Construction and optimization of a quantum analog of the Carnot cycle

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The quantum analog of Carnot cycles in few-particle systems consists of two quantum adiabatic steps and two isothermal steps. This construction is formally justified by use of a minimum work principle. It is then shown, using minimal assumptions of work or heat in nanoscale systems, that the heat-to-work efficiency of such quantum heat engine cycles can be further optimized via two conditions regarding the expectation value of some generalized force operators evaluated at equilibrium states. In general the optimized efficiency is system specific, lower than the Carnot efficiency, and dependent upon both temperatures of the cold and hot reservoirs. Simple computational examples are used to illustrate our theory. The results should be an important guide towards the design of favorable working conditions of a realistic quantum heat engine.

I. INTRODUCTION

The big *energy* challenge of this century calls for diversified energy research, including a bottom-up approach towards energy efficiency. Apart from two stimulating implementations of microscale heat engines [1,2], some theoretical aspects as well as possible realizations of nanoscale heat engines [3–17] have been studied. For purely quantum heat engines at the nanoscale where the working medium may consist of few particles only (e.g., few trapped ions) [6], both quantum fluctuations and thermal fluctuations become significant. General understanding of the design of such energy devices are also of fundamental interest to nanoscale thermodynamics [18–22]. In particular, as the size of the working medium shrinks to a quantum level, one must reexamine the implications of the second law of thermodynamics for the efficiency of quantum heat engines [23]. To that end, we construct and look into the quantum analog of Carnot cycles [24,25].

The construction of the quantum analog of a Carnot cycle is not as straightforward as it sounds. Consider first the two quasistatic isothermal steps during which the working medium is *in thermal equilibrium* with a reservoir. There, regardless of its size, the quantum medium has well-defined thermodynamic properties. As such isothermal steps can be directly carried over to the quantum case. However, translating the two adiabatic steps of a Carnot cycle into a quantum analog is by no means obvious. One intuition [3,9,10] is to replace quasistatic adiabatic steps in thermodynamics (without heat exchange) by quantum adiabatic processes (as defined in the celebrated quantum adiabatic theorem [26]). The starting point of this work is to formally justify such an intuitive construction by revealing a fundamental reason related to energy efficiency.

Below we simply call the above-defined quantum analog of a classical Carnot cycle (two quantum adiabatic processes, plus two isothermal quasistatic steps during which the system is at thermal equilibrium) as a quantum Carnot cycle. It is yet fundamentally different from a conventional Carnot cycle. During the two adiabatic steps, the working medium implementing the quantum Carnot cycle is generically not at equilibrium conditions (exceptions to be elaborated below).

Thus, it becomes important to lay out general designing principles concerning how the efficiency of a quantum Carnot cycle can be optimized, preferably using standard definitions of work and heat. The explicit optimization conditions will be presented in this work. Our theory also shows that in general the optimized efficiency attained by a quantum Carnot cycle is (i) lower than the standard Carnot efficiency, (ii) not a simple function of T_c/T_h but a function of both T_c and T_h, the temperatures of cold and hot reservoirs, and (iii) depends on the detailed spectrum of the working medium. These features will guide us in the design of favorable working conditions of a realistic quantum heat engine. Simple computational examples are used to illustrate our theory. Throughout this work we do not use recent microscopic interpretations or definitions of work or heat proposed for quantum systems, such as those introduced in Refs. [9,10,12,27]. Instead, we assume only that heat exchange is zero if the working medium is thermally isolated and work is zero if the system parameters of the working medium are fixed. This assumption is fully consistent with the understandings discussed in recent review articles [21,22].

II. EFFICIENCY OF QUANTUM HEAT ENGINE CYCLES AND THE SECOND LAW

We start with general considerations of a quantum heat engine cycle consisting of two steps of an isothermal system and two processes of a thermally isolated system. Figure 1 schematically depicts such a cycle. There $A \rightarrow B$ and $C \rightarrow D$ represent two isothermal processes during which the quantum medium is always at equilibrium with a reservoir, λ is assumed to be the only system parameter tunable in a cycle opeation, $\langle E \rangle$ is the mean energy of the system (that is, the quantum expectation value of the energy of the system obtained by many energy measurements), and $B \rightarrow C'$ and $D \rightarrow A'$ represent two thermally isolated and hence unitary processes. The symbols A' and C' indicate that right after a unitary process, the quantum medium is in general not at thermal equilibrium. States of A' and C' will reach thermal equilibrium states A and C after relaxation with a reservoir under fixed values of λ.

