dr} \eta_{mk}) + i \Pi^{2,3}_{km,mk}(\omega_{dr} \eta_{mk}) \right) \right\}$$

$$- \sum_{m,k=0,1(m\neq k)} S^{0,3}_{mk,km}(\omega_{dr} \eta_{km}) \hat{R}_{mm} + S^{1,3}_{mk,km}(\omega_{dr} \eta_{km}) \hat{R}_{kk}$$

(20)

In total there are $M$ number of terms similar to last line in Eq. (20) associated to similar diagrams at $M$ worlds. It is important to notice that these self-replica correlated terms are determined in fact only by physical correlations and they make already known results for the flow of von Neumann entropy in heat bath [30]. To see this more in more details, one can expand the summation and use the KMS relation and its generalized version in Eq. (19). After generalizing the result for $M$ replica, taking derivative with respect to $M$ and analytically continue the result to $M \rightarrow 1$ the incoherent part of flow in von Neumann entropy is

$$\left. \frac{dS^{(B)}}{dt} \right|_{\text{incoherent}} = - \frac{1}{T_B} \left( \Gamma^{(B)}_{\uparrow} p_0 - \Gamma^{(B)}_{\downarrow} p_1 \right)$$

(21)

with $\Gamma^{(B)}_{\uparrow} \equiv \tilde{\chi}(n_B (\omega_{dr}/T_B) + 1)$ and $\Gamma^{(B)}_{\downarrow} \equiv \tilde{\chi} n_B (\omega_{dr}/T_B)$, $\tilde{\chi} \equiv \tilde{\chi}_{10,01}$, and $p_n \equiv R_{nn}$. This is only self-interacting replicas, which is incomplete as ignores the following diagrams.
FIG. 9: Cross-replica interacting diagrams for a quantum system and a heat bath.

The new diagrams are the cross-world interactions. As discussed previously, cross-world diagrams cannot transfer physical quantities as they reply on the fact that entropy depends nonlinearly on density matrix and therefore it is not an a physical observable quantity. Some of these types of diagrams are shown in Fig. 9; for the case that one interaction takes place in the leftmost replica and the second interaction in the middle replica, thus leaving
the third replica intact.

\[
(e) : - \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t') \hat{R}_B \hat{R}_{mk} \hat{X}_{nl}^{(B)}(t' - \tau) \hat{R}_B \hat{R}_{nl} e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

\[
(f) : - \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t - \tau) \hat{R}_B \hat{R}_{mk} \hat{R}_B \hat{R}_{ln} \hat{X}_{ln}^{(B)}(t' - \tau) \hat{R}_B \hat{R}_{nl} e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

\[
(g) : \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t') \hat{R}_B \hat{R}_{mk} \hat{R}_B \hat{R}_{ln} \hat{X}_{ln}^{(B)}(t' - \tau) e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

\[
(h) : \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t' - \tau) \hat{R}_B \hat{R}_{mk} \hat{R}_B \hat{R}_{ln} \hat{X}_{ln}^{(B)}(t') e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

\[
(i) : \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t' - \tau) \hat{R}_B \hat{R}_{mk} \hat{R}_B \hat{R}_{ln} \hat{X}_{ln}^{(B)}(t') e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

\[
(j) : \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t' - \tau) \hat{R}_B \hat{R}_{mk} \hat{R}_B \hat{R}_{ln} \hat{X}_{ln}^{(B)}(t') e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

\[
(k) : - \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t' - \tau) \hat{R}_B \hat{R}_{mk} \hat{R}_B \hat{R}_{ln} \hat{X}_{ln}^{(B)}(t') e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

\[
(l) : - \int_0^\infty d\tau B \left\{ \sum_{m,n,k,l} \hat{X}_{mk}^{(B)}(t' - \tau) \hat{R}_B \hat{R}_{mk} \hat{R}_B \hat{R}_{ln} \hat{X}_{ln}^{(B)}(t') e^{-i\omega dt \eta n \tau} \delta_{Enl,Ekm} \hat{R}_B \right\} / \text{Tr}_B \left( \hat{R}_B^3 \right),
\]

where we used the following identity \( e^{i\omega dt (\eta n \tau + \eta q) t'} = \delta_{Enl,Eqp} \).

One can evaluate all diagrams associated to a general number of replica using above example. After careful analyzing all diagrams and proper simplifications —see [27]— the flow of Renyi entropy \( dS_M / dt \) in the heat bath B can be found, and consequently the so-called coherent part of entanglement (von Neumann) entropy can be found as follows:

\[
\frac{dS^{(B)}}{dt} \bigg|_{\text{coherent}} = - \frac{\Gamma^{(B)} - \hat{\Gamma}^{(B)}}{T_B} |R_{01}|^2
\]  

(22)

This is the new part of the entropy flow that comes from the generalized KMS correlations. We call this part the coherent part because it is nonzero for degenerate states or equivalently a two-level system driven by their detuning frequency.

