On the role of the quantum coherence in thermodynamic work

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Quantum coherence is commonly viewed as a quantum resource permitting to obtain processes classically inhibited. Here we study the role that the quantum coherence plays in performing thermodynamic work with processes generated through the external control of some parameters. In order to do this, we take in exam a general active quantum state and we isolate in its ergotropy the contribution coming from the initial quantum coherence with respect to the energy eigenstates. Such ergotropy coherence is shown to be related to the quantum relative entropy of coherence through an inequality which involves the completely passive state connected to the initial state. Finally, we extend the analysis to a general out-of-equilibrium process and we propose how take in account in the statistics of work the effects of the initial quantum coherence.

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Introduction – Thermodynamics of physical processes and how they are affected by the quantumness of the nature has received a big attention in the last decades [1,2]. In this context quantum coherence will undoubtedly play a fundamental role, it is strictly related to irreversible work [3,4], and makes it possible to create quantum correlations which can be employed in work extraction [5].

Recently quantum coherence has been studied and fully characterized as a genuine quantum resource in performing useful tasks, and it is commonly quantified by the so-called quantum relative entropy of coherence [6]. Certainly its role in thermodynamics has not be fully understood, and it has been also examined and exploited with the aim to acquire a gain otherwise classically inhibited [7,8].

We recall that in a typical out-of-equilibrium process performed by the control of an external parameter, the work done follows a statistics which is constrained by fluctuations theorems when certain initial conditions are satisfied [9,10]. For taking in account quantum fluctuations different schemes have been proposed, among which a two measurements scheme is commonly adopted [11]. It is well known [12] that in this invasive scheme the first measurement of the energy destroys the initial coherence in the energy eigenstates and quantum coherence does not disturb the statistics of the work.

On the other hand, a state with quantum coherence is active and it is characterized by a non zero quantum ergotropy [13], which is equal to the maximum work extractable by performing unitary cycles.

In this letter we aim to clarify the role played by the quantum coherence in the work performed in these processes. We take in exam an active state and we isolate a contribution to the ergotropy strictly related to the initial quantum coherence of the state with respect the energy eigenstates. In order to do that we consider the extraction of work through incoherent operations which do not change the quantum coherence. By maximizing the work extracted we isolate a residual amount of work which is not extracted through incoherent operations and we refer to it as ergotropy coherence. This work is as well related to the quantum relative of coherence though an inequality which involves the correspondent completely passive state [14]. Typically the equality is obtained only for a certain class of initial states which we have identified for the case of a three levels system. In conclusion, we observe how the problem incurring with the first measurement of the energy can be avoided and we show how the cycle that we have introduced allows to identify the contribution to the statistics of work coming from the initial quantum coherence in a general out of equilibrium process.

Work extraction – We consider a quantum system with the Hamiltonian $H$. If the system is prepared in the state $\rho$ the work that can be extracted by performing a unitary cycle, i.e. a cyclic control of the parameters of the system, cannot exceed the ergotropy $W(\rho)$, such that the work $W(\rho, U) = \text{Tr}\{\rho H\} - \text{Tr}\{U \rho U^\dagger H\} \leq W(\rho)$ for any unitary $U$.

The Hamiltonian $H$ and the state $\rho$ can be always expressed as

$$H = \sum_{k=1}^N \epsilon_k |k\rangle \langle k|, \quad \rho = \sum_{k=1}^N r_k |r_k\rangle \langle r_k|$$

with $r_k \geq r_{k+1}$ and $\epsilon_k \leq \epsilon_{k+1}$. If the energy is degenerate, we define the basis $|k\rangle$ so that $\rho$ is diagonal in every degenerate subspace.

The ergotropy can be written as

$$W(\rho) = \sum_{kj} r_k (|\langle j | r_k\rangle|^2 - \delta_{kj}) \epsilon_j$$

A unitary $U_E$ which allows to extract the ergotropy depends on the state $\rho$ and it remains defined at least of unitary transformations in the degenerate subspaces, defining an equivalence class of unitary transformations.

We start by study the relation between the ergotropy and the quantum coherence of the state $\rho$. 

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We recall that the quantum coherence of a state \( \rho \) in the reference basis \( \{|j\rangle\}_{j=1}^N \), can be quantified by considering the quantum relative entropy of coherence defined as\[^{[6]}\]

\[
C(\rho) = \min_{\eta \in I} D(\rho||\eta)
\]

(2)

where the quantum relative entropy \( D(\rho||\eta) \) is defined by \( D(\rho||\eta) = \text{Tr} \{ \rho (\ln \rho - \ln \eta) \} \), and \( I \) is the set of incoherent states, so that a generic \( \eta \in I \) reads \( \eta = \sum_k \eta_k |k \rangle \langle k | \). The state \( \eta \) minimizing the right side of Eq. (2) is the incoherent state \( \eta = \Delta(\rho) \), where \( \Delta \) is the dephasing operator defined by \( \Delta(\rho) = \sum_i |i \rangle \langle i | \langle i | \). In detail, the quantum relative entropy of coherence can be expressed in terms of the Von Neumann entropy \( S(\rho) = -\text{Tr} \{ \rho \ln \rho \} \), as \( C(\rho) = S(\Delta(\rho)) - S(\rho) \).

