A quantum mechanical open system as a model of a heat engine

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A quantum model of a heat engine is analyzed. This engine is constructed from two coupled oscillators in interaction with a warm and cold reservoir. Power is extracted by an external periodic driving force. As a function of control parameters a maximum in power is obtained, and a decline of thermodynamic efficiency below the ideal Carnot value. This irreversibility is a consequence of the mechanism devised to extract power in its perturbing the energy level structure of the engine. In the limit of weak coupling to the driving force the efficiency at maximum power obtains the value of $\eta = 1 - \sqrt{(T_a/T_b)}$.

I. INTRODUCTION

Real heat engines may be operated to maximize power by appropriate choice of parameters, and when they are so operated, they have efficiencies less than the ideal Carnot value for the same heat reservoirs. The Carnot value is obtainable only under reversible conditions which means that the power output is zero because transferring heat to work takes infinitely long.

A quantum model of a heat engine is presented in the present study. It is constructed to maximize power and therefore shows submaximum efficiency moreover the model shows that the efficiency falls as the coupling to the external world increases.

Empirical models for realistic heat engines are not new. Early work of Tolman[1] emphasized the irreversible character of the loss terms. More recent work[2–8] has established the field of thermodynamics in a finite time scale. In these models time enters through Newtons empirical heat transfer law, which is used to model the heat flow in and out of the engine. An examination of these models shows that the maximum in power and the decline in the thermodynamic efficiency, are not an intrinsic part of the engine but are a consequence of the heat transfer law. More recent work has examined models where there is an internal source of irreversiblity.[7–8] The common qualitative feature of all these models is the dependence of the power on the control parameters. The general scheme which is observed is that as a function of the control parameter the power starts from zero, reaches a maximum and declines again.

In the present research similarities exist between the present quantum model and the empirical thermodynamic models. For the limiting case when the coupling to the external driving force is weak the efficiency at maximum power obtains the value $\eta = 1 - \sqrt{(T_a/T_b)}$, which is the same value for efficiency at maximum power found by Curzon and Ahlborn.[2] Nevertheless different reasons of quantum origin for the maximum power phenomena have been found. The efficiency declines because the mechanism which is devised to extract power perturbs the energy level structure of the engine. Because of this perturbation new dissipative terms appear.

In the research, a model engine was set up whose mechanical part was constructed in a way similar to a quantum amplifier, out of two oscillators coupled to an external field.[9–11] The quantum model of the reservoirs was based on the development of the semigroup formalism for relaxation processes.[12] The quantum thermodynamic description which relates observables to thermodynamic quantities was adopted from the works of Lebowitz[13] and Alicki.[14] This paper describes the basics of the quantum mechanical heat engine.

II. THE BASIC MODEL

An abstract heat engine consists of four parts: the engine, the power output mechanism, and the warm and cold reservoirs.

(A) The engine: The mechanical part consists of two oscillators with frequencies ω_a and ω_b represented by the Hamiltonian

$$\hat{H}_0 = \omega_a \hat{a}^\dagger \hat{a} + \omega_b \hat{b}^\dagger \hat{b} \,. \tag{2.1}$$

The power source of the engine is a population inversion betwen the upper levels of oscillator a and the upper levels of oscillator b.

(B). The power output mechanism: The device that extracts the power, or the power output mechanism couples the engine to the external world. In this model it is accomplished by a periodic coupling which manipulates the population difference between the oscillators. This interaction can be realized by a classical electromagnetic field with circular polarization. The device is represented by the time dependent Hamiltonian

$$\hat{H}_I = \epsilon(\hat{a}^\dagger \hat{b} e^{i\nu t} + \hat{b}^\dagger \hat{a} e^{-i\nu t}), \tag{2.2}$$

where ν is the frequency of the driving force. (In the rest of this paper resonant conditions are chosen $\nu = \omega_a - \omega_b$.) The parameter ϵ measures the strength of the coupling to the external field and therefore is the main control parameter of the engine. A rotating scheme is chosen because steady state solutions of the equations of motion are obtained, making it unnecessary to average over the periodic cycle.

