# Quantum dynamical framework for Brownian heat engines

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(Received 5 March 2013; revised manuscript received 29 May 2013; published 23 July 2013)

We present a self-contained formalism modeled after the Brownian motion of a quantum harmonic oscillator for describing the performance of microscopic Brownian heat engines such as Carnot, Stirling, and Otto engines. Our theory, besides reproducing the standard thermodynamics results in the steady state, enables us to study the role dissipation plays in determining the efficiency of Brownian heat engines under actual laboratory conditions. In particular, we analyze in detail the dynamics associated with decoupling a system in equilibrium with one bath and recoupling it to another bath and obtain exact analytical results, which are shown to have significant ramifications on the efficiencies of engines involving such a step. We also develop a simple yet powerful technique for computing corrections to the steady state results arising from finite operation time and use it to arrive at the thermodynamic complementarity relations for various operating conditions and also to compute the efficiencies of the three engines cited above at maximum power. Some of the methods and exactly solvable models presented here are interesting in their own right and could find useful applications in other contexts as well.

DOI: 10.1103/PhysRevE.88.012130 PACS number(s): 05.30.−d, 05.70.Ln, 05.20.−y

## I. INTRODUCTION

In recent years there has been an upsurge of interest in the interface between thermodynamics and quantum mechanics [1], macro and nano or micro [2], leading to a thorough reexamination of the basic concepts and principles of thermodynamics with ramifications in biological processes and soft condensed matter systems. New paradigms for notions of work, thermal machines, etc., have emerged that provide deep insights into thermodynamics, which in turn help enlarge its scope far beyond that envisaged originally and open up new possibilities [3]. These developments force one to formulate questions concerning the efficiencies of various heat engines using appropriate microscopic considerations [4]. Indeed, one has even started considering quantum heat engines, which in principle have efficiency larger than Carnot efficiency, though such cases require nonequilibrium steady states. Such steady states can be reached via the use of the coherent laser fields or via quantum interference effects [5,6]. In a recent experiment [7] Blickle and Bechinger realized a microscopic Brownian heat engine [8–10]. The most important ingredient both in the work of Blickle and Bechinger [7] and in the proposals of Scully *et al.* [5] is the possibility that all the relevant parameters can be controlled very well experimentally; thus the heat engine cycle can be precisely realized and it becomes desirable to have exactly soluble models of microscopic heat engines.

In view of the way the experiments are carried out we need a fully dynamical model that should account for the way the system parameters such as potentials or the external parameters such as temperature are changed. Further, the behavior of the engine should depend on various time scales, for example, the time taken to reach an equilibrium state. Such a time would depend on the scales of the damping in the system. Motivated by these requirements, we develop in the present work an exactly soluble model of a microscopic Brownian heat engine. The model that we present is fully quantum mechanical. Our model enables us to examine many different possible experimental scenarios: (a) low-temperature behavior where quantum effects are likely to dominate, (b) behavior under different relaxation conditions, for example, the system could be underdamped or overdamped, (c) possibilities for the system to pass through nonequilibrium stages depending on the rate of change of the external parameters, and (d) nonequilibrium conditions because the experimental time scales are smaller than the time it takes for the system to reach steady state. Our formulation is based on the Wigner function and quantum Langevin equations for a harmonic oscillator whose frequency is modulated in time. We also assume that the temperature of the environment is time dependent as well. These time dependences are needed to implement the heat engine cycle realistically. We calculate the time-dependent Wigner function, all the fluctuation parameters, and the entropy. These enable us to calculate thermodynamic quantities such as work, heat, and internal energy.

A brief outline of the work is as follows. In Sec. II, for later reference, we briefly recapitulate the expressions for the efficiencies, both classical and quantum, for the three engines based on standard thermodynamic considerations with the usual assumptions regarding the speed with which the various steps are carried out. In Sec. III we present a quantum thermodynamic framework based on the Wigner phase-space description for quantum systems that contains the classical framework as a limiting case. In Sec. IV we develop a general setup for computing various quantities of interest and give two models of frequency modulation where the relevant equations are amenable to exact analytical results. In Sec. V we consider the situation when the diffusion constant is varied linearly and in Sec. VI analyze its ramifications on the efficiencies of Brownian heat engines. In Sec. VII we develop a systematic scheme for computing finite-time corrections to the efficiencies of classical and quantum Brownian motors and then use these results in Sec. VII to examine the role they play in determining the efficiency of the Stirling engine at

 

maximum power. Section IX contains our concluding remarks and further outlook. Motivated by the work of Blickle and Bechinger [7], we focus in this paper on the high-temperature regime $\hbar\omega/K_BT \ll 1$ (in Ref. [7], $\hbar\omega/K_BT \sim 10^{-6}$). We note that in the other extreme $\hbar\omega/K_BT \gg 1$, strong deviations from the standard thermodynamic behavior becomes very prominent [11]. For example, using the exact Langevin equations, Nieuwenhuizen and Allahverdyan [11] found that the Clausius inequality can be violated at low temperatures ($\hbar\omega/K_BT \gg 1$).

As noted above, our working model for a heat engine is based on a quantum harmonic oscillator with a frequency $\omega$ interacting with a thermal bath at temperature $T$. Three typical engines that have been discussed extensively in the literature based on varying $\omega$ and $T$ appropriately are the Stirling, Carnot, and Otto engines. Their cycles adapted to the harmonic oscillator model are schematically given as follows: For the Stirling engine [7],

$$\begin{array}{ccccc} \omega_1, T_c & & \text{isothermal} & & \omega_2, T_c \\ & 3 & \longrightarrow & 4 & \\ & & \tau_c & & \\ \text{isochoric} & \uparrow & & \downarrow & \text{isochoric} \\ & & \tau_h & & \\ & 2 & \longleftarrow & 1 & \\ \omega_1, T_h & & \text{isothermal} & & \omega_2, T_h \end{array} \tag{1}$$

with $\omega_2 > \omega_1$ and $T_h > T_c$; for the Carnot engine [9,12],

$$\begin{array}{ccccc} \omega_1, T_h & & \text{isothermal} & & \omega_2, T_h \\ & 1 & \longrightarrow & 2 & \\ & & \tau_h & & \\ \text{isentropic} & \uparrow & & \downarrow & \text{isentropic} \\ & & \tau_c & & \\ & 4 & \longleftarrow & 3 & \\ \omega_4, T_c & & \text{isothermal} & & \omega_3, T_c \end{array} \tag{2}$$

with $\omega_1 > \omega_2 > \omega_3 > \omega_4$, $T_h > T_c$, $\beta_h\omega_2 = \beta_c\omega_3$, and $\beta_h\omega_1 = \beta_c\omega_4$; and for the Otto engine [13],

$$\begin{array}{ccccc} \omega_c, T_2 & & \text{isentropic} & & \omega_h, T_h \\ & 4 & \longleftarrow & 3 & \\ & & \tau_1 & & \\ \text{isochoric} & \downarrow & & \uparrow & \text{isochoric} \\ & & \tau_2 & & \\ & 1 & \longrightarrow & 2 & \\ \omega_c, T_c & & \text{isentropic} & & \omega_h, T_1 \end{array} \tag{3}$$

for $\omega_h > \omega_c >$, $T_h > T_c$, $\beta_c\omega_c = \beta_1\omega_h$, and $\beta_h\omega_h = \beta_2\omega_c$. Here the $\tau$ indicate the time taken to carry out the indicated step and $\beta$ stands for $1/K_BT$. The calculations that we give in subsequent sections can be applied to any of these engines.

The three prototypical engines above thus involve suitable combinations of the following three steps: (a) isothermal, i.e., $\omega$ changing with $T$ fixed or (b) isochoric, i.e., $\omega$ held fixed with $T$ changing, or (c) isentropic, i.e., both $\omega$ and $T$ changing with $\omega/T$ fixed, and one needs an appropriate formalism to compute the efficiencies under specific physical circumstances in which these steps are actually executed in an experiment. The present work has this as its major objective. Our principal results include (i) development of a self-contained formalism for computing efficiencies of Brownian engines in both the classical and quantum contexts, (ii) an exact analysis of the role of damping in the process of coupling the system to a bath at a higher temperature and its influence on the performance of the Stirling engine, (iii) computation of the irreversible heat in isothermal processes and the derivation of complementarity relations, and (iv) a detailed analysis of the role of damping as well as finite-time corrections on the efficiency of the Stirling engine at maximum power.

