The Efficiency of Molecular Motors

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Abstract Molecular motors convert chemical energy into mechanical work while operating in an environment dominated by Brownian motion. The aim of this paper is to explore the flow of energy between the molecular motors and its surroundings, in particular, its efficiency. Based on the Fokker-Planck equation with either N or infinite chemical states, we find that the energy efficiency of molecular motors, whether the Stokes efficiency or the usual thermodynamic efficiency, is strictly less than one, because of the dissipation of the energy in both the overdamped surroundings and in the process of the chemical reaction.

Keywords Molecular motors · Fokker-Planck equation · Energy efficiency

1 Introduction

Molecular motors are biogenic force generators acting in the nanometer range [10]. Linear motors produce sliding movements along filamentous structures called protein tracks; for example, myosin slides along an actin filament [6, 9, 25], kinesin [4, 5, 8, 27, 30] and dynein [24, 29] along a microtubule. Many of molecular motors have the ability to rotate; for example, the bacterial flagellar motor [12] and F_0F_1-ATP synthase [17]. This movements and forces generated by the motors play essential roles in cellular functions. The linear motor kinesins are widely distributed in almost all eukaryotic cells. These motors are adenosine triphosphate (ATP)-driven walking machines that move in 8-nm steps toward the plus ends of the microtubule, turn over one ATP molecular per step under a range of loads [2, 10, 16, 32]. Kinesin has two motor domains called heads, each of which includes one ATP- and microtubule binding site [1, 13]. This motor steps mainly in the forward direction

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(to the plus end of the microtubule), but occasionally in the backward direction (to its minus end) [26].

The study of the energetics of molecular motors is relevant for several reasons. Firstly, the efficiency of molecule motors should be high enough to decrease the heat dissipation. Otherwise, the temperature of the surrounding would become higher and higher since the heat is difficult to be dissipated. Secondly, molecular motors are related to fundamental problems of thermodynamics and statistical mechanics. For instance, one of the first well-known Brownian motors was the ratchet-and-pawl setup studied by Feynman in his Lectures [23]. He calculated the efficiency of such an engine since his original purpose was to prove that an automatic demon cannot beat the second law of thermodynamics. Thirdly, many models of molecular motors proposed in the literature are based on nonequilibrium fluctuations without specifying their source. However, the study of the energetics of such models requires a more precise formulation, since one has to determine the physical nature of the external agent and verify that the motor is consistent with the second law of thermodynamics [19, 21].

Recently, Wang and Oster [31] have given the definition of the Stokes efficiency η_S (see (17)), and shown $\eta_S \leq 1$ through mathematical analysis of the Fokker-Planck equation with N chemical states. In [21], Qian have introduced a nonequilibrium potential function for a motor protein modelled by a rectified Brownian motion. Since the conservation of energy can be mathematically established, Qian's model provides a comprehensive theory for motor efficiency. In [19], the energetics of forced ratchets, chemical motors, and thermal motors has been discussed. The reasonable definitions of the energy efficiency of motors, which are compatible with the law of the thermodynamics, have also been reviewed.

In this research, we will discuss some properties of the energy efficiency of molecular motors in more details. Using the description of the Fokker-Planck equation with N or infinite chemical states, we obtain $\eta_S < 1$, $\eta_T < 1$. It is to say that the energy efficiency of molecular motors, either the Stokes efficiency [31] or the usual thermodynamic efficiency [19, 21], is strictly less than one, and any attempt to design a molecular motor that can convert the chemical energy into mechanical energy with efficiency one would fail. The movement of molecular motors satisfies the second law of the thermodynamics. It is why the Feynman ratchet doesn't work [22, 23]. But how is the chemical energy consumed in the movement of the molecular motors? In this paper, we'll find that the total energy released by the fuel molecules is consumed in three ways: to do mechanical work, to be dissipated into the surroundings, to be dissipated in the chemical reaction (see (41)). In fact, for motor proteins, such as kinesin, myosin and dynein, the heat dissipation in the surroundings is very important to keep the body temperature and a well-balanced body temperature is essential to the functions of the cell. So, not only mathematical analysis but also biophysical demand implies that the energy efficiency of the molecular motor should be strictly less than one. For motor proteins, the chemical energy is not only used to do mechanical work but also used to keep the body temperature. Of course, high efficient molecular motors are also very desirable in mechanical equipment.

