Strongly Coupled Quantum Heat Machines

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Accessibility
Quantum heat machines (QHMs) models generally assume a weak coupling to the baths. This supposition is grounded in the separability principle between systems and allows the derivation of the evolution equation for this case. In the weak coupling regime, the machine’s output is limited by the coupling strength, restricting their application. Seeking to overcome this limitation, we here analyze QHMs in the virtually unexplored strong coupling regime, where separability, as well as other standard thermodynamic assumptions, may no longer hold. We show that strongly coupled QHMs may be as efficient as their weakly coupled counterparts. In addition, we find a novel turnover behavior where their output saturates and disappears in the limit of ultra-strong coupling.

One of the basic tenets of standard thermodynamics is the principle of separability, which allows to clearly define and distinguish systems that interact with each other. When the surface to volume ratio is small, surface effects are negligible, and thermodynamic variables only depend on the volume and not on the shape. This argument implicitly assumes a weak coupling, restricting the interaction space to a small interface between the systems [1,3].

The assumption of weak coupling was essential for the development of open quantum system theory [4], in particular for the development of the Kossakowski-Lindblad master equation [4–6], that describes the evolution of a system interacting with a thermal bath. Quantum heat machines (QHMs) models [7–14] use this framework to describe the evolution of the “working fluid” under the influence of the hot and cold baths. Progress in this field has been recently reviewed [15, 16]. QHMs may operate either as engines, by extracting work power, or as refrigerators, by investing work power and cooling the cold bath. In both cases, quantum resources have been proposed [17–20] in order to boost their output and efficiency. Nevertheless, these models assume a weak coupling to the baths, resulting in limited QHMs outputs and consequently restricting their applications.

The potential technological implications of high-output QHMs, such as faster and more powerful laser cooling [21, 22], call for a prompt way to overcome the limitation set by the weak coupling assumption. However, the strong coupling limit has been virtually left unexplored due to the lack of theoretical tools to describe the “working fluid” evolution. One of the few exceptions [23] considers the case of Hamiltonian quench, which involves the switching “on” and “off” of the system-bath interaction Hamiltonian, introducing an energy and efficiency cost that reduces the machine efficiency below the Carnot bound. In this letter we take a different approach by putting forward a strongly coupled continuous QHM model (see Fig. 1), that does not require the coupling to and uncoupling from the baths, which may not be possible at nanoscale, where the system is totally embedded in thermal baths. We investigate its output and efficiency in order to determine its performance limits and which thermodynamic principles, e.g., Carnot bound, still hold at the strong coupling regime. Addressing these issues becomes more relevant in the light of the large progress achieved in the field of strongly coupled superconductors [24–27], which makes the realizations of strongly coupled QHMs potentially tractable in the near future.

Figure 1: Model of continuous quantum heat machine where the cold bath strongly interacts with the working fluid, while the hot bath is weakly coupled.

Model and analysis We employ a model for a continuous QHM similar to the one we studied previously in the weak coupling limit [28]. This system can operate either as an engine or a refrigerator depending on the spectrum of the reservoirs and the engine’s driving frequency. This model is comprised by a driven two-level quantum system, that represents the working fluid, permanently coupled to the heat baths (hot and cold). The evolution of this model is governed by the Hamiltonian

\[ H = \frac{\omega_0}{2} \sigma_z + \frac{\Omega}{2} \left( \sigma_+ e^{-i \omega t} + \sigma_- e^{i \omega t} \right) + \]

\[ \sigma_z \otimes \sum_k \xi_C (g_{C,k} a_k^\dagger + g_{C,k}^* a_k) + \]

\[ \sigma_x \otimes \sum_k \xi_H (g_{H,k} b_k^\dagger + g_{H,k}^* b_k) + \]

\[ \sum_k \omega_{C,k} a_k^\dagger a_k + \sum_k \omega_{H,k} b_k^\dagger b_k, \]  

