Towards fully quantum second laws of thermodynamics: limitations on the evolution of quantum coherences

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The second law of thermodynamics places a limitation on what states a system can evolve into. For closed systems, it says that a state can be transformed into another state, only if the course grained entropy increases. For systems in contact with a heat bath, it can be combined with the law of energy conservation, and it says that a system can only evolve into another if the free energy goes down. Here, the free energy is written in terms of the fine-grained entropy. Recently, it’s been shown that there are actually many second laws, and that it is only for large macroscopic systems that they all become equivalent to the ordinary one. These additional second laws also hold for quantum systems, and are in fact, often more relevant in this regime. They place a restriction on how the probabilities of energy levels can evolve. Here, we consider additional restrictions on how the coherences between energy levels can evolve. Coherences can only go down, and we provide a set of restrictions which limit the extent to which they can be maintained. We find that coherences over energy levels must decay at rates that are suitably adapted to the transition rates between energy levels. We show that the limitations are matched in the case of single qubit, in which case we obtain the full characterization of state-to-state transformations. For higher dimensions, we conjecture more severe constraints exist. The results are obtained in the paradigm of Thermal Operations, and we introduce a new class of thermodynamical operations which allow for greater manipulation of coherences and study its power with respect to Thermal Operations.

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I. INTRODUCTION

We consider a quantum system in state $\rho_5$ which can be put in contact with a reservoir at temperature $T$. The second law of thermodynamics, combined with the first law (conservation of energy) states that the free energy

$$F = \text{Tr}(H\rho_5) - TS(\rho_5) \quad (I.1)$$

can only decrease, where $S(\rho_5)$ is the von Neumann entropy $S(\rho) = -\text{Tr}\rho \log \rho$ and $H$ is the system’s Hamiltonian. Although this is a necessary constraint on what state transformation are possible, we now know that it is not sufficient. For transitions between two states, diagonal in the energy basis, there are a set of necessary and sufficient conditions which must be satisfied in order for a state to transform into another state. One has a family of free energies in the case of catalytic processes\textsuperscript{1} (i.e. where one is allowed an ancilla which can be returned to its original state in the spirit of Clausius-Planck formulation of the Second Law). For non-catalytic transformations, the set of necessary and sufficient conditions were proven to be majorization\textsuperscript{2} in the case when the Hamiltonian is $H = 0$ and thermo-majorization\textsuperscript{3} in general. It is only in the thermodynamic limit that all these conditions become equivalent to the ordinary second law of equation (I.1). However, for single finite systems (sometimes called the single-shot scenario), the full set of conditions are relevant. It is this finite regime which is more relevant for quantum systems or even in the meso-scopic regime, especially if long range interactions are present.

Regarding states which are not diagonal in the energy basis, thermo-majorization (or the generalised free energies of \textsuperscript{1} in the catalytic case) are still necessary conditions for state transformations and place conditions on the diagonal entries of the state $\rho_5$ (where we assume that $\rho_5$ is written in the energy eigenbasis). But these conditions do not say anything about how off-diagonal elements between different energies behave. This article is concerned with finding conditions for these coherences. Partial results were obtained in \textsuperscript{4,3} for the case where only the input state is non-diagonal and in \textsuperscript{4}, where relations between purity and quantum asymmetry in the spirit of coherences have been formulated. However finding a complete set of quantum limitations is still a challenge. Here, we will present a set of conditions, we will call Damping Matrix Positivity (DMP). Unlike the results of \textsuperscript{4,3}, they are not necessary and sufficient, although we will show that they are for the case of a qubit.

Here, we conduct our analysis using the resource theory of thermodynamics, so called Thermal Operations (TO), introduced in \textsuperscript{5} and applied later in \textsuperscript{3,6}. We will discuss these operations in Section \textsuperscript{1} and the restrictions they impose on state transformations in Section \textsuperscript{11}. In particular, our condition, DMP, is presented in Subsection \textsuperscript{11B}. Our discussion of this condition in
the case of a qubit is presented in Subsection II C where we see that DMP is a necessary and sufficient condition. As a result, we fully characterize the qubit-qubit case, as well as provide limitations for higher dimensional states. In Section IV we introduce a new class of operations we call Enhanced Thermal Operations, and study its power with respect to TO. They appear to be more powerful, in that for them, DMP are necessary and sufficient conditions for state transformations, while for Thermal Operations we believe DMP are not sufficient.

At least in the qubit case, TO can be describe by three conditions: completely positive trace preserving, some commutation relation, and preservation of the Gibbs state. We obtain a part of our findings by adapting results for studies of the weak-coupling between the system and the heat-bath, and dynamical semi-groups [7–10].

II. THERMODYNAMICS AS A RESOURCE THEORY AND THERMAL OPERATIONS

Let us start with recalling how thermodynamics can be viewed as a resource theory [2, 8–10]. This allows us to precisely define what thermodynamics is, as it will define what are the allowable class of operations in the theory. We can then exploit some mathematical machinery from information theory, for example, from single-shot information theory, where one does not have access to many copies of independent and identically distributed bits of information. In a resource theory, one considers some class of operations, and then asks how much of some resource can be used to perform the desired task and how this resource can be manipulated. In the case of thermodynamics, it is viewed as a theory involving state transformations in the presence of a thermal bath.

We want to obtain limitations, thus we allow any unitary. We also need to account for all sources of energy (work), that’s why we demand energy conservation (since all processes conserve total energy, the energy that is added or removed from the system and bath will be transferred to a work storage system. We will use then, so called, Thermal Operations, introduced in [5] (related, more broaden class has been studied earlier in [10]). Formally, under Thermal Operations one can

1. Bring in an arbitrary system in a Gibbs state with temperature T (free resource).
2. Remove (discard) any system.
3. Apply a unitary that commutes with the total Hamiltonian.

The class of Thermal Operations is generated by the unitaries $U$ (which act on the system, bath and other ancillas) which obey the energy conservation condition

$$[U, H_S + H_R + H_W] = 0, \quad (II.1)$$

where $H_W$ is a work system or a clock, or any other object under consideration besides the system and bath. Equation (II.1) is necessary and sufficient if we wish to ensure that energy is conserved on every input state. This is natural if we wish to apply our thermal machine on arbitrary unknown quantum states.

Thus, an arbitrary Thermal Operation is obtained by the implementation of an energy-preserving $U$ and tracing out the heat bath (see also, Fig. 1). Precisely, $\Lambda \in \text{Thermal Operations, when}$

$$\Lambda(\rho_S) = \text{Tr}_R(U\tau_R \otimes \rho_S U^\dagger). \quad (II.2)$$

As a remark, let us notice that one can derive laws of thermodynamics under Thermal Operations. The commutation relation from Eq. (II.1) is equivalent to the first law (energy conservation) and the unitarity (conservation of information) results in the second law (zeroth law). The third law can also be obtained in this framework. One can show that the only allowed state in (I) that can be brought in for free is the equivalent class of Gibbs states at temperature $T$. Allowing any other state would lead to the situation where there are simply no real limitations on possible transformations - every transformation is possible and there is no room for obtaining any bounds. This can be considered as the zeroth law which helps us to define the temperature. The assumption that a Gibbs state is the only possible free resource is crucial. Allowance of other states acting as a resource would lead to the situation where there are simply no real limitations on possible transformations - every transformation is possible and there is no room for obtaining any bounds.

It is worth noting that it is Equation (II.1) that prevents one from creating coherences over energy levels if one doesn’t already start with them. One can extend...
Thermal Operations to the case where one is allowed as a resource, a reference frame which acts as a source of infinite coherence, and in such a case, one can lift the superselection imposed by Equation (II.1)[13].

III. ALLOWED STATE-TO-STATE TRANSFORMATIONS UNDER THERMAL OPERATIONS

![Diagram](image)

**Fig. 2**: (Color online) The thermomajorization criteria is as follows: Consider probabilities $p(E, g)$ of the initial system $ρ_i$ to be in the $g$'th state of energy $E$. Now let us put $p(E, g)\exp(E)$ in decreasing order $p(E_1, g_1)\exp(E_1) \geq p(E_2, g_2)\exp(E_2) \geq p(E_3, g_3)\exp(E_3) ...$, we say that the eigenvalues are $β$-ordered. We can do the same for other system $ρ_j$ i.e. $\exp(E_1)q(E_1', g_1') \geq \exp(E_2)q(E_2', g_2') \geq \exp(E_3)q(E_3', g_3') ...$. Then the condition which determines whether we can transform $ρ_i$ into $ρ_j$ is depicted in the above figure. Namely, for any state, we construct a curve with points $k$ given by $\{\sum \exp(-βE)/Z, \sum p_i\}$. Then a thermodynamical transition from $ρ_i$ to $ρ_j$ is possible if and only if, the curve of $ρ_i$ lies above the curve of $ρ_j$. The Gibbs state $ρ_β$ always has the lowest possible cumulative plot. One can make a previously impossible transition possible by adding work $E$ which will scale each point by an amount $\exp(-E)$ horizontally. Based on this, in the figure, one can go from $ρ_1$ to any other state, but from $ρ_2$ it is possible to reach $ρ_4$ and $τ_β$ only, and so on.

It is known that Thermal Operations, due to the superselection rule that comes from Eq. (II.1), cannot create coherent superpositions between eigenstates and that they are outperformed by Gibbs preserving maps [14], but what are their ultimate power? In other words, what are the limitations for a general $(ρ, H_S) \rightarrow (σ, H_S)$ state-to-state transition? In [3] necessary and sufficient conditions, in terms of monotones, have been put forward for the block diagonal entries of a state written in the energy basis. These conditions are described in Fig. 2. Here, by noticing some general properties of Thermal Operations, we will provide bounds for off-diagonal elements - coherences under the assumption that the system Hamiltonian $H_S$ has non-degenerate Bohr spectrum, i.e., there are no degeneracies in the nonzero differences of energy levels of the Hamiltonian. To do that, we will adapt the results derived for open systems, and in particular, for Davies maps under weak-coupling [7,9].