(c) The reservoirs: A semigroup approach is chosen to describe the two reservoirs. In this approach additive dissipative terms are added to the equations of motion (in the Heisenberg picture), which now reads

$$\dot{\hat{X}} = L(\hat{X}) = L_H(\hat{X}) + L_{D_a}(\hat{X}) + L_{D_b}(\hat{X}), \tag{2.3}$$

where $L_H(\hat{X}) = i[\hat{H},\hat{X}]$. $\hat{X}$ is an aribitrary operator from the Hilbert space of the system, L_D is the dissipative part, and the a and b indexes represent the warm and cold reservoirs. The general dissipative operator has the form[4]

$$L_D(\hat{X}) = \sum_i \gamma_i\left(\hat{V}_i \hat{X}\hat{V}_i^\dagger - \frac{1}{2}\{\hat{V}_i \hat{V}_i^\dagger,\hat{X}\}\right). \tag{2.4}$$

The braces { } represent the anticommutator. Where the operators $\hat{V}$ are from the Hilbert space of the system and γ are positive constants. For a realistic model these constants determine the equilibrium state of the relaxing system and therefore the temperature. This form of the dissipative Liouville operator has also been derived in the weak coupling limit[15] and in the limit of a singular bath.[16] It has been argued[17,18] that the form (2.4) is more general than the derivation leading to it. (More explicit formulas for the constants γ_1 and γ_2 can be derived by approximating the behavior of the bath, e.g., by the weak coupling approximation.) For a single oscillator coupled to a reservoir the choice for $\hat{V}$ and γ in Eq. (2.4) is $\hat{V}_1 = \hat{a}$ for the down transition and $\hat{V}_2 = \hat{a}^\dagger$for the up transition. The detailed balance relation is $(\gamma_1/\gamma_2) = e^{(\hbar\omega/kT)}$. A similar reservoir exists for oscillator b.

These reservoirs represent a relaxation process with a nearest neighbor selection rule which brings each oscillator separately to a canonical equilibrium state of temperature T.[17,19]

III. THERMODYNAMIC RELATIONS

The basic equation by which the engine is examined is the conservation of energy equation:

$$\frac{d\langle E\rangle}{dt} = \langle L(\hat{H})\rangle + \dot{f}\langle\hat{V}\rangle. \tag{3.1}$$

In this equation $\hat{H}$ is partioned to $\hat{H} = \hat{H}_0 + \hat{V}f(t)$. Where $\hat{V}$ is the interaction potential and $f(t)$ is a time dependent function. Because $\hat{H}$ commutes with itself one gets

$$\frac{d\langle E\rangle}{dt} = \langle L_D(\hat{H})\rangle + \dot{f}\langle\hat{V}\rangle. \tag{3.2}$$

This partition, which is the time derivative of the first law of thermodynamics, is used to identify the power output as[13,14]

$$P = \dot{f}\langle\hat{V}\rangle. \tag{3.3}$$

Using the rotating scheme of Eq. (2.2), the power output for this model becomes

$$P = i\epsilon\nu(\langle\hat{a}^\dagger\hat{b}\rangle e^{i\nu t} - \langle\hat{b}^\dagger\hat{a}\rangle e^{-i\nu t}). \tag{3.4}$$

The heat flow is identified as

$$\dot{Q} = \langle L_D(\hat{H})\rangle. \tag{3.5}$$

The same basic identifications (3.2), (3.3), and (3.5) have been used to show the relation between line shapes in the linear response theory and exact calculations.[20] In this system the heat flow is partitioned to the contributions of each reservoir

$$\dot{Q} = \dot{Q}_a + \dot{Q}_b, \tag{3.6}$$

where $Q_i = \langle L_{D_i}(\hat{H})\rangle$. Under steady state operations the conservation of energy equation takes the form

$$P + \dot{Q}_a + \dot{Q}_b = 0. \tag{3.7}$$

The thermodynamic efficiency is defined as the ratio between the power output and the heat flow out of reservoir a:

$$\eta = \frac{P}{\dot{Q}_a}. \tag{3.8}$$

It now is left to find the steady state solutions of the expectation values of the operators participating in Eq. (3.7).

IV. A SECOND EXAMINATION OF THE RESERVOIRS

The simplest assumption concerning the reservoirs has been that they are each coupled to a single oscillator which is driven to thermal equilibrium. The temperature in the dissipative part of the Liouvillean is defined through the set of kinetic constants. For an isolated oscillator detailed balance means $(\gamma_1/\gamma_2) = e^{(\hbar\omega/kT)}$.[17,19] Solving for the power [Eq. (3.4)] under such an assumption leads to unphysical conclusions. The main one is that the power has no maximum for finite coupling coefficient ϵ. Also the efficiency stays constant $\eta = (\nu/\omega_1)$ regardless of changes in ϵ. The wrong conclusion is reached because the coupling between the oscillators is neglected in the relaxation terms. This coupling, which comes from the interaction to the external field, influences the reservoir relaxation constants.