2 Fokker-Planck Equation with N Chemical States

In this section, we'll discuss the energy efficiency η_S and η_T using the Fokker-Planck equation with N chemical states.

Let $\rho_i(x, t)$ be the probability density for finding the motor at position x in the ith chemical state at time t. The evolution of the probability density is governed by a set of coupled

Fokker-Planck equations that ensure the conservation of probability:

$$\frac{\partial \rho_i(x,t)}{\partial t} + \frac{\partial J_i(x,t)}{\partial x} = I_{i-\frac{1}{2}}(x,t) - I_{i+\frac{1}{2}}(x,t), \quad 1 \leq i \leq N. \tag{1}$$

Here J_i is the probability flux in the spatial direction for the ith chemical state, associated with convective transport and diffusion. $I_{i+1/2}$ is the probability flux density from state i to state $i+1$, N is the number of chemical states in one reaction cycle. For example, $N = 4$ is usually used in the motility cycle of ATP-driven motor proteins [28, 31].

In the ith state, the motor is driven by a periodic potential $\phi_i(x)$, and

$$
\begin{aligned}
J_i(x,t) = \rho_i(x,t)u_i(x,t) &= -\frac{\rho_i(x,t)}{\xi}\frac{\partial \Phi_i(x,t)}{\partial x} \\
&= -\frac{\rho_i(x,t)}{\xi}\frac{\partial \bar{\phi}_i(x)}{\partial x} - D\frac{\partial \rho_i(x,t)}{\partial x} \\
&= \underbrace{-\frac{\rho_i(x,t)}{\xi}\frac{\partial \phi_i(x)}{\partial x} + \frac{\rho_i(x,t)f_{\text{ext}}}{\xi}}_{\text{spatial drift flux}} \underbrace{-D\frac{\partial \rho_i(x,t)}{\partial x}}_{\text{spatial diffusion flux}}
\end{aligned}
\tag{2}
$$

$$I_{i+\frac{1}{2}}(x,t) = \rho_i(x,t)k_i^+ - \rho_{i+1}(x,t)k_{i+1}^- \quad \text{(flux along reaction coordinates)} \tag{3}$$

where $\Phi_i = \bar{\phi}_i + k_B T \ln \rho_i = \phi_i - f_{\text{ext}}x + k_B T \ln \rho_i$ is the enthalpy, ξ is the coefficient of viscous drag, D is the free diffusion coefficient, k_B is the Boltzmann constant, T is absolute temperature (D, ξ, k_B, T satisfy the Einstein relation $k_B T = \xi D$), f_{ext} is the external load ($f_{\text{ext}} \leq 0$), and k_i^+ is the transition rate from state i to state $i+1$, k_{i+1}^- is the transition rate from state $i+1$ to state i. k_i^+ and k_{i+1}^- satisfy

$$\frac{k_i^+}{k_{i+1}^-} = \exp\left(\frac{\phi_i(x) - \phi_{i+1}(x)}{k_B T}\right) \tag{4}$$

which ensures detailed balance at equilibrium.

Since the motor operates in a chemical and mechanical cycle, the boundary conditions for (1) in both the spatial direction and the reaction coordinate are periodical: $\rho_i(x+L,t) = \rho_i(x,t)$, $\rho_{i+N}(x,t) = \rho_i(x,t)$, $\phi_{i+N} = \phi_i - \triangle\mu$, where L is the step size of the motor ($L = 8.2$ nm for motor protein kinesin), $\triangle\mu > 0$ is the chemical free energy consumed in one reaction cycle. In physiological conditions, the hydrolysis free energy of ATP is $\triangle\mu \approx 25k_B T$ [10, 33, 34].