A. Properties of Thermal Operations

First of all, we need to ask, can we separate what happens to diagonal elements with the processing of the off-diagonal coherences? As we show in Supplementary Note [3] the answer is positive. Moreover, for systems having non-degenerated Bohr spectra, coherences are not mixed among themselves. We can thus say that Thermal Operations are block-diagonal, i.e., for an off-diagonal (diagonal) element $|i⟩_S⟨j| (|i⟩_S⟨i|)$ of state $ρ_S$ one gets

$$\Lambda(|i⟩_S⟨j|) = α_{ij}|i⟩_S⟨j|, i \neq j \quad (III.1)$$

and

$$\Lambda(|i⟩_S⟨i|) = \sum_{ij} p(i \rightarrow j)|j⟩_S⟨j|, \quad (III.2)$$

where $\Lambda$ is defined as in Eq. (II.2), $α_{ij}$ are factors by which the off-diagonal elements are multiplied (damped) during the transition, and $p(i \rightarrow j)$ is a transition probability of moving element $i$’s into $j$’s and $p(i)$ is a probability of occupying an energy state $i$. Thermal Operations are physical operations, so the dynamics should be implemented by completely positive trace preserving maps (CPTP maps). Together with the fact that under Thermal Operations, the Gibbs state is preserved, we have a set of properties fulfilled by Thermal Operations. It is known [7,8] that these properties are also satisfied by so called Davies maps appearing in the weak-coupling regime for Hamiltonians with non-degenerate Bohr spectra. Using the above properties, we obtain constraints for the behavior of coherences. We thus get bounds for off-diagonal elements which are determined by the probability for staying in the same energy-level.

B. Quantum states - second laws for off-diagonal elements

Imagine that we have one $d$—level state that we want to transform into another $d$—level state using Thermal Operations. From the properties of Thermal Operations, we then obtain two families of bounds, one for
diagonal elements of the states (thermo-majorization) and the second one for coherences.

Suppose now, that somehow we can transform diagonals of an input state into a state with some other diagonal entries. Since, we want to study the power of Thermal Operations and know which state-to-state transformations are possible, our question is then: How does this process affect coherences, i.e., the off-diagonal elements? Details of calculations are presented in Supplementary Note D.

We now use the properties of Thermal Operations provided in the previous section. As shown in Ref [7], the property of CPTP combined with formulas (III.1) and (III.2) imply that the following matrix must be positive:

\[
\begin{pmatrix}
    p(0 \to 0) & a_{01} & \ldots & a_{0n-1} \\
    a_{10} & p(1 \to 1) & \ldots & a_{1n-1} \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{n-10} & a_{n-12} & \ldots & p(n-1 \to n-1)
\end{pmatrix} \geq 0.
\]

(III.3)

See also, Fig. 3. We will call the above matrix the Damp-Matrix, and the above condition, Damping Matrix Positivity or DMP. Let us note, that the matrix is crucial for processing coherences. Indeed, positivity implies that the damping factors in particular satisfy

\[
|\alpha_{ij}| \leq \sqrt{p(i \to i)p(j \to j)}.
\]

(III.4)

Thus, the coherences must be damped at least by a factor \(\sqrt{p(i \to i)p(j \to j)}\) that comes from the \(2 \times 2\) minors of the matrix from Eq. (III.3). These formulas (introduced in the earlier version of our paper) were subsequently developed in [15]. In the subsequent section we will show that for qubits, this is the only constraint for processing coherences by Thermal Operations.

C. Qubit example

For qubits, there is only one bound for coherences transport and, as we show in Supplementary material Sec. D, the inequality can always be saturated, which implies that the criteria for qubits is necessary and sufficient. Thus given process on a diagonal, the damping factor can be always made equal to \(\sqrt{p(i \to i)p(j \to j)}\) from Eq. (III.4). We will determine this optimal factor for an arbitrary \(\rho \to \sigma\) transition. Going into details, consider two states \(\rho_S = \begin{bmatrix} p & \alpha \\ \alpha^* & 1-p \end{bmatrix}\) and \(\sigma_S = \begin{bmatrix} q & \chi \\ \chi^* & 1-q \end{bmatrix}\), written in the energy eigenbasis, on a system with a Hamiltonian \(H_S\), where \(\star\) stands for complex conjugation. We know that the evolution of diagonal elements can be separated from off-diagonal ones, so for diagonal elements one uses thermo-majorization obtaining four different situations, depending on the diagonal input/output and energies of the system, presented in Fig. 4. For coherences we obtain that their decaying rate is suitably adapted to the diagonal transition rates, so, in other words, the coherences damping factor depends only on diagonal elements of states and energies associated with the Hamiltonian of the system \(H_S\). Namely, we have that coherences obey the following inequality

\[
|\chi| \leq |\alpha|\kappa,
\]

(III.5)

where

\[
\kappa = \sqrt{(q - \tilde{p} e^{\beta \Delta E})(p - \tilde{q} e^{\beta \Delta E})} \left| p - \tilde{p} e^{\beta \Delta E} \right|
\]

(III.6)

\(\tilde{q} = 1 - q\), \(\tilde{p} = 1 - p\), \(e^{\pm \beta \Delta E} = e^{\pm \beta(E_j - E_i)}\) with \(E_i\) being the energy of the system and \(\beta\) the inverse temperature \(\beta = \frac{1}{T}\). Note that the phases commute with the total Hamiltonian of our setup, so we can restrict our attention only to moduli of the coherences. Summing up, we have necessary and sufficient conditions for an arbitrary qubit \(\rho \to \sigma\) transitions under Thermal Operations, where for \(a)\) diagonal elements we use thermo-majorization, \(b)\) for coherences, Eq. (III.5) (which can be achieved with equality).
IV. ENHANCED THERMAL OPERATIONS: A CLASS OF OPERATIONS WHICH SATURATE THE DMPCRITERIA

As we already have observed, in the case when one considers Hamiltonians with nondegenerated Bohr spectra, the properties of Thermal Operations are similar to those occurring when one studies Davies maps for many-level systems \[29\]. Basing on the properties showed in Sec. III we introduce a class of operations that is defined by these properties. We will call this class \textit{Enhanced Thermal Operations}.

We define Enhanced Thermal Operations (ETO) in the following way. \( \Lambda \in \text{ETO} \) when

1. \([\Lambda, \hat{H}] = 0\), where \( \hat{H}(X) = [H, X] \).
2. Is CPTP.
3. It preserves the Gibbs state.

ETO can be viewed as quantum channels which commute with the linear map \([H, \bullet] \) and preserve the Gibbs states associated to \( H \). The first property gives us that under Enhanced Thermal Operations, one is able to realize all possible transformations (and limitations) that arise from the matrix from Eq. (III.3). We will use this and the result for Thermal Operations from Sec. III to compare the power of these two classes.

We show that for qubits, Thermal Operations are equal to the new class and as a result we have laws for any state-to-state transition under Thermal Operations. Essentially, for qubits, Thermal Operations can already saturate the bound given by Eq. (III.3) and thus do no worse than Enhanced Thermal Operations. For qutrits, in Supplementary Note D.6 we provide a family of initial and final states \( \rho \) and \( \sigma \) that by Enhanced Thermal Operations, starting from \( \rho \) one can transform it into \( \sigma \) exactly, but it is not possible under Thermal Operations. Based on this, one can try to conclude that Thermal Operations are outperformed by Enhanced Thermal Operations, and what is more, state transitions by Thermal Operations are not equal to the ones under the new class (the latter statement is stronger; it could be that the set of Thermal Operations is smaller than enhanced one, but both classes lead to the same laws of transformations). Although, it is not a conclusive result, because one can try to approximate the channel that is used to realize the transition under Thermal Operations from Sec. III which may lead to the saturation of the bound for optimal coherences preservation.

At the end, let us stress, that we study thermodynamical operations for Hamiltonians with nondegenerate Bohr spectra, so it is worth to check what happens for the case of degenerate spectra. In both cases the thermodynamical classes should be extended to the wider ones since now, the coherences can be mixed between themselves during the evolution. This might lead to a larger class of second laws.

D. Sufficiency of the second laws?

It is clear that for an arbitrary transition, there are many stochastic maps that lead to the same final state and each such a map can be implemented by possibly many unitary transformations. We need such units that damp as little as possible, the off-diagonal elements of the density matrix - for which, the inequalities coming from the 2 \( \times \) 2 minors of the Choi map from Eq. (III.4) are all saturated. This would optimise the preservation of coherences. But, is it always possible under Thermal Operations? As we have shown, for qubits, for every state-to-state transition we have only one channel that realizes it and we can always implement it in the best way for optimal coherence preservation; we can always make the inequality that gives us a dumping factor for coherences tight. This uniqueness of channel may be not true anymore for higher dimensional states. Our belief relies on the fact that choosing a particular qutrit state-to-state transition \( (0, \frac{1}{2}, \frac{1}{2}) \rightarrow (e^{\frac{i\Delta_{23}}{2}}, 1 - e^{-\Delta_{23}}, 1 - e^{-\Delta_{20}}, 1 - e^{-\Delta_{120}}) \), which is indeed realized only by one channel for which the constrains for coherences reduce to these one for qubits, one is not able to find such a unitary map that at the same time realizes the exact states transition and leads to the saturation of bounds for coherence preservation under Thermal Operations. We also conjecture that this still holds in the case of approximate state-to-state processing.

FIG. 4: (Color online) Four cases that follows from different \( \beta \)-order are presented. In a) and b) there are the same \( \beta \)-order, in c) and d) different. Also in a) both states corresponding to the curves are less excited than Gibbs state, in b) more excited, in c) upper state - less excited, lower - more and in d) reverse. The lowest possible line corresponds to the Gibbs state.
FIG. 5: (Color online) Comparison of Thermal Operations (TO) and Enhanced Thermal Operations (ETO) for qubits ($d = 2$) and $d > 2$. In the case of the former, they are equal to, and from the Birkoff primitive, Thermal Operations can reproduce not only the extreme maps (when saturation happens) but any other from Enhanced Thermal Operations with an arbitrary precision; when for the latter, Enhanced Thermal Operations may be a wider class than Thermal Operations. However, we only have a "half-counterexample", i.e., we find a strict qutrit state-to-state transition than can be realized by ETO, but not by TO. Studies of approximate states transitions are needed to verify the possible gap between TO and ETO.