where \( \xi_C, \xi_H \) is the strength parameter of the cold (hot) bath, \( g_{i,k} \) is a dimensionless parameter that defines the relative coupling strength of the TLS to the mode i of the i-bath, \( \sigma_i \) are the standard Pauli matrices, and \( a_k^\dagger, a_k, b_k^\dagger, b_k \) are the creation and annihilation operator of the cold (hot) bath mode k. The election of the hot and cold bath is somehow arbitrary and a similar analysis could be performed if they are interchanged.
The coupling is considered weak if $\gamma \tau_{cor} \ll 1$, where $\gamma$ is the decay rate and is equivalent to the resonant coupling spectrum ($\gamma = G(\omega_0)$) and $\tau_{cor}$ is the bath correlation time [29]. Is it possible to extract work or to cool down in the strong coupling regime? To elucidate this question, consider that both couplings are strong. While the reduced dynamics is analytically solvable in the weak regime, in this case the perturbation expansion on the coupling strength contains infinite no-neglectable terms [30].

Nevertheless for $\mathcal{H}$, this obstacle may be overcome by solving the problem in a more appropriate basis, where the system is effectively weakly coupled to the two baths. This is achieved by using the polaron transformation [31-37], $e^S$, where $S = \sum_k (\alpha_k a_k^\dagger - \alpha_k^* a_k)$ and $\alpha_k = \xi C_{k,\omega_0}$.

The transformed Hamiltonian, $\tilde{\mathcal{H}} = e^S \mathcal{H} e^{-S}$, is

$$\tilde{\mathcal{H}} = \frac{\omega_0}{2} \sigma_z + \Omega l \left( \sigma_+ e^{-i\omega_l t} + \sigma_- e^{i\omega_l t} \right) + \Omega \left( e^{-i\omega_l \sigma_+} \otimes (A_+ - A) + e^{i\omega_l \sigma_-} \otimes (A_+ - A) \right) + (\sigma_+ \otimes A_+ + \sigma_- \otimes A_-) \sum_k \xi \tilde{H}(g_{H,k} b_k^\dagger + g_{H,k}^* b_k) + \sum_k \omega_{C,k} a_k^\dagger a_k + \sum_k \omega_{H,k} b_k^\dagger b_k, \quad (2)$$

where $A_\pm = \Pi_k D(\pm 2\alpha_k)$, $D(\alpha_k) = e^{\alpha_k a_k^\dagger - \alpha_k^* a_k}$ is the displacement operator, $A = (A_\pm) = e^{-2\xi G_1(\omega_0) \sum_k \beta \xi C_{k,\omega_0}^2 \coth(\beta C_{k,\omega_0})}$ and $\Omega l = \Omega A$. The terms on the Hamiltonian proportional to the identity have been neglected.

In the transformed Hamiltonian, the coupling operators are different. $A_+ - A$ and $A_- - A$, instead of $a_k^\dagger a_k$, $\alpha_k$ and extra terms are added to the hot bath coupling (see Eq. (2) and Suppl. A). As we show below, the new couplings may be effectively weak even for high values of the original coupling strengths, $\xi G_{1(H)}$. Therefore, the assumptions derived from the weak coupling are correct (e.g. the transformed baths remain at thermal equilibrium) and the master equation may be derived using standard techniques [4] for also values of $\xi G_{1(H)}$ that break the weak coupling assumption in the original basis [22,37].

The transformed cold bath, now interacts with the TLS through two different operators, $\tilde{F}_1(t) = \frac{\Omega}{2} (A_+(t) - A)$ and $\tilde{F}_2 = A_-(t) \otimes \sum_k \xi \tilde{H} \left( g_{H,k} b_k^\dagger + g_{H,k}^* b_k \right)$. The correlation function of the first is

$$\langle \tilde{F}_1(t) \tilde{F}_1(0) \rangle = \left( \frac{\Omega A_+}{2} \right)^2 \left( e^{4\xi \xi G_1(\omega_0) \sum_k \frac{\Delta(t)}{\xi}} - 1 \right), \quad (3)$$

where

![Figure 2: (Color online) Effects of the coupling strength. Main panel: Coupling spectrum in the original basis $G_1(\omega_0)$ (dotted line) and in the transformed basis $G_{1(\omega)}$ (continuous line) as a function of the coupling strength $\xi C \sim \xi H$. The weak coupling assumption holds only for coupling spectrum below the dashed line. Inset: Power for a QHM as a function of the coupling strength, $\xi C \sim \xi H$. A turnover is observed and the power decays for ultra-strong coupling. At this limit, the lack of system-bath separability prevents work extraction.](image-url)
with linear combinations of $\omega_0$ and $\omega_l$, the TLS and driving frequency, respectively [8].