In a realistic model, the two oscillators are coupled through the driving term. This means that the energy levels of the oscillators are perturbed[21] and therefore the dissipative terms have to be altered to ensure the correct equilibrium dependence.[22] Another important consequence of this coupling is that the operators $\hat{V}$ in the dissipative term of oscillator a, will have terms belonging to the Hilbert space of b.[22] Examining the Hamiltonian, it is convenient to employ a rotating scheme

$$\tilde{a} = \hat{Q}e^{i\omega_a t}, \quad \tilde{b} = \hat{b}e^{i\omega_b t}.$$

In this form the Hamiltonian is diagonalized by chosing

$$\tilde{A} = \tilde{a} + \tilde{b}, \quad \tilde{B} = \tilde{a} - \tilde{b}.$$

Rewriting the dissipative part of the Liouvillean, considering the interaction, one obtains the Liouville differential operator for a single reservoir

$$\begin{aligned} L_{D_i}(\hat{X}) &= k_1^{*i}(\tilde{A}^\dagger\hat{X}\tilde{A} - \tfrac{1}{2}\{\tilde{A}^\dagger\tilde{A},\hat{X}\}) + k_1^i(\tilde{A}\hat{X}\tilde{A}^\dagger - \tfrac{1}{2}\{\tilde{A}\tilde{A}^\dagger,\hat{X}\}) \\ &+ k_2^{*i}(\tilde{B}^\dagger\hat{X}\tilde{B} - \tfrac{1}{2}\{\tilde{B}^\dagger\tilde{B},\hat{X}\}) + k_2^i(\tilde{B}\hat{X}\tilde{B}^\dagger - \tfrac{1}{2}\{\tilde{B}\tilde{B}^\dagger,\hat{X}\}) \\ &+ k_3^{*i}(\tilde{A}^\dagger\hat{X}\tilde{B} - \tfrac{1}{2}\{\tilde{A}^\dagger\tilde{B},\hat{X}\}) + k_3^i(\tilde{A}\hat{X}\tilde{B}^\dagger - \tfrac{1}{2}\{\tilde{A}\tilde{B}^\dagger,\hat{X}\}) \\ &+ k_4^{*i}(\tilde{B}^\dagger\hat{X}\tilde{A} - \tfrac{1}{2}\{\tilde{B}^\dagger\tilde{A},\hat{X}\}) + k_4^i(\tilde{B}\hat{X}\tilde{A}^\dagger - \tfrac{1}{2}\{\tilde{B}\tilde{A}^\dagger,\hat{X}\}), \end{aligned} \tag{4.1}$$

where the kinetic rate constants in Eq. (4.1) still have to be determined. Equation (4.1) is just a generalization of Eq. (2.4).

There are two approaches which lead to the correct temperature dependence for the kinetic constants, which eventually lead to very similar results. The first approach used by Arimitsua *et al.*[22] was to apply perturbation theory.

The coupling term ϵ was used as the perturbation parameter for the kinetic constants. The result is mixing between the a and b oscillators through the relaxation. Explicit formulas for the kinetic constants of Eq. (4.1) are obtained which depend on ϵ. The temperature is introduced through the correlation function of the reservoir.

In this work a different approach which is an extension of the single oscillator approach is applied. For the single oscillator, the reservoir asymptotically has to bring the oscillator to thermal equilibrium. This imposes the detailed balance condition on the constants γ_1 and γ_2 so that only one free parameter is left which determines the rate at which equilibrium is reached. In the coupled oscillator case, the kinetic relaxation constants are determined through the requirement that each reservoir has to drive separately the coupled system to the correct equilibrium which includes the influence of the interaction. Moreover, when ϵ diminishes to zero the kinetic constants should approach the values obtained for a single oscillator coupled to the reservoir.