V. DISCUSSION AND OPEN QUESTIONS

We study the limit of state-to-state transformations under Thermal Operations, focusing mostly on coherences and their preservation and we compare its power to the newly introduced class - Enhanced Thermal Operations. A natural route of studies it to check the impact of these operations on quantum thermodynamics and study whether they really outperform Thermal Operations in the case of degenerate Bohr spectra, or for approximate transformations.

It would be also interesting to check how state transitions look like when one drops the energy conservation condition and allows the total Hamiltonian and unitaries just to nearly commute.

In our setup, Hamiltonians are fixed, so the natural question that arise is, can we relax the constraint of keeping the energy of the system fixed and allow the change of Hamiltonians $H_S \rightarrow H_S'$ during state transformations? The answer is probably positive, because it has been shown that for states diagonal in energy basis, one can add a qubit that switches between Hamiltonians, which makes the dynamics time dependent [3]. It is highly plausible to adapt that scenario also to arbitrary states.

Finally, we have seen that the second laws we have introduced in the form of the DMP criteria are not strictly necessary and sufficient limitations on thermodynamical transformations. This likely means that there are more second laws which have to be satisfied. Finding them is an interesting open question.

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Appendix A: (Q)Bit of notation and assumptions

Before proving and presenting in details the main results of our work, let us introduce some notation first. First, we will recall facts from [3] to which we will add some new assumptions and modifications in the end.

Let us define $\eta_X^E$ as a state of a system $X$ proportional to the projection on to a subspace of energy $E$ (according to the Hamiltonian $H_X$ on this system). In particular, $\eta_{E-E_S}^R$ is given by

$$
\eta_{E-E_S}^R = g(E - E_S)^{-1} \sum_\delta |E - E_S, \delta\rangle_R \langle E - E_S, \delta|
$$

where $\delta = 1, \ldots, g(E - E_S)$ are degeneracies, i.e. $\eta_{E-E_S}^R$ is the maximally mixed state of the reservoir with support on the subspace of energy $E_R = E - E_S$, $E_R$ are the energies of reservoir and $E_S$ of the system. We shall also use notation $\eta_K = \text{Id} / K$ where the identity acts on a $K$ dimensional space.

Let us note that the total space $\mathcal{H}_R \otimes \mathcal{H}_S$ can be decomposed as follows

$$
\mathcal{H}_R \otimes \mathcal{H}_S = \bigoplus_E \left( \bigoplus_{E_S} \mathcal{H}_R^{E-E_S} \otimes \mathcal{H}_S^{E_S} \right)
$$

Consider an arbitrary state $\rho_{RS}$ which has support within $E_{S \text{ max}}^S \leq E \leq E_R^{\text{max}}$. We can rewrite it as follows

$$
\rho_{RS} = \sum_{E} \sum_{\Delta} P_E \rho_{RS} P_{E+\Delta}
$$

Here $\Delta = -E_{S \text{ max}}, \ldots, E_{S \text{ max}}^S$. The blocks $P_E \rho_{RS} P_{E+\Delta}$ we can further divide into sub-blocks

$$
P_E \rho_{RS} P_{E+\Delta} = \sum_{E_S \in I_\Delta} \text{Id}_R \otimes P_{E_S} P_E \rho_{RS} P_{E+\Delta} \text{Id}_R \otimes P_{E+\Delta}^S
$$

where $I_\Delta = \{0, \ldots, E_{S \text{ max}} - \Delta\}$ for $\Delta \geq 0$ and $I_\Delta = \{-\Delta, \ldots, E_{S \text{ max}}^S\}$ for $\Delta \leq 0$. The sub-blocks map the Hilbert space $\mathcal{H}_R^{E-E_S} \otimes \mathcal{H}_S^{E+\Delta}$ onto $\mathcal{H}_R^{E-E_S} \otimes \mathcal{H}_S^{E_S}$

We can then extract the state $\rho_S$

$$
\rho_S = \sum_{E_S, E_S^S} P_{E_S} \rho_{S} P_{E_S}^S
$$

as follows:

$$
P_{E_S} \rho_{S} P_{E_S}^S = \sum_{E} \text{Tr}_{\mathcal{H}_R^{E-E_S}} (P_R^{E-E_S} \otimes P_{E_S} P_E \rho_{RS} P_{E+1-E_S} P_{E-E_S}^R \otimes P_{E_S}^R)
$$

Let us make some assumptions now.

We can assume that Hamiltonians of all systems of concern have minimal energy zero. Let $E_{R \text{ max}}$ and $E_{S \text{ max}}$ be the largest energy of the heat the bath and system, respectively (of course a typical heat the bath will have $E_{R \text{ max}} = \infty$).

Our heat the bath will be large, while our resource states will be small. This means that the system Hilbert space will be fixed, while the energy of the heat the bath (and other relevant quantities such as size of degeneracies) will tend to infinity. It is quite an important assumption, because when the energy spectrum of the bath is not highly degenerated, then the set of Thermal Operations is very small and restricted.

Remark 1 In principle, Thermal Operations need not satisfy detailed balance; they should merely preserve the Gibbs state as a whole.

The heat the bath is in a Gibbs state $\tau_R$ with inverse temperature $\beta$. Moreover there exists set of energies $\mathcal{E}_R$ such that the state of the heat the bath occupies energies from $\mathcal{E}_R$ with high probability, i.e. for the projector $P_{\mathcal{E}_R}$ onto the states with energies $\mathcal{E}_R$ we have

$$
\text{Tr} P_{\mathcal{E}_R} \rho_R \geq 1 - \delta
$$

and it has the following properties:
1. The energies \(E\) in \(\mathcal{E}_R\) are peaked around some mean value, i.e. they satisfy \(E \in \{\langle E \rangle - O(\sqrt{\langle E \rangle}), \ldots \langle E \rangle + O(\sqrt{\langle E \rangle})\}\).

2. For \(E \in \mathcal{E}_R\) the degeneracies \(g_R(E)\) scale exponentially with \(E\), i.e.
   \[g_R(E) \geq e^{E},\] (A.8)
   where \(\epsilon\) is a constant.

3. For any three energies \(E_R, E_S\) and \(E'_S\) such that \(E_R \in \mathcal{E}_R\) and \(E_S, E'_S\) are arbitrary energies of the system, there exist \(E'_R \in \mathcal{E}_R\) such that \(E_R + E_S = E'_R + E'_S\).

4. For \(E \in \mathcal{E}_R\) the degeneracies \(g_R(E)\) satisfy \(g_R(E - E_S) \approx g_R(E) e^{-\beta E_S}\), or more precisely:
   \[\left| \frac{g_R(E) e^{-\beta E'_S}}{g_R(E - E_S)} - 1 \right| \leq \delta\] (A.9)
   for all energies \(E_S\) of the system \(S\).

One can notice that a product \(\tau^n_R\) of many copies of independent Gibbs states satisfies the above assumptions. We then have:

**Theorem 2.** [3] We consider the set of energies
\[\mathcal{E} = \{E : E - E_S \in \mathcal{E}_R\}\] (A.10)
where \(\mathcal{E}_R\) satisfies assumptions for heat the bath listed above. Then
\[\forall E \in \mathcal{E} \quad \left| \frac{1}{p_E} P_E \rho_R \otimes \rho_S P_{E+\Delta} - \otimes \eta_{E-E_S} P_E \rho_S P_{E+\Delta} \right| \leq 2\delta\] (A.11)
and
\[\sum_{E \in \mathcal{E}} p_E \geq 1 - 2\delta\] (A.12)
where \(p_E = \text{Tr}(P_E \rho_R \otimes \rho_S)\).

All the above is sufficient, when one considers states that are diagonal in energy basis. To deal with coherences, our figure of merit, an additional assumption is needed.

Let us denote the minimal energy of the bath by \(E_{R_{\min}}\) and the maximal one by \(E_{R_{\max}}\).

1. Let us define a new set of energies \(\mathcal{E}'_R\) which is the set \(\mathcal{E}_R\) where we removed all energies that are less (greater) than \(E_{\min}'(E_{\max}') \pm \max E_S\). It has the property that for the projector \(P'_{\mathcal{E}'_R}\) onto the states with energies \(\mathcal{E}'_R\) we have
   \[\text{Tr} P'_{\mathcal{E}'_R} \rho_R \geq 1 - \delta'\] (A.13)

Theorem 2 also holds for this assumption, the only difference is that \(\delta\) needs to be replaced by \(\delta'\).

**Appendix B: Thermal Operations**

Let us, one more time, present the facts and properties of Thermal Operations. In Thermal Operations one can

1. Bring in an arbitrary system in a Gibbs state with temperature \(T\) (free resource).
2. Remove (discard) any system.
3. Apply a unitary that commutes with the total Hamiltonian.
Mathematically, the class of Thermal Operations on a system with \((\rho_S, H_S)\) can be viewed as

\[
(\rho_S, H_S) \mapsto (\text{Tr}_R[U(\rho_S \otimes \tau_R^{\text{th}}) U^\dagger], H_S) = (\sigma_S, H_S)
\]  

(B.1)

where \(\tau_R = e^{-\beta H_R}/Z_R\) is the thermal state of the reservoir for some reservoir Hamiltonian \(H_R\) at inverse temperature \(\beta\), \(\rho_S\) and \(\sigma_S\) are some initial and final states from \(H_S\). The class is generated by the unitaries \(U\) (which act on the system, bath...) which obey the (strong) energy conservation condition

\[
[U, H_S + H_R + H_W] = 0,
\]

(B.2)

where \(H_W\) is the term that a clock, a work system and other object under consideration besides the system and bath. Conservation of the total energy also implies the average energy conservation. In [3], the authors, provide an indication of how to generalize the above to the case of time-dependent system Hamiltonian, with the help of an auxiliary system \(S'\). Example: In the case, when one has only the system and the heat bath, the total Hamiltonian is

\[
H_{SR} = H_S \otimes I_R + I_S \otimes H_R,
\]

(B.3)

and from the energy conservation relation we have that

\[
[U, H_{SR}] = [U, H_S \otimes I_R] + [U, I_S \otimes H_R] = 0.
\]

(B.4)

It means that to have the non-trivial dynamics and state-to-state transitions

\[
[U, H_S \otimes I_R] = -[U, I_S \otimes H_R] \neq 0.
\]

(B.5)

When both commutators are equal to zero, everything trivialize.