Therefore the entanglement entropy flow is naturally separated onto two parts and there-
fore it is equal to the sum between the two parts:

$$\frac{dS^{(B)}}{dt} = \left. \frac{dS^{(B)}}{dt} \right|_{\text{incoherent}} + \left. \frac{dS^{(B)}}{dt} \right|_{\text{coherent}}$$

$$= -\frac{1}{T_B} (\Gamma_\uparrow p_0 - \Gamma_\downarrow p_1) - \frac{\Gamma_\downarrow - \Gamma_\uparrow}{T_B} |R_{01}|^2$$  \hspace{1cm} (23)$$

in which the first term in second line is what in textbook has been so far mistakenly taken as total entropy flow.

As we see in Eq. (23) is not directly related to energy flow —which here corresponds to the incoherent part. Instead of a finite flow that depends on the quantum coherence $(R_{01})^2$.

Considering that the two level system with energy difference $\omega_o$ is driven at the same frequency, i.e. $H = \Omega \cos(\omega_o t)$ and weakly coupled to two heat reservoirs at temperatures $T_A$ and $T_B$. From Eq. (1) of Ref. [27] one can find the following time evolution equations for density matrix and setting them to zero determines stationary solutions:

$$\frac{dR_{11}}{dt} = -\frac{i\Omega}{2} (R_{01} - R_{10}) - \Gamma_\downarrow R_{11} + \Gamma_\uparrow R_{00} = 0,$$

$$\frac{dR_{01}}{dt} = -\frac{i\Omega}{2} (R_{11} - R_{00}) - \frac{1}{2} (\Gamma_\downarrow + \Gamma_\uparrow) R_{01} = 0, \quad R_{00} + R_{11} = 1,$$

which finds the stationary ground state population $R_{00} = (\Gamma_\downarrow + \Gamma_\uparrow + \Omega^2)/((\Gamma_\downarrow + \Gamma_\uparrow)^2 + 2\Omega^2)$

and the stationary off-diagonal density matrix $R_{10} = -i\Omega(1 - 2R_{00})/(\Gamma_\downarrow + \Gamma_\uparrow)$, with $\Gamma_\downarrow \equiv \Gamma^{(A)}_\downarrow + \Gamma^{(B)}_\downarrow$ and $\Gamma_\uparrow \equiv \Gamma^{(A)}_\uparrow + \Gamma^{(B)}_\uparrow$. By considering that B is a probe environment with zero temperature, substituting all solutions in Eq. (22) the incoherent and coherent parts of entropy flow in the probe environment has been plotted in Fig. (10) for different driving amplitudes and $\omega_0/T_A$. 

FIG. 10: Entropy production in a probe bath that is kept at zero temperature and is coupled to a two level system depicted in Fig. (7). The entropy is the sum of two parts: the incoherent and the coherent parts. (a) The incoherent part of entropy is nothing new and can be determined by standard correlations. It is positive by the convention that entropy enters from a higher temperature bath (via the two level system); (b) The coherent part of entropy is previously unknown part as it comes from the informational correlations between different replicas. This part depends quadratically on the off diagonal density. Quite nontrivially this part of entropy has negative and summing it with the incoherent part will result in positive flow yet with much smaller magnitude for entropy at small driving amplitudes.

2. Example 2: Entropy in quantum 4-level photovoltaic cell

Scovil and Schulz-DuBois first introduced a quantum heat engine model (SSDB heat engine) in [35], where a single three-level atom consisting of a ground and two excited states are in contact with two heat baths. A large enough temperature difference can create population inversion between the two excited states and coherent light output. One hot photon is absorbed, one cold photon is emitted, therefore a laser photon is produced. The SSDB heat engine model gives a clear demonstration for the quantum thermodynamics. But we notice that some detailed properties of this lasing heat engine, e.g., the threshold behaviour and the statistics of the output light, is still not well studied. There are a number of modifications since then into this model, such as light-harvesting biocells, photovoltaic cells, etc.

Recently in Ref. [39] one of us studied entropy flow using the replica trick for a 4 level
photovoltaic cell with two degenerate ground states and two excited states, see Fig. 11. This heat engine was first proposed by Schully in [36] and recently studied in many further details by Schully and others [37, 38].

FIG. 11: A four level doubly degenerate photovoltaic cell.

