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PAPER

Non-equilibrium quantum heat machines

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Abstract

Standard heat machines (engine, heat pump, refrigerator) are composed of a system (working fluid) coupled to at least two equilibrium baths at different temperatures and periodically driven by an external device (piston or rotor) sometimes called the work reservoir. The aim of this paper is to go beyond this scheme by considering environments which are stationary but cannot be decomposed into a few baths at thermal equilibrium. Such situations are important, for example in solar cells, chemical machines in biology, various realizations of laser cooling or nanoscopic machines driven by laser radiation. We classify non-equilibrium baths depending on their thermodynamic behavior and show that the efficiency of heat machines powered by them is limited by the generalized Carnot bound.

1. Introduction

Quantum systems are rarely completely isolated from their environment, whose influence, positive or negative, should be considered. The theory of the open quantum system was developed [1–7] to achieve this goal and in particular to open the way to the study of quantum heat machines, such as engines and refrigerators [8–16]. These models generally assume the interaction between a system and an environment composed of several baths, each in thermal equilibrium, thereby termed heat baths. The efficiency of these machines is limited by the Carnot bound, requiring at least two baths at different temperatures in order to extract work.

Nevertheless, there are many examples in nature where at least part of the environment is not in thermal equilibrium, such as sunlight, continuous laser radiation, biological cells, etc. Our goal is to establish maximum efficiency bounds, as well as to determine the output (work power or cooling power) of quantum heat machines operating with non-equilibrium baths. Because the bath is not at thermal equilibrium, the second law does not demand the presence of a second bath for work extraction.

We study a micro-or mesoscopic externally driven quantum system, the working fluid, coupled to a large environment. On the relevant time-scale, which is longer than the scales of driving and of microscopic irreversible processes, *the basic parameters of the reservoir are constant*, hence the reference state of the environment *is a stationary state*. Such non-equlibrium stationary systems are well known in macroscopic thermodynamics and are usually described in terms of local equilibrium with space-dependent temperature, density, pressure, fluid velocity etc [17].

However, there are important situations where the non-equilibrium character of the environment state is not related to spatial non-homogeneity but rather to some internal properties of its state. For example, sunlight at the Earth's surface is a rather homogeneous environment; the shape of its spectrum roughly corresponds to the Planck distribution at the Sun's surface temperature T_s, but the photon density is much lower than the equilibrium one, and the absorption in the atmosphere creates 'holes' in the spectrum.

Another example is a laser radiation [18] in a continuous wave operation mode. For the idealized single mode situation it can be treated as a single quantum oscillator or even a classical monochromatic wave. For the multimode case with strong phase diffusion it acts on optically active centers like a non-equilibrium bath. Biological machines also provide examples of systems coupled to non-equilibrium baths either of a chemical nature or consisting of photons or different types of excitons. Non-equilibrium effects are also found in strongly coupled heat machines. Both the hot and cold baths undergo a mixing interaction, caused by their strong coupling to the system, and effectively produce a non-equilibrium bath [19].

In section 2 a general theory of non-equilibrium quantum heat machines, under the assumption of fast periodic driving is presented. The theory is based on the Markovian master equations (MMEs) derived using the Davies idea of weak coupling limit [1] and Floquet theory [20]. This theory is consistent with thermodynamics and yields a Carnot-like bound for the efficiency. In section 3 the physically important examples of stationary non-equilibrium bosonic baths are given and their local temperatures for linear interactions are computed. In the final section heat machines based on two-level systems (TLSs) are studied. Different examples of non-equilibrium baths are given and they are classified according to their effects on heat machine operation.

2. General theory of non-equilibrium quantum heat machines

We study a large class of open quantum systems with physical Hamiltonian $H_S(t) = H_S(t+\tau)$ under the assumption that the perturbation frequency $\Omega = 2\pi/\tau$ is comparable to or higher than the relevant Hamiltonian Bohr frequencies. Such fast driving is typically provided by a strong coherent laser field and appears in the thermodynamical approach to the theory of lasers [18, 21–23], various types of laser cooling [24, 25], optomechanical devices [26], etc. Potential applications include new light harvesting systems, both of a biological nature or man-made devices.

The theory of such systems, including the derivation of MMEs and thermodynamical analysis, has been presented in the unpublished tutorial [27] for the case of reservoir consisting of several independent heat baths. The idea of extending these results to non-equilibrium baths characterized by *local temperatures* has been proposed in the unpublished note [28] referring to the 'violation of Carnot bound' for non-equilibrium baths discussed in [29]. Here, we present a complete theory of such systems which are used to model quantum machines for the case of general stationary non-equilibrium baths. In particular, the laws of thermodynamics are derived and the Carnot-type bounds are obtained.

2.1. Master equations

We begin with a presentation of the canonical construction of the Markovian dynamics for an open system weakly coupled to a stationary, but generally non-equilibrium, environment. The special case of a periodically driven quantum optical system coupled to a photon bath at the vacuum state has already been discussed in [5]. The general theory has been developed in [30, 31] and applied in [13, 25, 32–35].

The system is assumed to be 'small' and described by the periodic in time physical Hamiltonian $H_S(t) = H_S(t+\tau)$ under the assumption that the perturbation frequency $\Omega = 2\pi/\tau$ is comparable to or higher than the relevant temporal Bohr frequencies. We assume that the Hamiltonian of the system already contains all Lamb-like shifts induced by interaction with the environment.

