A comment on a possible inadequacy of new redefinitions of heat and work in quantum thermodynamics

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We analyze the new redefinitions of heat Q and work W recently presented in [arXiv: 1912.01939; arXiv:1912.01983v5] in the quantum thermodynamics domain. According to these redefinitions, heat must be associated with the variation of entropy, while work must be associated with variation of state vectors. Analyzing the behavior of two specific examples, we show some peculiarities of these new redefinitions which, based on the counterexample presented, seems to point to a possible inadequacy of these redefinitions.

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I. INTRODUCTION

The pioneering work of Alicki [1], who introduced the concepts of heat Q and work W for a system interacting weakly with a Markovian reservoir, strongly boosted the area of quantum thermodynamics, not only with regard to its foundations but also concerning the study of thermal machines [2–4] and their definitive limits. For example, efficiency and performance coefficient have been extensively studied in different types of reservoirs [5–10]. The concepts of heat and work introduced by Alicki, however, needed to be revisited and expanded to include situations not foreseen in classical thermodynamics, as for example, initially correlated systems [11, 12] and generalized reservoirs [9, 11, 13, 14].

Although many of these formalisms have a sound theoretical appeal, as they are recent, the case study is important for verifying their compatibility with the framework of quantum thermodynamics as well as if they reproduce results in accordance with quantum thermodynamics. Recently, new redefinitions of heat and work, which aim to generalize the redefinitions as introduced by Alicki, were independently proposed by two groups [15, 16]. These redefinitions are based on the following pillars: (i) the changes that occur in a given system are taken into account in the corresponding reduced density operator. (ii) Changes arising only in the state vector are attributed to work, while changes arising from the entropy of the system are attributed to heat. (iii) To calculate heat the von Neumann entropy is to be used. In this work, we do a case study of these new redefinitions and show some peculiarities that may possibly be indicating an inadequacy of the formalism in [15, 16].

II. NEW REDEFINITIONS FOR WORK AND HEAT

According to the formalism introduced by the authors in Refs. [15, 16], the following protocol must be applied to a system interacting with its surroundings, which we will generally call by reservoir: (i) Given the initial states and the Hamiltonian, we evolve the composite system to find \( \rho_{AB}(t) \). (ii) From \( \rho_{AB}(t) \), we diagonalize \( \rho_A(t) \) to obtain the eigenvalues \( p_i(t) \) and eigenvectors \( |\psi_i(t)\rangle \) in accordance with \( \rho_A(t) = \sum_i p_i(t)|\psi_i(t)\rangle\langle\psi_i(t)| \). (iii) From the eigenvalues \( p_i(t) \) and eigenvectors \( |\psi_i(t)\rangle \) we calculate the work W and heat Q as given by \( dQ_A(t) = tr\sum_i dp_i(t)|\psi_i(t)\rangle\langle\psi_i(t)|H(t) \), and \( dW_A(t) = tr\sum_i p_i(t)d||\psi_i(t)\rangle\langle\psi_i(t)||H(t) \).

In this work we will focus on two simple models: (i) two qubits interacting off-resonance with each other and (ii) a qubit interacting weakly with its surrounding, as dictated by the standard master equation. As we shall show, these two simple examples display a peculiar behavior apparently not consistent with one would expect from a thermodynamics analysis of these interacting systems. In the following section we will explore these examples in details.

III. RESULTS

A. Two qubits interacting off-resonantly

The corresponding Hamiltonian model to the system A and B, including the off-resonant interaction, is

\[ H = \frac{\hbar \omega_0}{2} \sigma_z^A + \frac{\hbar \omega_0}{2} \sigma_z^B + \hbar \omega \sigma_z^A \otimes \sigma_z^B, \]

where \( \hbar \) is the reduced Planck constant, \( \sigma_z^{(A)} \) is the Pauli matrix to the qubit A (B), \( \omega_0 \) is the transition frequency between the two-level system, and \( q \) is the coupling constant of the interaction Hamiltonian. Note that this dispersive interaction do not change the internal energy of the qubits; instead, the interaction energy is stored in correlations produced during the time evolution.