In equilibrium one imposes

$$\langle \tilde{A}^\dagger \tilde{A} \rangle = N^i_A, \quad \langle \tilde{B}^\dagger \tilde{B} \rangle = N^i_B,$$
$$\langle \tilde{A}^\dagger \tilde{B} \rangle = 0, \quad \langle \tilde{B}^\dagger \tilde{A} \rangle = 0, \tag{4.2}$$

where i is the index of the reservoir and N is the occupation number in thermal equilibrium it reads

$$N^i_A = \frac{1}{e^{\frac{(\omega_i + \epsilon)}{kT_i}} - 1}, \tag{4.3}$$
$$N^i_B = \frac{1}{e^{\frac{(\omega_i - \epsilon)}{kT_i}} - 1}.$$

Inserting the operators $\tilde{A}^\dagger \tilde{A}, \tilde{B}^\dagger \tilde{B}, \tilde{A}^\dagger \tilde{B}$, and $\tilde{B}^\dagger \tilde{A}$ to Eq. (4.1) the result is

$$\frac{k^i_1}{K^i_1} = N^i_A, \quad \frac{k^i_2}{K^i_2} = N^i_B \tag{4.4}$$

and

$$\frac{k^i_t}{K^i_t} = \frac{1}{2}(N^i_A + N^i_B),$$

where $K_j = k^*_j - k_j$ is the total relaxation rate. The difference between reservoirs A and B is in the sign of k_t. k_t is positive for the A reservoir and negative for the B reservoir. These conditions ensure the correct asymptotic behavior. For simplicity the scheme $k_3 = k_4 = k_t$ and $k^*_3 = k^*_4 = k^*_t$ was chosen.

V. OPERATING THE ENGINE

Operating the engine means connecting both reservoirs and the time dependent interaction to the system. Assuming the reservoirs are independent their combined relaxation is obtained through Eq. (4.1) by adding the kinetic constants of each reservoir. The combined constants are then defined as

$$k_j = k^a_j + k^b_j, \tag{5.1}$$
$$K_j = K^a_j + K^b_j.$$

Solving Eq. (2.5) the equations of motion of the observables are obtained.

Defining for convenience the operators $\tilde{X} = \tilde{A}^\dagger \tilde{B} + \tilde{B}^\dagger \tilde{A}$ and $\tilde{Y} = i(\tilde{A}^\dagger \tilde{B} - \tilde{B}^\dagger \tilde{A})$, the result is

$$\dot{\overline{\tilde{A}^\dagger \tilde{A}}} = -K_1 \tilde{A}^\dagger \tilde{A} - \tfrac{1}{2} K_t \tilde{X} + k_1,$$
$$\dot{\overline{\tilde{B}^\dagger \tilde{B}}} = -K_2 \tilde{A}^\dagger \tilde{A} - \tfrac{1}{2} K_t \tilde{X} + k_2,$$
$$\dot{\tilde{X}} = -\tfrac{1}{2}(K_1 + k_2)\tilde{X} - \tfrac{1}{2} K_t(\tilde{A}^\dagger \tilde{A} + \tilde{B}^\dagger \tilde{B}) - \epsilon \tilde{Y}, \tag{5.2}$$
$$\dot{\tilde{Y}} = -\tfrac{1}{2}(K_1 + K_2)\tilde{Y} + \epsilon \tilde{X}.$$

In this work, only steady state solutions are of interest, so that Eq. (5.2) becomes a set of coupled linear equations in the observables. Solving for the power [Eq. (3.4)] the result is

$$P = \frac{\epsilon^2 \nu \left[k_t - \frac{1}{2} K_t \left(\frac{k_1}{K_1} + \frac{k_2}{K_2} \right) \right]}{(K_1 + K_2) \left[\frac{1}{4}(K_1 + K_2) - \frac{1}{4} K_t^2 \left(\frac{1}{K_1} + \frac{1}{K_2} \right) + \frac{\epsilon^2}{K_1 + K_2} \right]}. \tag{5.3}$$

Examining Eq. (5.3), it can be seen that as $K_t \to 0$, the power output increases. When $K_t = 0$ the total relaxation rates K_a and K_b of each reservoir are matched. Under these conditions Eq. (5.3) simplifies to

$$P = \frac{K \epsilon^2 \nu G}{K^2 + \epsilon^2}, \tag{5.4}$$

where

$$G = \frac{1}{2}(N^a_A + N^a_B - N^b_a - N^b_B)$$

and $K = K_a = K_b$. Examining Eq. (5.4), it is easy to understand the reason for the maximum in power as a function of ϵ and K. When ϵ is small, the power increases as ϵ^2. When ϵ becomes large, ϵ^2 in the nominator and denominator cancel and the power decreases because the adjusted gain G decreases with ϵ as is seen in Fig. 1. As a function of the relaxation rate, the power exhibits similar behavior. For small K the power increases because the pumping rate increases. For large K the relaxation reduces the power to zero because of the loss of phase. Figure 2 displays these features.