The system-bath interaction is parametrized as

$$H_{\mathrm{int}} = \sum_{\alpha} S_\alpha \otimes B_\alpha, \tag{1}$$

where S_α and B_α are hermitian operators of the system and bath, respectively. We sum over all the interactions between the system and the bath. The environment (bath) is assumed to be a large quantum system with a practically continuous Hamiltonian spectrum. The initial state of the bath is *stationary*, $[\bar{\rho}_B, H_B] = 0$, therefore it is invariant with respect to the free dynamics of the bath generated by the Hamiltonian H_B. Equilibrium states, $\bar{\rho}_B \propto \mathrm{e}^{-\beta H_B}$ are just a subset of the stationary states. To justify the Markovian approximation the multi-time correlation functions of relevant observables must satisfy certain Gaussian bounds [1] and a technical condition $\langle B_\alpha \rangle_B = 0$ holds, where $\langle \cdots \rangle_B$ denotes the average over the bath state. We assume also, for simplicity, that the cross-correlations between B_α and B_β vanish for $\alpha \neq \beta$.

Applying the Floquet theory, one obtains the following decomposition of the associated unitary propagator (we put $\hbar = 1$)

$$U(t) = \mathbb{T} \exp\left\{-\mathrm{i}\int_0^t H_S(s)\mathrm{d}s\right\} = P(t)\mathrm{e}^{-\mathrm{i}\bar{H}t}, \tag{2}$$

where $P(t) = P(t+\tau)$ is a periodic function taking values in the set of unitary operators. $\mathbb{T}$ is the time ordering operator [36] and $\bar{H}$ is the *averaged Hamiltonian* satisfying

$$U(\tau) = \mathrm{e}^{-\mathrm{i}\bar{H}\tau}. \tag{3}$$

The *Floquet operator* $U(\tau)$, and the averaged Hamiltonian $\bar{H}$ possess common eigenvectors $\{\phi_k\}$, i.e.,

$$\bar{H}\phi_k = \bar{\epsilon}_k\phi_k, \quad U(\tau)\phi_k = \mathrm{e}^{-\mathrm{i}\bar{\epsilon}_k\tau}\phi_k, \tag{4}$$

where $\{\epsilon_k\}$ are called *quasi-energies* of the system. These properties imply a particular form of the Fourier decomposition

$$S_\alpha(t) \equiv U(t)^\dagger S_\alpha U(t) = \sum_{\{\bar{\omega}_q\}} S_\alpha\left(\bar{\omega}_q\right)\mathrm{e}^{-\mathrm{i}t\bar{\omega}_q}, \tag{5}$$

where

$$\left\{\bar{\omega}_q\right\} = \left\{\bar{\omega} + q\Omega\right\}; \left\{\bar{\omega}\right\} = \left\{\bar{\epsilon}_k - \bar{\epsilon}_l\right\}, q \in \mathbb{Z}\Big\}, \tag{6}$$

i.e., it is a set of all sums of the *relevant Bohr quasi-frequencies* and all multiplicities of the modulation frequency. By $\{\bar{\omega}_q\}_+$ we denote the subset of $\{\bar{\omega}_q\}$ with non-negative relevant Bohr quasi-frequencies $\bar{\omega}$.

The operators $S_\alpha(\bar{\omega}_q)$ are subject to relations

$$\begin{aligned} S_\alpha\left(\bar{\omega}_q\right)^\dagger &= S_\alpha\left(-\bar{\omega}_q\right), \\ \left[\bar{H}, S_\alpha\left(\bar{\omega}_q\right)\right] &= -\bar{\omega}_q S_\alpha\left(\bar{\omega}_q\right). \end{aligned} \tag{7}$$

Physically, the harmonics $q\Omega$ correspond to the energy quanta which are exchanged with the external periodic driving.

Repeating the standard construction of the weak coupling generator in the interaction picture, one obtains

$$\mathcal{L} = \sum_\alpha \sum_{\{\bar{\omega}_q\}_+} \mathcal{L}^\alpha_{\bar{\omega}_q}, \tag{8}$$

with a single term defined as

$$\begin{aligned} \mathcal{L}^\alpha_{\bar{\omega}_q}\rho = \frac{1}{2}\Big\{ & G_\alpha\left(\bar{\omega}_q\right)\left(\left[S_\alpha\left(\bar{\omega}_q\right), \rho S_\alpha\left(\bar{\omega}_q\right)^\dagger\right] + \left[S_\alpha\left(\bar{\omega}_q\right)\rho, S_\alpha\left(\bar{\omega}_q\right)^\dagger\right]\right) \\ & + G_\alpha\left(-\bar{\omega}_q\right)\left(\left[S_\alpha\left(\bar{\omega}_q\right)^\dagger, \rho S_\alpha\left(\bar{\omega}_q\right)\right] + \left[S_\alpha\left(\bar{\omega}_q\right)^\dagger\rho, S_\alpha\left(\bar{\omega}_q\right)\right]\right)\Big\}. \end{aligned} \tag{9}$$

The bath coupling spectrum is defined as

$$G_\alpha(\omega) = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}t\omega}\left\langle B_\alpha(t)B_\alpha\right\rangle_B \mathrm{d}t, \tag{10}$$

where $B_\alpha(t) = \mathrm{e}^{\mathrm{i}H_B t}B_\alpha\mathrm{e}^{-\mathrm{i}H_B t}$.