Let us recall the properties of Thermal Operations that we introduce in Sec. III:

1. They are completely positive trace preserving maps (CPTP maps).
2. They preserve the Gibbs state.
3. During state-to-state transitions, the diagonal elements of an evolving state are not mixed with the off-diagonal ones, i.e., for any element \(|i\rangle_S\langle j|\) of a state \(\rho_S\),

\[
\Lambda(|i\rangle_S\langle j|) = \sum_{kl: E_k - E_i = E_j - E_l} a^{ij}_{kl} |k\rangle_S\langle l|,
\]

(B.6)

where \(\Lambda\) is Thermal Operations and \(a^{ij}_{kl}\) are factors by which state elements are multiplied after an evolution.
4. For Hamiltonians having non-degenerated Bohr spectra, the off-diagonal elements are also not mixed between themselves, i.e., for an off-diagonal element \(|i\rangle_S\langle j|\) one gets

\[
\Lambda(|i\rangle_S\langle j|) = \lambda_{ij}|i\rangle_S\langle j|, \ i \neq j
\]

(B.7)

\(\lambda_{ij}\) are factors by which the off-diagonal elements are multiplied (damped) during the transition.

Proof of the Properties 1-4. The first property comes from Eq. (B.1), since Thermal Operations are implemented by unital dynamics. The second property comes straightforwardly from the commutation relation between energy-preserving unitary matrices and the total Hamiltonian, \([U, H] = 0\) [3]. We need to focus in details on the last two from the above list. We will prove these attributes of Thermal Operations using the formalism from Sec. A.

Let us consider an evolution (under energy preserving unitary operation \(U\)) of an off-diagonal \(|i\rangle_S\langle j|\) element of a quantum state that acts on the system \(S\). Identifying the blocks of fixed energy \(E\) and using Eq. (A.3) we get:

\[
\bigoplus_{E} U_E \rho_R \otimes |i\rangle_S\langle j| U^\dagger \bigoplus_{E'} U^\dagger_{E'}.
\]

(B.8)

Let us now the state \(\rho_R\) in its energy-basis as

\[
\rho_R = \sum_{E_R} p(E_R) |E_R\rangle\langle E_R|,
\]

(B.9)
From Eq. (B.12), precisly, from the Kronecker deltas, we get that

\[
\langle E | \sum_{E} U_E \sum_{E'} p(E_R) | E_R \rangle \langle E_R | \otimes | i \rangle | S U^*_E \sum_{E'} p(E_R) \sum_{E'} U_{E'} | i \rangle S \langle E_R | \langle j | S U^*_E = \sum_{E} p(E_R) \sum_{E'} U_E | E_R \rangle | i \rangle S \langle E_R | \langle j | S U^*_E .
\]  

(B.10)

Let us examine now the action of \( U \) on matrix elements of states. The only elements that are going to remain are that whose total energy of the system and bath is equal to \( E \) \((E')\). It gives

\[
U_E | E_R \rangle | i \rangle S = \sum_k \alpha^{kl}_{E_R} E_R + E_i - E_k | k \rangle S \delta_{E, E_R + E_i},
\]

\[
\langle E_R | \langle j | S U^*_E = \sum_l \alpha^{lj}_{E_R} | (E_R + E_j - E_l) | l \rangle S \delta_{E', E_R + E_j}.
\]

(B.11)

where \( \delta_{E, E_R + E_i} \) and \( \delta_{E', E_R + E_j} \) are Kronecker deltas, \( E_x \) is the energy of an element \(| x \rangle \), and \( * \) stands for the complex conjugation. Inserting Eq. (B.11) into Eq. (B.10) leads to

\[
\sum_{E} p(E_R) \sum_{E'} \sum_k \alpha^{kl}_{E_R} \alpha^{lj}_{E_R} | E_R + E_i - E_k \rangle | k \rangle S \langle E_R + E_j - E_l | l \rangle S \delta_{E', E_R + E_j}.
\]

(B.12)

Using Kronecker deltas we get

\[
\sum_{E} p(E_R) \sum_{kl} \alpha^{kl}_{E_R} \alpha^{lj}_{E_R} | E_R + E_i - E_k \rangle | k \rangle S \langle E_R + E_j - E_l | l \rangle S.
\]

(B.13)

From Eq. (B.12), precisely, from the Kronecker deltas, we get that \( E' = E + E_j - E_i = E + \omega_{ij} \). From now on, we will denote \( E_x - E_y = \omega_{xy} \), meaning \( \omega_{xy} \) is the frequency between levels \( x \) and \( y \).

We can then rewrite Eq. (B.12) as

\[
\sum_{E} p(E_R) \left( \sum_{kl} \alpha^{kl}_{E_R} \alpha^{lj}_{E_R} | E_R + \omega_{ij} \rangle | k \rangle \otimes | k \rangle S \langle E_R + \omega_{ij} | E_R + \omega_{ij} \rangle \right).
\]

(B.14)

Applying the partial trave over the heat bath gives

\[
\sum_{E} p(E_R) \left( \sum_{kl} \alpha^{kl}_{E_R} \alpha^{lj}_{E_R} \langle E_R + \omega_{ij} \rangle \langle E_R + \omega_{kl} \rangle \right).
\]

(B.15)

To have non-zero scalar product, \( \omega_{ij} = \omega_{ij} \). Keeping in mind that \( \omega_{ij} = E_i - E_k \) and \( \omega_{ij} = E_j - E_l \), the scalar product is non-zero, iff \( E_k - E_i = E_j - E_l \). After the calculation, we get

\[
\sum_{kl: E_k - E_i = E_j - E_l} \left( \sum_{E} p(E_R) \alpha^{kl}_{E_R} \alpha^{lj}_{E_R} \right) | k \rangle \langle l | S = \sum_{kl: E_k - E_i = E_j - E_l} \alpha^{ij}_{kl} | k \rangle \langle l | S.
\]

(B.16)

This proves Eq. (B.6). But partcullary, for systems having non-degenerate Bohr spectra, we have \( E_i \neq E_j \) and \( E_k \neq E_l \), then \( E_k = E_i \) and \( E_j = E_l \) (it corresponds to the situation when both \( \omega \)'s are equal to 0), which changes Eq. (B.16) into

\[
\left( \sum_{E} p(E_R) \sum_{ij} \alpha^{ij}_{E_R} \alpha^{ij}_{E_R} \right) | i \rangle \langle j | S = \lambda_{ij} | i \rangle \langle j | S.
\]

(B.17)

We get that our off-diagonal element is, after evolution, multiplied by \( \Lambda_{ij} \) that depends only on \( | i \rangle \langle j | \) and not on any other off-diagonal element, which proves Eq. (B.7).

Property 3 implies the following

**Corollary 3.** For \( \Lambda \) being Thermal Operations as in Eq. (B.1), one has \([\Lambda, \hat{H}] = 0\), where \( \hat{H}(X) = |H, X\rangle \).

**Proof.** For \( \hat{H} \), we have that its eigenvalues are Bohr frequencies, and eigenspaces \( P \) with respect to \( \omega \) are given by \( P_\omega = \text{span} \{|k\rangle \langle l|, \omega = E_k - E_l\} \). From Property 3, we know that these eigenspaces are invariant for \( \Lambda \).
We take a product quantum state of the Gibbs states from the heat bath and the system’s state using Eq. \(\text{A.3}\). Since, we want to consider thermodynamical transitions, by means of Thermal Operations, we need to focus on energy preserving unitary transformations \(U\) acting in blocks of fixed total energy. We identify the blocks of fixed energies \(E^i = E^S_i + E^R_i\) and due to the assumption 3 about heat the bath, we know that there always exist two different combinations of a sum of system and the bath energies that gives the same energy \(E^i\), i.e., for the qubit with energies \(E^0_S\) and \(E^1_S\) one has \(E^i = E^0_S + E^0_R = E^1_S + E^1_R\). The unitary transformation acts in these sub-blocks that have the same energy total energy. Mathematically, we consider block-unitary transformations which can be written in the following form

\[
U = \bigoplus_i U_i, 
\]  

where each block acts on energy \(E^i\). Next we assume that an arbitrary unitary block \(U_k\) from the above sum has the structure

\[
U_k = \begin{pmatrix} A_k & B_k \\ C_k & D_k \end{pmatrix},
\]

where submatrices \(A_k\) and \(D_k\) are square matrices of dimensions \(d_k \times d_k\) and \(d_{k-1} \times d_{k-1}\) respectively, while submatrices \(B_k\) and \(C_k\) are rectangular matrices of dimensions \(d_k \times d_{k-1}\) and \(d_{k-1} \times d_k\) respectively.

Then, we let this unitary acts on our state, obtaining a structure presented in Fig. 6. In the next sections, we show that from detail studies of the action of energy-preserving unitaries on states, the main results of our paper can be obtained.

We need to fulfill our assumptions, so to model the energies in our setup, (for an arbitrary dimension of a state) we can use the multinomial distribution, so the assumption 1 is obeyed. We also need to work in a regime, where dimensions of degeneracies, in a region of energy distribution, are non-decreasing. Moreover, blocks of unitaries connect blocks of different bath energies, so to ensure we are in a proper regime (that fulfills all our assumptions), we first have to make a cut on system and the bath energies, using the Chernoff bound [16], so they fit blocks of unitary, and the assumption 3 is followed, and we have a non decreasing order of dimensions of degeneracies. In other words, in a general situation, we can identify 3 different steps:

- First, we make a cut, so the law about degeneracies is fulfilled.
- We move an energy by a value \(\max E^i\) into the direction of mean energy, where weight of energies are big.
- We want to have a unitary operation that acts on fully on blocks of set energies, so we take the projection from this regime, where all components of set energies (sum of systems and the bath energies), are from the region where to which we cut our energy distribution. Sometimes, to fulfill this, we need to include some energies which are already outside the cut area (by Chernoff bounds), but their weights are small, so we can take them to have all components of set energies.