Let us consider the following initial states for systems
A and B [15, 16]:

$$\rho_A(0) = \begin{pmatrix} p & c \\ \bar{c} & 1-p \end{pmatrix}, \quad \rho_B(0) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix},$$  \hspace{1cm} (2)

where in system A the parameter $c$ is only constrained by the positivity of $\rho_A(0)$.

Given these initial states, it is straightforward to obtain the reduced density matrix to the evolved systems $A$:

$$\rho_A(t) = \begin{pmatrix} p & c\cos(2gt) \\ \bar{c}\cos(2gt) & 1-p \end{pmatrix}, \quad \rho_B(t) = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} = \rho_B(0),$$  \hspace{1cm} (3)

For our purpose, we diagonalize this system for $p = \frac{1}{2}$ and $c = \bar{c} = \frac{1}{2}$. The eigenvalues and eigenvectors are found to be

$$\lambda_+(t) = p_1(t) = \sin^2 gt$$  \hspace{1cm} (4)

$$\lambda_-(t) = p_2(t) = \cos^2 gt$$  \hspace{1cm} (5)

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle),$$  \hspace{1cm} (6)

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle),$$  \hspace{1cm} (7)

and then, following the protocol described above we write $\rho_A(t)$ using its instantaneous eigenbasis:

$$\rho_A(t) = \sum_{i=1}^{2} p_i(t) |\psi_i\rangle \langle \psi_i| = \sin^2 gt |\psi_1\rangle \langle \psi_1| + \cos^2 gt |\psi_2\rangle \langle \psi_2|. \hspace{1cm} (8)$$

Note that, to these parameters, different from the eigenvalues, the eigenkets do not depend on time. Also, note that $\sigma_A^2 |\psi_{1(2)}\rangle = |\psi_{2(1)}\rangle$). Next, we calculate both $W$ and $Q$ according to Ref. [15, 16]. To the work $W$:

$$dW_A(t) = \sum_i p_i(t)d(|\psi_i|H_A|\psi_i|) = 0, \hspace{1cm} (9)$$

which is zero both because the eigenvector is time-independent and because $|\psi_i|H_A|\psi_i| = 0$. Therefore, as $W_A(t = 0) = W_A(t = T)$, $W_A$ is zero for all $t$’s. To the heat $Q$:

$$d(Q_A) = \sum_{i=1}^{2} dp_i(t)|\psi_i|H_A|\psi_i| = 0, \hspace{1cm} (10)$$

because $|\psi_i|H_A|\psi_i| = 0$. Therefore, as $Q_A(t = 0) = Q_A(t = T)$, $Q_A$ is zero for all $t$’s. Since the internal energy of each qubit is not varying, according to the first law $\Delta U = \Delta Q + \Delta W = 0$, we have the peculiar situation where two systems are interacting while neither heat nor work is being exchanged, which is precisely one of the examples used to criticize the Alick’s approach in Ref. [16]. It is important to note that this result ($\Delta U = \Delta Q = \Delta W$) is only true for the particular parameters we have used above; had one choose $p \neq 1/2$, although $\Delta U = 0$, one could find $\Delta Q = -\Delta W \neq 0$. Yet, from this example, it is to be noted that since $p_i(t)$’s vary, entropy is also varying. In fact, from differentiating von Neumann entropy to system A we find

$$dS_A = -\sum_i dp_i(t)\ln p_i(t), \hspace{1cm} (11)$$

or, after replacing $p_1(t) = \sin^2 gt$, $p_2(t) = \cos^2 gt$:

$$dS_A = -\sin(2gt)\ln(\tan^2 gt), \hspace{1cm} (12)$$

and, after integration:

$$S_A(t) = -2\ln|\cos(gt)| - \sin^2(gt)\ln[\sin^2(gt)] / \cos^2(gt). \hspace{1cm} (13)$$

This is another peculiar finds of this formalism: according to [15, 16], entropy variation is connected with exchange of heat; however, we have again this peculiar behavior where entropy varies without any heat being exchanged with the surroundings, thus pointing to a possible inadequacy of the formalism.