When the system at the nonequilibrium state C' starts heat exchange with the cold reservoir under fixed $\lambda = \lambda_C$, no work is done. Hence $\langle E_{C'} \rangle - \langle E_C \rangle$ is simply the heat dumped (which
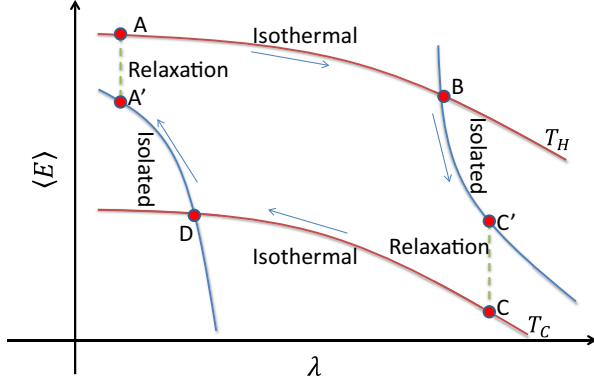
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FIG. 1. (Color online) A quantum heat engine cycle consisting of two isothermal steps and two thermally isolated and hence unitary steps. A, B, C, and D represent four equilibrium states, and C' and A' represent two nonequilibrium states at the end of two unitary steps, approaching, respectively, equilibrium states C and A after a relaxation step initiated by contact with the reservoirs. As shown in the text, for a quantum analog of the Carnot cycle, the two thermally isolated steps should be two quantum adiabatic processes.

could be negative). This thermal relaxation process is followed by the isothermal process from C to D. The total heat Q_{out} dumped to the cold reservoir ($Q_{\mathrm{out}} > 0$ indicates heat flowing from system to cold reservoir) is hence contributed by two terms, with

$$Q_{\mathrm{out}} = T_c(S_C - S_D) + \langle E_{C'}\rangle - \langle E_C\rangle, \qquad (1)$$

where S_C and S_D describe entropy of equilibrium states C and D. In the same fashion, the total heat absorbed from the hot reservoir, denoted by Q_{in} ($Q_{\mathrm{in}} > 0$ indicates heat flowing from hot reservoir to system), is given by

$$Q_{\mathrm{in}} = T_h(S_B - S_A) + \langle E_A\rangle - \langle E_{A'}\rangle. \qquad (2)$$

The efficiency of such a general quantum engine cycle is therefore $\eta_q = 1 - Q_{\mathrm{out}}/Q_{\mathrm{in}}$, i.e.,

$$\eta_q = 1 - \frac{T_c(S_C - S_D) + \langle E_{C'}\rangle - \langle E_C\rangle}{T_h(S_B - S_A) + \langle E_A\rangle - \langle E_{A'}\rangle}. \qquad (3)$$

To compare the above efficiency η_q with the Carnot efficiency $\eta_c \equiv 1 - T_c/T_h$, we first define $\Delta S_{B\to C}^{\mathrm{total}}$ and $\Delta S_{D\to A}^{\mathrm{total}}$, namely, the total entropy increase of the universe for the overall process $D \to A$ and $B \to C$. It is straightforward to obtain

$$\Delta S_{B\to C}^{\mathrm{total}} = (S_C - S_B) - \frac{1}{T_c}[\langle E_C\rangle - \langle E_{C'}\rangle],$$

$$\Delta S_{D\to A}^{\mathrm{total}} = (S_A - S_D) - \frac{1}{T_h}[\langle E_A\rangle - \langle E_{A'}\rangle]. \qquad (4)$$

By the second law of thermodynamics, both $\Delta S_{B\to C}^{\mathrm{total}}$ and $\Delta S_{D\to A}^{\mathrm{total}}$ cannot be negative. Let us now rewrite Eq. (3) as

$$\eta_q = 1 - \frac{T_c(S_B - S_D) + T_c\Delta S_{B\to C}^{\mathrm{total}}}{T_h(S_B - S_D) - T_h\Delta S_{D\to A}^{\mathrm{total}}}. \qquad (5)$$

Evidently then, if $\Delta S_{D\to A}^{\mathrm{total}}$ and $\Delta S_{B\to C}^{\mathrm{total}}$ in Eq. (5) is zero, then η_q would reduce exactly to the Carnot efficiency η_c. In general, η_q in Eq. (5) is seen to be *always lower* than η_c. In short, the

second law of thermodynamics requires that the efficiency of a quantum heat engine cycle described above should be in general lower than, and can only reach in exceptional cases, the Carnot efficiency.