The polaron transformation allows the derivation of the QHM evolution for a wide range of values of the coupling strengths. Nevertheless, this simplification entails other complications, as the loss of separability. In the transformed basis, the second correlation is far from standard. It involves exchange of excitation with both baths (the operators $b_{q,1}^{(t)}$ and $A_{q}$ for the hot and cold bath respectively). The lack of separability breaks the standard KMS condition, casting doubt on the validity of other thermodynamic principles, as the Carnot bound.

The answer to this question is obtained from the theory of non-equilibrium thermodynamics, which introduces the frequency dependent “local” temperatures, $\beta(\omega)$. They are analogous to the non-equilibrium position-dependent local temperatures [42]. In the non-equilibrium framework, the KMS condition is generalized (see Suppl. B): 

$$G_2(-\omega) = e^{-\beta(\omega)\omega}G_2(\omega),$$  
$$\beta(\omega) = \beta_C \lambda(\omega) + \beta_H (1 - \lambda(\omega)), \tag{5}$$ 

where $\lambda(\omega)$ measures the relative contribution of the transformed cold bath to $G_2(\omega)$ and may take any positive or negative value. Therefore $\beta(\omega)$ is not restricted to the range $[\beta_H, \beta_C]$. It depends on both baths coupling strength distribution and modes, making $\beta(\omega)$ frequency dependent, blurring its physical interpretation. As we show later, it allows to establish clear thermodynamic bounds to the efficiency of the QHMs and to relate them to the Carnot bound. The precise value taken by $\beta(\omega)$, depends on how the exchange energy $\omega$ is divided between the hot and the cold baths.

In a similar manner as $G_1(\omega), G_2(\omega)$ not only includes harmonics of the cold bath, but combinations of them with modes of the hot bath. Therefore, also the hot bath may be highly detuned from the TLS frequency (and from any linear combination with the driving frequency).

In the transformed basis, we use the standard weak coupling master equation based on the general Floquet theory of open systems [38]. We just stress the main steps, but the detailed derivation may be found in [28]. The reduced evolution of the TLS density matrix, $\rho$, is given by a linear combination of Lindblad generators obtained from the Fourier components in the interaction picture of the working fluid coupling operators $e^{\pm i\omega t} \sigma_{\pm}(t) = \sum_{q \in Z} \sum_{\omega} S_{q,0}(\omega)e^{-i(\omega+q\omega)t}$ and $\sigma_{\pm}(t) = \sum_{q \in Z} \sum_{\omega} S_{2,q}(\omega)e^{-i(\omega+q\omega)t}$. In the interaction picture,

$$\frac{d\rho}{dt} = \mathcal{L}\rho, \quad \mathcal{L} = \sum_{q,\omega} \mathcal{L}^1_{q,\omega} + \sum_{q,\omega} \mathcal{L}^2_{q,\omega},$$ 

$$\mathcal{L}^1_{q,\omega} = \frac{G^i(\omega + q\omega)}{2} \times \left( [S_{i,q}(\omega)\rho, S^\dagger_{i,q}(\omega)] + [S_{i,q}(\omega), \rho S^\dagger_{i,q}(\omega)] \right). \tag{6}$$

The TLS density matrix evolves until it reaches a steady state (limit cycle), $\mathcal{L}\rho = 0$. At this point any transient effect averages out and one may calculate the steady state work power and heat flows,

$$J_1 = \sum_{q,\omega} \text{sgn}(\omega) (\omega + q\omega) Tr \left[ \mathcal{L}^1_{q,\omega} \rho \right], \quad P = -J_1 - J_2, \tag{7}$$

where $\text{sgn}(\omega) = 1$ for $\omega > 0$ and $\text{sgn}(\omega) = -1$ for $\omega < 0$.