For a given coupling spectrum one can introduce the notion of *local temperature* $T_\alpha(\omega)$–a function of the frequency ω and the observable B_α defined by the formula (we put also $k_B \equiv 1$, hence angular frequency, energy and temperature have the same units)

$$\mathrm{e}^{-\omega/T_\alpha(\omega)} \equiv \frac{G_\alpha(-\omega)}{G_\alpha(\omega)}. \tag{11}$$

Notice that only in the case of the thermal bath the local temperature does not depend on the frequency and the choice of B_α and corresponds to the standard notion of temperature with the relation (11) being a direct consequence of the Kubo–Martin Schwinger (KMS) condition. The local temperatures can be measured by the 'thermometers' with a single working frequency ω like, for example, TLSs or linearly coupled harmonic oscillators. Upon 'equilibration' with the non-equilibrium bath, the ratio between consecutive state populations is $\rho_{j+1j+1}/\rho_{jj} = \mathrm{e}^{-\omega/T_\alpha(\omega)}$.

Due to (7) and (11), the structure of the local generator (9) is the same as the generator obtained in the weak coupling limit for the case of the system with the Hamiltonian $(\bar{\omega}_q/\bar{\omega})\bar{H}$ coupled to the heat bath at the temperature $T_\alpha(\bar{\omega}_q)$ [4, 5]. Hence, the corresponding *local stationary state of the system* possesses a Gibbs-like form [1]

$$\bar{\rho}^\alpha_{\bar{\omega}_q} = Z^{-1}\mathrm{e}^{-\left(\bar{\omega}_q/\bar{\omega}\right)\bar{H}/T_\alpha\left(\bar{\omega}_q\right)}, \tag{12}$$

with the local temperature $T_\alpha(\bar{\omega}_q)$ corresponding to the *coupling channel*$(\alpha, \bar{\omega}_q)$. The 'renormalizing' term $\bar{\omega}_q/\bar{\omega}$ in front of $\bar{H}$ in the Gibbs-like state takes into account the total energy exchange including $q\Omega$ corresponding to the external driving device. The properties (7) imply also that the generator (9) transforms independently the diagonal and off-diagonal elements of ρ computed in the eigenbasis of $\bar{H}$.

The MME in the *Schroedinger picture* possesses the following structure

$$\frac{d\rho_{sch}(t)}{dt} = -i[H_S(t), \rho_{sch}(t)] \tag{13}$$

where $\mathcal{U}(t)\rho = U(t)\rho U(t)^{\dagger}$. A very useful factorization property for the solution of (13) holds

$$\rho_{sch}(t) = \mathcal{U}(t)e^{t\mathcal{L}}\rho_{sch}(0), \tag{14}$$

which allows us to discuss separately the decoherence/dissipation effects described by $\mathcal{L}$ and the unitary evolution $\mathcal{U}(t)$.

2.2. The laws of thermodynamics

The structure of MMEs derived above and the introduced notion of local temperatures allow us to formulate the first and second law of thermodynamics in terms of energy, work, heat and entropy balance. The basic tool is the following inequality valid for any LGKS generator $\mathcal{L}$ with a stationary state $\bar{\rho}$ [7] and arbitrary ρ

$$\mathrm{Tr}\left(\mathcal{L}\rho\left[\ln\rho - \ln\bar{\rho}\right]\right) \leqslant 0. \tag{15}$$

This inequality is used to show positivity of entropy production under the assumption that the physical entropy of the system $S(t)$ is identified with the von Neumann entropy of its state in the Schroedinger or interaction picture

$$S(t) = -\mathrm{Tr}\,(\rho(t)\ln\rho(t)). \tag{16}$$

The early application of (15) to derive the laws of thermodynamics for an open system with a constant Hamiltonian coupled to several heat baths appeared in [7]. This idea was extended to heat engines with slow driving in [8] and recently to fast driving in unpublished notes [27]. These works do not analyze the case of baths out of equilibrium.

2.2.1. Entropy balance and local heat currents

In the case of fast driving there is no obvious definition of the temporal internal energy of the system because a fast exchange of energy quanta $q\Omega$ between the system and the external source of driving makes a temporal partition of energy between both systems ambiguous. The situation is different for the entropy balance because the entropy change is due to irreversible processes which are slow under the weak system–bath coupling assumption. The weak coupling scheme yields the coarse-grained in time effective dynamics described by the MME (13). This suggests the following definition of the local heat current $J_\alpha(\bar{\omega}_q)$

$$J^{\alpha}_{\bar{\omega}_q}(t) = \mathrm{Tr}\left[\rho(t)\left(\mathcal{L}^{\alpha}_{\bar{\omega}_q}{}^{*}\right)\left(\frac{\bar{\omega}_q}{\bar{\omega}}\bar{H}\right)\right] = \frac{\bar{\omega}_q}{\bar{\omega}}\mathrm{Tr}\left(\bar{H}\mathcal{L}^{\alpha}_{\bar{\omega}_q}\rho(t)\right), \tag{17}$$

where $\rho(t)$ is the system density matrix in the interaction picture and according to (13) given by

$$\rho(t) = e^{t\mathcal{L}}\rho(0). \tag{18}$$

The local heat current is the energy flow between the system and the environment composed of the bath and the external driving. It is the mean value of the time derivative of the energy operator, exclusively due to the given coupling channel. This action is described by the Heisenberg form of the relevant generator $\mathcal{L}^{\alpha}_{\bar{\omega}_q}{}^{*}$ applied to the renormalized averaged Hamiltonian $\frac{\bar{\omega}_q}{\bar{\omega}}\bar{H}$ which takes into account the energy supplied or extracted by the external driving. The fact that the state of the bath is stationary prevents the work exchange between the system and the bath, which requires the change of the bath state.