III. CONSTRUCTING A QUANTUM CARNOT CYCLE

To construct a quantum Carnot cycle, one must specify the two unitary processes $B \to C'$ and $D \to A'$. Reference [3] first proposed to consider quantum adiabatic processes for this purpose, mainly based on certain qualitative reversibility considerations [28]. Here we show that this intuitive construction is correct for a quantitative, and more fundamental, reason related to heat-to-work efficiency.

Before proceeding, we emphasize that adiabaticity in a quantum unitary process does not have the key feature of a thermal quasistatic adiabatic process in the Carnot cycle; i.e., the former does not result in equilibrium states in general but the latter does. As a result, quantities such as temperature and thermodynamic entropy are usually ill-defined for states C' and A'. Consider then the expression of η_q in Eq. (3). With four equilibrium states A, B, C, and D specified as in Fig. 1, only $\langle E_{C'}\rangle$ and $\langle E_{A'}\rangle$ may be varied by choosing different types of unitary processes $B \to C'$ and $D \to A'$. For processes of a thermally isolated system, there is no heat exchange, and as such, we have

$$\langle E_{C'}\rangle = \langle E_B\rangle + \langle W\rangle_{B\to C'},$$

$$\langle E_{A'}\rangle = \langle E_D\rangle + \langle W\rangle_{D\to A'}, \qquad (6)$$

where $\langle W\rangle_{B\to C'}$ and $\langle W\rangle_{D\to A'}$ represent the average work associated with $B \to C'$ and $D \to A'$. The meaning of the average work used here is fully consistent with the definition of average work discussed earlier for thermally isolated systems [21,22]. Remarkably, the minimal work principle [29,30] then takes us to a definite choice. In particular, for a quantum state initially prepared as a Gibbs equilibrium distribution (this specific requirement can be loosened) and for fixed initial and final λ values, a quantum adiabatic process (if implementable) is the one with the minimal average work. So if $D \to A'$ and $B \to C'$ are indeed quantum adiabatic processes, the minimal work principle ensures that the final mean energies $\langle E_{C'}\rangle$ or $\langle E_{A'}\rangle$ are minimized for fixed states B and D. Returning to the expression of η_q in Eq. (3), minimized $\langle E_{C'}\rangle$ and $\langle E_{A'}\rangle$ then yield the highest possible efficiency η_q. It is for this efficiency consideration that the quantum analog of Carnot heat engines must consist of two quantum adiabatic steps in addition to two isothermal steps. To our knowledge, this is an important and previously unknown insight [28].

IV. OPTIMIZING EFFICIENCY OF QUANTUM CARNOT CYCLES

With quantum Carnot cycles constructed and justified as above, we next seek specific design principles to further optimize η_q. The Hamiltonian of the working medium (when thermally isolated) is assumed to be $\hat{H}(\lambda)$ with energy levels $E_n(\lambda)$. The values of λ at B and D, namely, λ_B and λ_D, are assumed to be given. The focus question of this study is to show how to choose λ at states A and C, namely, λ_A and λ_C, such that η_q may be optimized.

It is interesting to first illustrate this optimization issue in systems possessing scale invariance [31,32] with λ. In such an exceptional case,

$$[E_n(\lambda_1) - E_m(\lambda_1)] = S(\lambda_1,\lambda_2)[E_n(\lambda_2) - E_m(\lambda_2)]. \quad (7)$$

Examples of this situation include a harmonic oscillator, with λ being the harmonic frequency, a particle in an infinitely deep square-well potential [3], where λ can be the width of the potential well, or simply a two-level quantum system [9]. Consider then the adiabatic step from B to C'. The initial state populations are given by $P_B(n) = e^{-\beta_h E_n(\lambda_B)}/Z_B$ (throughout Z represents equilibrium partition functions and β represents the inverse temperature). Upon reaching C', the final populations are still given by $P_{C'}(n) = e^{-\beta_h E_n(\lambda_B)}/Z_B$ due to the assumed quantum adiabaticity. Now given the assumed scale-invariance in Eq. (7), one can always define an effective temperature T_{eff} to reinterpret $P_{C'}(n)$, namely,

