

Single Particle Stochastic Heat Engine Confined in a Anharmonic Mexican Hat Potential

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Abstract—We combine the linear irreversible thermodynamics with stochastic energetics and study the stochastic heat engine for a Brownian particle confined in a anharmonic Mexican hat potential. Under the tight-coupling condition i.e., without heat leakage between the system and the reservoirs, we calculate the time at which the power is maximum and the corresponding efficiency.

1. INTRODUCTION

Carnot engine laid the foundation of thermodynamics, which convert heat into work. The efficiency of the Carnot heat engine, $\eta_c = 1 - T_c/T_h$ [1, 2], where T_h and T_c ($T_h > T_c$), are the temperature of the hot and cold reservoirs, respectively. It is the maximum efficiency attainable by the heat engines. Because of zero power output, Carnot engine has no practical use since all real engines have to operate with finite power output.

The efficiency at maximum power output usually have practical applications. Using an approximate analyzes, Curzon-Alhborn (CA) shown that the efficiency at maximum power of a finite-time Carnot heat engine as [3]

$$\eta_{CA} = 1 - \sqrt{T_c/T_h}. \quad (1)$$

Latter, Van den Broeck [4] studied the generic steady-state heat engine at maximum power output by using the linear irreversible thermodynamics (LIT) [5]. For a small temperature difference between the reservoirs, he obtained exactly η_{CA} for the tight-coupling condition [6], which has no heat leakage between the system and the reservoirs. Many models of heat engines and refrigerators were studied within the LIT [7-13] and also with the finite size reservoir(s) [14-17].

Recent experimental techniques allow us to investigate the small systems [18-21], which shows an eminent statistical fluctuation. If we are studying the system consists of a few molecules and the total energy of the system is in the order of $k_B T$, then the thermal fluctuation can lead to an observable large deviation from their average values [22].

Using the Langevin equation, Sekimoto developed the stochastic energetics [23] to study the stochastic heat engines [24, 25]. Microscopic analog of the Carnot heat engine were also studied at maximum power output in the overdamped [26] and underdamped cases [27]. Rana *et al.* also studied numerically the underdamped and overdamped cases [28]. Stochastic energetics also developed from the Kramers equation for the underdamped case [27, 29].

Many theoretical and experimental studies of stochastic heat engines are limited to the time-dependent harmonic oscillator [20-22, 24, 26-29] and the time-dependent log-harmonic potential [30, 31]. The power and the efficiency of stochastic engine also analyzed for the few anharmonic cases numerically and shown that the average power output and the average efficiency is decreasing while increasing the anharmonicity [28]. Their numerical results also showed that the efficiency at maximum power is model dependent and decreases as the potential becomes harder. In this work, we analytically investigate the effect of the time-dependent anharmonic Mexican hat potential on the efficiency at maximum power of the stochastic heat engines in the generalized framework.

This paper is organized as follows, In Section 2 and 3, we briefly review the framework of the linear irreversible thermodynamics [4] and stochastic energetics [27]. In Section 4, we investigate our model system and finally conclude the results.

2. LINEAR IRREVERSIBLE THERMODYNAMICS

If we consider the situation, where the system performs the work on the environment, $W = -Fx$, where F is the constant external force and x is the thermodynamic variable conjugate of F . Then the power output becomes $P = -F\dot{x}$. Where the dot denotes the time derivative of the quantity. We can write the thermodynamic force $X_w \equiv F/T$ and the flux $J_w \equiv \dot{x}$ for the power output as, $P = -T_c J_w X_w$ [4]. The heat flux $J_h \equiv \dot{Q}_h$, is absorbed by the system from the hot reservoir at temperature T_h and ejects the heat flux \dot{Q}_c to the cold reservoir

at temperature T_c corresponding thermodynamic force $X_h \equiv 1/T_c - 1/T_h$ [4]. In the linear response regime the fluxes can be written in terms of the thermodynamic forces as [4, 34]

$$J_w = L_{ww}X_w + L_{wh}X_h, \quad (2)$$

$$J_h = L_{hw}X_w + L_{hh}X_h, \quad (3)$$

where $L_{ij}(i, j = w, h)$ are the Onsager coefficients. The entropy production rate of the reservoirs,

$$\dot{\sigma} = \left(\frac{1}{T_c} - \frac{1}{T_h}\right) \dot{Q}_h - \frac{\dot{W}}{T_c}. \quad (4)$$