The definitions above allow us to formulate the second law which is again a consequence of (15) applied to each single coupling channel

$$\frac{d}{dt}S(t) - \sum_{\alpha}\sum_{\{\bar{\omega}_q\}_+}\frac{J^{\alpha}_{\bar{\omega}_q}(t)}{T_\alpha(\bar{\omega}_q)} = \sum_{\alpha}\sum_{\{\bar{\omega}_q\}_+}\sigma^{\alpha}_{\bar{\omega}_q}(t) \geqslant 0, \tag{19}$$

where $\sigma^{\alpha}_{\bar{\omega}_q}(t) \geqslant 0$ is an entropy production caused by a single coupling channel $(\alpha, \bar{\omega}_q)$ given by

$$\sigma^{\alpha}_{\bar{\omega}_q}(t) = \mathrm{Tr}\left(\mathcal{L}^{\alpha}_{\bar{\omega}_q}\rho(t)\left[\ln\rho(t) - \ln\bar{\rho}^{\alpha}_{\bar{\omega}_q}\right]\right) \geqslant 0. \tag{20}$$

For the case of an environment composed of several independent heat baths, the equation (19) reduces to the standard form of the second law for open systems with usual temperatures.

2.2.2. Steady state regime

Under natural ergodic conditions and due to (13), any initial state tends towards a limit cycle (or fixed point in particular cases), i.e.,

$$\rho_{\rm sch}(t) \to \bar{\rho}_{\rm sch}(t) = U(t)\bar{\rho}_{\rm sch}\, U(t)^{\dagger} = \bar{\rho}_{\rm sch}(t+\tau), \quad \text{where} \quad \mathcal{L}\bar{\rho}_{\rm sch} = 0. \tag{21}$$

Then the entropy $S(\bar{\rho}_{\rm sch}(t))$ is constant and in the formula for heat currents (17) the time dependence disappears leading to the following expression

$$\bar{J}^{\alpha}_{\bar{\omega}_q} = \frac{\bar{\omega}_q}{\bar{\omega}}\,{\rm Tr}\left(\bar{H}\mathcal{L}^{\alpha}_{\bar{\omega}_q}\bar{\rho}\right). \tag{22}$$

The second law now possesses a simplified form

$$\sum_{\alpha}\sum_{\left\{\bar{\omega}_q\right\}_+}\frac{\bar{J}^{\alpha}_{\bar{\omega}_q}}{T_{\alpha}\left(\bar{\omega}_q\right)} \leqslant 0. \tag{23}$$

The averaged internal energy of the system is constant in the limit cycle, and hence we can use the total energy conservation to write the first law in the form

$$\bar{P} = -\sum_{\alpha}\sum_{\left\{\bar{\omega}_q\right\}_+}\bar{J}^{\alpha}_{\bar{\omega}_q}, \tag{24}$$

where $\bar{P}$ is the stationary power and if it is negative, it is supplied to the source of external driving.

Remark 1. Each $\mathcal{L}^{\alpha}_{\bar{\omega}_q}$ transforms diagonal (in the $\bar{H}$ basis) elements of the density matrix into diagonal ones, and the stationary state $\bar{\rho}$ is diagonal. Therefore, the expressions for the stationary local heat currents and power involve only diagonal elements and the 'classical' transition probabilities between them.

2.3. Carnot bound at steady state

In the steady state regime the incoming and outgoing heat currents can be defined as follows

$$\bar{J}^{(+)} = \sum_{\left\{\alpha,\left\{\bar{\omega}_q\right\}_+;\bar{J}^{\alpha}_{\bar{\omega}_q}>0\right\}}\bar{J}^{\alpha}_{\bar{\omega}_q}, \quad \bar{J}^{(-)} = \sum_{\left\{\alpha,\left\{\bar{\omega}_q\right\}_+;\bar{J}^{\alpha}_{\bar{\omega}_q}<0\right\}}\left[-\bar{J}^{\alpha}_{\bar{\omega}_q}\right]. \tag{25}$$

In the standard situation of hot and cold heat baths, the heat current always flows from the hot to the cold one. In contrast, here different coupling channels to a single non-equilibrium bath can produce incoming or outgoing heat currents.

We can also introduce effective 'hot/cold bath temperatures' by averaging the inverse local temperatures with the weights proportional to incoming/outgoing heat currents

$$\frac{1}{T^{(+)}} = \sum_{\left\{\alpha,\{\omega_q\}_+;\bar{J}^{\alpha}_{\omega_q}>0\right\}}\left[\frac{\bar{J}^{\alpha}_{\omega_q}}{\bar{J}^{(+)}}\right]\frac{1}{T_{\alpha}(\omega_q)}, \quad \frac{1}{T^{(-)}} = \sum_{\left\{\alpha,\{\omega_q\}_+;\bar{J}^{\alpha}_{\omega_q}<0\right\}}\left[\frac{\bar{J}^{\alpha}_{\omega_q}}{\bar{J}^{(-)}}\right]\frac{1}{T_{\alpha}(\omega_q)}. \tag{26}$$

Combining now (23)–(26) and the standard notion of efficiency of a heat engine one obtains the generalized Carnot bound

$$\eta = \frac{-\bar{P}}{\bar{J}^{(+)}} \leqslant 1 - \frac{T^{(-)}}{T^{(+)}}, \tag{27}$$

which again coincides with the standard one in the case of an environment composed of two heat baths.

Remark 2. The derivation of the MME presented above is consistent only for the case of a stationary bath, i.e. being in the reference state commuting with the bath Hamiltonian. This condition corresponds to the *postulate of random phases* often used in quantum statistical mechanics [37]. This postulate seems to be well justified for large baths with various additional mechanisms of phase diffusion usually not included in the simplified Hamiltonian H_B (e.g. nonlinear effects in quantum oscillator models). However, if the experimental setting allows us to control at least initial phases of the bath, a direct injection of work from the bath is possible, but this effect is not included in the presented formalism.