### Appendix D: Seconds laws for coherences

Since we know that what happens of coherences can be separated on that what happens on a diagonal of a state, we can divide the full algorithm for state-to-state transitions into two steps

1. **Thermomajorization**

   There exist a necessary and sufficient method, derived in [3], called thermomajorization, to check whether a transition between states \((\rho_S, H_S) \rightarrow (\sigma_S, H_S)\) is possible, when both states commute with the Hamiltonian \(H\) of the total system, which means they are diagonal in the energy-basis. It is based on the majorization condition for state transformations, which is a necessary and sufficient condition for state transformations under permutation maps.
FIG. 6: (Color online) A qubit state $\rho_S = \begin{bmatrix} p & \alpha \alpha^* \end{bmatrix}$ with system energies $E^0_S$ and $E^1_S$, projected onto energy blocks $E^i_R$ of heat the bath with degeneracies of dimensions $d_i$. Darker squares correspond to blocks of set energies $E^i = E^i_S + E^i_R$, where a unitary $U = \bigoplus_i U_i$ acts to transform $\rho_S$ into other state.

The very brief idea is to write the eigenvalues of the state and heat bath, in terms of eigenvalues of only the state, order them in a nonincreasing way and compare integrals of the connected functions (some monotones).

To present the details, we will use the original formulation taken from [3].

Let $p_{E_S,g}$ be eigenvalues of $\rho$ and $q_{E_S,g}$ be eigenvalues of $\sigma$. The state $P_{E_R} \otimes \rho_S P_E$ after normalization is close to the state having the following eigenvalues:

$$e^{\beta E_S} p(E_S,g)$$

with multiplicity $g_R(E)e^{-\beta E_S}$, where $E_S$ runs over all energies of the system, and $g$ runs over degeneracies. Similarly, $P_{E_R} \otimes \sigma_S P_E$ has eigenvalues $e^{\beta E_S} g(E_S,g)$ with the same multiplicity.

The eigenvalues are very small, and they are collected in groups, where they are the same, hence the majorization amounts to comparing integrals. If one puts eigenvalues into decreasing order, one obtains a stair-case like function, and majorization in this limit will be to compare the integrated functions (which are then piece-wise linear functions).

To see how it works, we need to put the eigenvalues in nonincreasing order. The ordering is determined by the ordering of the quantities $e^{\beta E_S} p_{E_S,g}$. This determines the order of $p(E_S,g)$ (which in general will not be in decreasing order anymore). We shall denote such ordered probabilities as $p_i$, and the associated energy of the eigenstate as $E_i$. E.g. $p_1$ is equal to the $p(E_S,g)$ such that $e^{\beta E_S} p(E_S,g)$ is the largest. Note that for fixed $E_S$ the order
is the same as the order of \( p(E_S,g) \), while for different \( E_S \) it is altered by the Gibbs factor. We do the same for \( \sigma \), which results in \( q_i \).

The eigenvalues are thus ordered by taking into account Gibbs weights:

\[
\frac{p_1 e^{\beta E_1}}{d_E} \geq \frac{p_2 e^{\beta E_2}}{d_E} \geq \ldots
\]  

where \( d_E \) is a shorthand for \( g_R(E) \). We shall now ascribe to vector \( \{ p_i \} \) a function mapping interval \([0,Z]\) into itself. On the \( y \) axis, we put subsequent sums \( \sum_{l=1}^{i} p_i, l = 1, \ldots, d \) where \( d \) is the number of all probabilities, and on the \( x \) axis, we put sums \( \sum_{l=1}^{i} e^{-\beta E_i} \), with the final point being at \( x = Z \). This gives \( d+1 \) pairs: \((0,0),(p_1 e^{-\beta E_1}),(p_1 + p_2 e^{-\beta E_1} + e^{-\beta E_2}),\ldots,(Z,1)\). We join the points, and it will gives us a graph of a function, \( f_p(x) \). It is easy to see, that in the limit of large \( g_R(E) \), the eigenvalues of \( \rho \) majorize eigenvalues of \( \sigma \) if and only if \( f_p(x) \geq f_q(x) \) for all \( x \in [0,Z] \). The described scheme is also presented in Fig. 2.

2. Limitations for processing of coherences

Let us recall the bounds for coherences:

**Proposition 4.** When a transformation between two \( d \)-level system, initial - \( \rho_S \) and final - \( \sigma_S \) occurs, by means of Thermal Operations, the bounds for coherences transport come from the positivity of the Choi map that is associated with the energy preserving dynamics:

\[
\begin{pmatrix}
    p(0 \rightarrow 0) & \alpha_{11} & \cdots & \alpha_{1n} \\
    \alpha_{21} & p(1 \rightarrow 1) & \cdots & \alpha_{2n} \\
    \vdots & \vdots & \ddots & \vdots \\
    \alpha_{n1} & \alpha_{n2} & \cdots & p(n \rightarrow n)
\end{pmatrix},
\]  

where \( \alpha_{ij} \) are factors by which the off-diagonal elements are multiplied during the transition, and \( p(i \rightarrow i) \) are probabilities of staying in the same energy-level; \( p(i \rightarrow j) \) is a transition probability and \( p(i) \) is a probability of occupying an energy state \( i \).

It shows that the bounds for the transport of off-diagonal elements come from the minors of the matrix from Eq. (D.3). For example, for qubits, we have 2 minors to consider, one trivial (that probabilities \( p(i \rightarrow i) \) should be non-negative) and the one that really damps the coherences

\[
p(0 \rightarrow 0)p(1 \rightarrow 1) \leq \alpha^2.
\]  

Let us examine the qubit’s case in greater details.

3. Qubit example

For qubits, there is only one bound for coherences transport and the inequality is tight, which implies that the criteria for qubits is necessary and sufficient. To see that, consider two qubit states \( \rho_S = \begin{pmatrix} p & \alpha \\ \alpha^* & 1-p \end{pmatrix} \) and \( \sigma_S = \begin{pmatrix} q & \chi \\ \chi^* & 1-q \end{pmatrix} \), written in the energy eigenbasis, on a system with Hamiltonian \( H_S \), where \( * \) stands for complex conjugation. We know that the evolution of diagonal elements can be separated from off-diagonal ones, so for diagonal elements one uses thermomajorization obtaining four different situations, depending on the diagonal input and output and energies of the system.

\[
\frac{f}{1-f} \geq e^{\beta(E_1-E_0)},
\]  

where \( f \) is the order of \( p(E_S,g) \), while for different \( E_S \) it is altered by the Gibbs factor. We do the same for \( \sigma \), which results in \( q_i \).
or
\[
\frac{f}{1-f} \leq e^{\beta (E_1 - E_0)}, \tag{D.6}
\]
where \( f \) is \( p \) or \( q \), \( E_i \) is an energy of the system (of levels 1 and 0). Then, the state-to-state transformation \((\rho, H_5) \rightarrow (\sigma, H_5)\) by means of Thermal Operations is possible if and only if:

1. Diagonal elements - implied by thermomajorization.
   a: When both \( p \) and \( q \) fulfill D.5 then \( p \geq q \)
   b: when both \( p \) and \( q \) fulfill D.6 then \( p \leq q \)
   c: when \( p \) fulfills D.5 and \( q \) D.6 then \( q - p \geq r - q \)
   d: when \( p \) fulfills D.6 and \( q \) D.5 then \( p - q \leq r - q \).

2. Off-diagonal elements - fundamental bound for all cases from Eq. (D.4).
\[
|\chi| \leq |\alpha| \kappa,
\]
where \( \kappa = \sqrt{\frac{(q - p e^{\beta \Delta E})(q - \bar{q} e^{\beta \Delta E})}{|p - \bar{p} e^{\beta \Delta E}|}} \), \( \bar{q} = 1 - q \), \( \bar{p} = 1 - p \), \( e^{\pm \beta \Delta E} = e^{\pm \beta (E_j - E_i)} \) with \( E_i \) being energy of the system and \( \beta \) inverse temperature \( \beta = \frac{1}{kT} \). Remark. Since phases commute with the total Hamiltonian of our setup, we can restrict our attention only to moduli of the coherences.

4. Proof of the optimal coherence transport for qubits

It this subsection, we show that the qubits state-to-state transitions can be always implement by such an energy preserving \( U \) that the coherences are damped in a most friendly way for them, ie, that it is given by the equality from Eq. (D.4).

**Proposition 5.** For qubits, the bound from Proposition D.3, which gives Eq. (2), is tight.

Let us take two blocks \( D_k \) and \( A_{k-1} \) of a dimension \( d_{k-1} \), like in Figure 7. We assume here that matrices \( D_k \) and \( A_{k-1} \) have the diagonal form and satisfy constraints which follow from their trace norms
\[
\text{Tr} \left[ D_k D_k^\dagger \right] = \sum_{i=1}^{d_k} z_i^2 = d_{k-1} p(0 \rightarrow 0), \quad \text{Tr} \left[ A_{k-1} A_{k-1}^\dagger \right] = \sum_{i=1}^{d_{k-1}} x_i^2 = d_{k-1} p(1 \rightarrow 1). \tag{D.7}
\]

We would like to know the maximal value of
\[
\text{Tr} \left[ D_k A_{k-1}^\dagger \right] = \sum_{i=1}^{d_k} z_i x_i \tag{D.8}
\]
with constraints (D.7). We can treat diagonals of matrices of \( D_k \) and \( A_{k-1} \) like a vectors of length \( d_{k-1} \), so
\[
|\psi\rangle = |z_1, \ldots, z_{d_{k-1}}\rangle, \quad |\varphi\rangle = |x_1, \ldots, x_{d_{k-1}}\rangle \tag{D.9}
\]
with squared norms
\[
||\psi||^2 = d_{k-1} p(0 \rightarrow 0), \quad ||\varphi||^2 = d_{k-1} p(1 \rightarrow 1) \tag{D.10}
\]
and equation (D.8) reads \( \text{Tr} \left[ D_k A_{k-1}^\dagger \right] = \langle \psi | \varphi \rangle \). Thanks to this, maximization problem of \( \text{Tr} \left[ D_k A_{k-1}^\dagger \right] \) we can reformulate to \( \max \langle \psi | \varphi \rangle \) with constraints (D.10).
We consider two unitary blocks $U_k$ and $U_{k-1}$ and their subblocks $D_k$ and $A_{k-1}$ (red color) of dimensions $d_k \times d_k$. Our goal is to find maximal value of $\text{Tr} \left[D_k A_{k-1}^\dagger \right]$, when both matrices are diagonal and satisfy constraints $\text{Tr} \left[D_k D_k^\dagger \right] = d_k p(0 \to 0)$, $\text{Tr} \left[A_{k-1} A_{k-1}^\dagger \right] = d_{k-1} p(1 \to 1)$. By $p(0 \to 0)$ and $p(1 \to 1)$ we denote probability transitions between energy levels $0 \to 0$ and $1 \to 1$ respectively.