If the pumping rate is optimized to obtain maximum power Eq. (5.4) becomes

$$P = |\epsilon| \nu G. \tag{5.5}$$

Figure 3 expresses the power in optimized pumping conditions. A maximum in power is obtained as a function of ϵ.

Calculating the efficiency of the engine for the conditions of Eq. (5.4) one obtains

$$\eta = \frac{\nu}{\omega_a + \frac{(K^2 + \epsilon^2) G_2}{|\epsilon| G}}, \tag{5.6}$$

where

$$G_2 = \frac{1}{2}[(N^a_A - N^a_B) - (N^b_A - N^b_B)].$$

When both $k \to 0$ and $\epsilon \to 0$, the efficiency becomes: $\eta = (\nu/\omega_a) = 1 - (\omega_b/\omega_a)$. This value approaches the Carnot efficiency for zero gain.[10,11] [In this case, $(\omega_a/\omega_b) = (T_a/T_b)$.] In these conditions the power is zero as expected. Increasing ϵ or K decreases the efficiency. This decrease comes from the second term in the denominator. This term enters

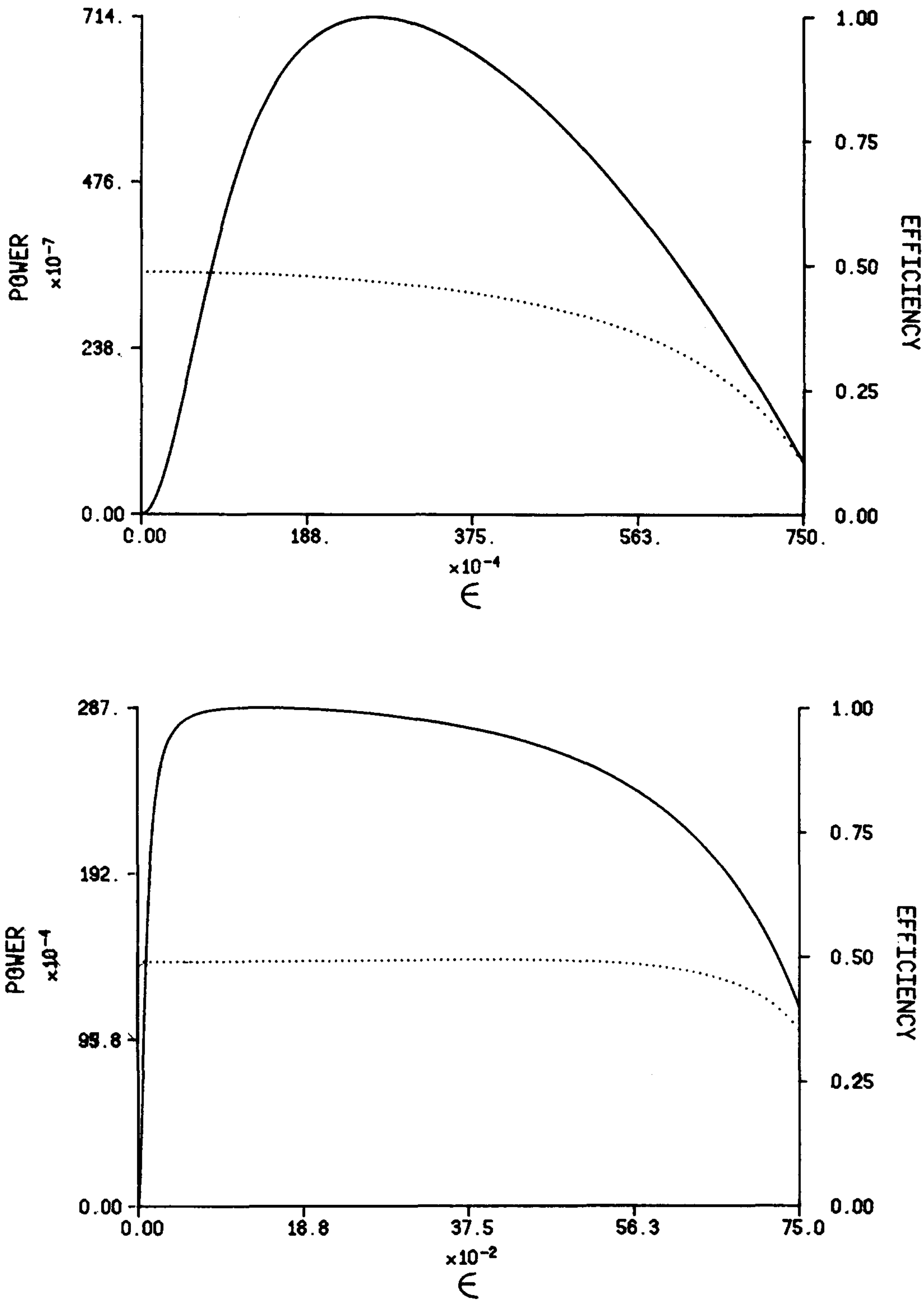

FIG. 1. (a) Power and efficiency as a function of ϵ. $\omega_a = 2.0$, $\omega_b = 1.0$, $kT_a = 2.01$, $kT_b = 1.0$, $K = 0.01$ ($\hbar = 1$). The solid line is the power and the dashed line is the efficiency. (b). Power and efficiency as a function of ϵ for high gain. $\omega_a = 2.0$, $\omega_b = 1.0$, $kT_a = 5.0$, $kT_b = 1.$, $K = 0.01$ ($\hbar = 1$).