At steady state, the dissipation rate Π_i corresponding to slide within the potential profile Φ_i (i.e. the dissipation rate in the ith chemical state) is [7, 18]

$$\Pi_i = -\int_0^L J_i \frac{\partial \Phi_i}{\partial x} dx, \quad 1 \leq i \leq N. \tag{5}$$

It can be readily verified that $\Pi_i = \int_0^L \frac{\rho(x)}{\xi}(\frac{\partial \Phi_i}{\partial x})^2 dx \geq 0$. Summing (5) over i and integral by part, we obtain the total spatial dissipation rate

$$\Pi = \sum_{i=1}^N \Pi_i = -\int_0^L \sum_{i=1}^N J_i \frac{\partial \Phi_i}{\partial x} dx = f_{\text{ext}} L \sum_{i=1}^N J_i(0) + \int_0^L \sum_{i=1}^N \frac{J_i(x)}{\partial x} \Phi_i(x) dx. \tag{6}$$

In view of (1), at steady state,

$$\frac{\partial J_i(x)}{\partial x} = I_{i-\frac{1}{2}}(x) - I_{i+\frac{1}{2}}(x). \tag{7}$$

Equations (6), (7) imply

$$\Pi = f_{\text{ext}} L \sum_{i=1}^{N} J_i(0) + \int_0^L \sum_{i=1}^{N} (I_{i-\frac{1}{2}}(x) - I_{i+\frac{1}{2}}(x)) \Phi_i(x) dx$$

$$= f_{\text{ext}} L \sum_{i=1}^{N} J_i(0) + \int_0^L \sum_{i=1}^{N} (\Phi_{i+1}(x) - \Phi_i(x)) I_{i+\frac{1}{2}}(x) dx$$

$$+ \int_0^L I_{\frac{1}{2}}(x)(\Phi_1(x) - \Phi_{N+1}(x)) dx$$

$$= f_{\text{ext}} L \sum_{i=1}^{N} J_i(0) + \Delta\mu \int_0^L I_{\frac{1}{2}}(x) dx + \int_0^L \sum_{i=1}^{N} (\Phi_{i+1}(x) - \Phi_i(x)) I_{i+\frac{1}{2}}(x) dx. \tag{8}$$

By (6) and (8), we obtain

$$f_{\text{ext}} L \sum_{i=1}^{N} J_i(0) + \Delta\mu \int_0^L I_{\frac{1}{2}}(x) dx$$

$$= \sum_{i=1}^{N} \int_0^L \left[\frac{\rho(x)}{\xi} \left(\frac{\partial \Phi_i}{\partial x} \right)^2 dx + (\Phi_i(x) - \Phi_{i+1}(x)) I_{i+\frac{1}{2}}(x) \right] dx. \tag{9}$$

Thanks to (7),

$$\frac{\partial}{\partial x} \left(\sum_{i=1}^{N} J_i(x) \right) \equiv 0, \qquad \int_0^L I_{\frac{1}{2}}(x) dx = \int_0^L I_{\frac{3}{2}}(x) dx = \cdots = \int_0^L I_{N+\frac{1}{2}}(x) dx \tag{10}$$

it is to say

$$L \sum_{i=1}^{N} J_i(0) = \sum_{i=1}^{N} \int_0^L J_i(x) dx = \int_0^L \sum_{i=1}^{N} \rho_i(x) u_i(x) dx =: V \tag{11}$$

$$\int_0^L I_{\frac{1}{2}}(x) dx = \frac{1}{N} \sum_{i=1}^{N} \int_0^L I_{i+\frac{1}{2}}(x) dx =: \nu \tag{12}$$

where V is the mean velocity of molecular motors, ν is the mean rate of the chemical reaction.

Due to (3) and (4)

$$I_{i+\frac{1}{2}}(x, t) = \rho_i(x, t) k_i^+ \left[1 - \frac{\rho_{i+1}(x, t) k_{i+1}^-}{\rho_i(x, t) k_i^+} \right]$$

$$= \rho_i(x, t) k_i^+ \left[1 - \frac{\rho_{i+1}}{\rho_i(x, t)} \exp \left(\frac{\phi_{i+1}(x) - \phi_i(x)}{k_B T} \right) \right]$$

$$= \rho_i(x,t)k_i^+ \left[1 - \exp\left(\frac{\bar{\phi}_{i+1}(x) - \bar{\phi}_i(x)}{k_B T} \right) \right]$$

$$= \rho_i(x,t)k_i^+ \left[1 - \exp\left(\frac{\Phi_{i+1}(x) - \Phi_i(x)}{k_B T} \right) \right] \tag{13}$$

so

$$\Phi_{i+1}(x) - \Phi_i(x) \geq 0 \ (\leq 0)$$

$$\implies \exp\left(\frac{\Phi_{i+1}(x) - \Phi_i(x)}{k_B T} \right) \geq 1 \ (\leq 1)$$

$$\implies I_{i+\frac{1}{2}}(x,t) \leq 0 \ (\geq 0) \implies (\Phi_i(x) - \Phi_{i+1}(x))I_{i+\frac{1}{2}} \geq 0. \tag{14}$$