$$P_{C'}(n) = e^{-\beta_h E_n(\lambda_B)}/Z_B = e^{-\beta_{\text{eff}} E_n(\lambda_C)}/Z_C, \quad (8)$$

where $\beta_{\text{eff}} \equiv 1/(k_B T_{\text{eff}}) = S(\lambda_B,\lambda_C)\beta_h$; that is, state C' has no difference from an equilibrium state with temperature T_{eff} under Hamiltonian $\hat{H}(\lambda_C)$. If we now choose λ_C to guarantee that $T_{\text{eff}} = T_c$, then state C' is already in thermal equilibrium with the cold reservoir at T_c. The relaxation process from C' to C as illustrated in Fig. 1 is no longer needed, resulting in $S_C = S_B$, $\langle E_C \rangle = \langle E_{C'} \rangle$ and hence $\Delta S_{B \to C}^{\text{total}} = 0$. Exactly the same analysis applies to the adiabatic process $D \to A'$. That is, by choosing an appropriate value of λ_A, we can set $\Delta S_{D \to A}^{\text{total}} = 0$. According to the expression of η_q in Eq. (5), η_q then yields the standard Carnot efficiency. This result also offers a clear perspective to explain why the Carnot efficiency can be obtained in some early studies of quantum heat engines [3,13].

We next lift the above scale-invariance assumption and proceed with optimizing η_q, by optimizing Q_{out} and Q_{in}. We first rewrite Q_{out} and Q_{in} in Eqs. (1) and (2) as the following:

$$Q_{\text{out}} = \langle E_{C'} \rangle - \langle E_D \rangle - k_B T_c \ln \frac{Z_D}{Z_C},$$

$$Q_{\text{in}} = \langle E_B \rangle - \langle E_{A'} \rangle + k_B T_h \ln \frac{Z_B}{Z_A}. \quad (9)$$

Interestingly, with states B and D fixed, only λ_C may affect Q_{out} via $\langle E_{C'} \rangle$ and Z_C; while only λ_A may affect Q_{in} via $\langle E_{A'} \rangle$ and Z_A. That is, to optimize η_q, minimizing Q_{out} and maximizing Q_{in} can be executed separately, which is a considerable reduction of our optimization task. For this reason, below we focus on minimizing Q_{out} and the parallel result concerning Q_{in} directly follows.

Accounting for quantum adiabaticity that maintains populations on each quantum level, one has

$$\langle E_{C'} \rangle = \frac{1}{Z_B} \sum_n e^{-\beta_h E_n(\lambda_B)} E_n(\lambda_C). \quad (10)$$

Note again that the level populations $\frac{1}{Z_B} e^{-\beta_h E_n(\lambda_B)}$ used above are in general not an equilibrium Gibbs distribution associated with $\hat{H}(\lambda_C)$ (because in general a system does not possess

scale invariance). Using Eqs. (9) and (10), we arrive at

$$\frac{\partial Q_{\text{out}}}{\partial \lambda_C} = \sum_n \left[\frac{e^{-\beta_h E_n(\lambda_B)}}{Z_B} - \frac{e^{-\beta_c E_n(\lambda_C)}}{Z_C} \right] \frac{\partial E_n(\lambda_C)}{\partial \lambda_C}. \quad (11)$$

The minimization of Q_{out} requires the condition $\partial Q_{\text{out}}/\partial \lambda_C = 0$, which indicates that

$$\sum_n \left[\frac{e^{-\beta_h E_n(\lambda_B)}}{Z_B} - \frac{e^{-\beta_c E_n(\lambda_C)}}{Z_C} \right] \frac{\partial E_n(\lambda_C)}{\partial \lambda_C} = 0. \quad (12)$$

Viewing the linear response in energy to a variation in λ as a generalized force, we define a general force operator $\hat{\mathcal{F}}_\lambda \equiv -\frac{\partial \hat{H}(\lambda)}{\partial \lambda}$. Then the condition in Eq. (12) can be cast in the following compact form,

$$\langle \hat{\mathcal{F}}_{\lambda_C} \rangle_C = \langle \hat{U}_{B \to C}^\dagger \hat{\mathcal{F}}_{\lambda_C} \hat{U}_{B \to C} \rangle_B, \quad (13)$$