Let us now turn our attention to system B. Since the evolved state remains unchanged for all times, this means that, different from system A, system B do not exchange neither work nor heat during its evolution. In other words: during systems A and B interaction there will be $dQ_A = -dW_A \neq 0$ flowing out/into the system A in general. The only explanation left is that the energy stored in the correlations flows only out/into the system A alone, and system B works as a catalyst in this process. Now, if we take the parameters to be $p = c = 1/2$, we have this peculiar situation: $dQ_B = dW_B = 0$, $dU_A = dQ_A = dW_A = 0$, at the same time that $S_A(t) \neq 0$, i.e., there is no energy flowing to any of the systems and yet the entropy of system A varies, which should lead to a no-null heat according to statement (ii) in Introduction.

**B. A single qubit dissipating**

The following master equation describes a qubit under a weak coupling with its reservoir in the interaction picture:

$$\dot{\rho} = -\frac{\gamma}{2}i[\sigma^+ \rho - \rho \sigma^- + \rho \sigma^+ \sigma^-] - \frac{\gamma}{2}i[\sigma^+ \rho - 2 \sigma \rho \sigma^+ + \rho \sigma^+ \sigma^-], \hspace{1cm} (14)$$
where $\sigma$ and $\sigma^+$ are the lowering and raising operators to the system, $\overline{\pi}$ is the reservoir average thermal excitation and $\gamma$ is the dissipation rate. This equation can be exactly solved, resulting

$$\rho_A(t) = \left( \begin{array}{cc} \rho_{ee}(t) & \rho_{eg}(t) \\ \rho_{eg}(t) & 1 - \rho_{ee}(t) \end{array} \right), \tag{15}$$

where

$$\rho_{ee}(t) = \frac{[(2\pi+1)\rho_{ee}(0)\pi - \pi]e^{-(2\pi+1)\gamma t} + \pi}{(2\pi+1)}, \tag{16}$$

and

$$\rho_{eg}(t) = \rho_{eg}(0)e^{-(\pi+\frac{1}{2})\gamma t}. \tag{17}$$

Next, we diagonalize Eq. (15) and find heat according to $dQ = \sum_{i=1}^2 dp_i(t)\langle \psi_i | H | \psi_i \rangle$, where $H = \hbar\omega\sigma_z$, and choose the qubit initial condition as being the following pure state:

$$\rho(0) = \frac{1}{2} \left( \begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right). \tag{18}$$

In Fig. (1) we plot $Q(t)$ versus $t$ for $T=0$. Note the following peculiar behavior: the heat of the system is greater than zero, thus the system is, for a while, drawing energy from the vacuum. One could argue that since according to the first law $\Delta U = \Delta Q + \Delta W$, and since $\Delta U < 0$ always, the net flux is from the system toward the reservoir, thus indicating that energy flows from the system to the vacuum reservoir. However, if we pay attention in what a true reservoir should be, i.e., an infinite collection of quantum harmonic oscillators as modeled by Eq. (14), the recurrence, which is the time to the energy goes back to the reservoir, should be infinite, and no energy should go from the system to the vacuum. [5–10].

**IV. CONCLUSION**

In this work we did two case studies in which we applied the formalism that introduces new definitions of heat and work in quantum thermodynamics as introduced in Refs. [15, 16]. One of the examples studied consists of two interacting qubits, a situation in which the concepts of heat and work are difficult to generalize, and there is currently no consensus on which formalism correctly describes the corresponding thermodynamic behavior, in particular the heat and work exchanged by the systems. The second example consists of qubit interacting weakly with a thermal reservoir in Born-Markov approximations, as described by the usual master equation, and where it is well known that the formalism developed by Alicki correctly describes heat and work. The analysis of the first example shows that, for certain initial conditions, the entropy of a system can vary without a counterpart in the heat variation, which is in apparent contradiction with one of the assertions on which the formalism [15, 16] is based. In the second example, the formalism [15, 16] shows a heat variation in the qubit that is apparently incompatible with what is expected of a genuine reservoir at zero absolute temperature, which must always absorb heat from the system in which it is in contact. These two examples seem to point to a possible inadequacy of the formalism in [15, 16].

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