After finding all extended Keldysh diagrams for an arbitrary $M$ Renyi degree, evaluating all self-interacting and cross interacting diagrams and simplifying, the von Neumann entropy flow in heat bath $A$ bath becomes [39]:

$$\frac{dS}{dt} \bigg|_A = \frac{1}{T_A} \left\{ \gamma p_4 - \omega_A \bar{x}_{42} \bar{n} \left( \frac{\omega_A}{T_A} \right) p_2 - \omega_A \bar{x}_{41} \bar{n} \left( \frac{\omega_A}{T_A} \right) p_1 - \bar{x}_{14,42} \left[ \omega_A \bar{n} \left( \frac{\omega_A}{T_A} \right) + \omega_A \bar{n} \left( \frac{\omega_A}{T_A} \right) \right] \text{Re} R_{12} - \frac{1}{2} \sum_{i=1,2} \omega_A \bar{x}_{14,42} |R_{12}|^2 \right\}$$

(24)

in which the first two lines can be found using physical correlations, however the last line which is essentially playing important role in the entropy evaluation can be obtained only through informational correlations. Here the state probabilities are $p_x \equiv R_{xx}$ for $x$ being 1, 2, 3, 4 depend on the characteristics of all heat baths, the dynamical response function is $\bar{x}_{ai} \equiv \bar{x}_{i\alpha,\alpha i}(\omega_{ia})$ with $i = 1, 2$ and $\alpha = 3, 4$, and $\bar{x}_{1\alpha,\alpha 2} = \sqrt{\bar{x}_{1\alpha} \bar{x}_{\alpha 2}}$. Moreover $\gamma \equiv \sum_{i=1,2} \left[ \bar{n} \left( \omega_A/T_A \right) + 1 \right] \omega_A \bar{x}_{3i}$.

In order to evaluate the stationary value of entropy flow in this heat bath, we must solve the quantum master equation for density matrix time evolution. This can be found in Ref. [39]. The solution is such that the coupling between environment and quantum system introduces decoherence in quantum states. Energy exchange between heat bath and a quantum system introduces a limited coherence time, namely $\tau_1$, for quantum state probabilities. Similarly, the phase of density matrix can fluctuate and depend on how noisy is the environment the off-diagonal elements of density matrix takes on a dephasing time, namely $\tau_2$ time. These two coherence times affects all elements of density matrix. From
solving the quantum master equation one can see that the only stationary solution of off-diagonal density matrix is $R_{12}$ (and its complex conjugate), whose imaginary part takes on an exponential decay due to dephasing: $\text{Im}R_{12} \sim \exp(t/\tau_2)$.

One can substitute the stationary solution of density matrix in Eq. (24) and depending on what is the dephasing time the flow of entropy in heat bath changes —see Fig. (2a,b) in [39]. In fact, increasing the dephasing time will improve the contribution of coherent flow of entropy, i.e. information correlations. This will reduce total entropy flow in the heat bath, which will equivalently increase the output power in this photovoltaic cell.

3. Example 3: Entropy in quantum resonator/cavity heat engine

Using a rather different technique —i.e. the correspondence between entropy and statistics of energy transfer that we discuss in next section— in [12, 13] we calculated entropy production for a resonator/cavity coupled two different environments that are kept at different temperatures. One of the two baths is probe environment at zero temperature for which we calculate the flow of entropy. One of the key aspect that makes resonator a key element in circuit design is the high-quality factor of a resonator and also how its Kerr interaction with qubits. Known how entropy flows as the result of interaction between resonator/cavity and other parts of the circuit can provide important information about the possibility of leakage or dephasing in the system and ultimately gives rise to modification in quantum circuits [4]. Another important aspect is that cavity/resonators are important to understand the nature of non-equilibrium quasiparticle poisoning in quantum circuits [40], so that tunnelling a quasiparticle can mark a jump in the entropy flow [41]. Given that entropy flow can be measured by the full counting statistics of energy transfer, see the next section, makes it important to keep track of entropy flow in a resonator.

![FIG. 12: A quantum cavity heat engine.](image)
Again we use the standard technique that we described above. Let us consider a single harmonic oscillator of frequency $\omega_0$ with Hamiltonian $\hat{H} = \omega_0(\hat{a}^\dagger \hat{a} + 1/2)$ is coupled to a number of environments at different temperatures with different coupling strength. We concentrate on a probe environment which is weakly coupled to the oscillator. In addition, the oscillator is driven by an external force at frequency $\Omega$. We calculate the Renyi and consequently von Neumann entropy flow of the probe environment. The coupling Hamiltonian between the harmonic oscillator and the probe reservoir is $\hat{H}(t) = \hat{X}(t)\hat{a}^\dagger(t) + h.c.$ with $\hat{X}$ being the probe reservoir operator. The Fourier transform of the correlator is:

$$S_{mn}(\omega) = \int \exp(-i\omega t)S_{mn}(t)d\omega/2\pi.$$ Due to the conservation of energy, the energy exchange occurs either with quantum $\Omega$ or with quantum $\omega_0$.