In the first step we change coordinates in the following way

\begin{align}
\sum_{i=1}^{d_{k-1}} z_i^2 &= d_{k-1} p(0 \to 0) \to \sum_{i=1}^{d_{k-1}} \bar{z}_i^2 = 1, \\
\sum_{i=1}^{d_{k-1}} x_i^2 &= d_{k-1} p(1 \to 1) \to \sum_{i=1}^{d_{k-1}} \bar{x}_i^2 = 1,
\end{align}

so we have $\lambda_1 z_i = \bar{z}_i$ and $\lambda_2 x_i = \bar{x}_i$, where $\lambda_1(2)$ are some numbers. Using norm invariance we calculate that

\begin{align}
\lambda_1 &= \frac{1}{\sqrt{d_{k-1} p(0 \to 0)}}, \quad \lambda_2 = \frac{1}{\sqrt{d_{k-1} p(1 \to 1)}}.
\end{align}

Finally we can write

\begin{align}
\max \langle \psi | \phi \rangle &= \max \left( \sum_{i=1}^{d_{k-1}} z_i x_i \right) = \frac{1}{\lambda_1 \lambda_2} \max \left( \sum_{i=1}^{d_{k-1}} \bar{z}_i \bar{x}_i \right) = \\
&= d_{k-1} \sqrt{p(0 \to 0) p(1 \to 1)} = \sqrt{\text{Tr} \left[D_k D_k^\dagger \right]} \sqrt{\text{Tr} \left[A_{k-1} A_{k-1}^\dagger \right]}.
\end{align}

From Eq. (D.13) we see that the maximum value of $\text{Tr} \left[D_k A_{k-1}^\dagger \right]$ is equal to the product $\sqrt{\text{Tr} \left[D_k D_k^\dagger \right]} \sqrt{\text{Tr} \left[A_{k-1} A_{k-1}^\dagger \right]} = d_{k-1} \sqrt{p(0 \to 0) p(1 \to 1)}$. One can see that in previous calculations we did not assume nothing about exact values of $x_i$ and $z_i$, where $1 \leq i \leq d_{k-1}$. We see that we saturate the inequality (D.13) when matrices $D_k$ and $A_{k-1}$ (respectively vectors $|\psi\rangle$, $|\phi\rangle$) are parallel.
It seems that for an arbitrary states transformation, there are many unitaries that realize some transition. We need the one that, which has the largest probabilities \( p(i \to j) \), as this would improve the transfer of coherences and possibly saturate bounds from Eq. (D.13). Then we can ask: Are we able to construct a unitary transformation \( U \) where every blocks \( D_k \) and \( A_{k-1} \) saturates the equality from Eq. (D.13)? The answer for this question in the case of a two-level system is like in Figure 8. One can note that there is also another possibility of constructing a block-unitary transformation \( U \) which saturates the inequality (D.13) and does not have the "brute" form, i.e. we do not put only zeros and ones on the diagonal in the block \( A_n \). It can be checked that filling the first block (left, upper corner) with \( \text{diag} \) and some transformation/damping of coherences, which comes from the energy conservation relation. From the preservation of the Gibbs state on a diagonal of input states, positivity of this channel, we get that the Gibbs state needs to be preserved and the coherences need to be damped.

We need to check what is the relation between \( p(0 \to 0) > p(1 \to 1) \). It is presented in the following lemma.

**Lemma 6.** For the qubit case one has:

\[
p(0 \to 0) > p(1 \to 1),
\]

and

\[
p(1 \to 0) > p(0 \to 1).
\]

**Proof.** From the preservation of the Gibbs state one has

\[
p(i \to j) \over p(j \to i) = e^{-\beta(E_j - E_i)} < 1,
\]

which immediately tells us that \( p(1 \to 0) > p(0 \to 1) \). Now, using a relation between \( p(0 \to 0) \) and \( p(1 \to 1) \):

\[
d_k p(1 \to 1) + (d_{k-1} - d_k) = d_{k-1} p(0 \to 0),
\]

where \( d_i \) are dimensions of degeneracies of the bath, we have that

\[
\begin{align}
d_{k-1} p(0 \to 0) - d_{k-1} &= d_k p(1 \to 1) - d_k p, \\
d_{k-1} (p(0 \to 0) - 1) &= d_k (p(1 \to 1) - 1), \\
\frac{d_{k-1}}{d_k} &= \frac{p(1 \to 1) - 1}{p(0 \to 0) - 1}.
\end{align}
\]

We know that Thermal Operations preserve the Gibbs state which equivalently means that \( \frac{d_{k-1}}{d_k} > 1 \) which gives \( p(0 \to 0) > p(1 \to 1) \) q.e.d.

The above lemma is used in the construction of the optimal unitary for coherences transport that is presented in Fig. 8.

---

5. Full characterization of qubits state-to-state transitions: classical channel analogy

In this section we give formulas which allow us to write probabilities \( p(i \to j) \) of the level transitions, in terms of initial and final state elements of our case-study example, written in the energy-basis, \( p, q, 1 - p, 1 - q \), using an analogy of the classical channel (we have a channel that preserves the Gibbs state on a diagonal of input states, and some transformation/damping of coherences, which comes from the energy conservation relation). From the positivity of this channel, we get that the Gibbs state needs to be preserved and the coherences need to be damped. To do this, let us consider a one block of the qubit in the initial state (see, Fig. 6). Due to the transformation \( U \) we obtain as a result, an output state in the form

\[
\sigma = \left( \frac{C p}{\bar{A}^{k-1}} + \frac{D p}{\bar{A}^{k-2}} \right) \otimes \left( \frac{p}{\bar{A}^{k-1}} + \frac{B p}{\bar{A}^{k-2}} \right),
\]

(D.18)
FIG. 8: (Color online) In this figure we present an optimal block-unitary transformation. We start our construction from unitary block $U_n$. Firstly on diagonal of submatrix $A_n$ we put some number of zeros and ones to satisfy constraint $\text{Tr} \left[A_n A_n^\dagger\right] = d_n p(1 \to 1)$. The numbers of zeros and ones tell us how much energy levels we want to move and leave untouched. On the off-diagonal blocks of $U_n$ we put ones to complete full block to unitary. Secondly, diagonal of submatrix $D_n$ we choose in such a way to obtain it parallel to diagonal of $A_n$, i.e. we rewrite diagonal of $A_n$ and put ones on the tail (we do not have more energy levels to move). The number of ones on diagonal of $D_n$ is equal to $d_n p(1 \to 1) + (d_{n-1} - d_n) = d_{n-1} p(0 \to 0)$. Now let us take submatrix $A_{n-1}$ in $U_{n-1}$. Diagonal of $A_{n-1}$ has to be parallel to diagonal of $D_n$ and of course satisfy condition $l_n \gamma^2 = d_{n-1} p(1 \to 1)$, where $l_n = d_{n-1} p(0 \to 0)$ is the number of ones in the submatrix $D_n$, so we have to choose $\gamma = \sqrt{\frac{p(1 \to 1)}{p(0 \to 0)}}$. We continue this procedure for the rest blocks in our unitary transformation. One can see that this construction is valid only in the regime $p(1 \to 1) < p(0 \to 0)$ (see, Lemma 6). In this figure $\gamma_1 = \sqrt{1 - \gamma}$ and $\gamma_2 = \sqrt{1 - \gamma^2}$.
In this figure we present an arbitrary block $U_k$ of a general block-unitary transformation from Fig. 8. Let us consider a submatrix $D_k$. The number of zeros is equal to the numbers of zeros in our starting point - submatrix $A_n$. Then number of $\gamma^k$ is equal to $l_n$, number of $\gamma^{k-1}$ is equal to $d_n - 2 - d_n - 1$ and finally number of 1’s in the tail is equal to $d_k - 1 - d_k$. We define $\gamma_i$ as $\sqrt{1 - \gamma_i}$.

where $A = A_{k-1}A_{k-1}^t$, $B = B_{k-1}B_{k-1}^t$, $C = C_kC_k^t$, $D = D_kD_k^t$, and $\bar{p} + p = 1$, $\bar{q} + q = 1$. Thanks to this and equation (D.18) we can write

$$
\frac{\bar{p}}{d_k} \text{Tr} C + \frac{p}{d_{k-1}} \text{Tr} D = q,
$$

$$
\frac{\bar{p}}{d_{k-1}} \text{Tr} A + \frac{p}{d_{k-2}} \text{Tr} B = \bar{q}.
$$

Now we can rewrite this in terms of probabilities $p_{ij}$ using the preservation of the Gibbs state relation obtaining

$$
q = p(0 \to 0) + \bar{p} e^{\beta \Delta E} p(0 \to 1),
$$

$$
\bar{q} = p e^{-\beta \Delta E} p(1 \to 0) + \bar{p} p(1 \to 1).
$$

(D.20)

Because of the constraints, coming from the unitarity of our block matrix, $p(1 \to 1) + p(1 \to 0) = 1$ and $p(0 \to 0) + p(0 \to 1) = 1$ we can easily express probabilities $p(i \to j)$ in terms of $\bar{p}, p, \bar{q}, q$

$$
p(0 \to 0) = \frac{1}{d_{k-1}} \text{Tr} D = \frac{q - \bar{p} e^{\beta \Delta E}}{p - \bar{p} e^{\beta \Delta E}},
$$

$$
p(1 \to 1) = \frac{1}{d_{k-1}} \text{Tr} A = \frac{\bar{q} - p e^{-\beta \Delta E}}{\bar{p} - p e^{-\beta \Delta E}}.
$$

(D.21)

Thanks to the above formulas we can rewrite the term $\sqrt{p(0 \to 0)p(1 \to 1)}$ from the condition (D.3) using probabilities $p, q$:

$$
\sqrt{p(0 \to 0)p(1 \to 1)} = \frac{\sqrt{(q - \bar{p} e^{\beta \Delta E})(p - \bar{q} e^{\beta \Delta E})}}{|p - \bar{p} e^{\beta \Delta E}|}.
$$

(D.22)

### 6. No-go for higher dimensional systems?

In this section we present results conjecturing that for higher dimension states ($d > 2$) it is impossible to saturate the bounds for processing of coherences. We do this by considering a class of Gibbs-preserving processes called
quasi-cycles from which we choose one particular as our case-study example. The quasi-cycle can be defined as follows, we choose an order of levels and put them on a circle, fixing a direction. The aim of the process is to take all states from the group of states with the largest energy and shift them to the states with the energy level in the chosen direction.