## II. STEADY STATE EFFICIENCIES FROM THERMODYNAMICS

To set the notation and for later reference we assemble here the standard thermodynamic considerations that enable us to compute the efficiencies for the three engines listed above in both classical and quantum contexts. These are (i) the thermodynamic conservation law or the energy balance relation $\Delta U = Q - W$, where $\Delta U$ is the change in the internal energy $U$, $Q$ is the heat absorbed by the system, and $W$ is the work done by the system; (ii) $Q$ in a reversible isentropic process $a \to b = 0$; (iii) work done in an isochoric process $a \to b = 0$ provided the only kind of work is via a change of volume (in the present context $\omega$); (iv) work done in an isothermal process $a \to b = -[F(b) - F(a)]$, where $F$ denotes the free energy of the system; (v) the expressions for $U$ and $F$ for the harmonic oscillator,

$$U = \begin{cases} 1/\beta, \ \beta \equiv \frac{1}{K_BT} & \text{(classical)} \\ \hbar\omega[n(\omega,T) + 1/2], \ n(\omega,T) \equiv \frac{1}{e^{\beta\hbar\omega}-1} & \text{(quantum)}, \end{cases} \tag{4}$$

$$F(\omega,T) = \begin{cases} l\frac{1}{\beta}\ln(\beta\hbar\omega) & \text{(classical)} \\ \frac{1}{\beta}\ln[2\sinh(\beta\hbar\omega/2)] & \text{(quantum)}; \end{cases} \tag{5}$$

and (vi) the expression for the entropy of a classical harmonic oscillator in equilibrium at a temperature $T$,

$$S = K_B\left[1 + \ln\left(\frac{1}{\beta\hbar\omega}\right)\right]. \tag{6}$$

In the quantum case, for the thermal state $\rho_{\text{th}}$,

$$\rho_{\text{th}} = \frac{e^{-\beta\hat{H}}}{\text{Tr}[e^{-\beta\hat{H}}]}, \tag{7}$$

where $\hat{H}$ denotes the Hamiltonian operator for a quantum harmonic oscillator, one has for the von Neumann entropy

$$S = K_B\{[n(\omega,T)+1]\ln[n(\omega,T)+1] - n(\omega,T)\ln n(\omega,T)\}. \tag{8}$$

From expressions (6) and (8) for $S$ above it follows that in both classical and quantum cases $S$ depends only on $\omega/T$ and further that the following relation, referred to as the entropy balance equation, holds:

$$dU = TdS + U\frac{d\omega}{\omega} \tag{9}$$

for isothermal reversible processes. It must, however, be borne in mind that its validity is restricted to thermodynamic changes such that the thermal state remains a thermal state all along. In a recent work, based entirely on the energy balance and the entropy balance relations, Beretta [14] examined the question of efficiencies of quantum thermodynamic Carnot- and Otto-like cycles modeled after a two-level system. The present work, though similar in spirit, largely addresses situations involving evolution of an initial thermal state into nonthermal states and its eventual relaxation to a different thermal state and this renders use of the entropy balance equation untenable.

With this preparation we now proceed to compute the efficiencies of the three engines mentioned earlier in both the classical and quantum cases. These would then be compared with the results obtained from the microscopic theory developed later.

*(a) Stirling engine*. The efficiency $\eta_S$ of the Stirling engine is defined as

$$\eta_S = \frac{W}{Q_{T_h}},$$

where $W$ denotes work done by the system and $Q_{T_h}$ denotes heat flow into the system at $T_h$. In the classical case the work done by the engine is given by

$$\begin{aligned} W_{1\to 2} + W_{3\to 4} &= -[F(\omega_1,T_h) - F(\omega_2,T_h)] \\ &\quad - [F(\omega_2,T_c) - F(\omega_1,T_c)] \\ &= K_B(T_h - T_c)\ln\left(\frac{\omega_2}{\omega_1}\right) \end{aligned} \tag{10}$$

and the heat absorbed at $T_h$ by

$$\begin{aligned} &W_{1\to 2} + \Delta U_{1\to 2} + \Delta U_{4\to 1} \\ &= -[F(\omega_1,T_h) - F(\omega_2,T_h)] + 0 + \frac{1}{2}\left(\frac{1}{\beta_h} - \frac{1}{\beta_c}\right) \\ &= K_B T_h \ln\left(\frac{\omega_2}{\omega_1}\right) + \frac{1}{2}K_B(T_h - T_c). \end{aligned} \tag{11}$$

[Note the factor of $\frac{1}{2}$ in the second term on the right-hand side (rhs) of Eq. (11). We will return to this later.] Hence

$$\eta_S^{\rm cl} = \frac{\eta_C}{1 + \eta_C \big/ \left[\ln\left(\frac{\omega_2^2}{\omega_1^2}\right)\right]}, \quad \eta_C = 1 - \frac{T_c}{T_h}. \tag{12}$$

Proceeding as before and using the expressions for $U$ and $F$ appropriate to the quantum case, we have for the work done

$$\begin{aligned} &W_{1\to 2} + W_{3\to 4} \\ &= -[F(\omega_1,T_h) - F(\omega_2,T_h)] - [F(\omega_2,T_c) - F(\omega_1,T_c)] \\ &= K_B T_h \ln\left(\frac{\sinh(\beta_h\hbar\omega_2/2)}{\sinh(\beta_h\hbar\omega_1/2)}\right) \\ &\quad - K_B T_c \ln\left(\frac{\sinh(\beta_c\hbar\omega_2/2)}{\sinh(\beta_c\hbar\omega_1/2)}\right) \end{aligned} \tag{13}$$

and for the heat absorbed at $T_h$

$$\begin{aligned} &W_{1\to 2} + \Delta U_{1\to 2} + \Delta U_{4\to 1} \\ &= -[F(\omega_1,T_h) - F(\omega_2,T_h)] + \left\{\hbar\omega_1\left[n(\omega_1,T_h) + \tfrac{1}{2}\right]\right. \\ &\quad \left. -\hbar\omega_2\left[n(\omega_2,T_h) + \tfrac{1}{2}\right]\right\} + \tfrac{1}{2}\left(\left\{\hbar\omega_2\left[n(\omega_2,T_h) + \tfrac{1}{2}\right]\right]\right. \\ &\quad \left. - \left[\hbar\omega_2\left[n(\omega_2,T_c) + \tfrac{1}{2}\right]\right]\right\}\Big), \end{aligned} \tag{14}$$

hence

$$\begin{aligned} &\eta_S^q = \frac{1 - Y/X}{1 + Z/X}, \\ &X = \ln\left(\frac{\sinh(\beta_h\hbar\omega_2/2)}{\sinh(\beta_h\hbar\omega_1/2)}\right), \quad Y = \frac{\beta_h}{\beta_c}\ln\left(\frac{\sinh(\beta_c\hbar\omega_2/2)}{\sinh(\beta_c\hbar\omega_1/2)}\right), \\ &Z = \frac{\beta_h}{2}\left[\hbar\omega_1\coth(\beta_h\hbar\omega_1/2) - \frac{\hbar\omega_2}{2}\{\coth(\beta_h\hbar\omega_2/2)\right. \\ &\quad \left. + \coth(\beta_c\hbar\omega_2/2)\}\right]. \end{aligned} \tag{15}$$

In the limit $\beta\omega \ll 1$, $\eta_S^{\rm q}$ goes over to the classical efficiency $\eta_S^{\rm cl}$ as expected.

*(b) Carnot engine*. For the Carnot engine the efficiency defined as before

$$\eta_C = \frac{W}{Q_{T_h}}$$

turns out to be the same in both the classical and quantum cases and is given by

$$\eta_C^{\rm cl} = \eta_C^q = \eta_C = \left(1 - \frac{T_c}{T_h}\right). \tag{16}$$

*(c) Otto engine*. Here again the efficiency defined as

$$\eta_O = \frac{W}{Q_{2\to 3}}$$

turns out to be the same in both the quantum and classical cases and is given by

$$\eta_O^{\rm cl} = \eta_O^q = 1 - \frac{U(4) - U(1)}{U(3) - U(2)} = \left(1 - \frac{\omega_c}{\omega_h}\right). \tag{17}$$

The expressions for efficiencies for the three engines, realized here through a harmonic oscillator by appropriate changes of its frequency (or equivalently its spring constant) and the ambient temperature, hold for idealized operating conditions as stipulated in equilibrium thermodynamics. These, for instance, demand that the isothermal changes of frequency involved in the Stirling or the Carnot cycles be carried out quasistatically, i.e., so slowly that at each instance the oscillator remains in the state of equilibrium at that temperature and frequency. Such conditions are hardly ever met in practice and particularly in the light of the experimental work reported in [7] there is an obvious need for developing a framework that brings into play aspects of the approach to equilibrium, in both classical and quantum contexts, and is capable of furnishing a self-contained scheme for computing the efficiencies under realistic conditions. We develop such a scheme in the next section.