We note that the time dependence of the average of two operators can be written as $\langle \hat{a}^\dagger(t)\hat{a}(t') \rangle = \langle \langle \hat{a}^\dagger \hat{a} \rangle \rangle e^{i\omega_0(t-t')} + \langle \hat{a}(t) \rangle \langle \hat{a}^\dagger(t') \rangle$, where the $\langle \hat{a}(t) \rangle$ is due to the driving force and therefore oscillates at frequency $\Omega$: $\langle \hat{a}(t) \rangle = \langle a \rangle_+ \exp(i\Omega t) + \langle a \rangle_- \exp(-i\Omega t)$. This corresponds to the fact that the oscillator can oscillates both at its own frequency and at the frequency of external force.

Obtaining the entropy flows from the extended Keldysh correlators are straightforward. The generalized KMS relation in Eq. (19) helps to describe the correlators in the thermal bath $B$ in terms of its dynamical susceptibility. Result can be summarized as follows:

$$\frac{dS_{BM}}{dt} = \frac{M\bar{n}(M\omega_0/T_B)}{\bar{n}((M-1)\omega_0/T_B)} \left\{ \langle \langle \hat{a}^\dagger \hat{a} \rangle \rangle e^{\omega_0/T_B} - \langle \langle aa^\dagger \rangle \rangle \right\}.$$ Here we defined $T_{\text{resonator}}$ to be the effective temperature of the harmonic oscillator $\langle \langle aa^\dagger \rangle \rangle = \bar{n}(\omega_0/T_{\text{resonator}}) + 1$ and $\langle \langle \hat{a}^\dagger \hat{a} \rangle \rangle = \bar{n}(\omega_0/T_{\text{resonator}})$. Taking derivative with respect to $M$ and analytically continuing the result to the limit of $M \to 1$ will determine the thermodynamic entropy flow:

$$\frac{dS_{M}}{dt} = \frac{1}{T_B} \left\{ \bar{n} (\omega_0/T_{\text{resonator}}) - \bar{n} (\omega_0/T_B) \right\} (25)$$

The entropy flow changes sign at the onset temperature $T_{\text{resonator}} = T_B$. Moreover one should notice that after exact evaluation the incoherent part of entropy flow contains some terms proportional to $\langle a \rangle$ and $\langle a^\dagger \rangle$. These terms oscillates with the external drive and are nonzero, however they are all cancelled out by the coherent part of entropy flow such that the overall flow will only depends on temperatures, and not driving force. Therefore the entropy flow is robust in the sense that it only depends on the probe and harmonic oscillator temperatures and completely insensitive to the external driving force.
An insensitive entropy flow in external driving force is an interesting quantity that can put coherent entropy flow into an experiment: In the absence of cross-replica correlators the thermodynamic entropy of a probe environment coupled to a thermal bath via a resonator will dramatically depend on the amplitude of external driving. If no such a dependence of driving amplitude is found it indicates the absence they are in fact eliminated by quantum coherence!

IV. LINKING INFORMATION TO PHYSICS; A NEW CORRESPONDENCE

As discussed above, the Renyi entropies in quantum physics are considered unphysical, i.e. non-observable quantities, due to their nonlinear dependence on the density matrix. Such quantities cannot be determined from immediate measurements; instead, their quantification seems to be equivalent to determining the density matrix. This requires reinitialization of the density matrix between many successive measurements. Therefore, the Renyi entropy flows between the systems are conserved measures of nonphysical quantities. An interesting and nontrivial question is as follows: Is there any relation between the Renyi entropy flows and the physical flows?

An idea of such a relation was first put forward by Levitov and Klich in [19], where they proposed that entanglement entropy flow in electronic transport can be quantified from the measurement of the full counting statistics (FCS) of charge transfers [18, 31, 32, 32]. The validity of this relation is restricted to zero temperature and obviously to the systems where interaction occurs by means of charge transfer. Recently we presented a relation that is similar in spirit [12]. We derived a correspondence for coherent and incoherent second-order diagrams in general time-dependent situation. This relation gives an exact correspondence between the informational the measure of Renyi entropy flows and physical observables, namely, the full counting statistics of energy transfers [34].

