A quantum dynamical framework for Brownian heat engines

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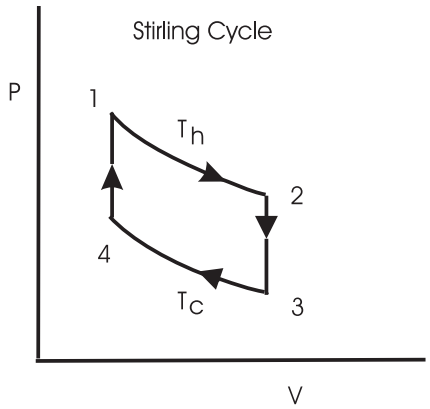
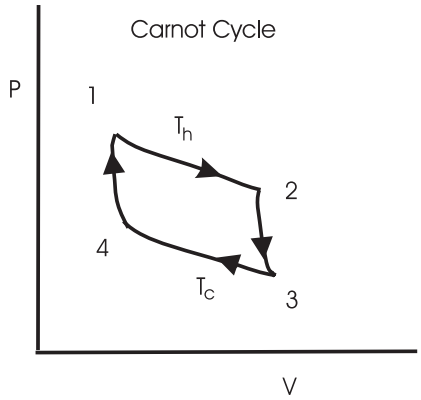
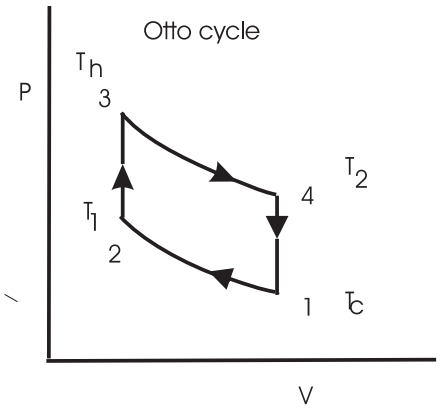
Some important heat engines