## III. EFFICIENCIES BEYOND THE STEADY STATE: A DYNAMICAL MODEL

To go beyond the standard thermodynamic assumptions regarding the rate at which various steps in a heat engine are carried out so that one can evaluate the performance of an engine under actual laboratory conditions, we need a framework that treats the system modeling the engine as an open system and permits proper inclusion of dissipative effects and the possibility of varying the system potential and the ambient temperature. In the present context, such a framework

is provided by the dynamics of a quantum Brownian oscillator of frequency $\omega$ in contact with a heat bath at temperature $T$ and is described by the master equation [15]

$$\frac{\partial}{\partial t}\rho = -\frac{i}{\hbar}\left[\hat{p}^2/2m + \frac{1}{2}m\omega^2\hat{q}^2,\rho\right] - \frac{2\kappa m\omega}{\hbar}[n(\omega,T)+1/2]([\hat{q},[\hat{q},\rho]]) - \frac{i\kappa}{\hbar}([\hat{q},\{\hat{p},\rho\}]), \tag{18}$$

where $\hat{q}$ and $\hat{p}$ denote the position and momentum operators obeying the commutation relations $[\hat{q},\hat{p}] = i\hbar$.

For reasons given later it proves expedient to transcribe the quantum dynamics described by the master equation using the Wigner phase space description of quantum systems [16, 17], which associates with a density operator $\rho$ a phase space function $W(q,p)$ of classical variables $q,p$ as follows:

$$\hat{\rho} \mapsto W_{\hat{\rho}}(q,p) = \mathrm{Tr}\{\hat{\rho}\hat{W}(q,p)\}, \quad \hat{W}(q,p) = \frac{1}{(2\pi\hbar)}\int_{-\infty}^{\infty} dq' \left|q+\tfrac{1}{2}q'\right\rangle\left\langle q-\tfrac{1}{2}q'\right| e^{ipq'/\hbar}. \tag{19}$$

We note here that we prefer to use the Wigner phase space description over other phase space descriptions for three reasons: (a) It associates a real phase space function with every Hermitian operator, (b) it maps the quantum mechanical average of a product of two operators to the phase space average of the corresponding Wigner functions, and (c) its moments $\langle q^m p^n\rangle$ correspond to quantum averages of the symmetrized operator $(\hat{q}^m\hat{p}^n)_S$. For example, $\langle q^2 p\rangle$ corresponds to the expectation value of the operator $(\hat{q}^2\hat{p}+\hat{q}\hat{p}\hat{q}+\hat{p}\hat{q}^2)/3$. Although we prefer to work with real phase space functions, Beretta [18] has pointed out the usefulness of complex phase space functions based on the Blokhintzev map for a phase space description of quantum kinematics.

Use of the Wigner description turns the master equation into a Fokker-Planck equation (FPE) for $W(q,p)$ [17],

$$\frac{\partial}{\partial t}W(q,p,t) = \left\{-\frac{\partial}{\partial q}\left(\frac{p}{m}\right) + \frac{\partial}{\partial p}\left[2\kappa p + \left(\frac{\partial V(q,a)}{\partial q}\right)\right] + D\frac{\partial^2}{\partial p^2}\right\} W(q,p,t),$$

where

$$V(q,a) = \tfrac{1}{2}aq^2, \quad a \equiv m\omega^2 \tag{20}$$

and

$$D = 2m\hbar\omega\kappa\left[n(\omega,T)+\tfrac{1}{2}\right], \quad n(\omega,T) = (e^{\beta\hbar\omega}-1)^{-1}. \tag{21}$$

In the following the parameter $a$, the spring constant, will be taken to be controlled externally.

The Langevin equations equivalent to the above FPE read

$$\dot{q} = \frac{p}{m}, \tag{22}$$

$$\dot{p} = -2\kappa p - \frac{\partial}{\partial q}V(q,a) + f(t), \tag{23}$$

$$\langle f(t)f(t')\rangle = 2D\delta(t-t'). \tag{24}$$

The Langevin equations (22)–(24) lend themselves to a nice thermodynamic interpretation [8]: Rewriting (23) as

$$-[-2\kappa p + f(t)] + \dot{p} + \frac{\partial}{\partial q}V(q,a) = 0, \tag{25}$$

multiplying it by $dq$, and using

$$dV = \frac{\partial V(q,a)}{\partial q}dq + \frac{\partial V(q,a)}{\partial a}da, \tag{26}$$

one obtains

$$-[-2\kappa p + f(t)]dq + d[p^2/2m + V(q,a)] - \frac{\partial V(q,a)}{\partial a}da. \tag{27}$$

The three terms in Eq. (27) may now be identified in an intuitively plausible manner as

$$\mathcal{Q} = [-2\kappa p + f(t)]dq, \quad d\mathcal{U} = d(p^2/2m + V), \quad \mathcal{W} = -\frac{\partial V(q,a)}{\partial a}da, \tag{28}$$

leading to the energy balance equation

$$-\mathcal{Q} + d\mathcal{U} + \mathcal{W} = 0, \tag{29}$$

with $\mathcal{Q}$ $(-\mathcal{Q})$ understood as the heat flow into (out of) the system and $\mathcal{W}$ $(-\mathcal{W})$ as the work done by (on) the system. The stochastic averages of these quantities denote by $Q$, $dU$, and $W$, respectively, relate directly to the corresponding thermodynamic quantities and capture the thermodynamic conservation laws. This self-contained approach is clearly more microscopic than thermodynamics as it provides a framework for computing not only the averages of these quantities but their probability distributions as well.

We note here that while it is certainly possible to transcribe the master equation dynamics directly into equivalent quantum Langevin equations for the operators $\hat{q}$ and $\hat{p}$, owing to their noncommutativity, the crucial step (27) needed to obtain a clear thermodynamic interpretation of such Langevin equations would now involve terms such as $\hat{p}d\hat{q}$ and would therefore be fraught with ordering ambiguities.

The scheme described above for computing $Q$, $dU$, and $W$ together with the expression for von Neumann entropy

$$S = K_B[(\sigma+1)\ln(\sigma+1) - \sigma\ln\sigma], \quad \sigma = \sqrt{\mathrm{Det}[\mathcal{V}]} - \tfrac{1}{2} \tag{30}$$

for Gaussian states [19] (which is what we would exclusively deal with), i.e., states $\rho$ for which the Wigner distribution is a Gaussian:

$$W(q,p) = \frac{1}{\sqrt{(2\pi)^2\mathrm{Det}[\mathcal{V}]}}\exp\left[-\frac{x^T\mathcal{V}x}{2\,\mathrm{Det}[\mathcal{V}]}\right], \quad x \equiv \begin{pmatrix} q \\ p \end{pmatrix}, \tag{31}$$

provides all that we need for the considerations below. Here $V$ stands for the variance matrix

$$\mathcal{V} = \begin{pmatrix} \langle q^2\rangle & \langle qp\rangle \\ \langle qp\rangle & \langle p^2\rangle \end{pmatrix} \tag{32}$$

and angular brackets denote the average with respect to the Wigner distribution. The uncertainty relations require that $\sigma$

be positive. Note that the set of Gaussian states contains the set of harmonic oscillator thermal states $\rho_{\rm th}$ as a special case.

Before proceeding further it is instructive to check that the Wigner description above together with the thermodynamic interpretation implied by (28) in the steady state does indeed reproduce the results given earlier for the efficiencies of the three engines using standard thermodynamic considerations. Thus, for instance, calculation of the efficiency of the Stirling engine involves computing $W_{1\to 2}$, $W_{3\to 4}$, $\Delta U_{1\to 2}$, and $\Delta U_{4\to 1}$, which in the present framework are given by

$$W_{1\to 2} = \int_1^2 W = -\int_{\omega_2}^{\omega_1} m\omega\langle q^2\rangle_{T=T_c} d\omega, \tag{33}$$

$$W_{3\to 4} = \int_3^4 W = -\int_{\omega_1}^{\omega_2} m\omega\langle q^2\rangle_{T=T_h} d\omega, \tag{34}$$

$$\Delta U_{1\to 2} = \int_1^2 dU = \left(\frac{\langle p^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle q^2\rangle\right)_2 - \left(\frac{\langle p^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle q^2\rangle\right)_1, \tag{35}$$

$$\Delta U_{4\to 1} = \int_4^1 dU = \left(\frac{\langle p^2\rangle_1}{2m} - \frac{\langle p^2\rangle_4}{2m}\right). \tag{36}$$

Further, from the FPE or the Langevin equations it follows that in the steady state

$$\langle p^2\rangle = D/2\kappa, \quad m\omega^2\langle q^2\rangle = D/2m\kappa. \tag{37}$$

On using $D = 2m\kappa\omega[n(\omega,T) + \frac{1}{2}]$ these equations then give

$$W_{1\to 2} = -\int_{\omega_2}^{\omega_1}\left[n(\omega,T_h) + \tfrac{1}{2}\right]d\omega = K_B T_h \ln\left(\frac{\sinh(\beta_h\omega_2/2)}{\sinh(\beta_h\omega_1/2)}\right) = F(1) - F(2), \tag{38}$$

$$W_{3\to 4} = -\int_{\omega_1}^{\omega_2}\left[n(\omega,T_c) + \tfrac{1}{2}\right]d\omega = -K_B T_c \ln\left(\frac{\sinh(\beta_c\omega_2/2)}{\sinh(\beta_c\omega_1/2)}\right) = [F(3) - F(4)], \tag{39}$$

$$\Delta U_{1\to 2} = \left\{\omega_1\left[n(\omega_1,T_h) + \tfrac{1}{2}\right\} - \left\{\omega_2\left[n(\omega_2,T_h) + \tfrac{1}{2}\right]\right\}, \tag{40}$$

$$\Delta U_{4\to 1} = \tfrac{1}{2}\left(\left\{\omega_2\left[n(\omega_2,T_h) + \tfrac{1}{2}\right]\right\} - \left\{\omega_2\left[n(\omega_2,T_c) + \tfrac{1}{2}\right]\right\}\right), \tag{41}$$

which are the same expressions as before and therefore one recovers the expression for efficiency given in Sec. II. (Note here that in computing $\Delta U_{4\to 1}$ we considered only the contribution from $\langle p^2\rangle$ and not from $\langle q^2\rangle$, a question that will be examined in greater detail later.)