Finally, (9), (11), (12) and (14) mean

$$f_{\text{ext}}V + v\triangle\mu = \sum_{i=1}^{N} \int_0^L \left[\frac{\rho(x)}{\xi} \left(\frac{\partial \Phi_i}{\partial x} \right)^2 + (\Phi_i(x) - \Phi_{i+1}(x))I_{i+\frac{1}{2}}(x) \right] dx$$

$$= \sum_{i=1}^{N} \int_0^L \left[\underbrace{\xi\rho(x)u_i^2(x)}_{I} + \underbrace{(\Phi_i(x) - \Phi_{i+1}(x))I_{i+\frac{1}{2}}(x)}_{II} \right] dx \geq 0 \tag{15}$$

where I is the dissipation corresponding to slide within the potential profile Φ_i, II is the dissipation corresponding to transitions between two chemical states. Formula (15) is the second law of the thermodynamics.

By (15), the thermodynamic efficiency

$$\eta_T := -\frac{f_{\text{ext}}V}{v\triangle\mu} \leq 1 \tag{16}$$

the Stokes efficiency

$$\eta_S := \frac{\xi V^2}{f_{\text{ext}}V + v\triangle\mu} = \frac{\xi\left(\int_0^L \sum_{i=1}^{N} \rho_i(x)u_i(x)dx \right)^2}{f_{\text{ext}}V + v\triangle\mu}$$

$$\leq \frac{\xi \int_0^L \sum_{i=1}^{N} \rho_i(x)u_i^2(x)dx}{f_{\text{ext}}V + v\triangle\mu} = \frac{\sum_{i=1}^{N} \int_0^L \frac{\rho(x)}{\xi} \left(\frac{\partial \Phi_i}{\partial x} \right)^2 dx}{f_{\text{ext}}V + v\triangle\mu}$$

$$\leq 1. \tag{17}$$

In view of (14)

$$\sum_{i=1}^{N} \int_0^L (\Phi_i(x) - \Phi_{i+1}(x))I_{i+\frac{1}{2}}(x)dx = 0$$

$$\iff (\Phi_i(x) - \Phi_{i+1}(x))I_{i+\frac{1}{2}}(x) \equiv 0, \quad \forall i, \ 1 \leq i \leq N, \ 0 \leq x \leq L$$

$$\iff \Phi_i(x) \equiv \Phi_{i+1}(x), \quad \forall i, \ 1 \leq i \leq N, \ 0 \leq x \leq L$$

$$\iff \Phi_i(x) \equiv \Phi_j(x), \quad \forall i, j, \ 1 \leq i, j \leq N, \ 0 \leq x \leq L$$

$$\implies \triangle\mu = 0. \tag{18}$$

Therefore, if $\triangle\mu \neq 0$, then $\sum_{i=1}^{N}\int_0^L (\Phi_i(x) - \Phi_{i+1}(x))I_{i+\frac{1}{2}}(x)dx \neq 0$, which implies (see the inequality (15) and the definitions (16) and (17))

$$\eta_T < 1, \qquad \eta_S < 1. \tag{19}$$

If $\triangle\mu = 0$, then the mean velocity $V \leq 0$ (see (15)). It is to say that no useful mechanical work can be done by molecular motors if there is no input of the energy. If the mean velocity $V > 0$, i.e., molecular motors do useful work against the external load $f_{ext} < 0$, then $\triangle\mu \neq 0$, which implies $\sum_{i=1}^{N}\int_0^L (\Phi_i(x) - \Phi_{i+1}(x))I_{i+\frac{1}{2}}(x)dx \neq 0$, consequently $\eta_T < 1$, $\eta_S < 1$ (see (15)–(18)). Therefore, there always exists energy dissipation as long as the input energy $\triangle\mu \neq 0$.