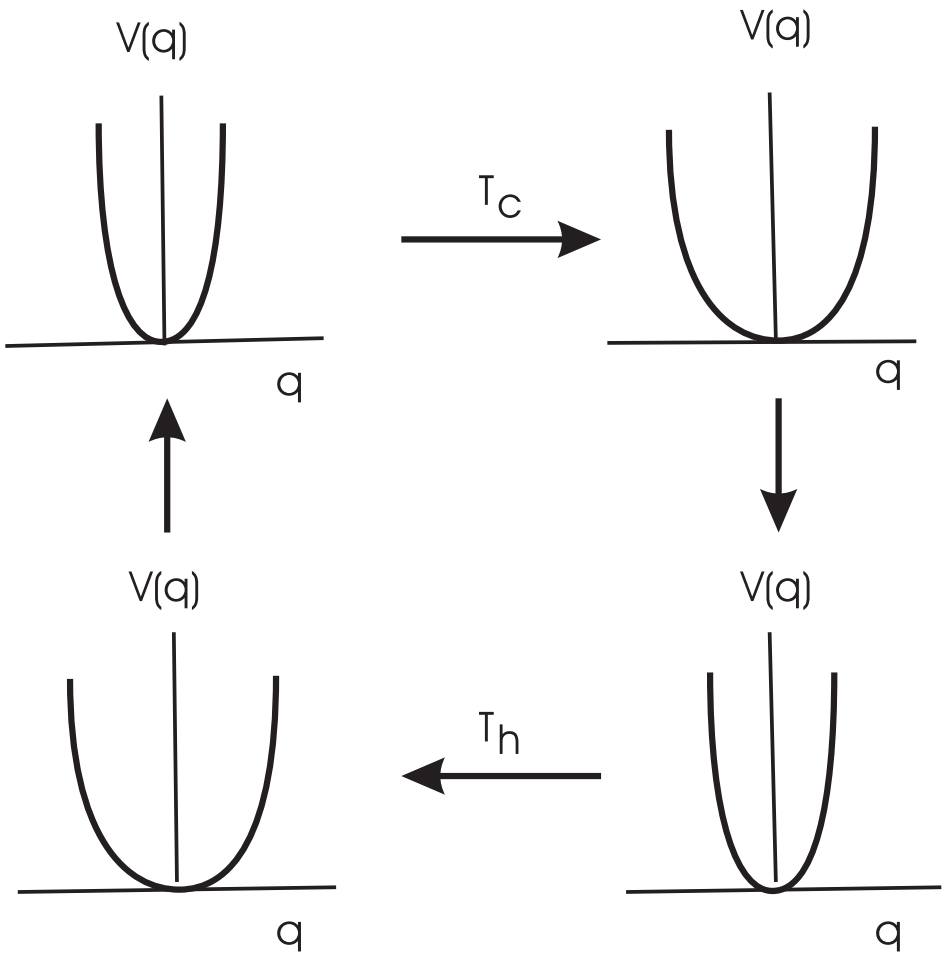




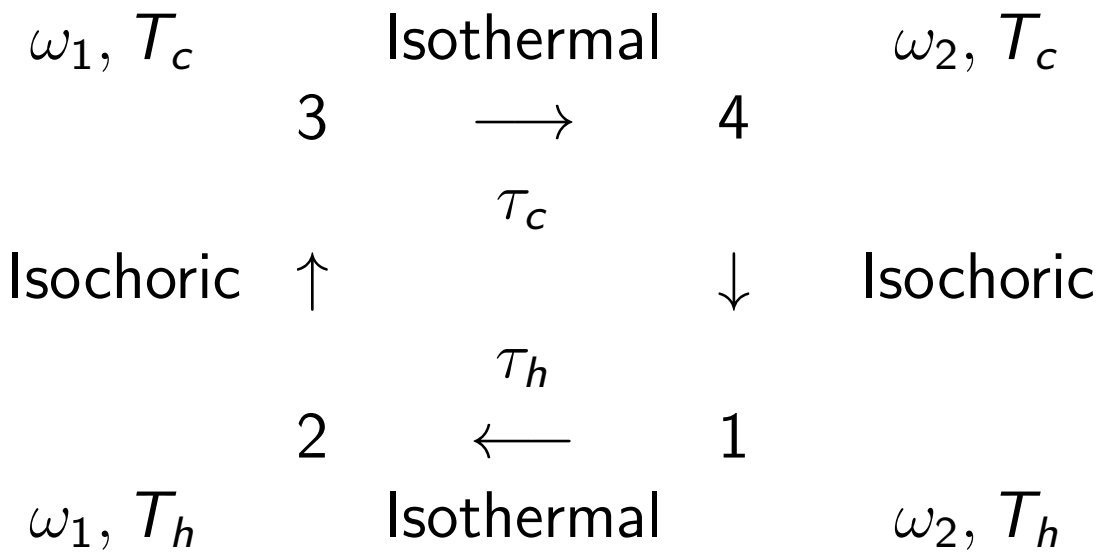


- Stirling engine: Originally conceived in 1816 by Robert Stirling, a scottish inventor, as a rival to the steam engine.
- Carnot engine: A theoretical thermodynamic cycle proposed by Nicolas Léonard Sadi Carnot in 1823.
- Otto engine : The earliest prototype four stroke engine developed by Nikolaus August Otto in Cologne, Germany in 1876.

Stirling cycle: Harmonic oscillator realization



A microscopic realization of the Stirling Engine



$$\omega_2 > \omega_1, \;\; T_h > T_c \qquad ,$$

Realized experimentally by Blickle and Bechinger [Nature Physics **8** 143-146 (2012)] through a single colloidal particle in an optical laser trap. The expression for the efficiency η_s^{cl} of the Stirling engine given in their work reads

$$\eta_s^{\mathrm{cl}} = \frac{\eta_c}{1 + \frac{1}{2}\eta_c / \ln(\frac{\omega_2}{\omega_1})}, \quad \eta_c = 1 - \frac{T_c}{T_h}.$$

To get this formula one is obliged to take the change in the internal energy in the isochoric step from T_h to T_c to be $K_B(T_h - T_c)/2$ rather than $K_B(T_h - T_c)$ as one would naively expect for a one dimensional harmonic oscillator. Why should that be so? A query with the authors revealed that this factor arises from the fact that one is dealing with an overdamped harmonic oscillator. This then raises two questions

- What happens when we are in the weak dissipation regime?
- What is the status of this formula in the regime where quantum effects are expected to be important?