In particular we are interested in the ultra-strong coupling regime ($\xi_C \sim \xi_H \gg \omega_0$) to find out if QHMs may have an ultra-high output. Nevertheless at this limit, and assuming a weak driving with positive detuning ($\delta = \omega_0 - \omega_l \gg \Omega_r > 0$), the work power dependence on the coupling strength goes as (see Suppl. C)

$$P \propto \omega_l \frac{A_C^2 (e^{-\beta C \delta} - e^{-\beta(\omega_0)\omega_0})}{\xi_C^2} \propto e^{-4\xi_C^2 \sum_k \| \frac{\text{sgn}(\omega_k^0)}{\omega_k} \| ^2 \coth \left( \frac{\beta(\omega_k^0)}{2} \right)}. \tag{8}$$

The conditions for work extraction ($P < 0$),

$$\frac{\omega_l}{\omega_0} < 1 - \frac{\beta(\omega_0)}{\beta_C},$$

is derived from Eq. (8). The heat currents to the baths are:

$$J_1 \propto \delta \frac{A_C^2 (e^{-\beta C \delta} - e^{-\beta(\omega_0)\omega_0})}{\xi_C^2} < 0;$$

$$J_2 \propto -\omega_0 \frac{A_C^2 (e^{-\beta C \delta} - e^{-\beta(\omega_0)\omega_0})}{\xi_C^2} > 0. \tag{9}$$

For ultra-strong coupled baths, the work power will decay with the coupling strength as shown in Eq. (8). The exact counterpart of Eq. (8) for any value of $\xi_C \sim \xi_H$ is plotted on figure 2. Inset. Opposite to what may be expected from previous results in the weak coupling regime, work power does not increase indefinitely with the coupling strength. Not only it saturates, but at some point, decays and vanishes. At the ultra-strong limit, the system and the baths are no longer independent, preventing work extraction which requires some degree of separability.

The determination of the engine efficiency, as well as the cooling power (in the refrigerator operation mode), is a more subtle issue. A naive guess would be to consider $J_2$, which is positive, as the incoming heat flow from the hot bath and to define the efficiency as

$$\eta = -\frac{P}{J_2} = \frac{\omega_l}{\omega_0} \leq 1 - \frac{\beta(\omega_0)}{\beta_C}. \tag{10}$$

which can take any value, even above Carnot limit. Nevertheless, the lack of separability complicates the determination of how much energy is exchanged with each bath through the
conducting flux qubit with tunable gap \[46\], where the main point (\[43, 44\]) has been recently achieved \[43, 44\], showing astounding \(\xi_i/\omega_0\) ratios of around 0.12. Moreover, recent theoretical studies have shown that a \(\sigma_x\)-coupling between quantum microwaves and artificial Josephson-based atoms can be pushed up to \(\xi_i/\omega_0 \sim 2\) \[45\], which is well beyond the critical point \((\xi_i/\omega_0 = 1)\) at which the power efficiency is maximum. Our proposal consists of a periodically driven superconducting flux qubit with tunable gap \[46\], where the main loop is coupled to the hot bath (\(\sigma_x\) coupling), and the \(\alpha\)-loop is coupled to the cold bath (\(\sigma_z\) coupling). In order to bring the \(\sigma_x\) coupling to the strong regime, we galvanically couple the \(\alpha\)-loop to the open transmission line that plays the role of the cold bath.

Conclusions The possibility of work extraction and cooling in the strong coupling regime was shown. Even though some thermodynamic principles, as the standard KMS condition, do not longer hold at this regime due to the lack of separability between the baths, the operation of the QHMs may be described in a non-equilibrium framework. This is advantageous because it shows that important principles, as the Carnot bound, still hold in the strong coupling regime. The introduction of frequency-local temperatures, that account for the different baths contributions to the heat flows, are useful to determine how the heat flows are divided between baths and to correctly calculate the QHMs efficiency. As we have shown, continuous strongly coupled QHMs, as their weakly coupled counterparts, avoid the efficiency reduction due to the coupling turning on and off and keep the Carnot bound which can be reached under the appropriate driving frequency.