Remark 3. In the derivation of the MME we assume that the bath average $\langle B_{\alpha}\rangle = 0$ for all bath operators entering the system–bath interaction Hamiltonian. This can always be assumed for stationary baths because we can replace B_{α} by $B_{\alpha} - \langle B_{\alpha}\rangle$ and add the term $\langle B_{\alpha}\rangle S_{\alpha}$ to the system Hamiltonian (this is the mean 'external potential' produced by the bath). If the bath is in a time-dependent state, then the additional external potential $\langle B_{\alpha}(t)\rangle S_{\alpha}$ can also be time-dependent and cause exchange of work with the system.

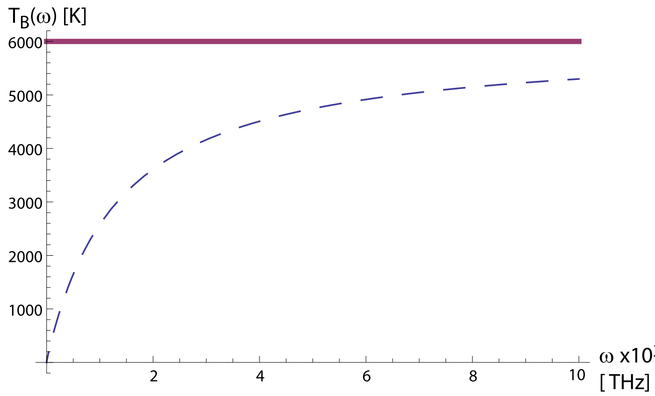

Figure 1. Local temperature of a TLS coupled to sunlight. The continuous line corresponds to the case of thermal radiation at the temperature of the Sun's surface $T_s \simeq 6000\ K$, while the dashed line relates to sunlight out of equilibrium due to a geometrical factor, $\lambda = 2.5 \times 10^{-5}$ (see main text).

3. Examples of harmonic oscillator non-equilibrium baths

Baths like electromagnetic radiation or vibration modes of a material are just a collection of independent quantum oscillators with a quasi-continuous spectrum of frequencies [5]. Baths could also be composed of fermions (e.g., spin-baths), but even then by suitable transformations (e.g. Holstein–Primakoff Hamiltonian) they can often be approximated by bosonic baths. The bosonic bath free Hamiltonian is given by

$$H_B = \sum_k \omega_k\, b_k^+ b_k, \quad \left[b_k, b_l^+\right] = \delta_{kl}. \tag{28}$$

In most applications the bath operator that couples to the system is linear in creation and annihilation operators

$$B = \sum_k \left\{g_k b_k + \bar{g}_k b_k^+\right\}. \tag{29}$$

The state of the bath is assumed to be stationary and hence diagonal in the particle number basis. Then, the coupling spectrum yields

$$G_B(\omega) = \begin{Bmatrix} \sum_k \left|g_k\right|^2 \left(n_k + 1\right) \delta(\omega_k - \omega), & \omega > 0 \\ \sum_k \left|g_k\right|^2 n_k \delta(\omega_k - \omega), & \omega < 0 \end{Bmatrix}, \tag{30}$$

where $n_k = \mathrm{Tr}(\rho_B b_k^+ b_k)$ is the k-mode population, and the upper (lower) line in (30) is the emission (absorption) rate. The local temperature is given by

$$T_B(\omega) = \frac{\omega}{\ln\left[\dfrac{G_B(\omega)}{G_B(-\omega)}\right]} \tag{31}$$

or

$$\mathrm{e}^{-\omega/T_B(\omega)} = \frac{n(\omega)}{n(\omega) + 1}, \tag{32}$$

where $n(\omega) = \frac{\sum_k |g_k|^2 n_k \delta(\omega_k - \omega)}{\sum_k |g_k|^2 \delta(\omega_k - \omega)}$ denotes the average population number for the frequency ω.

As we show below, the frequency dependence of the local temperature determines whether work can be extracted from the single non-equilibrium bath.

3.0.1. Sunlight

The Sun is a thermal source, emitting thermal radiation at $T_s = 6000\ K$. Due to geometrical considerations [38, 39], just a small fraction of the emitted photons reach the Earth, reducing the effective mode population and thereby $n(\omega) = \lambda[\mathrm{e}^{\omega/T_s} - 1]^{-1}$, where $\lambda = 2.5 \times 10^{-5}$ is a geometric factor equal to the angle subtended by the Sun seen from the Earth. Effectively, sunlight on Earth is out of equilibrium, and systems with different frequencies, will 'equilibrate' to different temperatures. Figure 1 shows the equilibration temperature, as a function of the thermometer's frequency. Moreover, the atmosphere acts like a filter and produces a more complicated shape of $n(\omega)$ with many 'holes'.