The positivity of the entropy production rate $\dot{\sigma} = J_w X_w + J_h X_h \geq 0$ impose the constraint on the Onsager coefficients,

$$L_{ww} \geq 0; L_{hh} \geq 0; L_{ww}L_{hh} - L_{wh}L_{hw} \geq 0, \quad (5)$$

with the Onsager reciprocity relation

$$L_{wh} = L_{hw}, \quad (6)$$

From Eq. (3) we can rewrite the work flux and the corresponding force as

$$J_w = \frac{L_{ww}}{L_{hw}} J_h - L_{wh} \left(\frac{1-q^2}{q^2}\right) X_h, \quad (7)$$

$$X_w = \frac{J_h - L_{hh} X_h}{L_{hw}}, \quad (8)$$

where $q^2 \equiv L_{wh}^2 / L_{ww}L_{hh}$. The efficiency is given by

$$\eta = \frac{-T_c X_w J_w}{J_h}. \quad (9)$$

From Eqs. (7) and (8), the power and the efficiency can be written as

$$P = T_c \left[\left(\frac{2-q^2}{q^2}\right) J_h X_h - L_{hh} \left(\frac{1-q^2}{q^2}\right) X_h^2 - \frac{J_h^2}{L_{hh} q^2} \right], \quad (10)$$

$$\eta = T_c \left[\left(\frac{2-q^2}{q^2}\right) X_h - L_{hh} \left(\frac{1-q^2}{q^2}\right) \frac{X_h^2}{J_h} - \frac{J_h}{L_{hh} q^2} \right]. \quad (11)$$

3. STOCHASTIC ENERGETICS

A particle immersed in a liquid and confined in one dimensional time-dependent potential $U(x, \lambda(t))$, which is a function of both x and the time-dependent external control parameter $\lambda(t)$. The dynamics of a Brownian particle can be studied by using the Langevin equation [33],

$$\dot{x} = p; \dot{p} = -\gamma p - \frac{\partial U(x, \lambda(t))}{\partial x} + \xi(t), \quad (12)$$

where m is the mass of a Brownian particle which we set to be 1, γ is the frictional coefficient of the medium, x and p are the dynamical variable of the system, respectively, the position

and its conjugate momentum. $\xi(t)$ is random force which is assumed to be a Gaussian white noise obeying the relations,

$$\langle \xi(t) \rangle = 0; \langle \xi(t) \xi(t') \rangle = C \delta(t - t'), \quad (13)$$

where $C = 2\gamma k_B T$, k_B is the Boltzmann constant and T is the temperature of the reservoir. The symbol $\langle \dots \rangle$, denotes the average over the ensembles. The Hamiltonian of the system is given by

$$H = \frac{p^2}{2} + U(x, \lambda(t)). \quad (14)$$

The differential of the above Hamiltonian is

$$dH = (\dot{p}p + \dot{x} \frac{\partial U(x, \lambda(t))}{\partial x}) dt + \left(\dot{\lambda} \frac{\partial U}{\partial \lambda}\right) dt, \quad (15)$$

and the energy difference of the system between the final Hamiltonian $H(t_f)$ to the initial Hamiltonian $H(t_i)$ is

$$\Delta e \equiv H(t_f) - H(t_i). \quad (16)$$

The work done by the system is defined as [24, 25]

$$w \equiv \int_{t_i}^{t_f} dt \dot{\lambda} \frac{\partial U}{\partial \lambda}, \quad (17)$$

and the heat absorbed by the system is

$$q \equiv \int_{t_i}^{t_f} dt (\dot{p}p + \dot{x} \frac{\partial U}{\partial x}). \quad (18)$$

From the law of energy balance [24]

$$\Delta e = w + q. \quad (19)$$

The probability distribution function $\rho(x, p, t)$ of a Brownian particle evolves according to the Kramers equation [33]

