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Thermodynamics of a qubit undergoing dephasing

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Abstract. The thermodynamics of a qubit undergoing dephasing due to the coupling with the external environment is discussed. First of all, we assume the dynamics of the system to be described by a master equation in Lindblad form. In this framework, we review a standard formulation of the first and second law of thermodynamics that has been known in literature for a long time. After that, we explicitly model the environment with a set of quantum harmonic oscillators choosing the interaction such that the global dynamics of system and bath is analytically solvable and the Lindblad master equation is recovered in the weak-coupling limit. In this generalized setting, we can show that the correlations between system and bath play a fundamental role in the heat exchange. Moreover, the internal entropy production of the qubit is proven to be positive for arbitrary coupling strength.

1. Introduction

Standard thermodynamics is a phenomenological theory describing transformations of macroscopic systems in equilibrium according to few simple laws [1]. In particular, the first law of thermodynamics deals with the conservation of total energy that can be exchanged in the form of heat or work. The second law of thermodynamics instead regards the entropy, a state function that can never decrease in isolated systems, thus providing an arrow of time.

In the last years many attempts have been made to study the fate of thermodynamics when the system of interest can no longer be considered macroscopic and is out of equilibrium. This research is motivated by the high degree of control reached in many experimental setups such as ultracold atoms [2], optomechanical systems [3] and trapped ions [4], that allows to test the laws of thermodynamics in a completely new scenario. At the nanoscale quantum effects are expected to become important and the formulation of a consistent theory of quantum thermodynamics has recently attracted lot of attention [5]. From a fundamental point of view, one can address the issue of equilibration and thermalization in closed systems [6]. Moreover, it is interesting to study how the phenomenological laws of thermodynamics emerge from the underlying microscopic dynamics and in what sense they can be generalized beyond the usual thermodynamic limit [7].

In the following, we discuss two different approaches to quantum thermodynamics by means of an explicit example, namely a qubit undergoing dephasing due to the interaction with the external environment. In Section 2 a master equation in Lindblad form is used to describe the time-evolution of the qubit and the thermodynamic formalism developed in [8] for a driven open quantum system is reviewed. In this case the environment is taken implicitly into account. In Section 3 an explicit model for the interaction between the qubit and a bath of harmonic oscillators is introduced, such that the unitary dynamics of the global system is analytically solvable [9] and the Lindblad master equation for the qubit alone is recovered in the weak-coupling limit. In this more general framework we can highlight



the important role of bipartite correlations in the heat balance following the definitions given in [10]. Moreover, we can show that the internal entropy production for the qubit is positive without resorting to the weak-coupling approximation.

2. Lindblad master equation

Consider a qubit evolving in time according to the following master equation in Lindblad form [11, 12]

$$\partial_t \varrho(t) = -i \left[\frac{\omega_0}{2} \sigma_z, \varrho(t) \right] + \frac{\gamma}{2} (\sigma_z \varrho(t) \sigma_z - \varrho(t)), \quad (1)$$

whose solution is easily found to be

$$\varrho(t) = \varrho_{00}|0\rangle\langle 0| + \varrho_{11}|1\rangle\langle 1| + e^{-\gamma t} (\varrho_{10} e^{i\omega_0 t} |1\rangle\langle 0| + \varrho_{01} e^{-i\omega_0 t} |0\rangle\langle 1|), \quad (2)$$

where $\sigma_z |\ell\rangle = (-)^{\ell} |\ell\rangle$, with $\ell \in \{0, 1\}$. This is a model for dephasing, since the populations remain constant while coherence decays exponentially in time. The thermodynamics of this quantum system can be studied using the standard formulation presented in [8]. In particular, the first law of thermodynamics for a driven open quantum system with Hamiltonian $H(t)$ reads

$$\partial_t \mathbb{U}(t) = \partial_t \mathbb{Q}(t) + \partial_t \mathbb{W}(t), \quad (3)$$

where the internal energy $\mathbb{U}(t)$, the heat flux $\partial_t \mathbb{Q}(t)$ and the work power $\partial_t \mathbb{W}(t)$ are defined respectively

$$\mathbb{U}(t) := \text{Tr} [\varrho(t) H(t)], \quad (4)$$

$$\partial_t \mathbb{Q}(t) := \text{Tr} [\partial_t \varrho(t) H(t)], \quad (5)$$

$$\partial_t \mathbb{W}(t) := \text{Tr} [\varrho(t) \partial_t H(t)]. \quad (6)$$

This separation between work and heat contributions to the energy variation is quite reasonable. Indeed, the work power (Eq. (6)) is vanishing as expected in absence of an external field modelled by a time-dependent Hamiltonian, while the heat flux (Eq. (5)) is zero for the unitary dynamics generated by $H(t)$, namely if the system is closed.