where $\hat{U}_{B \to C}$ is the unitary transformation that transforms an arbitrary nth eigenstate of $\hat{H}(\lambda_B)$ to the nth eigenstate of $\hat{H}(\lambda_C)$. That is, the expectation value of a generalized force operator at λ_C over equilibrium state C should be identical with that of a mapped force operator over equilibrium state B. Needless to say, the condition for Q_{in} to be maximized is given by

$$\langle \hat{\mathcal{F}}_{\lambda_A} \rangle_A = \langle \hat{U}_{D \to A}^\dagger \hat{\mathcal{F}}_{\lambda_A} \hat{U}_{D \to A} \rangle_D, \quad (14)$$

where $\hat{U}_{D \to A}$ transforms an arbitrary nth eigenstate of $\hat{H}(\lambda_D)$ to the nth eigenstate of $\hat{H}(\lambda_A)$.

Unlike a previous interesting suggestion [33], the two explicit conditions in Eqs. (13) and (14) to optimize η_q are not about matching the mean energy between states C' and C (A' and A). Attempts to match information entropy between states C' and C (A' and A) do not optimize η_q, either. Rather, the conditions found here are about a more subtle and more involving matching of the expectation values of some generalized force operators through equilibrium states. We now take Eq. (12) as the example to digest the optimization conditions. For the exceptional case of a scale-invariant medium, due to the existence of a $\beta_{\text{eff}} = \beta_c$ at C', one can achieve $\frac{e^{-\beta_h E_n(\lambda_B)}}{Z_B} - \frac{e^{-\beta_c E_n(\lambda_C)}}{Z_C} = 0$ for arbitrary n. Then Eq. (12) can be easily satisfied, independent of the details of $\frac{\partial E_n(\lambda_C)}{\partial \lambda_C}$. For a general working medium, the condition of Eq. (12) may be still satisfied after setting the sum of all the terms $\frac{\partial E_n(\lambda_C)}{\partial \lambda_C} \left[\frac{e^{-\beta_h E_n(\lambda_B)}}{Z_B} - \frac{e^{-\beta_c E_n(\lambda_C)}}{Z_C} \right]$ to zero.

V. NUMERICAL EXAMPLES

We adopt a simple model system that is not scale-variant with λ, with $E_n(\lambda) = \lambda n + \alpha n^2 + \text{const}$ (all variables in dimensionless units). For our purpose here there is no need to specify the explicit form of the Hamiltonian. If α is comparable to λ, then the ratio $[E_n(\lambda_1) - E_m(\lambda_1)]/[E_n(\lambda_2) - E_m(\lambda_2)]$ does depend strongly on n and m, a clear sign of breaking the scale invariance. Cases of a very small α would resemble the behavior of a harmonic oscillator at low temperatures. To guarantee quantum adiabaticity, we exclude cases with level crossings. This is achieved by requiring $\lambda > -\alpha$ such that $E_n > E_m$ if $n > m$. Other physical considerations for the cycle to operate as a meaningful heat engine suggests that λ_A should be the largest and λ_C the smallest among λ_A, λ_B, λ_C, and λ_D. Our computational details confirm that (i) minimization
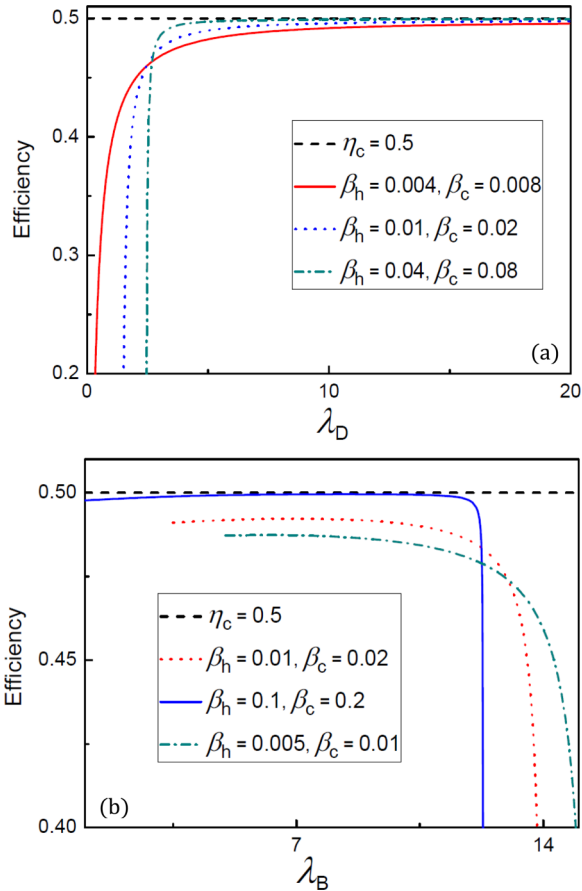
FIG. 2. (Color online) Behavior of heat-to-work efficiency η_q optimized under given λ_B, λ_D, T_c and T_h, with λ_A and λ_C chosen according to Eqs. (13) and (14). (a) η_q vs λ_D if $\lambda_B = 6.0$ for three sets of T_c and T_h and (b) η_q vs λ_B if $\lambda_D = 6.0$, also for three sets of T_c and T_h. In all the shown cases the Carnot efficiency $\eta_c = 0.5$ (top dashed curve). All variables are in dimensionless units. The energy levels of the working medium are assumed to be $E_n(\lambda) = \lambda n + \alpha n^2$ with $\alpha = 0.1$.