The appearance of the “non-equilibrium” temperatures is related to the loss of separability. Even though both baths, in the transformed basis, are in equilibrium, the heat flows mixes the contribution of both of them, causing an effective deviation from equilibrium.

There are similarities between weakly and strongly coupled QHMs, but the differences should not be overlooked. While weakly coupled QHMs require baths with modes resonant to the TLS (or linear combinations with the driving frequency), strongly coupled QHMs operate also for highly detuned baths, because harmonics of the strongly coupled bath modes also contribute to both coupling spectra. An important feature of strongly coupled QHMs is that, differently to their weakly coupled counterpart, where the outputs are proportional to the square of the coupling strength, work and cooling power saturate at some point and for ultra-strongly coupled machines they fall down as the coupling strength increases. This is a consequence of the loss of separability as the coupling strength increases, and shows that QHMs require some degree of separability to operate.

In order to optimize QHMs output the “right” coupling strength is needed, resembling the quantum Goldilocks effect \[47\] found in photosynthetic systems. The latter should be further investigated to determine if evolution fine-tuned the coupling strength to the baths in order to maximize their chemical power output. Alternatively, the turnover behavior may be corroborated experimentally using superconducting qubits \[23, 27\].

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Supplementary Information

A. System-Bath coupling

In the original basis the system-bath coupling operators are:

\[ \sigma_z \otimes \sum_k \xi_C (g_{C,k} a_k^\dagger + g_{C,k}^* a_k), \]
\[ \sigma_x \otimes \sum_k \xi_H (g_{H,k} b_k^\dagger + g_{H,k}^* b_k), \]  
(S1)

where \( \sigma_i \) are Pauli matrix and operate on the system. \( a_k^\dagger \) and \( a_k \) \( (b_k^\dagger \) and \( b_k \)) are the cold (hot) bath operators.

In the transformed basis, the system-bath coupling operators are

\[ \frac{\Omega}{2} (e^{-i\omega t} \sigma_+ \otimes (A_+ - A) + e^{i\omega t} \sigma_- \otimes (A_- - A) ), \]
\[ (\sigma_+ \otimes A_+ + \sigma_- \otimes A_-) \otimes \sum_k \xi_H (g_{H,k} b_k^\dagger + g_{H,k}^* b_k), \]  
(S2)

where

\[ A_\pm - A = \Pi_k e^{\pm 2\alpha_\pm a_k^\dagger a_k} - e^{-2\alpha_\pm \sum_k \| \frac{a_k^\dagger a_k}{\xi_k} \|^2 \coth(\frac{\beta \xi_k}{2})}, \]
\[ A_\pm = \Pi_k e^{\pm 2\alpha_\pm a_k^\dagger a_k}. \]  
(S3)

B. Generalized KMS condition

As mentioned in the main text, the coupling spectrum \( \tilde{G}_2(\omega) \) contains contributions from both baths. The frequency sum of the contributing hot and cold bath modes should match the spectrum frequency, \( \omega = \omega_{H,i} + \omega_{C,j} \). There are many combinations of modes that match the spectrum frequency, therefore

\[ \tilde{G}_2(\omega) = \sum_{i,j} \tilde{G}_2(\omega_{H,i} + \omega_{C,j}). \]  
(S4)

Due to the non-linearity of the cold bath coupling operators in the transformed basis, its mode harmonics also contribute to the sum on Eq. (S4). The \( \tilde{G}_2(\omega_{H,i} + \omega_{C,j}) \) physical meaning is an energy exchange, where an excitation \( \omega \) of the system is interchanged with the \( \omega_{H,i} \) and \( \omega_{C,j} \) modes of the hot and cold baths, respectively. They keep a modified KMS condition

\[ \tilde{G}_2(-\omega_{H,i} - \omega_{C,j}) = e^{-\beta H \omega_{H,i} - \beta C \omega_{C,j}} \tilde{G}_2(\omega_{H,i} + \omega_{C,j}). \]  
(S5)