For the qubit described in equation (2), the preservation of populations implies that the internal energy, namely the mean value of $\sigma_z \omega_0 / 2$, is constant in time. Moreover, the work power is zero, since there is no time-dependence in the Hamiltonian, and as a consequence the heat exchange with the environment is also vanishing. Up to now, it seems that dephasing happens without energy transfer; however, we will come back to this point later on, when we explicitly consider the presence of the bath.

For an open quantum system interacting with a thermal bath at inverse temperature β , the internal entropy production σ can be defined as the difference between the total variation of the entropy and the entropy flux due to the heat exchange [13]

$$\sigma(t) := \partial_t \mathbb{S}(t) - \beta \partial_t \mathbb{Q}(t), \quad (7)$$

where \mathbb{S} is the von Neumann entropy

$$\mathbb{S}(t) := -\text{Tr} [\varrho(t) \log \varrho(t)]. \quad (8)$$

The second law of thermodynamics states that $\sigma \geq 0$. In our model there is no heat exchange, so that the internal entropy production equals the variation of the von Neumann entropy and the second law reads $\partial_t \mathbb{S}(t) \geq 0$. Such a property is easily verified using the eigenvalues $(1 \pm r(t))/2$ of the density matrix $\varrho(t)$:

$$\partial_t \mathbb{S}(t) = -\frac{1}{2} \log \left(\frac{1+r(t)}{1-r(t)} \right) \partial_t r(t) \geq 0, \quad (9)$$

where

$$r(t) = \sqrt{1 - 4(\varrho_{00}\varrho_{11} - e^{-2\gamma t} |\varrho_{01}|^2)}, \quad \partial_t r(t) = -\frac{4\gamma e^{-2\gamma t} |\varrho_{01}|^2}{r(t)}. \quad (10)$$

3. Explicit model for the environment

Instead of considering the thermodynamics of the qubit alone, a complete thermodynamic description of the qubit and the environment together could be given, in order to include possible effects due to the correlations between them. Indeed, as shown in [10], in a generic bipartite quantum system the correlations between the subsystems play a fundamental role and a consistent formulation of the first and second law of thermodynamics explicitly accounting for that can be given.

In the following, we study the exactly solvable model of a qubit in interaction with a thermal bosonic bath presented in [9]. In the weak-coupling limit the dynamics of the qubit is given by equation (1), but this more general approach highlights some interesting thermodynamic features. For instance, we show that due to correlations a non zero heat flux in the bath can happen without changing the internal energy of the qubit. Moreover, the internal entropy production of the qubit is found to be positive for an arbitrary coupling strength λ , namely without performing the standard Markov approximations.

3.1. The model

Consider a total Hamiltonian given by $H_{\text{tot}} = H_S + H_B + H_{\text{int}}$ with

$$H_S = \frac{\omega_0}{2} \sigma_z, \quad H_B = \sum_{k=1}^{\infty} \omega_k a_k^\dagger a_k, \quad H_{\text{int}} = \lambda \sigma_z \otimes \sum_{k=1}^{\infty} (f_k^* a_k + f_k a_k^\dagger),$$

where a_k is the bosonic annihilation operator of mode k , satisfying the canonical commutation relations $[a_k, a_j^\dagger] = \delta_{kl}$, and the complex parameters f_k are such that $\sum_{k=1}^{\infty} |f_k|^2 < \infty$. We assume that the initial state of the total system can be written as $\varrho_{SB}(0) = \varrho_S(0) \otimes \varrho_B^\beta$, where $\varrho_S(0)$ is the initial state of the qubit and ϱ_B^β is the Gibbs state of the thermal bath at inverse temperature β ,

$$\varrho_S(0) = \sum_{\ell, \ell'=0}^1 \varrho_{\ell\ell'} |\ell\rangle \langle \ell'|, \quad \sigma_z |\ell\rangle = (-)^\ell |\ell\rangle, \quad \varrho_B^\beta = \frac{e^{-\beta \sum_k \omega_k a_k^\dagger a_k}}{\text{Tr} \left[e^{-\beta \sum_k \omega_k a_k^\dagger a_k} \right]}. \quad (11)$$