3.0.2. Multimode laser radiation

A multimode laser radiation in a continuous wave operation mode may be modeled as a bosonic bath at the phase average, $\bar{\rho}_B$, of the multimode coherent state ρ_B,

$$\rho_B = U_z \left|\text{vac}\right\rangle\left\langle\text{vac}\right| U_z^\dagger, \quad \left|\text{vac}\right\rangle\left\langle\text{vac}\right| = \underset{k}{\otimes} \left|0_k\right\rangle\left\langle 0_k\right|, \tag{33}$$

where $U_z^\dagger$ is the displacement operator

$$U_z^\dagger b_k U_z = b_k - z(\omega_k). \tag{34}$$

We now average over the phases,

$$\bar{\rho}_B = \sum_{\vec{i}} \left|\vec{i}\right\rangle\left\langle\vec{i}\right| \rho_B \left|\vec{i}\right\rangle\left\langle\vec{i}\right| \tag{35}$$

where $|\vec{i}\rangle$ is just the energy basis of the bath free Hamiltonian. Notice, that in order to compute the local temperature we do not need to compute explicitly the state $\bar{\rho}_B$ but it is enough to compute the average population number $n(\omega_k)$. Therefore, we apply the unitary map (34) to the particle number operator $b_k{}^\dagger b_k$, neglect the terms which are not invariant with respect to phase rotation (called *gauge transformation*) and compute the average of the remaining ones with respect to the initial coherent state. The bath in this stationary, phase averaged state, will not exchange work with the system and will drive the thermometer, with a single working Bohr frequency ω, to a Gibbs state with the local temperature

$$T_B(\omega) = \frac{\omega}{\ln\left(1 + |z(\omega)|^{-2}\right)}, \tag{36}$$

as follows from equations (31) and (32). For large $|z(\omega)|$ (36) yields

$$T_B(\omega) \simeq \omega\, |z(\omega)|^2. \tag{37}$$

Therefore, for a constant shift, z, for all the modes, the local temperature is a linearly increasing function of the frequency.

3.0.3. Squeezed thermal bath

The state of a stationary squeezed thermal bath is the phase average (compare with [29, 40] where a non-stationary squeezed bath is used), $\bar{\rho}_B$, of the following density matrix

$$\rho_B = Z^{-1} S_r\, \mathrm{e}^{-H_B/T_{\text{eq}}}\, S_r^\dagger, \tag{38}$$

where S_r is the squeezing unitary operator defined by

$$S_r^\dagger b_k S_r = \cosh(r(\omega)) b_k + \sinh(r(\omega)) b_k^+, \tag{39}$$

and $r(\omega)$ is the squeezing parameter for the mode ω.

As for the multimode laser state, we assume that the bath is in a phase averaged state, see equation (35). Similarly, we do not need to compute explicitly the state $\bar{\rho}_B$ but only the average population number $n(\omega_k)$ applying (39) to $b_k{}^\dagger b_k$ and leaving the gauge invariant terms only. The local temperature is given by the expression

$$T_B(\omega) = \frac{\omega}{\ln\left\{1 + \left[n_{\text{eq}}(\omega) + \left(2n_{\text{eq}}(\omega) + 1\right)\sinh^2(r(\omega))\right]^{-1}\right\}}, \tag{40}$$

where $n_{\text{eq}}(\omega) = [\mathrm{e}^{\omega/T_{\text{eq}}} - 1]^{-1}$, is the mode population without squeezing. In the high temperature limit, $\frac{\omega}{T_{\text{eq}}} \ll 1$,

$$T_B(\omega) \simeq \frac{T_{\text{eq}}}{1 + \sinh^2(r(\omega))}. \tag{41}$$

Applying this result to a modified Otto cycle, where the hot bath is in a thermal squeezed state, the efficiency bound (equation (27)), found in [29, 40] is recovered. For large r (40) reduces to

$$T_B(\omega) \simeq \frac{\omega}{4}\left(2n_{\text{eq}}(\omega) + 1\right)\mathrm{e}^{2r}. \tag{42}$$

The notion of local temperature explains the meaning of 'violation of Carnot bound' for the engine with a squeezed hot bath observed in [29] (see [28]).

4. TLS heat machines coupled to different baths

In order to illustrate the particular properties of heat machines powered by non-equlibrium stationary baths we discuss the simplest implementation: a TLS-based system driven by the the *diagonal* periodic perturbation. We compare different examples of baths and discuss various scenarios of work extraction.

The working fluid (TLS) Hamiltonian is the following

$$H(t) = \left(\omega_o + \omega(t)\right)\frac{\sigma_z}{2}, \quad \omega\left(t + \frac{2\pi}{\Omega}\right) = \omega(t) \tag{43}$$

with Pauli matrices σ_i; $i = x, y, z$, and the conditions

$$\omega_o \geqslant 0, \quad \int_0^{2\pi/\Omega} \omega(t)\mathrm{d}t = 0. \tag{44}$$

The coupling to the bath is combined in a single term

$$H_{\text{int}} = \sigma_x B \tag{45}$$

with a single coupling spectrum $G(\omega)$.

The averaged Hamiltonian of the system coincides with the unperturbed one

$$\bar{H} = \frac{1}{2}\omega_o\sigma_z \tag{46}$$

and therefore (compare Remark 1), to analyze the stationary case it is enough to use the rate equation for the diagonal matrix elements in the H_o basis. The rate equation has the form

$$\dot{\rho}_{ee} = \sum_{q\in Z} P_q\left(G(-\omega_q)\rho_{gg} - G(\omega_q)\rho_{ee}\right), \quad \omega_q \equiv \omega_o + q\Omega, \tag{47}$$

where ρ_{gg} and $\rho_{ee} = 1 - \rho_{gg}$ are populations of the ground and excited state, respectively. The probability distribution $P_q = P_{-q} = |\xi_q|^2$ is obtained from the Fourier series $\mathrm{e}^{-\mathrm{i}\int_0^t \omega(t')\mathrm{d}t'} = \sum_{q\in Z} \xi_q \mathrm{e}^{-\mathrm{i}q\Omega t}$.