Then we consider the constrain that in the work extraction cycles the coherence quantified by the relative entropy \( C(\rho) \) remains unchanged. Due to this constrain the ergotropy cannot be always obtained, and the cy-


gers.

\[ \eta = \Delta(\rho), \]

We proceed with the analysis by considering two simple models, which are a two and a three levels system.

**Examples:** We consider a qubit having energies \( \epsilon_1 = 0 \) and \( \epsilon_2 = 1 \). In this case we note that the equality in Eq. (5) holds, furthermore the ergotropy coherence \( W_c \) can be also related to the \( l_1 \) norm of coherence \( \| \) which results to be \( C_{l_1}(\rho) = \| (1|\rho \rangle \| ) \) through the equation

\[
W_c(\rho) = \frac{1}{2} \left( \sqrt{2P(\rho)} - 1 - \sqrt{2P(\rho) - 1} - C_{l_1}^2(\rho) \right)
\]

(6)

where \( P(\rho) = \text{Tr} \{ \rho^2 \} \) is the purity of the state \( \rho \).

The work \( W_C(\rho) \) is maximum if and only if \( \rho \) is a maximally coherent state with \( C_{l_1} = 1 \) and \( P = 1 \). From Eq. (6) we note that the inequality \( W_c(\Lambda(\rho)) \leq W_c(\rho) \) is not satisfied for every incoherent operations \( \Lambda \), such that \( W_c(\rho) \) is not a monotone of coherence \( \| \). For a given value of the purity \( P \), the coherence takes its maximum value for mixed states \( \rho \) such that \( p_1 = p_2 = 1/2 \), for which we have \( P = (1 + C_{l_1}^2)/2 \) and \( W_c = C_{l_1}/2 \).

We proceed by investigating the relation with the relative entropy \( C(\rho) \) expressed by the inequality in Eq. (4). We consider a three levels system with energy levels \( \epsilon_1 = 0 \), \( \epsilon_2 = \epsilon \) and \( \epsilon_3 = 1 \) and the difference of the two sides of the inequality \( \Delta W_c = \beta^{-1} \left( C(\rho) + \sum_k p_k \ln \left( \frac{p_k}{\sigma_k} \right) \right) - W_C(\rho) \geq 0 \). This difference can be written as \( \Delta W_c = r_2 \epsilon + r_3 - \frac{\epsilon e^{-\beta \epsilon} + e^{-\beta \epsilon}}{1 + e^{-\beta \epsilon}} \) where the inverse temperature \( \beta \) is a solution of the non-linear equation \( \beta (e^{-\beta \epsilon} + e^{-\beta \epsilon})/Z = S - \ln Z \), where \( S = -\sum_k \ln r_k \) is the von Neumann entropy and \( Z = 1 + e^{-\beta \epsilon} + e^{-\beta \epsilon} \) the partition function. By numerically solving the non linear equation it results that \( \Delta W_c \) is equal to zero only for a certain set of initial states (see Fig. 1).

**Work statistics** - Having analysed the role of quantum coherence in an active state \( \rho \), we now take in exam a general out-of-equilibrium process with time evolution \( U(t) \) generated by the time dependent Hamiltonian \( H(t) = \sum_k \epsilon_k(t) |k(t) \rangle \langle k(t) | \) with \( H(0) = H \) trough the external control of some system parameters. When the initial state \( \rho \) is a stationary state, i.e. such that
[\rho, H] = 0$, the average work done can be expressed in terms of a distribution probability $p(w)$ as

$$
\langle w \rangle = \text{Tr} \{H(t)\rho(t)\} - \text{Tr} \{H\rho\} = \int p(w)wdw
$$

where $\rho(t) = U(t)\rho U^\dagger(t)$ and the distribution probability of the work is $p(w) = \sum_k p_\sigma(k) \langle k(t)|U(t)|j(t)\rangle^2 \delta(w - \epsilon_k(t) + \epsilon_j)$. Obviously if the initial state $\rho$ is not stationary the relation does not hold.

Anyway it can be always connected to a stationary state $\rho_d$ such that $[\rho_d, H] = 0$ through a unitary cycle $V$, such that $\rho = V^\dagger \rho_d V$, and for instance we will consider $V = U_g = U_1 U_c U_1$. In particular the transformation $U_g$ has the following geometrical meaning: by considering the subset $I_g(\rho) \subset I$ of the incoherent states that are unitarily connected to $\rho$, the transformation $U_g$ is the unitary $U$ that minimizes the quantum relative entropy $D(\rho||U\rho U^\dagger)$ such that $U\rho U^\dagger \in I_g(\rho)$.