## IV. QUANTUM DYNAMICS UNDER TIME-DEPENDENT CHANGES OF TEMPERATURE AND POTENTIAL

We have seen in the preceding section that the Langevin equations equivalent to the Fokker-Planck equation obeyed by the Wigner distribution lend themselves to a direct and transparent thermodynamic interpretation and that this interpretation in the steady state limit reproduces the standard thermodynamic results. To prepare the groundwork for going beyond the steady state limit we now analyze the structure of the solutions of the Langevin equations at hand, allowing for an arbitrary time dependence in the potential and the diffusion coefficients and apply this framework to arrive at the exact solutions of the Langevin equations for three fairly realistic models.

The Langevin equations, which in the present case are linear stochastic equations with additive noise, may be solved to yield

$$\begin{pmatrix} q(t)\\ p(t)\end{pmatrix} = M(t)\begin{pmatrix} q(0)\\ p(0)\end{pmatrix} + \int_0^t dt' M(t)M(t')^{-1}\begin{pmatrix} 0\\ \sqrt{2D(t')}f(t')\end{pmatrix}, \tag{42}$$

where

$$M(t) \equiv \begin{pmatrix} u(t) & v(t)\\ m\dot{u}(t) & m\dot{v}(t)\end{pmatrix} \tag{43}$$

solves the homogeneous equations

$$\frac{d}{dt}\begin{pmatrix} q(t)\\ p(t)\end{pmatrix} = \begin{pmatrix} 1/m & 0\\ -m\omega^2 & -2\kappa\end{pmatrix}\begin{pmatrix} q(t)\\ p(t)\end{pmatrix}. \tag{44}$$

From (22) for the variance matrix

$$\mathcal{V}(t) \equiv \begin{pmatrix} \langle q^2(t)\rangle & \langle q(t)(p(t)\rangle\\ \langle q(t)p(t)\rangle & \langle p^2(t)\rangle\end{pmatrix} \tag{45}$$

one has

$$\mathcal{V}(t) = M(t)\left[\mathcal{V}(0) + \int_0^t dt' M^{-1}(t')\times\begin{pmatrix} 0 & 0\\ 0 & 2D(t')\end{pmatrix}M^{T-1}(t')\right]M^T(t). \tag{46}$$

It is therefore clear that finding explicit solutions for the variances in situations where both $\omega$ and $T$ depend on time depends on our ability to solve for $M(t)$. We list below three physically meaningful cases for which this is indeed possible.

*Case I: $\omega$ independent of time.* For this familiar case the functions $U(t)$ and $V(t)$, which determine the matrix $M(t)$, are explicitly given by

$$u(t) = \frac{\lambda_+ e^{-\lambda_- t} - \lambda_- e^{-\lambda_+ t}}{\lambda_+ - \lambda_-}, \quad v(t) = \frac{e^{-\lambda_- t} - e^{-\lambda_+ t}}{m(\lambda_+ - \lambda_-)}, \quad \lambda_\pm = \kappa \pm \sqrt{\kappa^2 - \omega^2}. \tag{47}$$

Further, owing to the time translation available in this case, we have $M^{-1}(t) = M(-t)$ and $M(t)M(t') = M(t+t')$ and (45) simplifies to

$$\mathcal{V}(t) = M(t)\mathcal{V}(0)M^T(t) + \int_0^t dt' M(t')\begin{pmatrix} 0 & 0\\ 0 & 2D(t-t')\end{pmatrix}M^T(t'). \tag{48}$$

*Case II: $\omega^2(t) = \omega_0^2(1 + \frac{\mu t}{T})$, $0 \leqslant t \leqslant T$.* In this case investigated in [20], the functions $u(t)$ and $v(t)$ in the range $0 \leqslant t \leqslant T$ are given by

$$u(t) = \left[\frac{f_+(t)\dot{f}_-(0) - f_-(t)\dot{f}_+(0)}{f_+(0)\dot{f}_-(0) - f_-(0)\dot{f}_+(0)}\right], \quad v(t) = m\left[\frac{f_+(t)f_-(0) - f_-(t)f_+(0)}{\dot{f}_+(0)f_-(0) - \dot{f}_-(0)f_+(0)}\right]; \tag{49}$$

$$f_{\pm}(t) = e^{-\kappa t}(t+a)^{1/2} J_{\pm 1/3}\left[\tfrac{2}{3} b^{1/2}(t+a)^{3/2}\right], \qquad a = \left(1 - \frac{\kappa^2}{\omega_0^2}\right)\frac{T}{\mu}, \quad b = \frac{\omega_0^2 \mu}{T}. \tag{50}$$

*Case III:* $\omega^2(t) = \omega_0^2 e^{\mu t/T}$, $0 \leqslant t \leqslant T$. In this case the functions $f_+(t)$ and $f_-(t)$ in (50) are again given in terms of Bessel functions as

$$f_{\pm}(t) = e^{-\kappa t} J_{\pm\alpha}(a e^{\mu t/2T}), \quad a = \frac{2T\omega_0}{\mu}, \quad \alpha = \frac{2T\kappa}{\mu}. \tag{51}$$

Having dealt with some exactly solvable cases where the frequency is changed in a specific way but the temperature may be varied arbitrarily, we now illustrate how the formalism developed above lends itself to useful exact or approximate calculations leading to finite-time corrections.

## V. LINEAR VARIATION OF THE DIFFUSION CONSTANT

We first consider the case in which the harmonic oscillator with frequency $\omega$ is in equilibrium with a bath at temperature $T_0$ characterized by a diffusion constant $D_0$. With $\omega$ held fixed, the diffusion coefficient is changed linearly from its initial value $D_0$ appropriate to temperature $T_0$ to its final value $D_1$ appropriate to temperature $T_1$ in a time $\tau$ and then kept at that value thereafter. For $\omega$ held fixed,

$$D(t) = \begin{cases} D_0 + (D_1 - D_0)\frac{t}{\tau}, & 0 \leqslant t \leqslant \tau \\ D_1, & t > \tau. \end{cases} \tag{52}$$

This situation pertains to the isochoric step in the Brownian engines and is relevant for discussions on aspects of decoupling the system from a heat bath at one temperature and recoupling it to another heat bath at a different temperature.

For the case at hand, with $\mathcal{V}(0)$ chosen to be the variance matrix corresponding to the oscillator being at equilibrium with the bath at temperature appropriate to $D_0$,

$$\mathcal{V}(0) = \begin{pmatrix} \frac{D_0}{2\kappa m} & 0 \\ 0 & \frac{D_0}{2\kappa m^2\omega^2} \end{pmatrix}, \tag{53}$$

we have from (48)

$$\langle q^2(t)\rangle = \frac{D_0}{2\kappa}\left(\frac{u^2(t)}{m^2\omega^2} + v^2(t)\right) + 2\int_0^t dt' v^2(t-t')D(t'), \tag{54}$$

$$\langle q(t)p(t)\rangle = 2\int_0^t dt' v(t-t')\dot{v}(t-t')D(t'), \tag{55}$$

$$\langle p^2(t)\rangle = \frac{mD_0}{2\kappa}\left(\frac{u(t)\dot{u}(t)}{m^2\omega^2} + v(t)\dot{v}(t)\right) + 2m^2\int_0^t dt' \dot{v}^2(t-t')D(t'). \tag{56}$$