It follows immediately that the steady state population, $\dot{\rho}_{ee} = 0$, ratio reads

$$w = \left(\frac{\bar{\rho}_{ee}}{\bar{\rho}_{gg}}\right) = \frac{\sum_{q\in\mathbb{Z}} P_q G(-\omega_q)}{\sum_{q\in\mathbb{Z}} P_q G(\omega_q)} \tag{48}$$

which is just the expression for the detailed balance population for driven states. The local heat currents and power defined by the general formulas (22), (24) reduce to

$$\bar{J}_q = \frac{\omega_q P_q}{w + 1}\left(G(-\omega_q) - G(\omega_q)w\right), \tag{49}$$

$$\bar{P} = -\sum_{q\in Z} \bar{J}_q. \tag{50}$$

In (49) ω_q is the energy quantum exchanged between the bath and the system and the driving. The rest of the equation is the rate of population flow.

Classification of non-equilibrium baths

The functional dependence of $T_B(\omega)$ can be used to classify non-equilibrium baths. It depends on the coupling channel composed of the bath state, coupling to the system and frequency. Using equations (48) and (49) we can write the expression for power supplied to the system as

$$\bar{P} = z^{-1} \sum_{\{q_1 > q_2 \in \mathbb{Z}\}} \left(q_1 - q_2\right)\Omega P_{q_1} P_{q_2} G(\omega_{q_1}) G(\omega_{q_2})\left(\mathrm{e}^{-\omega_{q_2}/T_B(\omega_{q_2})} - \mathrm{e}^{-\omega_{q_1}/T_B(\omega_{q_1})}\right), \tag{51}$$

where

$$z = \sum_{q\in\mathbb{Z}} P_q G(\omega_q)\left[1 + \mathrm{e}^{-\omega_q/T_B(\omega_q)}\right]. \tag{52}$$

A sufficient condition

$$\omega_{q_2}/T_B(\omega_{q_2}) > \omega_{q_1}/T_B(\omega_{q_1}), \quad \text{for} \quad \left\{q_1 > q_2\right\}, \tag{53}$$

assures that $\bar{P} < 0$ and hence the engine extracts work from the bath.

4.0.4. Non-equilibrium but passive

We define the *passivity function* as $f(\omega) \equiv \frac{\mathrm{d}}{\mathrm{d}\omega}(\omega/T_B(\omega))$. According to (51) if for all frequencies $f(\omega) > 0$, no work can be extracted. We term such coupling channels as *passive*. This is in analogy to passive states [35, 41–43] which do not allow for work extraction by unitary transformations. Here, the transformation is non-unitary due to the presence of a bath; nevertheless, work extraction is still not allowed. Previous examples, based on linear coupling to bosonic baths, are passive if we consider only frequency independent deformations of a thermal bath (constant filtering, displacement or squeezing). From equation (51) we deduce that work extracted from a single non-equilibrium bath depends on the coupling spectrum shape and requires the passivity function $f(\omega)$ to be negative in some ranges of frequencies.

4.0.5. Two equilibrium baths as a single non-equilibrium one

As a first example of a non-passive bath, we consider the TLS quantum heat engine where the working fluid interacts with two independent baths at equilibrium (hot and cold). The coupling operator $B = B_h + B_c$ is a sum of two terms with negligible cross-correlations. Due to a generic cross-talking between baths induced by the system–bath coupling, we can treat them as a single non-equilibrium bath with a continuous local temperature function obtained from the coupling spectrum being a sum of two bath spectra. Therefore, the local temperature of this composed bath satisfies the following relation

$$\mathrm{e}^{-\omega/T_B(\omega)} = \frac{\mathrm{e}^{-\omega/T_h}G^h(\omega)}{G^h(\omega) + G^c(\omega)} + \frac{\mathrm{e}^{-\omega/T_c}G^c(\omega)}{G^h(\omega) + G^c(\omega)} = \mathrm{e}^{-\omega/T_h}(1 - m(\omega)) + \mathrm{e}^{-\omega/T_c}m(\omega), \quad 0 \leqslant m(\omega) \leqslant 1,$$

where we use the fact that both baths are in equilibrium and the standard KMS condition holds. The effective Boltzmann factor is a weighted average of two Boltzmann ones, where the weights depend on the strength of the working fluid coupled to each bath at the given frequency. Therefore, $T_h \geqslant T_B(\omega) \geqslant T_c$. For the sake of simplicity, we assume that the bath coupling spectrum overlaps with only two harmonic frequencies ($\omega_{q_1} > \omega_{q_2}$). As shown in [34] this condition is required in order to achieve high efficiency. Work extraction requires the hot bath being coupled more strongly to the high frequency mode ($G^h(\omega_{q_1}) \gg G^c(\omega_{q_1})$) and the opposite for the low frequency mode ($G^h(\omega_{q_2}) \ll G^c(\omega_{q_2})$) [34]. The efficiency of the engine is given by the Carnot-type formula

$$\eta = 1 - \frac{T_B(\omega_{q_2})}{T_B(\omega_{q_1})} \leqslant 1 - \frac{T_c}{T_h}.$$

The extreme case, where the engine reaches the maximum efficiency, the Carnot bound, is when the baths are spectrally separated, i.e. $T_B(\omega_{q_1}) \simeq T_h$ and $T_B(\omega_{q_2}) \simeq T_c$. This example, called in [34] *universal quantum machine*, provides the closest analog to the standard heat machine alternately coupled to a hot and a cold bath.

