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Efficiency bounds of molecular motors under a trade-off figure of merit

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HIGHLIGHTS

- The optimization of molecular motors under a trade-off figure of merit criterion is studied.
- The efficiencies of molecular motors at two different optimization configurations are calculated.
- The upper and lower bounds for the efficiency of molecular motors are determined.
- The optimal efficiencies at the two different optimization configurations are always larger than 1/2.

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ABSTRACT

On the basis of the theory of irreversible thermodynamics and an elementary model of the molecular motors converting chemical energy by ATP hydrolysis to mechanical work exerted against an external force, the efficiencies of the molecular motors at two different optimization configurations for trade-off figure of merit representing a best compromise between the useful energy and the lost energy are calculated. The upper and lower bounds for the efficiency at two different optimization configurations are determined. It is found that the optimal efficiencies at the two different optimization configurations are always larger than 1/2.

1. Introduction

Molecular motors are a class of biological molecular machines that convert biochemical energy generated typically from ATP hydrolysis to perform directed motion and mechanical work in living organisms [1–4]; these machines work in a thermal environment at a constant temperature. The energy conversion efficiency of molecular motors is a central figure of merit in the biological world and has been studied from a thermodynamic point of view [5–9]. According to the first law of thermodynamics, the maximum efficiency of such molecular motors is equal to 1 [10]. However, the maximum efficiency can only be reached in an equilibrium situation corresponding to a vanishing power [11]. This is not the case for real living organisms. It is intuitive that the organisms follow the economic principles between the power and the efficiency [12–15]. The ability of motor proteins to convert chemical energy into mechanical work is a particularly striking example of molecular motors that is ubiquitous and highly optimized in nature [1]. Therefore, the high efficiency of molecular motors is one of their most intriguing attributes from an ecological viewpoint. The study of two-state molecular motor model indicated that the high efficiency of molecular motors can be achieved only when the chemical and mechanical cycles of the motors are suitably designed [10]. Thus, the thermodynamic optimization of molecular motors has attracted considerable attention in recent years [16–19].

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On the basis of biodiversity, it is a possible explanation from the viewpoint of thermodynamic optimization that the organisms in different survival environments can follow a variety of optimization criteria. In a number of recent papers, the efficiency at the maximum power of molecular motors was investigated as one of the possible thermodynamic optimizations [20–26]. However, this optimization focuses only on the maximum power, while the corresponding efficiency may be larger or smaller than 1/2 [20]. Thus, it is a natural question to determine at what conditions an optimal efficiency larger than 1/2 at a certain power can be achieved. This implies that the useful energy that is absorbed by an organism is greater than the lost energy that is discharged by the organism. To answer this question, we focus on the analysis of the optimization of molecular motors under the trade-off figure of merit criterion, which represents the best compromise between the useful energy and the lost energy. It is easy for any energy converter to implement both isothermal and nonisothermal processes [27,28]. An important feature of the trade-off figure of merit criterion is that it gives an optimal efficiency that lies between the maximum efficiency and the efficiency at the maximum power [27,28]. Recently, it was further proved that the trade-off figure of merit criterion is equivalent to the ecological optimization criterion [29].

Therefore, in the present study, we introduce a trade-off figure of merit as another possible optimization criterion to study the optimization performance of molecular motors. We first study the optimization efficiency of two different configurations in the linear response region. We then extend our analysis to the nonlinear regime, derive the universal expression of the optimization efficiency, and determine the upper and lower bounds of the efficiency at the two different optimization configurations.

2. Molecular motors in the linear response region

We consider an elementary model of molecular motors [4,20,26] as shown in Fig. 1(a). The transition between the next-neighbor discrete states M_n ($n = 0, \pm1, \pm2, \ldots$) with a periodic structure and a repeat unit of length L is driven by hydrolyzing ATP into the products ADP and inorganic phosphate P, i.e.,

$$\mathrm{ATP} + M_n \underset{k^-}{\overset{k^+}{\rightleftharpoons}} M_{n+1} + \mathrm{ADP} + \mathrm{P}, \tag{1}$$

where k^+ and k^- are the forward and backward reaction rates, respectively. The molecular motor was brought out of the equilibrium by the chemical gradient, which was derived from the difference between the chemical potential μ_{ATP} of ATP molecules and the chemical potentials μ_{ADP} and μ_P of ADP and P molecules, respectively, i.e., $\Delta\mu = \mu_{ATP} - \mu_{ADP} - \mu_P$. To perform useful mechanical work, the molecular motor should move against an opposing but weaker external loading force F_{ext} in each step. The action of these forces leads to motion and fuel consumption, characterized by the average reaction velocity J_1 from fuel or reactant state ATP to product state ADP+P and the average reaction velocity J_2 from ADP+P to ATP. This nonequilibrium steady-state process is characterized by a steady entropy production rate as

$$\dot{S} = J_1 \frac{F_{ext}}{T} + J_2 \frac{\Delta\mu}{T}, \tag{2}$$

where T is the temperature. For an energy converter, the entropy production rate consists of two parts. We can define that the first term on the right-hand side of Eq. (2) is the loading process with negative entropy production. Thus, the power in each step can be defined as

$$P = -J_1 F_{ext}. \tag{3}$$

The second term on the right-hand side of Eq. (2) corresponds to the driving process with positive entropy production, and the chemical energy consumption is $J_2\Delta\mu$. The efficiency defined as the ratio of the power to the chemical energy consumption can be expressed as

$$\eta = -\frac{J_1 F_{ext}}{J_2 \Delta\mu}. \tag{4}$$

The efficiency of such a system may obviously reach the maximum efficiency, i.e., $\eta_{\max} = 1$, for a reversible process with zero entropy production. Within the framework of linear irreversible thermodynamics, the linear relationship between the average reaction velocities (J_1, J_2) and forces $(F_{ext}, \Delta\mu)$ can be expressed as [5,30,31]

$$\begin{aligned} J_1 &= L_{11} F_{ext} + L_{12}\Delta\mu \\ J_2 &= L_{21} F_{ext} + L_{22}\Delta\mu. \end{aligned} \tag{5}$$

The second law of thermodynamics requires that the entropy production rate (2) is non-negative. This implies for the Onsager coefficients L_{ij} that $L_{11} \geq 0$, $L_{22} \geq 0$, and $4L_{11}L_{22} - (L_{12} + L_{21})^2 \geq 0$. Furthermore, the Onsager symmetry resulting from the time reversibility of the microscopic dynamics stipulates $L_{12} = L_{21}$.

The trade-off figure of merit (Ω criterion) representing a compromise between energy benefits and losses for a specific job was first proposed as a unified optimization criterion for energy converters by Hernández et al. [27]. This criterion is easy to implement for any energy converter (isothermal or nonisothermal), without the requirement of the explicit evaluation