3 Fokker-Planck Equation with Continuous Chemical Coordinates

In this section, we'll discuss the energy efficiency η_S and η_T using the Fokker-Planck equation with infinite chemical states.

Following [11, 20], we denote y as the coordinate of the internal conformational space of the motor protein, and x as its center of mass with respect to the linear track. Let $\rho(x, y, t)$ be the probability density for finding the motor at position x and chemical coordinate y at time t, $\Phi(x, y)$ be the potential. Due to (13), in the large N limit,

$$
\begin{aligned}
I_{i-\frac{1}{2}}(x) - I_{i+\frac{1}{2}}(x) &= -\frac{\partial}{\partial y}\left[\frac{1}{\zeta}\rho(x, y, t)\frac{\partial \Phi(x, y)}{\partial y}\right] \\
&= -\frac{\partial}{\partial y}\left[\frac{D_y}{k_B T}\rho(x, y, t)\frac{\partial \Phi(x, y)}{\partial y}\right]
\end{aligned}
\tag{20}
$$

where

$$D_y = \lim_{N \to \infty}\frac{k^+(y \to y + \frac{1}{N})}{N^2} \quad \text{and} \quad \zeta = \frac{k_B T}{D_y}.$$

Let $u(x, y) = -\frac{1}{\xi}\frac{\partial \Phi(x,y)}{\partial x}$, $v(x, y) = -\frac{1}{\zeta}\frac{\partial \Phi(x,y)}{\partial y}$, in the large N limit, (1) arrives

$$\frac{\partial \rho(x, y, t)}{\partial t} + \frac{\partial J(x, y, t)}{\partial x} + \frac{\partial I(x, y, t)}{\partial y} = 0, \quad 0 \leq x \leq L, \ 0 \leq y \leq 1 \tag{21}$$

where $J = \rho u$, $I = \rho v$.

At the steady state, the mean velocity of the movement is

$$V = \langle u \rangle = \int_0^1\int_0^L \rho(x, y)u(x, y)dxdy = \int_0^1\int_0^L J(x, y)dxdy \tag{22}$$

the mean rate of the chemical reaction is

$$v = \langle v \rangle = \int_0^1\int_0^L \rho(x, y)v(x, y)dxdy = \int_0^1\int_0^L I(x, y)dxdy. \tag{23}$$

Define

$$\Pi = \int_0^L\int_0^1 \left[\underbrace{-J(x, y)\frac{\partial \Phi(x, y)}{\partial x}}_{I'} \underbrace{-I(x, y)\frac{\partial \Phi(x, y)}{\partial y}}_{II'}\right]dydx \tag{24}$$

where I' is the dissipation rate along the spatial coordinate x, II' is the dissipation rate along the reaction coordination y. So Π is the total dissipation rate of molecular motors.

It is easy to find

$$\Pi = \int_0^1 \int_0^L \rho \left(\frac{\Phi_x^2}{\xi} + \frac{\Phi_y^2}{\zeta} \right) dxdy = \int_0^1 \int_0^L \rho \left(\xi u^2 + \zeta v^2 \right) dxdy \geq 0 \qquad (25)$$

at the same time

$$-\int_0^1 \int_0^L J(x, y)\Phi_x(x, y)dxdy$$

$$= -\int_0^1 \left[J(x, y)\Phi(x, y) \Big|_{x=0}^{x=L} - \int_0^L J_x(x, y)\Phi(x, y)dx \right] dy$$

$$= f_{\text{ext}}L \int_0^1 J(L, y)dy + \int_0^1 \int_0^L J_x(x, y)\Phi(x, y)dxdy$$

$$= f_{\text{ext}}L \int_0^1 J(L, y)dy - \int_0^1 \int_0^L I_y(x, y)\Phi(x, y)dxdy$$

$$= f_{\text{ext}}L \int_0^1 J(L, y)dy - \int_0^L \left[I(x, y)\Phi(x, y) \Big|_{y=0}^{y=1} - \int_0^1 I(x, y)\Phi_y(x, y)dy \right] dx$$

$$= f_{\text{ext}}L \int_0^1 J(L, y)dy + \Delta\mu \int_0^L I(x, 1)dx + \int_0^1 \int_0^L I(x, y)\Phi_y(x, y)dxdy \qquad (26)$$

so

$$\Pi = f_{\text{ext}}L \int_0^1 J(L, y)dy + \Delta\mu \int_0^L I(x, 1)dx. \qquad (27)$$