through the dissipation of the interaction part of the Hamiltonian. The coupling splits the levels of the oscillators and as a consequence energy is stored in the engine. This stored energy is dissipated to the cold bath which is the loss mechanism responsible for the decline in efficiency. When ϵ becomes too large the stored energy dissipation exceeds the power output so that the engine absorbs power and dissipates it to the reservoirs.

VI. RELATION TO THE NEWTONIAN HEAT ENGINES

In the Newtonian heat engines the source of irreversibility is in the heat transfer law which is also responsible for the time dependence. In these models it is assumed that once the heat has been transferred to and from the engine it is converted to work by an ideal Carnot engine. If the temperature of the hot and cold reservoirs are T_a and T_b the ideal internal

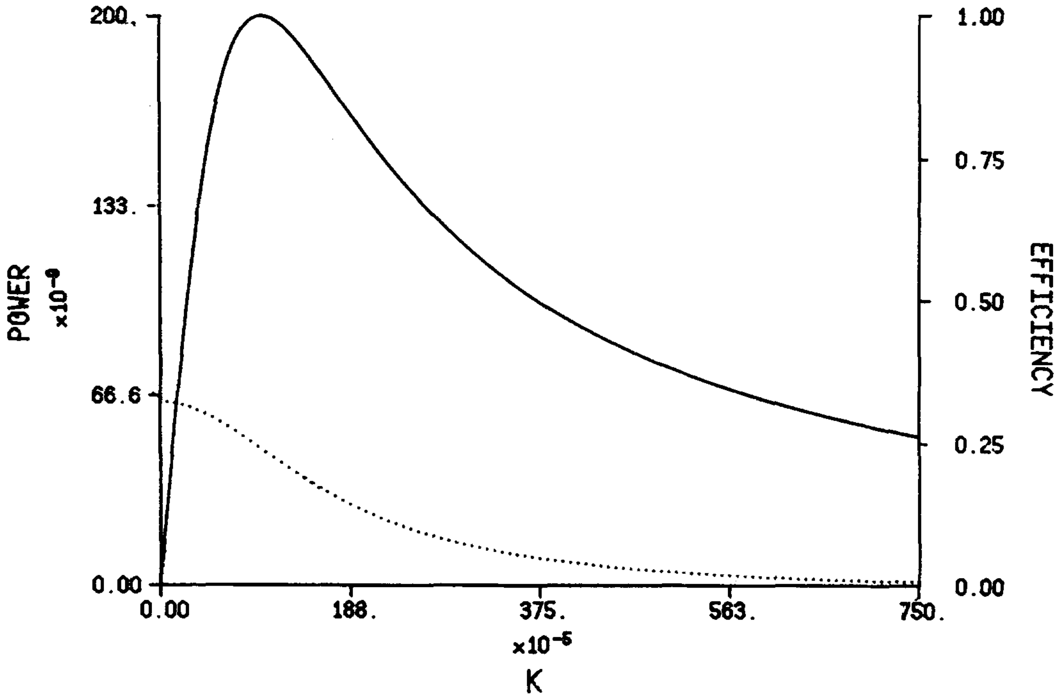

FIG. 2. Power and efficiency as a function of K. $\omega_\alpha = 1$, $\omega_b = 0.05$, $kT_a = 2.001$, $kT_b = 1$, $\epsilon = 0.001$ $(\hbar = 1)$.