Indeed the eigenvalues of $\rho$ are invariant under unitary transformations, then a state $\eta \in I_g(\rho)$ can be expressed as $\eta = \sum_k r_\pi(k)|k\rangle \langle k|$. The quantum relative entropy can be expressed as $D(\rho||\eta) = -S(\rho) - \sum_k p_\pi(k) \ln(r_\pi(k))$ such that by choosing $\pi(k) = s(k)$ it takes its minimum value. We have indicated this state with $\rho_d = \sum_k r_\pi(k)|k\rangle \langle k|$, and it is straightforward to show that $\rho_d = U_g\rho U_g^\dagger$ with $U_g = U_1 U_c U_1$.

The two works performed in the processes $\rho_d \rightarrow \rho$ with unitary $V^\dagger$ and $\rho_d \rightarrow \rho(t)$ with unitary $V^\dagger U(t)$ can be obtained from the distributions $p_\sigma(w_c)$ and $p_{\text{tot}}(w_{\text{tot}})$ with obvious definitions. Then the work in the real process $\rho \rightarrow \rho(t)$ with unitary $U(t)$ can be thought as the random variable $w = w_{\text{tot}} - w_c$ having distribution $p(w) = \int p_\sigma(u) p_{\text{tot}}(w + u)du$, where we expect that the work $w_c$ is intimately related to the initial quantum coherence of the state. We note that when $\rho_d$ is a Gibbs state $\rho_d \propto e^{-\beta H}$ the work done $w$ satisfies the fluctuation relation $\langle e^{-\beta(w + w_c)} \rangle = e^{-\beta \Delta F}$ where $\Delta F$ is the usual Helmholtz free energy difference calculated between the final equilibrium state with Hamiltonian $H(t)$ and the initial one which is equal to $\rho_d$.

**Conclusions** - Resuming we have take in exam the contribution in the extractable work which comes from the initial quantum coherence with respect to the energy eigenstates. This led to the definition of a quantum coherence quantifier based on the ergotropy. We have shown that the ergotropy coherence is related to the quantum relative entropy of coherence. Furthermore we have investigate how the statistics of the work is affected by the initial coherence.

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1. M. Campisi, P. Hänggi, and P. Talkner, Rev. Mod. Phys. 83, 771 (2011)
2. S. Vinjanampathy, J. Anders, Contemporary Physics, 57, 545 (2016)
3. G. Francica, J. Goold and F. Plastina, Phys. Rev. E 99, 042105 (2019)
4. J.P. Santos, L.C. Céleri, G.T. Landi and M. Paternostro, npj Quantum Inf 5, 23 (2019)
5. NPJ Quantum Information, 3, 12 (2017)
6. A. Streltsov, G. Adesso and M. B. Plenio, Rev. Mod. Phys. 89, 041003 (2017)
7. K. Korzekwa, M. Lostaglio, J. Oppenheim and D. Jennings, New J. Phys. 18 023045 (2016)
8. M.O. Scully, M.S. Zubairy, G.S. Agarwal, H. Walther, Science 299 862 (2003)
9. C. Jarzynski, Phys. Rev. Lett. 78, 2690 (1997)
10. G. E. Crooks, Phys. Rev. E 60, 2721 (1999)
11. P. Talkner, E. Lutz, and P. Hänggi, Phys. Rev. E 75, 050102(R) (2007)
12. Phys. Rev. Lett. 118, 070601 (2017)
13. A. E. Allahverdyan, R. Balian and Th. M. Nieuwenhuizen EPL 67 565 (2004).
14. R. Alicki and M. Fannes, Phys. Rev. E 87, 042123 (2013)
15. Y. Peng, Y. Jiang, and H. Fan, Phys. Rev. A 93, 032326 (2016).
16. In order to show the inequality of Eq. (1), we note that $W_C(\rho) \leq E(\rho_c) - E(\sigma_C(\beta)) = \sum_k (p_k - \sigma_k) \epsilon_k$. Since $\epsilon_k = -\beta^{-1} \ln \sigma_k + \text{const}$, we have that $W_C \leq \beta^{-1} \sum_k (\sigma_k - p_k) \ln \sigma_k$. Since $S(\sigma_C(\beta)) = S(\rho)$, we have that $W_C \leq \beta^{-1} \sum_k (\sigma_k \ln r_k - p_k \ln \sigma_k)$, from which follows Eq. (1). If $\rho_c = \sigma_C(\beta)$, then $W_C(\rho) = E(\rho_c) - E(\sigma_C(\beta))$, and since $\sigma_k = r_k$ we have Eq. (5).
17. For the qubit system under consideration, we have that $W_C(\rho) = (p_2 - r_2)\epsilon_c$. The smaller eigenvalue of $\rho$ is $r_2 = (1 - \sqrt{1 - 4\det P})/2$, and since the purity reads $P = 1 - 2 \det \rho$, it follows that $r_2 = (1 - \sqrt{2P - 1})/2$. Furthermore $\det P = P_1^2 - P_1^2/4$, from which the smaller population of $\rho$ is $p_2 = (1 - \sqrt{2P - 1 - C_1^2})/2$, and so it follows the Eq. (2).