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}, \quad (20)$$

$$\mathbf{J} = p\rho \hat{x} - \rho \left(\gamma p + \frac{\partial U}{\partial x} + \frac{\gamma T}{\rho} \frac{\partial \rho}{\partial p} \right) \hat{p}, \quad (21)$$

where $\nabla \equiv \frac{\partial}{\partial x} \hat{x} + \frac{\partial}{\partial p} \hat{p}$. The average energy difference is given as [34],

$$\Delta E = \int dx \int dp (H\rho) \Big|_{t_i}^{t_f}. \quad (22)$$

The average work done by the system is

$$W = \int_{t_i}^{t_f} dt \int dx \int dp \rho \dot{\lambda} \frac{\partial U}{\partial \lambda}, \quad (23)$$

and the average heat absorbed from the medium is given by [27],

$$Q = - \int_{t_i}^{t_f} dt \int dx \int dp \gamma p \left(p + \frac{T}{\rho} \frac{\partial \rho}{\partial p} \right) \rho. \quad (24)$$

4. THE EFFICIENCY AT MAXIMUM POWER OUTPUT

We consider a Brownian particle confined in the time-dependent anharmonic Mexican hat potential and its Hamiltonian is given by

$$H = \frac{p^2}{2} + U(x, \lambda(t), k(t)), \quad (25)$$

with

$$U(x, t) = -\lambda(t)x^2/2 + k(t)x^4/4, \quad (26)$$

where $\lambda(t)$ and $k(t)$ are the external time- dependent control parameters. We assume the initial probability distribution of the system is Gaussian with mean zero, variance $\alpha(t) \equiv \langle x^2 \rangle$ and $\beta(t) \equiv \langle p(t)^2 \rangle$ which is given by

$$\rho(x, p) = \frac{1}{\sqrt{4\pi^2\alpha\beta}} \exp\left(-\frac{x^2}{2\alpha} - \frac{p^2}{2\beta}\right). \quad (27)$$

This probability evolves according to the Kramers equation (20). Multiplying Eq. (20) by x^2 , p^2 , and xp then integrating we get, respectively, the following equations

$$\dot{\alpha} = 0, \quad (28)$$

$$\dot{\beta} = -2\gamma\beta + 2\gamma T, \quad (29)$$

$$\beta = -\lambda\alpha + 3k\alpha^2, \quad (30)$$

Eq. (28) shows that the width of the position is independent of time and the value of the external control parameter. The momentum distribution depends on the external control parameters through Eq. (30). If $\lambda(t)$ or $k(t)$ is increases the width of momentum distribution is increase and vice versa. The increase (decrease) of the width of momentum distribution mimics the increase (decrease) of volume in the macroscopic engines.

Using the above Eq. (29), the time evolution of the variance of momentum $\beta(t)$ with the initial momentum independent of $\beta(0)$ (see appendix

$$\beta(t) = T + (\beta_0 - T)e^{-2\gamma t}. \quad (31)$$

Using Eq. (24) the rate of heat flow from the hot reservoir to the system is obtained as (see appendix B)

$$J_h = \gamma(T_h - \beta). \quad (32)$$

Substituting Eqn. (31) in Eq. (32) we get the heat flux as

$$J_h = \gamma(T_h - \beta_0)e^{-2\gamma t}. \quad (33)$$

The system work as a heat engine for $\beta_0 < T_h$ and work as a refrigerator for $\beta_0 > T_h$. Under the condition $q^2 = 1$, so called the tight-coupling condition, the heat leakage term vanishes [10, 14] and hence the power and efficiency becomes

$$P = \eta_C J_h - \frac{T_c}{L_{hh}} J_h^2, \quad (34)$$

$$\eta = \eta_C - \frac{T_c}{L_{hh}} J_h. \quad (35)$$

It has to be noted from the above equation that for the finite heat flux J_h , the efficiency of a heat engine is always less than the Carnot efficiency. Substituting Eq. (33) in Eqs. (34) and (35), we get the power output and the efficiency as

$$P = \eta_C \gamma (T_h - \beta_0) e^{-2\gamma t} - \frac{\gamma^2 T_c}{L_{hh}} (T_h - \beta_0)^2 e^{-4\gamma t}, \quad (36)$$

$$\eta = \eta_C - \frac{\gamma T_c}{L_{hh}} (T_h - \beta_0) e^{-2\gamma t}. \quad (37)$$