Using the relations

$$v^2 = -\frac{1}{2\kappa}\frac{1}{2}\frac{d}{dt}\left(\frac{u^2}{m^2\omega^2} + v^2\right), \tag{57}$$

$$v\dot{v} = -\frac{1}{2\kappa}\frac{d}{dt}\left(\frac{u\dot{u}}{m^2\omega^2} + v\dot{v}\right), \tag{58}$$

$$\dot{v}^2 = -\frac{1}{2\kappa}\frac{1}{2}\frac{d}{dt}\left(\frac{\dot{u}^2}{m^2\omega^2} + \dot{v}^2\right), \tag{59}$$

which follow from

$$\dot{v} = -2\kappa v + \frac{u}{m}, \quad \dot{u} = -m\omega^2 v, \tag{60}$$

we obtain for $t > \tau$

$$\langle q^2(t)\rangle = \alpha(t)\langle q^2\rangle_0 + (1-\alpha(t))\langle q^2\rangle_1, \tag{61}$$

$$\langle p^2(t)\rangle = \beta(t)\langle p^2\rangle_0 + (1-\beta(t))\langle p^2\rangle_1, \tag{62}$$

where

$$\alpha(t) = \frac{1}{\tau}\int_{t-\tau}^t dt'[m^2\omega^2 v^2(t') + u^2(t')], \tag{63}$$

$$\beta((t) = \frac{1}{\tau}\int_{t-\tau}^t dt'\left[m^2\dot{v}^2(t') + \frac{\dot{u}^2(t')}{\omega^2}\right]. \tag{64}$$

In the limit $t \to \infty$ both $\alpha(t)$ and $\beta(t)$ go to zero and hence $\langle q^2\rangle$ and $\langle p^2\rangle$ assume their respective equilibrium values. The parameters $\alpha(t)$ and $\beta(t)$ thus interpolate between the initial and the final equilibrium values of $\langle q^2\rangle$ and $\langle p^2\rangle$ and quantify the approach to equilibrium. In the following we consider the case when $t = \tau$, i.e., the situation that is obtained immediately after the bath has reached the state characterized by the final value of the diffusion coefficient. Evidently, as far as the system is concerned, we are dealing here with a nonequilibrium state as the system has not yet had time to equilibrate with the final bath.

By setting $t = \tau$ in (63) and (64) and denoting $\alpha(\tau)$ and $\beta(\tau)$ simply as $\alpha$ and $\beta$ we obtain on substituting for $u$ and $v$ from (47) and carrying out the relevant integrals

$$\alpha = \frac{1}{(x-y)^2}\left[(x+y)\left(\frac{x}{2y}(1-e^{-2y}) + \frac{y}{2x}(1-e^{-2x})\right) - \frac{4xy}{x+y}(1-e^{-(x+y)})\right], \tag{65}$$

$$\beta = \frac{1}{(x-y)^2}\left[(x+y)\left(1 - \frac{e^{-2y}+e^{-2x}}{2}\right) - \frac{4xy}{x+y}(1-e^{-(x+y)})\right], \tag{66}$$

where $x = [\kappa + \sqrt{\kappa^2 - \omega^2}]\tau$ and $y = [\kappa - \sqrt{\kappa^2 - \omega^2}]\tau$. We now examine the behavior of $\alpha$ and $\beta$ in the overdamped and weak dissipation regimes, respectively.

In the overdamped regime, i.e., $\kappa \gg \omega$, $x \approx 2\kappa\tau \gg 1$, and $y \approx \frac{\omega^2\tau}{2\kappa} \ll 1$ one finds that

$$\alpha \approx \frac{1-e^{-2y}}{2y} \to 1 \quad \text{as } y \to 0, \tag{67}$$

$$\beta \approx \frac{1-e^{-2x}}{2x} \to 0 \quad \text{for } x \gg 1. \tag{68}$$

In contrast, in the weak dissipation regime $\kappa \ll \omega$, $x \approx \kappa + i\omega$, and $y \approx \kappa - i\omega$, we have in the limit $\kappa\tau \to 0$

$$\alpha \approx \left[\frac{1-e^{-2\kappa\tau}}{2\kappa\tau} + \kappa\tau\left(\frac{\sin\omega\tau}{\omega\tau}\right)^2\right] \tag{69}$$

$$\approx 1 - \kappa\tau\left[1 - \left(\frac{\sin\omega\tau}{\omega\tau}\right)^2\right], \tag{70}$$

$$\beta \approx \left[\frac{1-e^{-2\kappa\tau}}{2\kappa\tau} - \kappa\tau\left(\frac{\sin\omega\tau}{\omega\tau}\right)^2\right] \tag{71}$$

$$\approx 1 - \kappa\tau\left[1+\left(\frac{\sin\omega\tau}{\omega\tau}\right)^2\right]. \tag{72}$$

Note that $\alpha > \beta$ in both cases. In fact, this is always true: It can easily be shown that with $x,y$ defined as before

$$\alpha - \beta = \frac{x+y}{x-y}\int_0^1 dt[e^{-2xt} - e^{-2yt}] \tag{73}$$

and hence $\alpha > \beta$ by virtue of the fact that the integrand is always positive.

We conclude this section with a general remark to put the contents of this section in a larger perspective. Standard thermodynamic considerations assume that the external parameters such as frequency and temperature are changed so slowly that the system goes continuously from one equilibrium state to another. The situation is different if at any stage the system goes out of thermodynamic equilibrium and the one discussed here is a case in point. Here the system does go through out-of-equilibrium states [see (61) and (62)] and our analysis shows that the damping parameter is crucial in determining the out-of-equilibrium states, although the state in thermodynamic equilibrium does not depend on the damping parameter. In situations where the intermediate state depends on damping, the changes considered are not reversible.

## VI. EFFECT OF TIME SCALES ON EFFICIENCIES OF BROWNIAN MOTORS

We recall that in the calculation of the efficiency of the Stirling engine from standard thermodynamic considerations presented in Sec. II we had drawn attention to the factor of $\frac{1}{2}$ in the expression for $\Delta U_{4\to1}$. Likewise, in the computation of the Stirling engine using the quantum stochastic thermodynamics in the steady state we had noted that in computing $\Delta U_{4\to1}$ only $\langle p^2\rangle/2m$ contributes to $\Delta U_{4\to1}$ and not $m\omega^2\langle q^2\rangle/2$. This seemingly *ad hoc* prescription can now be understood at a deeper level in the light of the analysis in Sec. V leading to Eqs. (61)–(64). It is clear from the discussion therein that, in general, the expression for $\Delta U_{4\to1}$ should be taken to be

$$\Delta U_{4\to1} = (1-\beta)\left(\frac{\langle p^2\rangle_1}{2m} - \frac{\langle p^2\rangle_4}{2m}\right) + (1-\alpha)m\omega^2\left(\frac{\langle q^2\rangle_1}{2} - \frac{\langle q^2\rangle_4}{2}\right), \tag{74}$$

where $\alpha$ and $\beta$ depend on various time scales involved. Indeed, in the overdamped regime $\alpha \to 1$ and $\beta \to 0$ and one recovers the earlier results. The mystery behind the factor of $\frac{1}{2}$ in (11) and that behind retaining the contribution from $\langle p^2\rangle/2m$ in (36) alone is thus resolved. In contrast, in the weak dissipation regime, where both $\alpha$ and $\beta$ are close to 1, the situation is very different and this has significant consequences for the relative magnitude of classical and quantum efficiencies under the same operating conditions as discussed later. Further, since for a harmonic oscillator $\langle p^2\rangle/2m = m\omega^2\langle q^2\rangle/2$, we can rewrite Eq. (74) as

$$\Delta U_{4\to1} = 2\mu\left(\frac{\langle p^2\rangle_1}{2m} - \frac{\langle p^2\rangle_4}{2m}\right), \quad \mu = 1 - \frac{\alpha+\beta}{2}. \tag{75}$$

Using this expression in the calculations of the classical and quantum efficiencies for the Stirling engine given earlier, we obtain

$$\eta_S^{\rm cl} = \frac{\eta_C}{1+\eta_C\mu\big/\ln\left(\frac{\omega_2}{\omega_1}\right)} \tag{76}$$

and

$$\eta_S^q = \frac{1-Y/X}{1+Z/X},$$
$$X = \ln\left(\frac{\sinh(\beta_h\hbar\omega_2/2)}{\sinh(\beta_h\hbar\omega_1/2)}\right),$$
$$Y = \frac{\beta_h}{\beta_c}\ln\left(\frac{\sinh(\beta_c\hbar\omega_2/2)}{\sinh(\beta_c\hbar\omega_1/2)}\right),$$
$$Z = \frac{\beta_h}{2}\{\hbar\omega_1\coth(\beta_h\hbar\omega_1/2) - \hbar\omega_2[(1-\mu)\coth(\beta_h\hbar\omega_2/2) + \mu\coth(\beta_c\hbar\omega_2/2)]\}. \tag{77}$$

The appearance of the parameter $\mu$ here may be viewed as a phenomenological way of incorporating nonequilibrium effects arising from decoupling of the system from one bath and recoupling it to another.