of Q_{out} and maximization of Q_{in} indeed occur precisely at those locations predicted by Eqs. (13) and (14), and (ii) the optimized η_q can be markedly higher than that obtained by matching the mean energy or information entropy between states C' and C (A' and A). Optimization of η_q as outlined above is hence indeed doable and necessary.

The rather specific conditions to optimize η_q (under fixed λ_B and λ_D) indicates that the η_q thus optimized will be highly system specific. To see this, we present in Fig. 2 optimized η_q as a function of λ_D (λ_B) with fixed λ_B (λ_D), under different temperatures T_c and T_h. From Fig. 2(a) it is seen that the optimized η_q can be way below, but nevertheless quickly approaches, the Carnot efficiency η_c as λ_D increases. This is because a larger λ_D leads to an even larger λ_A due to the

optimization requirement, both facts pushing the system closer to a scale-invariant system under fixed temperatures. Note also that even though the three η_q curves in Fig. 2(a) are for the same ratio T_c/T_h, their η_q values are much different. This shows that the optimized η_q is no longer a simple function of T_c/T_h, but a function of both T_c and T_h. Figure 2(b) shows that our optimized η_q may not be always a monotonous function of λ_B with a fixed λ_D. Interesting effects of T_c and T_h under a common T_c/T_h are again observed there. The shown ranges of λ_B or λ_D in Fig. 2 vary with the chosen temperatures because we exclude level crossing situations. The sharp change of η_q in Fig. 2(a) [Fig. 2(b)] with a decreasing (increasing) of λ_D (λ_B) under a given λ_B (λ_D) is simply because the optimized cycle is about to cease to operate as a heat engine (which requires $Q_{in} > Q_{out} > 0$).

VI. DISCUSSIONS AND CONCLUSIONS

Several previous studies investigated quantum Otto cycles [6,11,16,34] consisting of two thermally isolated steps and two isochoric processes that are simply relaxation processes with a hot or a cold reservoir. Such cycles can be regarded as a special case of the quantum heat engine cycles considered here, by removing the isothermal process $A \rightarrow B$ or $C \rightarrow D$. That is, by setting $\lambda_A = \lambda_B$ and $\lambda_C = \lambda_D$ in Fig. 1, we obtain the quantum Otto cycles. One can now also justify the use of quantum adiabatic steps to construct energy efficient quantum Otto cycles via the minimum work principle again [29]. Because in our efficiency optimization under fixed λ_B and λ_D, the obtained λ_A (λ_C) in general differs from λ_B (λ_D), one deduces that the optimized η_q here is generically higher than the efficiency of the corresponding quantum Otto cycles. This fact strengthens the importance of quantum Carnot cycles we have optimized.

Our analysis does not really demand the two adiabatic steps to be executed slowly, so long as the final-state populations agree with those given by the quantum adiabatic theorem. This understanding encourages the use of shortcuts to adiabaticity [32,34–37] or even an optimal control approach [38] to implement quantum Carnot cycles within a shorter time scale, thus boosting the heat engine power.

In conclusion, using minimal assumptions about work and heat in nanoscale systems, we have shown how to construct and optimize the quantum analog of Carnot cycles. The heat-to-work efficiency can be optimized if two conditions regarding some generalized force operators evaluated at some equilibrium states are met. In general the optimized efficiency is system specific and lower than the Carnot efficiency.

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