Since

$$\frac{\partial}{\partial x} \left[\int_0^1 J(x, y)dy \right] = \int_0^1 \frac{\partial}{\partial x} J(x, y)dy = -\int_0^1 \frac{\partial}{\partial y} I(x, y)dy = 0 \qquad (28)$$

$$\frac{\partial}{\partial y} \left[\int_0^L I(x, y)dx \right] = \int_0^L \frac{\partial}{\partial y} I(x, y)dx = -\int_0^L \frac{\partial}{\partial x} J(x, y)dx = 0 \qquad (29)$$

one knows

$$\int_0^1 J(x, y)dy = \int_0^1 J(L, y)dy, \qquad \int_0^L I(x, y)dx = \int_0^L I(x, 1)dx \qquad (30)$$

therefore

$$L \int_0^1 J(L, y)dy = \int_0^L \int_0^1 J(x, y)dydx = V \qquad (31)$$

$$\int_0^L I(x, 1)dx = \int_0^1 \int_0^L I(x, y)dxdy = v \qquad (32)$$

Finally, (25), (27), (31) and (32) imply

$$\Pi = f_{\text{ext}}V + v\triangle\mu = \int_0^1\int_0^L \rho\left(\xi u^2 + \zeta v^2\right)dxdy \geq 0 \tag{33}$$

this is the second law of the thermodynamics. By (33), the thermodynamic efficiency

$$\eta_T = -\frac{f_{\text{ext}}V}{v\triangle\mu} = 1 - \frac{\Pi}{v\triangle\mu} \leq 1 \tag{34}$$

the Stokes efficiency

$$\eta_S = \frac{\xi V^2}{f_{\text{ext}}V + v\triangle\mu} = \frac{\xi\left(\int_0^L\int_0^1 \rho(x,y)u(x,y)dydx\right)^2}{f_{\text{ext}}V + v\triangle\mu}$$

$$\leq \frac{\xi\int_0^L\int_0^1 \rho(x,y)u^2(x,y)dydx}{f_{\text{ext}}V + v\triangle\mu}$$

$$= 1 - \frac{\zeta\int_0^L\int_0^1 \rho(x,y)v^2(x,y)dydx}{f_{\text{ext}}V + v\triangle\mu} \leq 1. \tag{35}$$

Similar as (18)

$$\zeta\int_0^L\int_0^1 \rho(x,y)v^2(x,y)dydx = 0$$

$$\Longleftrightarrow \quad v(x,y) = 0, \qquad 0 \leq x \leq L,\ 0 \leq y \leq 1$$

$$\Longleftrightarrow \quad \Phi(x,y) = \Phi(x,z), \quad 0 \leq x \leq L,\ 0 \leq y, z \leq 1$$

$$\Longrightarrow \quad \triangle\mu = \Phi(x,0) - \Phi(x,1) = 0. \tag{36}$$

So, if $\triangle\mu \neq 0$, then $\zeta\int_0^L\int_0^1 \rho(x,y)v^2(x,y)dydx \neq 0$, which means the inequalities (19) hold true.

Moreover, applying the Cauchy-Schwarz inequality, and using the constraint

$$\int_0^L\int_0^1 \rho(x,y)dydx = 1,$$

one obtains

$$\int_0^L\int_0^1 \rho(x,y)u^2(x,y)dydx \geq \left(\int_0^L\int_0^1 \rho(x,y)u(x,y)dydx\right)^2 = V^2$$

$$\int_0^L\int_0^1 \rho(x,y)v^2(x,y)dydx \geq \left(\int_0^L\int_0^1 \rho(x,y)v(x,y)dydx\right)^2 = v^2 \tag{37}$$

so

$$\eta_T = -\frac{f_{\text{ext}}V}{v\triangle\mu} \leq 1 - \frac{\xi V^2 + \zeta v^2}{v\triangle\mu} = 1 - \frac{(\xi L^2 + \zeta)V}{\triangle\mu L} \tag{38}$$

$$\eta_S = \frac{\xi V^2}{f_{\text{ext}}V + v\triangle\mu} \leq \frac{\xi V^2}{\xi V^2 + \zeta v^2} = \frac{\xi L^2}{\xi L^2 + \zeta} = 1 - \frac{\zeta}{\xi L^2 + \zeta}. \tag{39}$$

Here the equalities hold true if and only if $u(x, y) \equiv V$, $v(x, y) \equiv v$. Obviously $\eta_T < 1$, $\eta_S < 1$.