We consider reservoir B and quantum system q. We assume that B is infinitely large and is kept in thermal equilibrium at a temperature $T_B$. System q is arbitrary as it may carry several degrees of freedom as well as infinitely many of those. It does not have to be in thermal equilibrium and in general, is subject to time-dependent forces. It is convenient to assume that these forces are periodic with a period of $\tau$; However, the period does not explicitly enter the formulation of our result, which is also valid for aperiodic forces. The only
requirement is that the flows of physical quantities have stationary limits. The stationary limits are determined after averaging instant flows over a period — for aperiodic forces by averaging over a sufficiently long time interval. In the case of energetic interactions, energy transfer is statistical. The statistics can be described by a generating function, the so-called full counting statistics (FCS) generating function the so-called ‘FCS Keldysh actions’.

Recently in Ref. [12] we proved that the flow of entanglement (von Neumann), as well as Renyi entropy between two heat baths via a quantum system, is exactly equivalent to the difference between two FCS Keldysh actions of incoherent and coherent energy transfers. In the limit of long $\tau$ and for a typical reservoir $B$ with temperature $T_B$ the incoherent and coherent FCS Keldysh actions are $f_i(\xi, T_B)$ and $f_c(\xi, T_B)$, with $\xi$ being the counting field of energy transfer. These generating functions can be determined using Keldysh diagrams, see [13]. After their evaluations one finds the statistical $m$-th cumulant function $C_m$ by taking derivative of the generating function in the limit of zero counting function, i.e. $C_m = \lim_{\xi \to 0} \partial^m f / \partial \xi^m$.

In fact, any physical quantity should depend on the cumulants and consequently to zero counting field, however, informational measures are exceptional. Detailed analysis shows that the flow of Renyi entropy of degree $M$ in the reservoir $B$ at equilibrium temperature $T_B$ is exactly and unexpectedly the following: $dS_{M}(T_B)/dt = M \left[ f_i(\xi^*, T_B/M) - f_c(\xi^*, T/M) \right]$ with $\xi^* \equiv i(M - 1)/T_B$. Notice that in this correspondence the temperature in the left side is $T_B$ while it is $T_B/M$ on the right side. Also, it is important to notice the entropy is evaluated by using the generating function of full counting statistics at nonzero counting field $\xi^*$. This relation is valid in the weak-coupling limit, where the interaction between the systems can be treated perturbatively. There is an obvious classical limit in the case where the quantum system $B$ is considered classical and in that case, the coherent flow vanishes, otherwise, coherent flow is of the same order as the incoherent one.

V. DISCUSSION

Currently ‘time’ does not play any essential role in quantum information theory. In this sense quantum theory is underdeveloped similar to how quantum physics without Schrödinger equation. In this review article, we discuss a fascinating extension of the Keldysh formalism that consistently copes with the problem of time at least for one of the central
quantities in quantum information theory, entropy. We characterised the flows of conserved entropies (both Renyi and von Neumann) and illustrate them diagrammatically to introduce new correlators that so far have been absent in the literature.

Given that entropies are not accessible indirect measurement because they are nonlinear functions of the density matrix, one can think of directly measuring density matrix for a probe environment and determining the reduced density matrix of an infinite system. This requires the complete and precise reinitialization of the initial density matrix. In this review, we showed that entropy as well as its flow as functions of density matrix can be evaluated by substituting density matrix; however, in the light of the new correspondence, we claim that entropy flow in a probe environment can be directly measured in the lab using the statistical cumulants of transferred energy in experimental data. This can be done equally well for imaginary and real values of the characteristic parameter. The measurement procedures may be complex, yet feasible and physical. The correspondence can have many other advantages; for instance, a complete understanding of entropy flows may help to identify the sources of fidelity loss in quantum communications and methods to prevent or control them.

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[42] Let us clarify that what we study in this paper is the flow of thermodynamic Renyi and von Neumann entropies between the heat baths and quantum system $q$, therefore other entropies are beyond the scope of this paper.
[43] Some authors prefer to multiply the right side of Eq. (2) by the constant $1/(1 - M)$ and call this rescaled quantity the Renyi entropy. For the purpose of this paper, which is finding the flow of Renyi entropy, one needs to take the time derivative of log function. This makes the flow of Renyi entropy insensitive to any constant prefactor. Therefore we prefer not to confuse our readers by including the prefactor.
[44] It might be useful to further comment that the Renyi entropy without the logarithm has many names such as Tsallis entropy or power entropy etc. However in what we call the Renyi entropy the presence of logarithm is necessary because otherwise one can see $\lim_{M \to 1} Tr p^M = 0$, which cannot be a true measure of information at this important limit.