The dynamics of the total system can be analytically solved (see [9] or [10] for all the details) and it turns out that the density matrix $\varrho_{SB}(t)$ can be written as follows

$$\varrho_{SB}(t) = \sum_{\ell, \ell'=0}^1 \varrho_{\ell\ell'} e^{-i\omega_0 \zeta_{\ell\ell'} t/2} |\ell\rangle \langle \ell'| \otimes D_\ell(g_t) \varrho_B^\beta D_{\ell'}^\dagger(g_t), \quad (12)$$

where $\zeta_{\ell\ell'} = (-)^\ell - (-)^{\ell'}$ and $D_\ell(g_t)$ is the displacement operator

$$D_\ell(g_t) = e^{(-)^\ell \lambda \sum_k [g_k(t) a_k^\dagger - g_k^*(t) a_k]}, \quad g_k^*(t) = f_k^* (e^{-i\omega_k t} - 1) / \omega_k. \quad (13)$$

By partial tracing one can obtain the reduced density matrices of the two subsystems

$$\varrho_S(t) = \varrho_{00} |0\rangle \langle 0| + \varrho_{11} |1\rangle \langle 1| + e^{-8\lambda^2 \Gamma(t)} (\varrho_{10} e^{i\omega_0 t} |1\rangle \langle 0| + \varrho_{01} e^{-i\omega_0 t} |0\rangle \langle 1|), \quad (14)$$

$$\varrho_B(t) = \sum_{\ell=0}^1 \varrho_{\ell\ell} D_\ell(g_t) \varrho_B^\beta D_\ell^\dagger(g_t), \quad (15)$$

where $\text{Tr} [D_\ell(g_t) \varrho_B^\beta D_{\ell'}^\dagger(g_t)] = e^{-8\lambda^2 \Gamma(t)}$ for $\ell \neq \ell'$, with

$$\Gamma(t) = \sum_k \frac{|f_k|^2}{\omega_k^2} \coth(\beta \omega_k / 2) \sin^2(\omega_k t / 2). \quad (16)$$

The bath at any time is described by a convex combination of displaced thermal states, while the dynamics of the qubit is similar to that one in equation (2) but with a time-dependent damping $\Gamma(t)$.

It is possible to recover equation (2) from equation (14) in the so called weak-coupling limit. First of all, we should substitute the discrete sum in equation (16) with the following integral

$$\Gamma(t) = \int_0^\infty d\omega \frac{1}{\omega} \coth(\beta\omega/2) \sin^2(\omega t/2) e^{-\epsilon\omega}, \quad \epsilon \geq 0 \quad (17)$$

where a regularized Ohmic spectral density given by $f_k \simeq \sqrt{\omega} e^{-\omega\epsilon/2}$ has been used as in [9]. Then, a new time scale τ is defined such that $t = \tau/\lambda^2$ and in the limit $\lambda \rightarrow 0$ one finds $\lambda^2 \Gamma(\tau/\lambda^2) \simeq \pi\tau/(2\beta)$. The solution of the Lindblad master equation (1) is immediately found identifying the constant damping rate $\gamma = 4\pi/\beta$.

3.2. Heat balance

Using the model above, we can exploit an interesting feature of bipartite quantum systems related to the heat balance. The total energy of the composite system \mathbb{U}_{tot} defined as follows

$$\mathbb{U}_{\text{tot}} := \text{Tr} [H_{\text{tot}} \varrho_{SB}(t)] \quad (18)$$

is conserved, so that its time derivative is vanishing $\partial_t \mathbb{U}_{\text{tot}} = 0$. Explicitly, one can write

$$\begin{aligned} \partial_t \mathbb{U}_{\text{tot}} &= \text{Tr} [H_{\text{tot}} \partial_t \varrho_S(t) \otimes \varrho_B(t)] + \text{Tr} [H_{\text{tot}} \varrho_S(t) \otimes \partial_t \varrho_B(t)] + \text{Tr} [H_{\text{tot}} \partial_t \chi(t)] = \\ &= \text{Tr} [\partial_t \varrho_S(t) H'_S(t)] + \text{Tr} [\partial_t \varrho_B(t) H'_B(t)] + \text{Tr} [H_{\text{int}} \partial_t \chi(t)] = 0, \end{aligned} \quad (19)$$

where the operator $\chi(t) := \varrho_{SB}(t) - \varrho_S(t) \otimes \varrho_B(t)$ has been introduced to describe the amount of correlations between S and B , and a modified Hamiltonian has been defined for each subsystem

$$H'_{S,B}(t) := H_{S,B} + \text{Tr}_{B,S} [\varrho_{B,S}(t) H_{\text{int}}]. \quad (20)$$

The first two terms in the second line of equation (19) can be associated to heat exchanged by S and B respectively, indeed they are formally similar to equation (5). However, the modified Hamiltonians appear instead of the free Hamiltonians H_S and H_B ; this is expected since the interaction Hamiltonian should contribute to the internal energy of each subsystem. Given the second line of equation (19) and defining a binding energy as

$$\mathbb{U}_\chi(t) := \text{Tr} [\chi(t) H_{\text{int}}], \quad (21)$$

the heat balance can be stated as follows

$$\partial_t \mathbb{Q}_S(t) + \partial_t \mathbb{Q}_B(t) = -\partial_t \mathbb{U}_\chi(t). \quad (22)$$

The binding energy is interpreted as an amount of energy stored in the correlations between S and B that can be exchanged with both subsystems in the form of *heat* [10].