In terms of dimensionless quantities $a,b,c$ such as

$$\beta_c\hbar\omega_1 = a, \quad \frac{\omega_2}{\omega_1} = b, \quad \frac{\beta_h}{\beta_c} = c, \tag{78}$$

the expression above for the efficiencies $\eta_S^q$ and $\eta_S^{\rm cl}$ in the classical and quantum read

$$\eta_S^{\rm cl}(b,c) = \frac{1-c}{1+\mu\frac{(1-c)}{\ln b}}, \tag{79}$$

$$\eta_S^q(a,b,c) = \frac{\ln\left(\frac{\sinh(abc/2)}{\sinh(ac/2)}\right) - c\ln\left(\frac{\sinh(ab/2)}{\sinh(a/2)}\right)}{\ln\left(\frac{\sinh(abc/2)}{\sinh(ac/2)}\right) + \frac{ac}{2}\coth(ac/2) - \frac{abc}{2}[(1-\mu)\coth(abc/2) + \mu\coth(ab/2)]}. \tag{80}$$

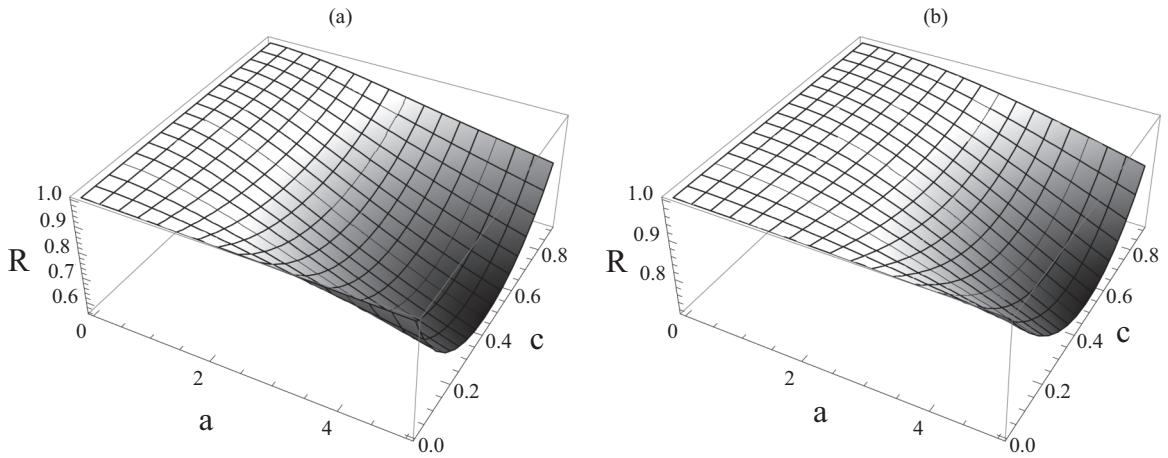


FIG. 1. Ratio $R = \eta_S^q/\eta_S^{\rm cl}$ plotted as a function of $a = \beta_c\hbar\omega_1$ and $c = \beta_h/\beta_c$ for $\omega_2/\omega_1 = 2.05$.

In the experiments of Blickle and Bechinger [7]

$$a = 9.500\,65 \times 10^{-7}, \quad b = 2.049\,22, \quad c = 0.845\,272. \tag{81}$$

With $b$ fixed at this value, we plot in Fig. 1 the ratio $R = \eta_S^q/\eta_S^{\rm cl}$ as a function of $a$,$c$ for two representative values of $\mu$.

## VII. FINITE-TIME CORRECTIONS: COMPLEMENTARITY RELATIONS

We next consider the situation when the system starts out at equilibrium with a bath at temperature $T$ and the frequency is changed from its initial value $\omega_0$ to its final value $\omega_1$ in a finite time either isothermally ($T$ held fixed) or isentropically ($\omega/T$ held fixed) and focus on computing finite-time corrections to the standard thermodynamic results. Referring to (1)–(3), we recall that while Stirling and Carnot engines involve the former operation, Carnot and Otto engines involve the latter. The scheme for computing finite-time corrections developed below is similar in spirit to the adiabatic approximation in quantum mechanics and is a variant of the method formulated in [21] in the context of the Fokker-Planck equation adapted to the equations for the moments themselves.

The equations for the second moments that follow from the Langevin or the Fokker-Planck equation may be written as

$$\frac{d}{dt}X(t) = A(t)X(t) + Y(t), \tag{82}$$

where

$$X(t) = \begin{pmatrix} \langle q^2\rangle \\ \langle qp\rangle \\ \langle p^2\rangle \end{pmatrix}, \quad A(t) = \begin{pmatrix} 0 & \frac{2}{m} & 0 \\ -m\omega^2(t) & -2\kappa & \frac{1}{m} \\ 0 & -2m\omega^2 & -4\kappa \end{pmatrix},$$
$$Y(t) = \begin{pmatrix} 0 \\ 0 \\ 2D(t) \end{pmatrix}. \tag{83}$$

(At this stage, as indicated, we allow the frequency and the diffusion coefficients to be independent functions of $t$; later, however, we would specialize to situations appropriate to isothermal or isentropic variation of the frequency.) Setting $t = s\tau$ and expanding $X(t)$ as

$$X(t) = X^{(0)}(s) + \frac{1}{\tau}X^{(1)}(s) + \cdots, \tag{84}$$

we obtain

$$A(s)X^{(0)}(s) + Y(s) = 0 \Rightarrow X^{(0)}(s) = -A^{-1}(s)Y(s), \tag{85}$$

$$X^{(1)}(s) = A^{-1}(s)\frac{d}{ds}X^{(0)}(s). \tag{86}$$

Equation (85) can be taken to describe the situation where the system is in the steady state corresponding to the instantaneous values of $\omega$ and $D$ and Eq. (86) as describing deviations from this steady state. These equations then give

$$\langle q^2(s)\rangle^{(0)} = \frac{D(s)}{2m^2\omega^2(s)\kappa}, \quad \langle q(s)p(s)\rangle^{(0)} = 0,$$
$$\langle p^2(s)\rangle^{(0)} = \frac{D(s)}{2\kappa} \tag{87}$$

and

$$\langle q^2(s)\rangle^{(1)} = -\left[\frac{8\kappa^2 + 2\omega^2(s)}{8\kappa\omega^2(s)}\frac{d}{ds}\langle q^2(s)\rangle^{(0)} + \frac{1}{m\omega^2(s)}\frac{d}{ds}\langle q(s)p(s)\rangle^{(0)} + \frac{1}{4\kappa m^2\omega^2(s)}\frac{d}{ds}\langle p^2(s)\rangle^{(0)}\right], \tag{88}$$

$$\langle q(s)p(s)\rangle^{(1)} = \frac{m}{2}\frac{d}{ds}\langle q^2(s)\rangle^{(0)}, \tag{89}$$

$$\langle p^2(s)\rangle^{(1)} = -\left[\frac{m^2\omega^2(s)}{4\kappa}\frac{d}{ds}\langle q^2(s)\rangle^{(0)} + \frac{1}{4\kappa}\frac{d}{ds}\langle p^2(s)\rangle^{(0)}\right]. \tag{90}$$

These equations together with (87) give finite-time corrections to the variances. As the diffusion coefficient is a function of both $\omega$ and $T$, we now specialize to the situations where $\omega$ is time dependent and $T$ is held fixed (the isothermal case) and $\omega$ and $T$ both are time dependent but $\omega/T$ is held fixed (the isentropic case). With this in mind, we may rewrite the

expression for $\langle q^2(s)\rangle^{(1)}$ (which we will need shortly) as

$$\langle q^2(s)\rangle^{(1)} = \frac{\hbar}{4\kappa m\omega^2}\left[\left(\frac{4\kappa^2}{\omega^2}\right)\left(n(\omega,T)+\frac{1}{2}\right)\frac{d\omega}{ds} - \left(\frac{4\kappa^2}{\omega^2}+2\right)\omega\frac{d}{ds}\left(n(\omega,T)+\frac{1}{2}\right)\right]. \quad (91)$$

In the isothermal case both terms on the rhs contribute. In contrast, in the isentropic case only the first term contributes as during this process $\omega/T$ and hence $n(\omega,T)$ are held constant. In the following we confine ourselves to the isothermal case and give the results for two physically interesting limiting cases corresponding to the overdamped and weak dissipation regimes: In the overdamped regime $\kappa \gg \omega$,

$$\langle q^2(s)\rangle^{(1)} = \frac{\kappa}{m\omega^5\beta}\left[\left(\frac{\beta\hbar\omega}{2}\right)\coth\left(\frac{\beta\hbar\omega}{2}\right) + \left(\frac{\beta\hbar\omega}{2}\right)^2\operatorname{cosech}^2\left(\frac{\beta\hbar\omega}{2}\right)\right]\left(\frac{d\omega}{ds}\right) \quad (92)$$

and in the weak dissipation regime $\kappa \ll \omega$,

$$\langle q^2(s)\rangle^{(1)} = \frac{1}{2\kappa m\omega^3\beta}\left[\left(\frac{\beta\hbar\omega}{2}\right)\operatorname{cosech}\left(\frac{\beta\hbar\omega}{2}\right)\right]^2\left(\frac{d\omega}{ds}\right). \quad (93)$$