Clearly there is a need for a quantum dynamical framework which permits proper inclusion of dissipative effects and is capable of accommodatiing variation of the ststem potential

Beyond standard thermodynamics

The desired framework is provided by the dynamics of a quantum Brownian oscillator of frequency ω in contact with a heat bath at temperature T is described by the master equation [G. S. Agarwal, Phys. Rev. A **4**, 739 (1971)]:

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

where $\hat{q}$ and $\hat{p}$ are denote the position and momentum operators obeying the commutation relations $[\hat{q}, \hat{p}] = i\hbar$. This master equation enjoys the property of evolving a Gaussian state into a Gaussian state.

For reasons that will become clear later, it proves expedient to transcribe the quantum dynamics described by the master equation into a Fokker-Planck equation using the Wigner phase space description of quantum systems

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

where

$$V(q,a) = \frac{1}{2}aq^2, \qquad a \equiv m\omega^2,$$

and

$$D = 2m\hbar\omega\kappa(n(\omega,T) + \frac{1}{2}), \quad n(\omega,T) = (e^{\beta\hbar\omega} - 1)^{-1}.$$

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:

$$\dot{q} = \frac{p}{m}, \tag{1}$$

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

$$< f(t) f(t') >= 2D\delta(t - t'). \tag{3}$$

The Langevin equations lend themselves to a nice thermodynamics intepretation [K. Sekimoto and Shin-ichi Sasa, J. Phys. Soc. Jpn, **66**, 3326 (1997)]: Multiplying the second by dq, after some algebraic manipulations, one obtains

$$-(-2\kappa p + f(t))dq + d(p^2/2m + V(q, a)) - \frac{\partial V(q, a)}{\partial a} da = 0.$$

The three terms may now be identified as :

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

leading to the energy balance equation:

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

with $\mathcal{Q}$ (-$\mathcal{Q}$) understood as the heat flow into of (out) the system and $\mathcal{W}$ (-$\mathcal{W}$) as the work done by (on) the system.

The stochastic averages of these quantities denoted 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.

Technical Details I

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

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

where

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

solves the homogeneous equations

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

For the variance matrix

$$\mathcal{V}(t) \equiv \begin{pmatrix} < q^2(t) > & < q(t)(p(t) > \\ < q(t)p(t) > & < p^2(t) > \end{pmatrix},$$

one has

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

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

Three exactly solvable models

Case I: ω independent of time

For this familiar case the functions $U(t)$ and $V(t)$ which determine the matrix $M(t)$ are explicitly given by

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

Further, owing to time translation available in this case, we have $M^{-1}(t) = M(-t)$, $M(t)M(t') = M(t+t')$, and (4) simplifies to

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

Case II : $\omega^2(t) = \omega_0^2\left(1 + \frac{\mu t}{T}\right),\ 0 \leq t \leq T$

In this case the functions $u(t)$ and $v(t)$ in the range $0 \leq t \leq T$ are given by

$$u(t) = \left[\frac{f_+(t)\dot{f}_-(0) - f_-(t)\dot{f}_+(0)}{f_+(0)\dot{f}_-(0) - f_-(0)\dot{f}_+(0)}\right],$$

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

$$f_\pm(t) = e^{-\kappa t}(t+a)^{1/2} J_{\pm 1/3}\left(\frac{2}{3}b^{1/2}(t+a)^{3/2}\right),$$

$$a = \left(1 - \frac{\kappa^2}{\omega_0^2}\right)\frac{T}{\mu},\ b = \frac{\omega_0^2\mu}{T}.$$

Case III : $\omega^2(t) = \omega_0^2 e^{\frac{\mu t}{T}},\ 0 \leq t \leq T$

In this case the functions $f_+(t)$ and $f_-(t)$ are again given in terms of Bessel functions as

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

Origin of the factor of 1/2 and its generalisation

A detailed analysis of the Langevin equations for the case when the diffusion the diffusion coefficient is changed linearly from D_0 appropriate to temperature T_0 to D_1 appropriate to temperature T_1 in a time τ and then kept at that value thereafter,

$$D(t) = \begin{array}{ll} D_0 + (D_1 - D_0)\dfrac{t}{\tau}, & 0 \leq \ t \ \leq \ \tau \\ \\ D_1, \quad & t > \tau. \end{array}$$

one is able to resolve the mystery behind the factor of 1/2. The general formulae for the classical and quantum efficiencies turn out to be given by

$$\eta_s^{\mathsf{cl}} = \frac{\eta_c}{1 + \eta_c \mu / \ln\left(\dfrac{\omega_2}{\omega_1}\right)} \ ,$$