Our case-study example is a three-level system and a quasi-cycle from Figure 10.

![Figure 10](image)

**Fig. 10:** (Color online) A $0 \rightarrow 1 \rightarrow 2$ three-level quasi-cycle (with energy level 0, 1 and 2) for which it is showed that the fundamental limit for coherences transport can not be reached. The quasi-cycle is set so forbidden transitions are $2 \rightarrow 2$, $0 \rightarrow 2$, $2 \rightarrow 1$ and $1 \rightarrow 0$, which means that their corresponding probabilities $p_{22}, p_{21}, p_{10}$ and $p_{02}$ are equal to zero, and the probability of transition $2 \rightarrow 0$, $p_{20}$, is equal to 1.

At the beginning, let us show that there is a least one family of initial and final states (with given diagonal elements) for which the realization of the quasi-cycle from Fig. 10 is unique.

**Fact 7.** No other process has the same effect for a qutrit-to-qutrit transition between a family of states with given diagonal elements $(0, \frac{1}{2}, \frac{1}{2}) \rightarrow (e^{-\beta \Delta E_{21}}/2, 1-e^{-\beta \Delta E_{21}}/2, 1-e^{-\beta \Delta E_{20}}/2)$ as the quasi-cycle from Fig. 10.

Before proving this, let us observe the following

**Lemma 8.** In the quasi-cycle from Fig. 10 all probabilities are constrained and fixed. The are

\[
p(2 \rightarrow 2) = 0, p(2 \rightarrow 1) = 0, p(2 \rightarrow 0) = 1, \\
p(1 \rightarrow 2) = e^{-\beta \Delta E_{21}}, p(1 \rightarrow 1) = 1 - e^{-\beta \Delta E_{21}}, p(1 \rightarrow 0) = 0, \\
p(0 \rightarrow 2) = 0, p(0 \rightarrow 1) = e^{-\beta \Delta E_{20}}, p(0 \rightarrow 0) = 1 - e^{-\beta \Delta E_{20}}. 
\]  
(D.23)

**Proof.** Let us start with writing conditions for probabilities of level transitions coming from the unitarity constrains

\[
p(2 \rightarrow 2) + p(2 \rightarrow 1) + p(2 \rightarrow 0) = 1, \\
p(1 \rightarrow 2) + p(1 \rightarrow 1) + p(1 \rightarrow 0) = 1, \\
p(0 \rightarrow 2) + p(0 \rightarrow 1) + p(0 \rightarrow 0) = 1. 
\]  
(D.24)

From the preservation of a Gibbs state, we also have that

\[
p(2 \rightarrow 2) + p(1 \rightarrow 2) e^{-\beta \Delta E_{12}} + p(0 \rightarrow 2) e^{-\beta \Delta E_{02}} = 1, \\
p(2 \rightarrow 1) e^{-\beta \Delta E_{21}} + p(1 \rightarrow 1) + p(0 \rightarrow 1) e^{-\beta \Delta E_{01}} = 1, \\
p(2 \rightarrow 0) e^{-\beta \Delta E_{20}} + p(1 \rightarrow 0) e^{-\beta \Delta E_{10}} + p(0 \rightarrow 0) = 1, 
\]  
(D.25)

where $\Delta E_{ij}$ is an energy difference between levels $i$ and $j$ of a qutrit. Comparing Eq. (D.24) with (D.25) we obtain
Lemma 10. That

\[ p(1 \to 2) e^{-\beta \Delta E_{12}} + p(0 \to 2) e^{-\beta \Delta E_{02}} = p(2 \to 1) + p(2 \to 0), \]
\[ p(2 \to 1) e^{-\beta \Delta E_{21}} + p(0 \to 1) e^{-\beta \Delta E_{01}} = p(1 \to 2) + p(1 \to 0), \]
\[ p(2 \to 0) e^{-\beta \Delta E_{20}} + p(1 \to 0) e^{-\beta \Delta E_{10}} = p(0 \to 2) + p(0 \to 1). \] (D.26)

For our quasi-cycle, \( p(2 \to 2), p(2 \to 1), p(1 \to 0), \) and \( p(0 \to 2) = 0, \) which immediately imposes \( p(2 \to 0) = 1. \) Then, inserting it into Eqs. (D.24, D.25, D.26) and solving them, we get that all other probabilities are fixed too and given by

\[ p(2 \to 2) = 0, p(2 \to 1) = 0, p(2 \to 0) = 1, \]
\[ p(1 \to 2) = e^{-\beta \Delta E_{21}}, p(1 \to 1) = 1 - e^{-\beta \Delta E_{21}}, p(1 \to 0) = 0, \]
\[ p(0 \to 2) = 0, p(0 \to 1) = e^{-\beta \Delta E_{20}}, p(0 \to 0) = 1 - e^{-\beta \Delta E_{20}}. \] (D.27)

q.e.d. It implies that there is no freedom in choosing the rest of probabilities, the ones that are set to 0 and 1 already constrain and fix the rest.

With the above, the proof of Fact 7 is quite straightforward. From the relation \( \sum_i d_i p(i \to j) = d_j \) [2], we can build a stochastic matrix with probabilities \( p(i \to j), \) which tells us whether, under a given input, the Gibbs state is preserved on the diagonal of a state. This effectively tells us which state-to-state transformations are possible under a given quasi-cycle from the point of view of their diagonal inputs (preservation of the Gibbs state). For our state we have,

\[
\begin{bmatrix}
  p(2 \to 2) & p(2 \to 1) & p(2 \to 0) \\
  p(1 \to 2) & p(1 \to 1) & p(1 \to 0) \\
  p(0 \to 2) & p(0 \to 1) & p(0 \to 0)
\end{bmatrix}
\begin{bmatrix}
  0 \\
  1 \\
  1
\end{bmatrix}
= \begin{bmatrix}
  e^{-\beta \Delta E_{21}} \\
  1 - e^{-\beta \Delta E_{21}} + e^{-\beta \Delta E_{20}} \\
  1 - e^{-\beta \Delta E_{20}}
\end{bmatrix},
\]

where, to obtain the final values, we put the probabilities from Eq. (D.23).

Due to the constrains on the matrix from the proof of Lemma 8 (and the unitary matrix, constructed later in the text, from \( p(i \to j) \) from Eq. (D.31)), there is no freedom in changing \( p(i \to j), \) which proves the uniqueness.

Before going further with the analyze of the state-to-state transitions, let us recall some auxiliary lemma proved by von Neumann [12] and Fan [13], which will appear to be crucial in our further considerations. The lemma gives a maximization over \( \text{Tr} X Y^\dagger \), where \( X, Y \) are some matrices, with respect to all possible rotations over \( X \) and \( Y \).

Lemma 9. If \( X \) and \( Y \) are \( n \times n \) complex matrices, \( W \) and \( V \) are \( n \times n \) unitary matrices, and \( \sigma_1 \geq \cdots \geq \sigma_n \geq 0 \) denotes ordered singular values, then

\[ |\text{Tr} WXY| \leq \sum_{i=1}^{n} \sigma_i(X)\sigma_i(Y) \] (D.28)

and

\[ \sup_{W,Y} |\text{Tr} WXY| = \sum_{i=1}^{n} \sigma_i(X)\sigma_i(Y). \] (D.29)

We are ready now to summarize our findings in the following

Lemma 10. Consider a unitary matrix \( U = \bigoplus_k U_k \), written in the block form, where for a fixed block \( k \), one has

\[
U_k = \begin{pmatrix}
  u_{(22)}^k & u_{(21)}^k & u_{(20)}^k \\
  u_{(12)}^k & u_{(11)}^k & u_{(10)}^k \\
  u_{(02)}^k & u_{(01)}^k & u_{(00)}^k
\end{pmatrix},
\]

where, for each \( k, u_{(ij)}^k \) is a matrix of dimension \( d_i \times d_j \). Assuming that the dimensions are such that \( d_0^k > d_1^k > d_2^k \), and \( u_{(22)}^k = 0, u_{(21)}^k = 0, u_{(10)}^k = 0, u_{(02)}^k = 0 \), and \( \text{Tr} u_{00}^k u_{00}^\dagger \neq \text{Tr} u_{11}^k u_{11}^\dagger \), there is no such a \( U \) that saturates the Cauchy-Schwarz...
inequality of the form $\text{Tr} u_{(00)}^k u_{(11)}^{k+l} \leq \sqrt{\text{Tr} u_{(00)}^k u_{(00)}^\dagger \text{Tr} u_{(11)}^{k+l} u_{(11)}^{k+l}}$, where $l$ is an integer, such that $d_0^k = u_1^{k+l}$, one always has a strict inequality.

Lemma 10 implies the following:

**Corollary 11.** There is no such an energy-preserving unitary $U$ that commutes with the total Hamiltonian of the system-bath setup, where one has a generic heat bath that follows assumptions from Secs A and C from Appendix and realizes the state-to-state from transition from Fact 7 in a precise way (no disturbance and approximations in reaching the final state) that leads to the best possible processing of coherences, which means saturation of the bounds from Proposition 4 (in that case $|\alpha| = \sqrt{p(0 \rightarrow 0)p(1 \rightarrow 1)}$).