For the model of interest, denoting the qubit polarization at time $t = 0$ by $\langle \sigma_z \rangle$ and using equations (14) and (15), the modified qubit Hamiltonian takes the form

$$H'_S(t) = \left(\frac{\omega_0}{2} - 4\lambda^2 \langle \sigma_z \rangle \Delta(t) \right) \sigma_z, \quad (23)$$

where $\Delta(t)$ corresponds to

$$\Delta(t) = -\frac{\text{Tr} \left[\varrho_B(t) \sum_k (f_k^* a_k + f_k a_k^\dagger) \right]}{4\lambda \langle \sigma_z \rangle} = \sum_k \frac{|f_k|^2}{\omega_k} \sin^2(\omega_k t/2), \quad (24)$$

while $H'_B(t)$ reads

$$H'_B(t) = \sum_k \omega_k a_k^\dagger a_k + \lambda \langle \sigma_z \rangle \sum_k \left(f_k^* a_k + f_k a_k^\dagger \right). \quad (25)$$

As a consequence, the heat fluxes for both S and B can be explicitly computed and turn out to be

$$\partial_t Q_S(t) = 0, \quad (26)$$

$$\partial_t Q_B(t) = 4\lambda^2 (1 - \langle \sigma_z \rangle^2) \partial_t \Delta(t). \quad (27)$$

Notice that the heat exchanged by the qubit is vanishing even in this more general situation, because the modified Hamiltonian is proportional to σ_z and $\text{Tr} [\partial_t \rho_S(t) \sigma_z] = 0$ since populations are preserved (see Eq. (14)). Nevertheless, the heat transfer for the bath of harmonic oscillators does not vanish as expected, indeed the correlations built in during the time-evolution effectively act as a third subsystem exchanging energy with B in the form of heat according to equation (22).

3.3. Entropy production

Another interesting comparison between the present model and the weak-coupling limit discussed in Section 2 regards the internal entropy production for the qubit. Again, the internal entropy production equals the time derivative of the von Neumann entropy because $\partial_t Q_S(t) = 0$. Using equation (14), the entropy variation of the qubit $\partial_t \mathcal{S}_S$ can be calculated from the eigenvalues $(1 \pm r_S(t))/2$ of $\rho_S(t)$ with

$$r_S(t) = \sqrt{1 - 4 (\rho_{00}\rho_{11} - e^{-16\lambda^2\Gamma(t)} |\rho_{01}|^2)}. \quad (28)$$

Explicitly, one finds

$$\partial_t \mathcal{S}_S(t) = -\frac{1}{2} \log \left(\frac{1 + r_S(t)}{1 - r_S(t)} \right) \partial_t r_S(t) = \lambda^2 \frac{16 |\rho_{01}|^2 e^{-16\lambda^2\Gamma(t)}}{r_S(t)} \log \left(\frac{1 + r_S(t)}{1 - r_S(t)} \right) \partial_t \Gamma(t); \quad (29)$$

therefore, the sign of $\partial_t \mathcal{S}_S(t)$ corresponds to the sign of $\partial_t \Gamma(t)$. The behaviour of the latter can be studied considering the integral expression in equation (17). By means of the substitution $\omega t = \tilde{\omega}$ and taking the derivative inside the integral it turns out that

$$\partial_t \Gamma(t) = \int_0^\infty d\tilde{\omega} \frac{1}{\tilde{\omega}} \sin^2(\tilde{\omega}/2) \partial_t \left[\coth(\beta\tilde{\omega}/2t) e^{-\epsilon\tilde{\omega}/t} \right] \geq 0. \quad (30)$$

The second law of thermodynamics in the form $\partial_t \mathcal{S}_S(t) \geq 0$ is hence satisfied without invoking the weak-coupling limit.

4. Conclusions

We compared two different approaches to study the thermodynamics of a quantum system. In particular, a qubit undergoing dephasing has been firstly analyzed in the Markovian regime where the time evolution is well described by a Lindblad master equation and the paradigm of [8] can be used. After that, an explicit model for the environment has been introduced such that the global dynamics of system and bath is analytically solvable and the previous qubit dynamics is recovered in the weak-coupling limit. In this more general framework, the important role of correlations in the heat balance has been highlighted using the definitions given in [10]. Moreover, the second law of thermodynamics for the qubit has been proven to hold independently of the coupling strength.

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