Finally, by (33) and the definitions of the energy efficient η_S, η_T, we can get the following interesting relationship

$$\xi V^2 = \eta_S (1 - \eta_T) v \triangle \mu \tag{40}$$

$$\triangle \mu = -f_{\text{ext}} L + \xi V L + \left[\frac{L}{V} \int_0^1 \int_0^L \rho \left(\xi u^2 + \zeta v^2 \right) dx dy - \xi V L \right]$$

$$= \eta_T \triangle \mu + \eta_S (1 - \eta_T) \triangle \mu + (1 - \eta_S)(1 - \eta_T) \triangle \mu. \tag{41}$$

From (41), we can know how the energy is consumed in the movement of molecular motors: where $\eta_T \triangle \mu = f_{\text{ext}} L$ is the energy used to do useful work against the external force f_{ext}, $(1 - \eta_T) \triangle \mu$ is the total energy dissipation, $\eta_S (1 - \eta_T) \triangle \mu$ is the energy dissipation due to the overdamping surroundings, $(1 - \eta_S)(1 - \eta_T) \triangle \mu$ is the energy dissipation during the chemical reaction.

Though the 2D Fokker-Planck equation (21) is the large N limit of (1), most of the results in Sect. 3 can't be obtained directly by the limitation of the corresponding ones in Sect. 2 (for $\eta = \lim_{n \to +\infty} \eta_n$ and $\eta_n < 1$, it is not always correct that $\eta < 1$). Moreover, through the detailed discussion in Sect. 3, the relationship between the parameters in (1) and the parameters in (21) is clarified, and how the energy is consumed in the movement of the molecular motor is also clarified easily. Equations (1) might be more physical, but it might be more convenient to get detailed results using (21).

4 Conclusions

In this paper, we have given a detailed discussion of the energy efficiency of molecular motors. We find that the energy efficiency of molecular motors, whether the usual thermodynamic efficiency or Stokes efficiency, is strictly less than one. This result is sharper than in previous work [21, 31], where $\eta_S \leq 1$ and $\eta_T \leq 1$ were proved. In each step of a molecular motor, the total energy released by the fuel molecules is consumed in three ways: to do mechanical work, to be dissipated in the surroundings, or to be dissipated in the chemical reaction. According to the second law of the thermodynamics (33), the faster the molecular motors move, the more the energy is dissipated. Theoretically, the highest energy efficiency only can be achieved when the movement of the molecular is a quasi-static process, which is more like the Carnot heat engine.

For the multiple pathways case [3, 14, 15], the results in this paper are also correct. The only difference is that the energy efficiency (or the energy used to do mechanical work, the velocity) in different pathways might be different. Regardless of the pathways, the efficiency of molecular motors is always strictly less than one.

Finally, similar theoretical analysis can be used to describe the backward stepping case of motor protein kinesin [5]. If fuel molecules are resynthesized in the backward stepping process, then $f_{\text{ext}} < 0$, $V < 0$, $\triangle \mu < 0$ and $f_{\text{ext}} V + v \triangle \mu > 0$. So the energy efficiency of fuel molecules resynthesizing $\eta = -\frac{v \triangle \mu}{f_{\text{ext}} V}$ is strictly less than one. Generally, in each backward step of a molecular motor, the total external energy ($f_{\text{ext}} V$) is consumed in three ways: to resynthesize fuel molecules ($-v \triangle \mu$), to be dissipated in the surroundings ($\int_0^1 \int_0^L \rho \xi u^2 dx dy$), or to be dissipated in the chemical reaction ($\int_0^1 \int_0^L \rho \zeta v^2 dx dy$): $f_{\text{ext}} V = -v \triangle \mu + \int_0^1 \int_0^L \rho (\xi u^2 + \zeta v^2) dx dy$. Where $\triangle \mu < 0$ means fuel molecules are resynthesized, and $\triangle \mu > 0$ means fuel molecules are consumed.

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