Combining all the terms, the effective frequency-local temperature may be defined as

\[ e^{-\beta(\omega)} = \frac{\tilde{G}_2(-\omega)}{\tilde{G}_2(\omega)} = \sum_{i,j} e^{-\beta H \omega_{H,i} - \beta C \omega_{C,j}} K_{\omega_{H,i} + \omega_{C,j}}, \]
\[ K_{\omega_{H,i} + \omega_{C,j}} = \frac{\tilde{G}_2(\omega_{H,i} + \omega_{C,j})}{\sum_{i,j} \tilde{G}_2(\omega_{H,i} + \omega_{C,j})}, \]  
(S6)

where \( K_{\omega_{H,i} + \omega_{C,j}} \) is the relative weight of the \( \tilde{G}_2(\omega_{H,i} + \omega_{C,j}) \) component.

C. Heat currents and power

For a weak driving and positive detuning, the heat currents and power are (see [28])
\[ J_1 = \delta \frac{\tilde{G}_1(\delta)\tilde{G}_2(\omega_0)}{G_1(\delta) + G_2(\omega_0)} (e^{-\beta_C \delta} - e^{-\beta(\omega_0)\omega_0}), \quad (S7) \]
\[ J_2 = -\omega_0 \frac{\tilde{G}_1(\delta)\tilde{G}_2(\omega_0)}{G_1(\delta) + G_2(\omega_0)} (e^{-\beta_C \delta} - e^{-\beta(\omega_0)\omega_0}), \quad (S8) \]
\[ P = \omega_0 \frac{\tilde{G}_1(\delta)\tilde{G}_2(\omega_0)}{G_1(\delta) + G_2(\omega_0)} (e^{-\beta_C \delta} - e^{-\beta(\omega_0)\omega_0}), \quad (S9) \]

where \( \tilde{G}_i(\omega) = \int_{-\infty}^{\infty} e^{it\omega} \langle \tilde{F}_i(t)\dagger\tilde{F}_i(0) \rangle dt. \)

We assume that the main contribution to the coupling spectrum comes from few modes. For the sake of simplicity we present the calculation assuming that this contribution is due to one mode. Then,
\[
\langle \tilde{F}_1(t)\dagger\tilde{F}_1(0) \rangle = \left( \frac{\Omega A}{2} \right)^2 \left( e^{4\xi^2 \sum_k \frac{\Lambda_k(t)}{\omega_k^2}} - 1 \right) \approx \left( \frac{\Omega A}{2} \right)^2 \left( e^{4\xi^2 \sum_k \frac{\Lambda_k(t)}{\omega_k^2}} - 1 \right) \approx \left( \frac{\Omega A}{2} \right)^2 \left( \frac{4\xi^2 \sum_k \frac{\Lambda_k(t)}{\omega_k^2}}{\omega_k^2} - 1 \right) \approx \left( \frac{\Omega A}{2} \right)^2 \left( \frac{4\xi^2 \sum_k \frac{\Lambda_k(t)}{\omega_k^2}}{\omega_k^2} - 1 \right). \quad (S10)\]

where Bessel and modified Bessel functions have been used to expand the exponential. Using the Fourier transformation and taking the asymptotic limits of the Bessel and modified Bessel functions:

\[
\tilde{G}_1(\delta) \propto e^{-4\xi^2 \sum_k \frac{\|g_{C,k}\|}{\omega_k^2} \coth(\frac{\beta_C \omega^2}{2})}. \quad (S11)\]

\( \tilde{G}_2(\omega_0) \) has a similar dependence. Therefore, for \( \xi_C \to \infty, P \propto \frac{4\xi^2 \sum_k \frac{\|g_{C,k}\|}{\omega_k^2} \coth(\frac{\beta_C \omega^2}{2})}{\xi_C}. \)