We now compute expressions for the irreversible heat $Q_{\rm irr}$,

$$Q_{\rm irr} = F(i) - F(f) - W_{i\to f}, \quad (94)$$

in an isothermal process at temperature $T$ from $i \to f$ arising from finite-time corrections. Recalling that

$$W_{i\to f} = -\int_{\omega_i}^{\omega_f} m\omega\langle q^2\rangle d\omega = -\int_{\omega_i}^{\omega_f} m\omega\left(\langle q^2\rangle^{(0)} + \frac{1}{\tau}\langle q^2\rangle^{(1)}\right)d\omega \quad (95)$$

and

$$-\int_{\omega_i}^{\omega_f} m\omega\langle q^2\rangle^{(0)} d\omega = F(i) - F(f), \quad (96)$$

we have

$$Q_{\rm irr} = \frac{1}{\tau}\int_{\omega_i}^{\omega_f} m\omega\langle q^2\rangle^{(1)} d\omega \equiv T\frac{\Sigma}{\tau}. \quad (97)$$

From the way the quantity $\Sigma$ is defined above it is clear that it would in general depend on both $T$ and the manner in which $\omega$ is varied from its initial value $\omega_i$ to its final value $\omega_f$ in the time $\tau$. We now turn to the question as to what would be the minimum value of $Q_{\rm irr}$ and hence that of $\Sigma$ in the weak dissipation and overdamped regimes.

Using (92) and (93) and parametrizing $\omega(s)$ such that $\omega(0) = \omega_i$ and $\omega(1) = \omega_f$ we have

$$Q_{\rm irr} = \begin{cases} l\frac{2\kappa}{\beta\tau}\int_0^1 ds\, g(\omega(s))\left(\frac{d\omega}{ds}\right)^2 & (\kappa \gg \omega) \\ \frac{1}{2\kappa\beta\tau}\int_0^1 ds\, g(\omega(s))\left(\frac{d\omega}{ds}\right)^2 & (\kappa \ll \omega), \end{cases} \quad (98)$$

where

$$g(\omega) = \begin{cases} \frac{1}{2\omega^4}\left[\left(\frac{\beta\hbar\omega}{2}\right)\coth\left(\frac{\beta\hbar\omega}{2}\right) + \left(\frac{\beta\hbar\omega}{2}\right)^2\operatorname{cosech}^2\left(\frac{\beta\hbar\omega}{2}\right)\right] & (\kappa \gg \omega) \\ \frac{1}{\omega^2}\left[\left(\frac{\beta\hbar\omega}{2}\right)\operatorname{cosech}\left(\frac{\beta\hbar\omega}{2}\right)\right]^2 & (\kappa \ll \omega). \end{cases} \quad (99)$$

The expression $Q_{\rm irr}$ involves the functional

$$I[\omega] = \int_0^1 ds\, g(\omega(s))\left(\frac{d\omega}{ds}\right)^2. \quad (100)$$

If we define $\Omega = f(\omega)$ and its inverse as $\omega = h(\Omega)$ and choose $f(\omega)$ to satisfy

$$\frac{df(\omega)}{d\omega} = \sqrt{g(\omega)}, \quad (101)$$

then we find that the curve $\omega(s)$ $(0 \leqslant s \leqslant 1)$, which minimizes $I[\omega]$, is given by

$$\omega(s) = h(f(\omega(0))(1-s) + f(\omega(1))s) \quad (102)$$

and its minimum value by

$$I_{\rm min}[\omega] = [f(\omega(1)) - f(\omega(0))]^2. \quad (103)$$

In the classical limit $\beta\hbar\omega \lll 1$, in the strong damping regime $\kappa \gg \omega$ we have

$$g(\omega) = \frac{1}{\omega^2} \Rightarrow f(\omega) = -\frac{1}{\omega}, \quad h(\Omega) = -\frac{1}{\Omega} \quad (104)$$

and hence

$$Q_{\rm irr}^{\rm min} = \frac{2\kappa K_B T}{\tau}\left[\frac{1}{\omega(1)} - \frac{1}{\omega(0)}\right]^2, \quad (105)$$

in agreement with the results of Sekimoto and Sasa [21] (modulo an erroneous factor of $\frac{1}{4}$ in the value of $Q_{\rm irr}^{\rm min}$ as quoted). This minimum value is realized along the curve

$$\omega(s) = \left[\frac{s}{\omega(0)} + \frac{1-s}{\omega(1)}\right]^{-1}, \quad 0 \leqslant s \leqslant 1. \quad (106)$$

Thus, in the classical limit, in the overdamped regime, we obtain the following inequality for the product of the irreversible heat and the time taken to execute the step:

$$\tau \times Q_{\rm irr} \geqslant 2\kappa K_B T\left[\frac{1}{\omega(1)} - \frac{1}{\omega(0)}\right]^2. \quad (107)$$

Such a relation is referred to in the literature as a thermodynamic complementarity relation, an analog, in both spirit and form, of the energy-time uncertainty relations in quantum mechanics. It should, however, be noted that the rhs of the above complementarity relation is independent of $\hbar$.

Again in the overdamped regime, but now in the low-temperature limit, i.e., $\beta\hbar\omega \to 0$, we find that $g(\omega) \approx \beta\hbar/4\omega^3$ and the complementarity relation becomes

$$\tau \times Q_{\rm irr} \geqslant \hbar(2\kappa)\left[\frac{1}{\sqrt{\omega(1)}} - \frac{1}{\sqrt{\omega(0)}}\right]^2. \tag{108}$$

One finds that $\hbar$ now does appear on the rhs as one would expect in the limit of low temperature where quantum effects become significant.

Turning to the weak dissipation case, one finds that the expression for $g(\omega)$ is such that the relevant integral in (101) can be given in a closed form leading to the following complementarity relation:

$$\tau \times Q_{\rm irr} \geqslant \frac{K_B T}{2\kappa}\left[\ln\left(\frac{\tanh(\beta\hbar\omega(1)/4)}{\tanh(\beta\hbar\omega(0)/4)}\right)\right]^2, \tag{109}$$

valid for all values of $T$. In particular, in the classical limit it becomes

$$\tau \times Q_{\rm irr} \geqslant \frac{K_B T}{2\kappa}\left[\ln\left(\frac{\omega(0)}{\omega(1)}\right)\right]^2 \tag{110}$$

and the curve $\omega(s)$ $(0 \leqslant s \leqslant 1)$, which minimizes $Q_{\rm irr}$, now turns out to be

$$\omega(s) = \omega(0)^{(1-s)/2}\omega(1)^{s/2}. \tag{111}$$

We emphasize here that though we have presented explicit expressions for $Q_{\rm irr}$ for the weak and strong damping regimes, the results in (87) and (88) enable us to derive expressions for $Q_{\rm irr}$ for both classical and quantum cases without any specific assumptions on the relative magnitudes of $\kappa$ and $\omega$. Further, in the classical limit we find that for an isothermal process from $i \to f$ carried out in a finite time $\tau$, $Q_{\rm irr}$ has the structure

$$Q_{\rm irr} = T\frac{\Sigma}{\tau}, \tag{112}$$

where $\Sigma$ is independent of $T$. On using the fact that for an isothermal process $F(i) - F(f) = T\Delta S_{i\to f}$, we may rewrite (94) as

$$W_{i\to f} = T\left(\Delta S_{i\to f} - \frac{\Sigma_{i\to f}}{\tau_{i\to f}}\right). \tag{113}$$

This provides a convenient and physically useful way of parametrizing deviations from quasistaticity in that in the limit $\tau_{i\to f} \to \infty$ one recovers the familiar results of equilibrium thermodynamics.

## VIII. EFFICIENCY OF THE STIRLING ENGINE AT MAXIMUM POWER

In this section we use the results of the preceding section to analyze the efficiency of the Stirling engine at maximum power very much in the spirit of the earlier works in the context the Carnot cycle. We closely follow the works of Schmiedl and Seifert [9] and Esposito *et al.* [12], who analyzed the question of the efficiency of the Carnot cycle at maximum power in the limit of low dissipation from fairly general considerations. In particular, in [12] it was shown that the Carnot efficiency at maximum power $\eta_C^*$ is bounded below by $\eta_C/2$ and above by $\eta_C/(2-\eta_C)$ and that while the Curzon-Ahlborn efficiency [22] is reached in the limit of symmetric dissipation, the upper bound is realized in a completely asymmetric limit and coincides with the universal upper bound derived in [23,24] from somewhat different considerations.