4.0.6. An example of a non-equilibrium and non-passive bosonic bath

As shown above, frequency independent deformation of a thermal bosonic bath with linear coupling, creates passive baths. Therefore, work extraction requires the use of '*selective*' transformations. As an illustration we analyze the case where the deviation from equilibrium is obtained through selective filters. This scenario can be implemented in optical setups, where the photon bath is 'filtered' with the use of optical filters. Other possible deviations from equilibrium may be obtained by other transformations, such as displacement or squeezing, but its detailed analysis is beyond the scope of this work. In order not to contradict the second law of thermodynamics, which forbids work extraction from a single thermal bath, this selective filter should involve the presence of other baths, non-equilibrium processes or a hidden work injection.

Assume a single bosonic bath at the equilibrium temperature T_{eq} and linearly coupled to the system. If a selective filter, $\lambda(\omega)$, is applied, the local temperature satisfies

$$\mathrm{e}^{-\omega/T_B(\omega)} = \frac{\lambda(\omega)n_{\mathrm{eq}}(\omega)}{\lambda(\omega)n_{\mathrm{eq}}(\omega) + 1}, \tag{54}$$

with $n_{\mathrm{eq}}(\omega) = (\mathrm{e}^{\omega/T_{\mathrm{eq}}} - 1)^{-1}$. What are the conditions required for this filter to allow work extraction?

Consider again the bath coupling spectrum which overlaps with only two harmonic frequencies ω_{q_1}, ω_{q_2} with $q_1 > q_2$. Assume that we reduce the population of the mode ω_{q_2} ($\lambda(\omega_{q_2}) < 1$), and we do not filter the other mode ($\lambda(\omega_{q_1}) = 1$). In order to allow work extraction ($\bar{P} < 0$, see equation (51)), the filter should satisfy the following condition

$$\lambda(\omega_{q_2}) < e^{\frac{(q_2 - q_1)}{2T_{\mathrm{eq}}}\Omega}\frac{\sinh\left(\frac{\omega_{q2}}{2T_{\mathrm{eq}}}\right)}{\sinh\left(\frac{\omega_{q1}}{2T_{\mathrm{eq}}}\right)} < 1.$$

As paradoxical it may sound, by reducing a specific mode population, we can extract work from a single thermal bath! The filtering lowers the effective temperature $T_B(\omega_{q_2})$, reducing the excitations that are emitted to this mode, and 'saving' energy, which is ultimately transformed into work. The efficiency of this machine is bounded by a generalized Carnot limit

$$\eta = \frac{-\bar{P}}{\bar{J}_H} \leqslant 1 - \frac{T_B(\omega_{q_2})}{T_{\text{eq}}},$$

where T_{eq} and $T_B(\omega_{q_2})$ play the role of the effective hot and cold bath temperature, respectively.

4.0.7. Deviation from equilibrium of an engineered bath

Using the selective filtering introduced in the last section, we can engineer a non-equilibrium bosonic bath from an equilibrium one, and characterize its deviation from equilibrium by the parameter

$$D = 1 - \lambda(\omega_{q_2}).$$

For the equilibrium bath $D = 0$, and when we start reducing the population of the modes with frequencies around ω_{q_2}, the bath will go away from equilibrium, producing some non-equilibrium effects, such as frequency dependent equilibration temperature. Nevertheless, work extraction will be possible only when the bath is far enough from equilibrium, i.e.

$$D > n_{\text{eq}}(\omega_{q_1})\left(\mathrm{e}^{\omega_{q_1}/T_{\text{eq}}} - \mathrm{e}^{\omega_{q_2}/T_{\text{eq}}}\right). \tag{55}$$

When the deviation from equilibrium increases, the local temperature of the lower frequency mode reduces and the efficiency of the quantum heat engine rises. For $D < 0$ the bath is also out of equilibrium. But, in this case, instead of the mode population reducing, it is being increased by some external mechanism (for example, selective concentration of light). The equilibration temperature of the system will depend on the frequency, but for $D < 0$, work cannot be extracted. Again, paradoxically, the increase of energy in 'incorrect modes' reduces the possibility of work extraction. The bath is taken away from thermal equilibrium, but in the 'opposite direction' to that leading to work extraction.

5. Conclusions

We showed that quantum machines weakly coupled to a single non-equilibrium stationary environment, and subject to fast periodic driving by work reservoirs, can be described by the thermodynamical principles and bounds which are very similar to the standard ones if only the definitions of the basic notions, which are consistent with thermodynamics, are used. In particular, the notion of local temperature which depends not only on the state of environment but also on the form of system–environment coupling is crucial.

The developed non-equilibrium theoretical framework may be used also to describe the standard heat engine model with two thermal baths including cross-talking effects. Such machines can be effectively treated as coupled to a single non-equilibrium bath.

Starting from a bosonic thermal bath we showed how to obtain non-equilibrium baths by using different engineering methods such as filtering, energy concentration, displacement or squezeeing operations. We discovered that such non-equilibrium baths may be divided into two different types: (i)*Passive*, which equilibrate systems to different temperatures depending on their working frequencies but cannot drive heat engines. Such baths can be obtained by frequency independent transformations of equilibrium ones. (ii) *Non-passive*, which, besides producing local equilibration temperatures, allow work extraction from a single bath and, in the case of bosonic reservoirs, can be engineered by frequency dependent transformations of equilibrium states. They are also farther away from equilibrium than passive baths.

A case where a non-equilibrium bath is not stationary but, for example, is also perturbed by an external periodic driving is another interesting topic with possible applications. A natural example is a spin-1/2 coupled to a spin-bath, both periodically perturbed by an external magnetic field. It seems that the theory presented above can be extended to these cases as well.

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