engine operates between the temperatures T'_a and T'_b. The heat flows are defined by Newtons heat transfer law $\dot{Q}_\alpha = \kappa(T_a - T'_a)$ and $\dot{Q}_b = \kappa(T_b - T'_b)$. T'_a and T'_b are the control parameters of the engine. In order to find an analogous quantum engine the internal conversion of heat to work has to become reversible. This is achieved in the limit $\epsilon \to 0$. The control parameters of the quantum model are the frequencies ω_α and ω_b. The frequencies ω_α and ω_b play a similar role as the internal temperatures T'_a and T'_b. Examining Eq. (5.4) the gain G increases when the difference $\nu = \omega_\alpha - \omega_b$ decreases. Eventfully the power has to reach a maximum because it is proportional to ν (which also defines the time scale). Writing the gain in the limit of $\epsilon \to 0$ and the high temperature limit[23] (which corresponds to the classical limit) one obtains

$$G = \frac{kT_\alpha}{\omega_\alpha} - \frac{kT_b}{\omega_b}. \tag{6.1}$$

Maximizing Eq. (5.4) with respect to ω_α using Eq. (6.1) for the gain one obtains

$$\frac{\omega_\alpha}{\omega_b} = \sqrt{\frac{T_\alpha}{T_b}}. \tag{6.2}$$

Inserting Eq. (6.2) into Eq. (5.6) and taking the limit $\epsilon \to 0$ the

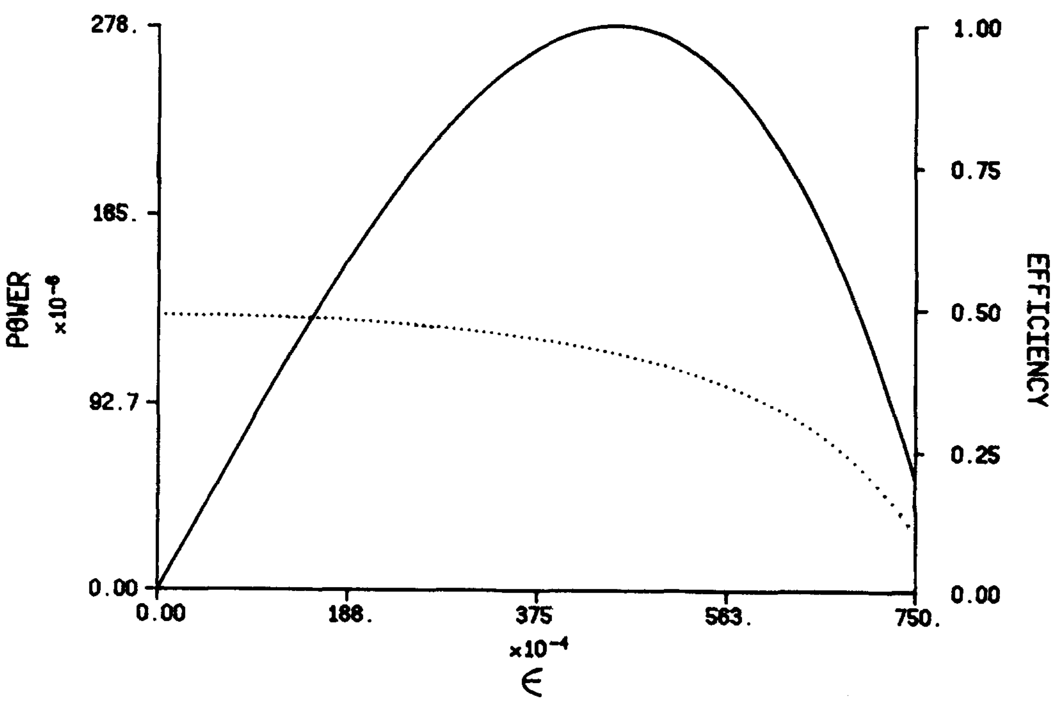

FIG. 3. Power and efficiency as a function of ϵ for optimal pumping conditions. $\omega_\alpha = 2.0$, $\omega_b = 1.0$, $kT_a = 2.01$, $kT_b = 1$.