To prove Corollary 11, one needs to adapt the mathematical structures from Lemma 10 to states transitions under Thermal Operations and connect it with the facts already shown in this section.

1. The unitary matrix from Lemma 10 can be treated as an energy-preserving matrix that is used to implement state-to-state transitions under Thermal Operations as in Eq. (B.1).

2. The channel that realizes state-to-state transition from Fact 7 is unique, and its transition probabilities $p(i \rightarrow j)$ correspond to terms $\text{Tr} u_{ij} u_{ij}^\dagger$ from Lemma 10.

3. The generic heat bath (laws of degenerations from Secs A and C) gives that the dimensions of blocks ($d_0^k > d_1^k > d_2^k$) should be strict inequalities.

4. The Cauchy-Schwarz inequality can be identity with the bounds from Proposition 4 (since, in this state-to-state transition, $p(2 \rightarrow 2)$, there is only one bound that one can try to saturate $\pm |\alpha| = \sqrt{p(0 \rightarrow 0)p(1 \rightarrow 1)}$).

**Proof of Lemma 10.** Let us fix $k^{th}$ energy block, then a general unitary transformation has a form

$$U_k = \begin{pmatrix}
    u_{(22)}^k & u_{(21)}^k & u_{(20)}^k \\
    u_{(12)}^k & u_{(11)}^k & u_{(10)}^k \\
    u_{(02)}^k & u_{(01)}^k & u_{(00)}^k
\end{pmatrix},$$  \hspace{1cm} (D.31)

where numbers in the brackets correspond to transitions between levels of our system. To obtain the result, we need a simpler form of the matrix $U_k$. Thanks to Lemma 9, we know that the maximal value of $\text{Tr} u_{(00)}^k u_{(11)}^{k+l}$ is equal to $\sum_i \sigma_i \left(u_{(00)}^k\right) \sigma_i \left(u_{(11)}^{k+l}\right)$, where singular values are taken is a non-increasing order. This allows us to consider only singular values of $u_{(00)}^k$ and $u_{(11)}^{k+l}$, because we want to know maximal possible values of trace and compare it with the bound that comes from Proposition 4. From the general theory we know that it saturates when either the first or the second vector is a multiple of the other. So, to obtain the result, we have to show that the vector constructed from non-increasing ordered singular values of $u_{(00)}^k$ is not proportional to the vector constructed in the same way from the block $u_{(11)}^{k+l}$. We show this using an explicit form of our quasicycle from Figure 10 and unitary constraints $U_k U_k^\dagger = U_k^\dagger U_k = 1$. From the form of our quasicycle one can see that blocks which correspond to zero probabilities of transition are represented by zero matrices. Indeed constraints $\text{Tr}(u_{(ij)}^k (u_{(ij)}^k)^\dagger) = 0$ implies that $u_{(ij)}^k = O$, where $O$ denotes zero matrix. In our case we have that $u_{(22)}^k = u_{(21)}^k = u_{(10)}^k = u_{(20)}^k = O$ and the matrix $U_k$ form (D.31) looks like

$$U_k = \begin{pmatrix}
    O & O & u_{(20)}^k \\
    u_{(12)}^k & u_{(11)}^k & O \\
    O & u_{(01)}^k & u_{(00)}^k
\end{pmatrix}.$$  \hspace{1cm} (D.32)

In the next step we use singular value decomposition (SVD) to $u_{(11)}^k$ and $u_{(00)}^k$. Thanks to this we can write $u_{(11)}^k = A_{(11)}^k \Sigma_{(11)}^k (B_{(11)}^k)^\dagger$ and $u_{(00)}^k = A_{(00)}^k \Sigma_{(00)}^k (B_{(00)}^k)^\dagger$, where $A_{(ii)}^k, B_{(ii)}^k$ for $i = 0, 1$ are rectangular, unitary matrices and $\Sigma_{(00)}, \Sigma_{(11)}$ are square, diagonal matrices with singular values as entries. Using SVD we can define
new unitary matrix $\tilde{U}_k$ which gives us the same probability transitions (since $\text{Tr} \ u_{ij} u_{ij}^\dagger = \text{Tr} \ Sigma_{ij} \Sigma_{ij}$), but it is simpler to analysis:

$$\tilde{U}_k = \begin{pmatrix}
(A_{22}^k)^\dagger & O & O & O \\
O & (A_{11}^k)^\dagger & O & O \\
O & O & (A_{00}^k)^\dagger & O \\
O & O & O & \Sigma_{00}^k \\
\end{pmatrix} \begin{pmatrix}
O & u_{12}^k & O & (B_{22}^k)^\dagger \\
O & u_{11}^k & O & B_{11}^k \\
O & u_{01}^k & u_{00}^k & B_{00}^k \\
\end{pmatrix}$$

Indeed such transformation ensures that main blocks of $\tilde{U}_k$ have diagonal form, namely all diagonal blocks are equal to $\Sigma_{(ii)}^k$.

Now we show that singular values of the main blocks are equal to zero or one. Because now we deal with nonzero probabilities it is obvious that some of the singular values of the main have to be strictly positive. It is also important to mention that without lose of generality we rearrange rows of $\tilde{U}_k$ in such a way that singular values are in decreasing order. We also interpret rows and columns of matrix $\tilde{U}_k$ as a vectors $|r_i\rangle$ and $|c_l\rangle$ respectively. Because of unitarity conditions these vectors have to be orthonormal, i.e. $\langle r_i | r_j \rangle = \delta_{ij}$ and $\langle c_l | c_j \rangle = \delta_{lj}$. Let us take row $|r_i\rangle$ which posses nonzero singular value $\sigma_i$, for example from main block $\Sigma_{11}^k$. Computing scalar product of this vector $|r_i\rangle$ with any other row vector $|r_j\rangle$, where $d_k + d_{k-1} < j \leq d_k + d_{k-1} + d_{k-2}$, together with above mentioned condition $\sigma_i \neq 0$ we can conclude that column vector which contains singular value $\sigma_i$ has only one nonzero element which is our $c_l$. Using normalization constraint $\langle r_i | r_i \rangle = 1$ we have that $\sigma_i = 1$. This same argumentation can be used to the rest of nonzero singular values and see that only possible values of all singular values are zero or one.

In the last step we have to show that vector constructed from non-increasing ordered singular values of $u_{00}^k$ is not proportional to vector constructed in the same way, but from the block $u_{11}^k$. We know that these two blocks determine different probabilities $p_{00}$ and $p_{11}$ which due to equation (D.23) have to be different. Together with knowledge that all positive singular value are equal to one we can say that vectors constructed in an aforementioned way have different length so they cannot saturate the bound form Eq. (4).

**Remark 12** One can notice that one of the possible realization of unitary transformation $U_k$ in Eq. (D.31) for the quasi-cycle from Fig. 10 is a realization in the so-called "brute" form. It means that all nonzero elements of $U_k$ are equal to one. Then every such a transformation can be written as a direct sum of permutation matrices

$$U_k = \left( \bigoplus_{\pi} V(\pi) \right) \oplus 1$$

for a certain $\pi \in S(3)$. The identity in Eq. (D.34) follows from the fact that some of the levels are untouched. Of course, that realization is quite harmful for coherences, and is far from saturating the inequality.

In the end, we want to conjecture the following

**Conjecture 13.** Corrolary 11 is true also if the transition $\rho \rightarrow \sigma$ is realized in the perturbed way, and instead of the final state $\sigma$ one obtains a state $\sigma'$, such that $|\sigma - \sigma'| < \delta$, where $\delta$ is small, i.e. probabilities of transitions $p(i \rightarrow j)$ that previously were equal to 0, now are equal to $p(i \rightarrow j) = \epsilon$, and other probabilities are also respectively change. Summing up, there is no such a channel that realizes the state-to-state transition from Fact 7 in the most friendly way for coherences, one is not able to reach the fundamental limit for a limimal coherences damping.

The probabilities look then as follows

**Fact 14.** When we set the probabilities $p(2 \rightarrow 2), p(2 \rightarrow 1), p(1 \rightarrow 0)\text{and}p(0 \rightarrow 2)$ (that previously, in the exact state-to-state transition were equal to 0) to be all equal to $\epsilon$, where $\epsilon$ is small, the other probabilities of the perturbed version of the
quasi-cycle $2 \rightarrow 1 \rightarrow 0$ from Fig. 10 are all fixed and equal to

\begin{align*}
p(2 \rightarrow 2) &= \epsilon, p(2 \rightarrow 1) = \epsilon, p(2 \rightarrow 0) = 1 - 2\epsilon, \\
p(1 \rightarrow 2) &= e^{-\beta \Delta E_{21}} (1 - \epsilon) - e^{-\beta \Delta E_{10}} \epsilon, p(1 \rightarrow 1) = (1 - e^{-\beta \Delta E_{21}})(1 - \epsilon) - e^{\beta \Delta E_{10}} \epsilon, p(1 \rightarrow 0) = \epsilon, \\
p(0 \rightarrow 2) &= \epsilon, p(0 \rightarrow 1) = (e^{-\beta \Delta E_{20}})(1 - 2\epsilon) + (e^{-\beta \Delta E_{10}} - 1)\epsilon, p(0 \rightarrow 0) = 1 - \epsilon - (1 - \epsilon)e^{-\beta \Delta E_{20}} + e^{\beta \Delta E_{10}} \epsilon. \\
\end{align*}

This construction is sufficient to search for a counterexample (that in this quasi-cycle, the previously impossible saturation of the bound for coherences is possible). We examine many construction, which should be the most crude forms of a perturbation of the unitary matrix, ie, in blocks $U_{ij}^k$ of $U$ that correspond to probabilities equal to zero, we put some number of perturbation represented by $\sqrt{\epsilon}$ on a diagonal of the block, and this constructions always lead us to the previously considered case (the one without the perturbation), since the matrix elements of the unitary matrix $U$ are then equal to 0 or 1, or are $\epsilon$-closed. Of course, a deeper analysis is needed to find a counter-example, or to analytically verify our conjecture.

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