and

$$\eta_s^{\mathrm{q}} = \frac{1 - Y/X}{1 + Z/X} \quad ,$$

$$X = \ln\left(\frac{\sinh(\beta_h \hbar\omega_2/2)}{\sinh(\beta_h \hbar\omega_1/2)}\right), \quad Y = \frac{\beta_h}{\beta_c} \ln\left(\frac{\sinh(\beta_c \hbar\omega_2/2)}{\sinh(\beta_c \hbar\omega_1/2)}\right) \quad ,$$

$$Z = \frac{\beta_h}{2}\left[\hbar\omega_1 \coth\left(\beta_h \hbar\omega_1/2\right) - \hbar\omega_2\{(1-\mu)\coth\left(\beta_h \hbar\omega_2/2\right) + \mu \coth\beta_c \hbar\omega_2/2\,)\}\right].$$

The appearance of the parameter μ appearing here (for which one has an exact expression) may be viewed as a phenomenological way of incorporating non equilibrium effects arising from decoupling of the system from one bath and recoupling it to another. Further, in the overdamped regime it does approach 1/2.

Technical Details II

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

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

where

$$X(t) = \begin{pmatrix} < q^2 > \\ < qp > \\ < p^2 > \end{pmatrix}, A(t) = \begin{pmatrix} 0 & \frac{2}{m} & 0 \\ -m\omega^2(t) & -2\kappa & \frac{1}{m} \\ 0 & -2m\omega^2 & -4\kappa \end{pmatrix},$$

$$Y(t) = \begin{pmatrix} 0 \\ 0 \\ 2D(t) \end{pmatrix}.$$

(At this stage, as indicated, we allow the frequency and the diffusion coefficients to be independent functions of t)

Putting $t = s\tau$ and expanding $X(t)$ as

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

we obtain

$$A(s)X^{(0)}(s) + Y(s) = 0 \Rightarrow X^{(0)}(s) = -A^{-1}(s)Y(s),$$
$$X^{(1)}(s) = A^{-1}(s)\frac{d}{ds}X^{(0)}(s).$$

The first of these equations can be taken to describe the situation where the system is in the steady state corresponding to the instantaneous values of ω and D and the second as describing deviations from this steady state.

Finite time corrections: Complementarity relations

Using this simple algebraic method applied to the moment equations that follow from the Langevin equations we are able to derive finite time corrections and hence the quantum analogues of the complementarity relations such as

$$Q_{\text{irr}} \times \tau \geq \frac{2\kappa K_B T}{\tau} \left[\frac{1}{\omega(1)} - \frac{1}{\omega(0)} \right]^2 ,$$

obtained by Sekimoto and Sasa in the classical case .

Efficiency of the Stirling engine at maximum power

In the spirit of the earlier works in the context the Carnot cycle by Schmiedl et al and Esposito et al. we find the efficiency for the Stirling engine at maximum power is given by

$$\eta_s^{\mathrm{cl}*} = \frac{\eta_c \left(1+\sqrt{\frac{T_c\Sigma_c}{T_h\Sigma_h}}\right)}{\left(1+\sqrt{\frac{T_c\Sigma_c}{T_h\Sigma_h}}\right)^2 + \frac{T_c}{T_h}\left(1-\frac{\Sigma_c}{\Sigma_h}\right) + \frac{2\mu\eta_c}{\log\left(\frac{\omega_2}{\omega_1}\right)}}.$$

We now consider two cases:

Case A $\mu = 0$

In the extreme weak dissipation regime i.e. $\mu = 0$, one recovers results similar to those in the context of the Carnot cycle :

1. In the symmetric case i.e $\Sigma_c/\Sigma_h = 1$, $\eta_s^{\mathrm{cl}*}$ equals the Curzon-Ahlborn efficiency $\eta_{CA} = 1 - \sqrt{T_c/T_h}$:

$$\frac{\Sigma_c}{\Sigma_h} = 1 : \qquad \eta_s^{\mathrm{cl}*} = \eta_{CA}.$$

2. $\eta_s^{\mathrm{cl}*}$ is bounded by $\eta_c/2$ and $\eta_c/(2-\eta_c)$

$$\eta_c/2 \leq \eta_s^{\mathrm{cl}*} \leq \eta_c/(2-\eta_c).$$

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

Case B $\mu \neq 0$

For small but non zero $\mu < \frac{1}{2}\log(\omega_2/\omega_1)$ these results get modified to those given below