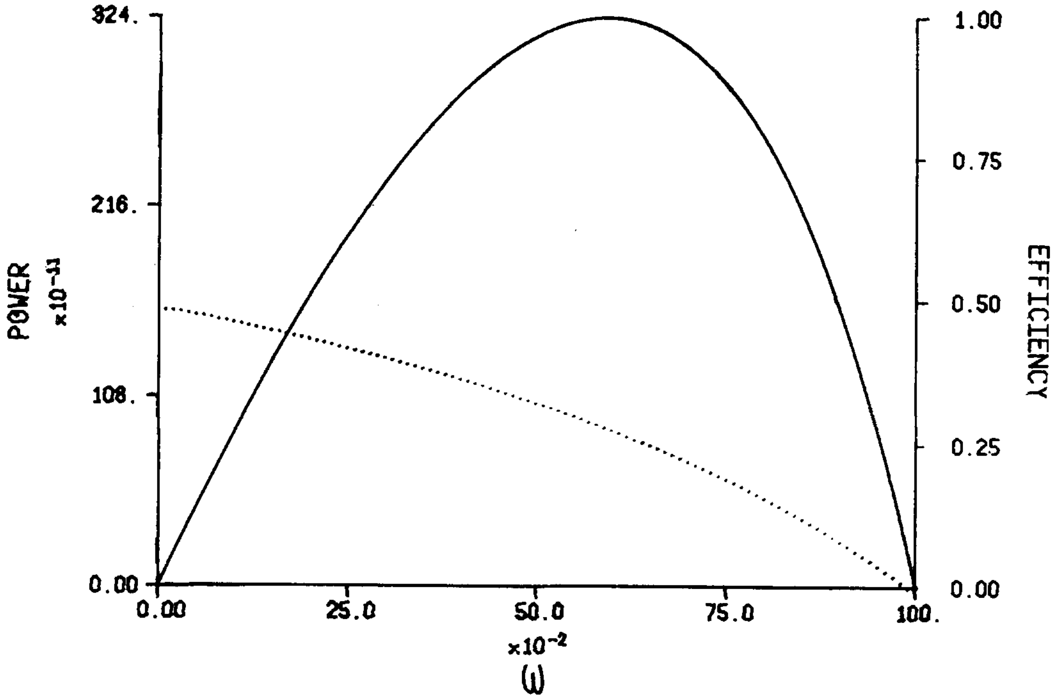

FIG. 4. Power and efficiency as a function of ω which is the deviation of ω_a from zero gain conditions. $\omega_b = 1$, $kT_a = 2$, $kT_b = 1$, $\epsilon = 0.0001$, and $K = 0.01$.

efficiency becomes

$$\eta = 1 - \sqrt{\frac{T_b}{T_a}}, \tag{6.3}$$

which is the value obtained for the Newtonian engine.[2] Figure 4 shows the power and efficiency as ω_α decreases from the zero gain value.

VII. CONCLUSIONS

The quantum mechanical heat engine displays qualitative behavior similar to the models analyzed in the work on finite time thermodynamics. The power reaches a maximum as a function of the control parameters, and the efficiency declines below the ideal reversible value. Nevertheless the quantum engine is more complicated and has unique features. In this model only the variations in the control parameters ϵ, K, ω_α, and ω_b have been studied. Additional control parameters as ν the driving frequency (which was constrained to resonance conditions), and individual relaxation constants can also be varied. Considering ϵ, K, ω_α, and ω_b, each has a unique influence on the operation of the engine. As has been shown in Sec. VI ω_a and ω_b are closely related to the internal temperatures of the Newtonian engine T'_α and T'_b. In the limit when $\epsilon \to 0$ the decline in efficiency is a consequence of the irreversibility in the heat transfer.

When the coupling to the external field is nonzero ($\epsilon \neq 0$) new sources of irreversibility appear, energy is stored in the engine. This can be seen by calculating the expectation value of the interaction energy Eq. (2.2) which increases with ϵ. This stored energy is dissipated directly to the reservoirs, with the result of short circuiting the engine. The maximum in power is a result of a balance between conflicting effects. On the one hand increasing the coupling extracts more power but simultaneously the levels of the engine are split. As a result the gain which respresents the population inversion is reduced. The influence of K is different. In the Newtonian engine an increase in κ the heat conductivity increases the power. In the quantum engine increasing the pumping rate supplies more power but this also increases the relaxation rate resulting in relaxation of the phase relation between the oscillators.[20] Without this phase relation no power can be extracted.

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