Consider the situation when the isothermal steps $1 \to 2$ and $3 \to 4$ are carried out in finite times $\tau_h$ and $\tau_c$, respectively, as indicated in (1). Power generated during the Stirling cycle is then

$$P = \frac{W_{1\to2} + W_{3\to4}}{\tau_c + \tau_h}. \tag{114}$$

Also, as we have seen in Sec. VI, the expression for the efficiency for the Stirling engine can be written as

$$\eta_S^{\rm cl} = \frac{W_{1\to2} + W_{3\to4}}{\mu K_B(T_h - T_c) + W_{1\to2}}, \tag{115}$$

where $\mu \approx 0$ in the weak coupling regime and $\mu = \frac{1}{2}$ in the overdamped regime.

Using (113) and setting $\Sigma_{1\to2} \equiv \Sigma_h, \Sigma_{3\to4} \equiv \Sigma_c, \Delta S_{1\to2} = -\Delta S_{3\to4} = \Delta S$, (114) and (115) become

$$P = \frac{(T_h - T_c)\Delta S - T_h\Sigma_h/\tau_h - T_c\Sigma_c/\tau_c}{\tau_c + \tau_h}, \tag{116}$$

$$\eta_S^{\rm cl} = \frac{(T_h - T_c)\Delta S - T_h\Sigma_h/\tau_h - T_c\Sigma_c/\tau_c}{\mu K_B(T_h - T_c) + T_h\Delta S - T_h\Sigma_h/\tau_h}. \tag{117}$$

Maximizing $P$ with respect to $\tau_h$ and $\tau_c$, one finds that $P$ attains its maximum value for

$$\tau_h = \tau_h^* = 2\frac{T_h\Sigma_h}{(T_h - T_c)\Delta S}\left(1 + \sqrt{\frac{T_c\Sigma_c}{T_h\Sigma_h}}\right), \tag{118}$$

$$\tau_c = \tau_c^* = 2\frac{T_c\Sigma_c}{(T_h - T_c)\Delta S}\left(1 + \sqrt{\frac{T_h\Sigma_h}{T_c\Sigma_c}}\right). \tag{119}$$

Substituting these values for $\tau_h$ and $\tau_c$ in (117), one finds that the efficiency for the Stirling engine at maximum power is given by

$$\eta_S^{\rm cl*} = \frac{\eta_C\left(1 + \sqrt{\frac{T_c\Sigma_c}{T_h\Sigma_h}}\right)}{\left(1 + \sqrt{\frac{T_c\Sigma_c}{T_h\Sigma_h}}\right)^2 + \frac{T_c}{T_h}\left(1 - \frac{\Sigma_c}{\Sigma_h}\right) + \frac{2\mu\eta_C}{\ln(\frac{\omega_2}{\omega_1})}}. \tag{120}$$

We now consider two cases.

*Case A:* $\mu = 0$. In the extremely weak dissipation regime, i.e., $\mu = 0$, one recovers results similar to those in [9,12] in the context of the Carnot cycle: In the symmetric case, i.e., $\Sigma_c/\Sigma_h = 1$, $\eta_S^{\rm cl*}$ equals the Curzon-Ahlborn efficiency $\eta_{CA} = 1 - \sqrt{T_c/T_h}$,

$$\eta_S^{\rm cl*} = \eta_{CA}, \tag{121}$$

and for the case in which $\eta_S^{\rm cl*}$ is bounded by $\eta_C/2$ and $\eta_C/(2-\eta_C)$,

$$\eta_C/2 \leqslant \eta_S^{\rm cl*} \leqslant \eta_C/(2-\eta_C). \tag{122}$$

The upper and lower bounds correspond to $\Sigma_c/\Sigma_h \to 0$ and $\Sigma_c/\Sigma_h \to \infty$, respectively.

*Case B:* $\mu \neq 0$. For small but nonzero $\mu < \frac{1}{2}\ln(\omega_2/\omega_1)$ these results get modified to the following: In the symmetric case, i.e., $\Sigma_c/\Sigma_h = 1$, $\eta_S^{\rm cl*}$ is less than the Curzon-Ahlborn

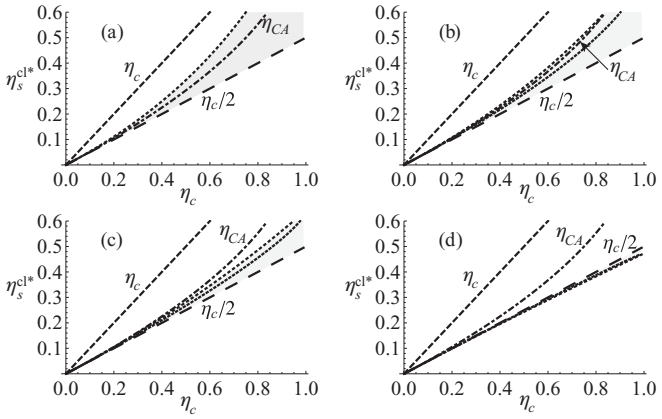


FIG. 2. Efficiency $\eta_S^{cl*}$ of the Stirling engine at maximum power as a function of the Carnot efficiency $\eta_C$. The graph $\eta_S^{cl*}$ versus $\eta_C$, for all values of $\Sigma_c/\Sigma_h$, lies in the shaded regions given for $\omega_2/\omega_1 = 2.05$ and (a) $\mu = 0.001$, (b) $\mu = 0.1$, (c) $\mu = 0.2$, and (d) $\mu = 0.4$. The graphs of $\eta_C$, $\eta_{CA}$, and $\eta_C/2$ versus $\eta_C$ are displayed for comparison. While in (a)–(c) $\mu < \frac{1}{2}\ln(\omega_2/\omega_1)$, (d) corresponds to the case for $\mu > \frac{1}{2}\ln(\omega_2/\omega_1)$ when there is no lower boundary. The unmarked curve (b) and (c) within and (d) outside the shaded regions is $\eta_S^{cl*}$ for $\Sigma_c/\Sigma_h = 1$ [Eq. (123)].

efficiency [22] $\eta_{CA} = 1 - \sqrt{T_c/T_h}$,

$$\eta_S^{cl*} = \frac{\eta_{CA}}{1 + \left(\frac{\mu}{\ln(\omega_2/\omega_1)}\right)\left(\frac{2\eta_{CA}}{2-\eta_{CA}}\right)} < \eta_{CA}, \tag{123}$$

and in the case in which $\eta_S^{cl*}$ is bounded by $\eta_C/2$ and $\eta_S/(2-\eta_S)$,

$$\eta_C/2 \leqslant \eta_S^{cl*} \leqslant \frac{\eta_C}{2 - \eta_C\left(1 - \frac{2\mu}{\ln(\omega_2/\omega_1)}\right)}. \tag{124}$$

As before, the upper and lower bounds correspond to $\Sigma_c/\Sigma_h \to 0$ and $\Sigma_c/\Sigma_h \to \infty$, respectively. In contrast, if $\mu > \frac{1}{2}\ln(\omega_2/\omega_1)$, one finds that

$$\eta_S^{cl*} \leqslant \eta_C/2. \tag{125}$$

In Fig. 2 we display the bounds on $\eta_S^{cl*}$ for $\mu = 0.001, 0.1, 0.2, 0.4$ with $\omega_2/\omega_1$ taken to be 2.05; we also give the plots for $\eta_C$, $\eta_{CA}$, and $\eta_c/2$ for comparison.

## IX. CONCLUSION

In this work we have developed a microscopic framework for computing the efficiencies of quantum and classical Brownian motors realized by a harmonic oscillator. Two exactly solvable models for frequency modulation are presented. In the context of the Stirling engine, we have analytically treated the question of coupling the system at equilibrium with a bath at low temperature to a bath at higher temperature and the role that various time scales play in this process and have shown that these have a strong influence on its efficiency. Further, we have developed a procedure for computing finite-time corrections to the quantities of interest needed for calculating the efficiency of the three engines considered—Stirling, Carnot, and Otto—and have derived the thermodynamic complementarity relations in the overdamped and underdamped situations in both the high- and low-temperature limits. In the spirit of the works reported in [9,12] on the Carnot engine, we have analyzed in detail the efficiency of the Stirling engine at maximum power and have investigated the role of dissipation parameters thereon. Though in this work we have exclusively considered interactions between the system and a thermal bath, the formalism can easily be extended to situations where the thermal bath is replaced by a squeezed thermal bath bringing with it new parameters and thereby ushering in new possibilities that have no classical analogs.

In the present work we have modeled the three heat engines after the quantum harmonic oscillator. It is of interest to carry out a similar analysis for finite-state quantum systems. Indeed, the entire perspective on heat pumps, refrigerators, and heat engines developed in [3] is based on the simplest of quantum systems: a qubit. Though in that context a convenient Fokker-Planck framework would no longer be available, we expect that the methodology developed here applied directly to the master equation would be useful there as well. We hope to return to this and related questions in the near future.

## ACKNOWLEDGMENT

One of (S.C.) gratefully acknowledges the hospitality extended to him by the Department of Physics, Oklahoma State University, Stillwater, where a large part of this work was carried out.

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