1. In the symmetric case i.e $\Sigma_c/\Sigma_h = 1$, η_s^{cl*} is less than the Curzon-Ahlborn efficiency $\eta_{CA} = 1 - \sqrt{T_c/T_h}$:

$$\frac{\Sigma_c}{\Sigma_h} = 1: \qquad \eta_s^{cl*} = \frac{\eta_{CA}}{1 + \left(\frac{\mu}{\log(\omega_2/\omega_1)}\right)\left(\frac{2\eta_{CA}}{2-\eta_{CA}}\right)} < \eta_{CA}.$$

2. η_s^{cl*} is bounded by $\eta_c/2$ and $\eta_s/(2-\eta_s)$

$$\eta_c/2 \leq \eta_s^{cl*} \leq \eta_s/(2-\eta_s).$$

As before, the upper and the lower bounds respectively correspond to $\Sigma_c/\Sigma_h \to 0$ and $\Sigma_c/\Sigma_h \to \infty$

On the other hand if $\mu > \frac{1}{2}\log(\omega_2/\omega_1)$, one finds that

$$\eta_s^{\mathrm{cl}*} \leq \eta_c/2.$$

In the figures below we display the bounds on $\eta_s^{\mathrm{cl}*}$ for $\mu = 0.001, 0.1, 0.2, 0.4$ with ω_2/ω_1 taken to be 2.05 where we also give the plots for η_c, η_{CA} and $\eta_c/2$ for comparison.

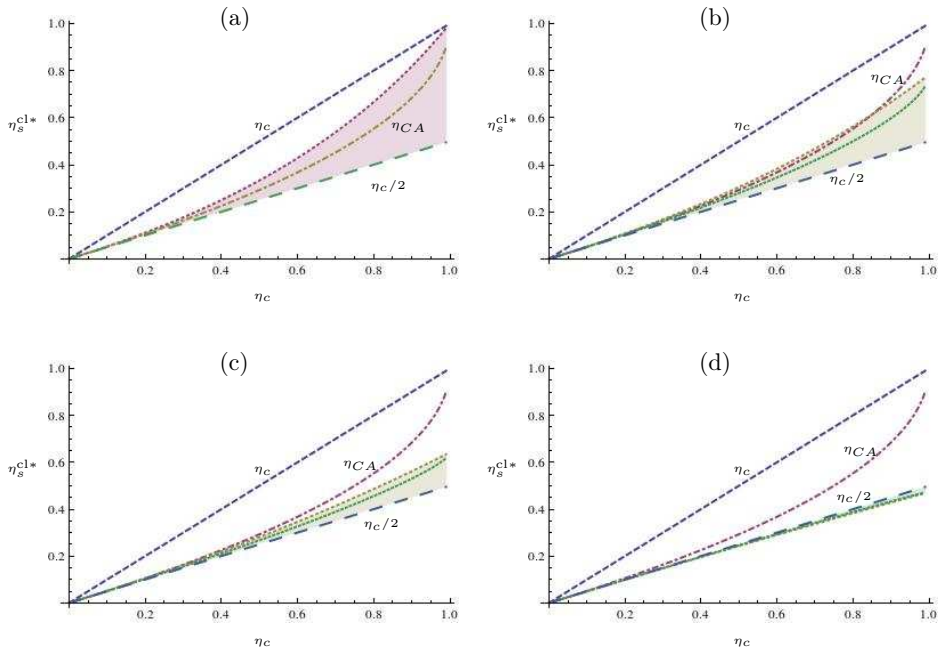


Fig.2 Efficiency η_s^{cl*} of the Stirling engine at maximum power as a function of the Carnot efficiency η_c. The graph η_s^{cl*} versus η_c, for all values of Σ_c/Σ_h, lies in the shaded regions given here for $\omega_2/\omega_1 = 2.05$ and (a) $\mu = 0.001$ (b) $\mu = 0.1$ (c) $\mu = 0.40$ and (d) $\mu = 0.4$. The graphs of η_c, η_{CA} and $\eta_c/2$ versus η_c are displayed for comparison. While in (a)–(c), $\mu < \frac{1}{2}\log(\omega_2/\omega_1)$, (d) corresponds to the case when $\mu > \frac{1}{2}\log(\omega_2/\omega_1)$.

References

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