When $t \rightarrow \infty$, $P \rightarrow 0$ and the efficiency $\eta \rightarrow \eta_C$. Optimizing the power output with respect to time, we get the optimal time as (see appendix C)

$$t^* = \frac{1}{2\gamma} \ln \frac{\eta_C L_{hh}}{2\gamma T_c (T_h - \beta_0)}. \quad (38)$$

Substituting Eq. (38) in Eq. (37), we get the efficiency at maximum power as

$$\eta^* = \frac{\eta_C}{2}. \quad (39)$$

This result has been obtained for the Brownian particle confined in a anharmonic Mexican hat potential. Rana *et al.* numerically shown that, when an anharmonicity is increased the efficiency at maximum power is decreases [28]. When we incorporating the linear irreversible thermodynamics, our analytical result showed that the efficiency at maximum power of a single particle stochastic heat engine does not dependence on the potential.

5. CONCLUSION

We have obtained the efficiency at maximum power of a single particle Brownian heat engine confined in a anharmonic Mexican hat potential. We used the framework of the linear irreversible thermodynamics combined with stochastic energetics and showed that for the tight-coupling condition, the efficiency at maximum power is independent of $\beta(0)$ (see appendix B) and it is always equal to half of the Carnot efficiency.

APPENDIX A

Consider the Eqn. (29)

$$\dot{\beta} + 2\gamma\beta = 2\gamma T,$$

solving the above equation using integrating factor, we get

$$e^{\int_0^t 2\gamma d\tau} = e^{2\gamma t}$$

$$\beta e^{2\gamma t} = 2\gamma T \int_0^t e^{2\gamma \tau} d\tau + c$$

$$\beta = T(1 - e^{-2\gamma t}) + c e^{-2\gamma t}$$

At time $t = 0$, $\beta(0) = \beta_0$, which gives $c = \beta_0$. Therefore

$$\beta = T(1 - e^{-2\gamma t}) + \beta_0 e^{-2\gamma t}.$$

By rewriting the above equation, we get

$$\beta = T + (\beta_0 - T)e^{-2\gamma t}.$$

Appendix B

Starting from Eqns. (24) and (27),

$$\begin{aligned} \dot{Q}_h &= -\gamma \int dx \int dp p \left(p + \frac{T_h}{\rho} \frac{\partial \rho}{\partial p} \right) \rho, \\ &= \frac{-\gamma}{\sqrt{4\pi^2\alpha\beta}} \int dx \int dp \exp\left(\frac{-x^2}{2\alpha} - \frac{p^2}{2\beta}\right) \left(p^2 - \frac{T_h p^2}{\beta}\right), \\ &\int dz z^{2n} \exp(-az^2) = \frac{\Gamma(n + \frac{1}{2})}{a^{n+\frac{1}{2}}}. \end{aligned}$$

Using the above Gamma integration first integrating with respect to p , we get

$$\dot{Q}_h = -\frac{\gamma}{\sqrt{2\pi\alpha}} \int dx (\beta - T_h) \exp\left(-\frac{x^2}{2\alpha}\right)$$

again integrating with respect to x , we get

$$\dot{Q}_h = \gamma(T_h - \beta).$$

APPENDIX C

Let $x = e^{-2\gamma t}$ in Eqn. (36), the power becomes

$$P = \eta_C \gamma (T_h - \beta_0) x - \frac{\gamma^2 T_c}{L_{hh}} (T_h - \beta_0)^2 x^2,$$

maximizing with respect to x , we get

$$x = \frac{\eta_C L_{hh}}{2\gamma T_c (T_h - \beta_0)}$$

from above equation we get the optimized time

$$t^* = \frac{1}{2\gamma} \ln \frac{\eta_C L_{hh}}{2\gamma T_c (T_h - \beta_0)},$$

substituting above t^* in equation (37), we get

$$\eta^* = \frac{\eta_C}{2}.$$

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