Energetics and efficiency of a molecular motor model

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Abstract. The energetics and efficiency of a linear molecular motor model proposed by Mogilner \textit{et al} are analyzed from an analytical point of view. The model, which is based on protein friction with a track, is described by coupled Langevin equations for the motion in combination with coupled master equations for the ATP hydrolysis. Here the energetics and efficiency of the motor are addressed using a many body scheme with focus on the efficiency at maximum power (EMP). It is found that the EMP is reduced from about 10\% in a heuristic description of the motor to about 1 per mille when incorporating the full motor dynamics, owing to the strong dissipation associated with the motor action.

Keywords: stochastic processes (theory), molecular motors (theory)

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1. Introduction

There is currently an interest in the energetics and efficiency of molecular motors and nanoengines. Molecular motors are energy-consuming, non-equilibrium nanoscale engines encountered in various dynamical processes on the intra- and intercellular level [1, 2]; for a recent review of the more physical aspects see, for instance, [3]. Linear motor proteins like myosin or kinesin are driven by the hydrolysis of ATP into ADP and move along linear polar tracks like actin filaments or microtubules. The motors typically work in an isothermal environment at ambient temperatures subject to viscous forces.

Modern experimental techniques in biology and biophysics, in particular single biomolecule manipulation by, for example, optical tweezers or micro-needles, and single particle tracking methods, have yielded considerable insight into the mechanism and the relevant physical scales in molecular motor behavior, see e.g. [4]. The typical size of a molecular motor is of order 10–20 nm, moving with a step size of order 8 nm, e.g., kinesin on microtubules, with one ATP molecule hydrolyzed on average per step. The velocities of molecular motors range from nm s$^{-1}$ to µm s$^{-1}$ and the maximum load is of the order of several pN. The time scale of the chemical cycle is a few ms and the average energy input from the ATP–ADP cycle is of order 15–20$kT$. Here $kT$ is the energy scale of thermal motion at temperature $T$.

A molecular motor constitutes an interesting non-equilibrium system operating in the classical regime and is thus directly amenable to analysis using methods in statistical physics. Physical modeling of molecular motors has thus been studied intensively in recent years, both from the point of view of the fundamental underlying physical principles and with regard to the specific modeling of concrete motors [5]–[16]. The most common
statistical approach to molecular motors is the ratchet model [3, 10], modeling the periodically alternating energy landscape felt by the motor during its cycle. An alternative motor model can be based on protein friction, where the motor during its cycle is in contact with a track [6, 10], [17]–[20].

In recent work Mogilner et al [21] have studied a specific protein friction model. The motor is represented by two coupled overdamped oscillators driven by a two-step Markov process alternating between a relaxed and a strained state of the oscillators. The motor is embedded in a thermal environment represented by additive white noise. The subprocesses are associated with internal conformational changes of the motor protein. One subprocess is slow, allowing protein friction to act, while the other is fast and only subject to solvent friction. By means of a numerical analysis Mogilner et al show that the system acts like a motor and can carry a load. However, unlike ratchet models, which operate with an attachment to a periodic polar protein filament, the model of Mogilner et al only needs a ‘passive’ groove in order to perform directed motion. The motion comes about due to the asymmetric internal velocity fluctuations which are then rectified by protein friction. In that sense, it is a robotic model of molecular motors.

Recently, there has been an interest in the efficiency of molecular motors and nanoengines [9], [22]–[29]. Unlike heat engines where the efficiency is bounded by Carnot’s law, see e.g. [30], molecular motors work in an isothermal environment at ambient temperatures and the efficiency can in principle reach unity. The efficiency of a motor is given by

$$\eta = \frac{p}{\epsilon_{\text{in}}} \quad (1.1)$$

where $p$ is the output power, i.e., the work done per unit time on the surroundings. Likewise, $\epsilon_{\text{in}}$ is the input energy rate. Conservation of energy implies

$$\epsilon_{\text{in}} = p + q_{\text{out}} \quad (1.2)$$

where $q_{\text{out}}$ is the dissipation rate. Here $\epsilon_{\text{in}}$ refers to the energy input to the motor arising from the ATP hydrolysis, whereas $q_{\text{out}}$, the dissipation rate, refers to the frictional effects during the motor operation. $\epsilon_{\text{in}}$ and $q_{\text{out}}$ refer to two different energy reservoirs and there is thus no conflict with the second law of thermodynamics. The theoretical upper limit $\eta = 1$ requires the absence of irreversible processes, i.e., $q_{\text{out}} = 0$, and can thus only be attained by infinitely slow driving, corresponding to vanishing power. A more relevant measure of efficiency is therefore, for example, the efficiency at maximum power (EMP), i.e.,

$$\eta_{\text{emp}} = \frac{p_{\text{max}}}{\epsilon_{\text{in}}} \quad (1.3)$$

In a recent paper [31] we analyzed the motor model by Mogilner et al from a purely analytical point of view and derived explicit expressions for the motion of the motor and the velocity–load relationship. In this paper we return to the analytical solution of the Mogilner model and focus on the energetics and efficiency of the model; these aspects were not considered in [31].

The paper is organized in the following manner. In section 2 we review the Mogilner model and the analytical solution. In section 3 we address the energetics and derive an expression for the efficiency. In section 4 we discuss the efficiency of the motor in detail. Section 5 is devoted to a brief summary.
2. Model

We consider a minimal power stroke model of a motor molecule or nanoengine operating in an isothermal environment. We assume that the motor is driven by ATP hydrolysis. During a cycle an ATP molecule is attached to the motor releasing the free energy $\Delta \mu$. The motor is composed of two sections or heads, an active head and a passive head. During a conformational change the positions of the heads change. Denoting the equilibrium distance between the heads by $L$ we assume that the motor can exist in only two geometrical conformations, corresponding to the values $L_r$ and $L_s$. During a power stroke induced by the attachment of an ATP molecule to the motor and the subsequent hydrolysis of ATP the motor undergoes a conformational change from a relaxed state R with geometrical parameter $L_r$ to a strained state S with parameter $L_s$. We, moreover, characterize the elastic states of the motor by two spring constants $k_r$ and $k_s$, referring to the relaxed and strained states, respectively.

The state of the motor is driven by the ATP hydrolysis. This two-step stochastic process is modeled by two coupled master equations for the respective probabilities $P_s$ and $P_t$,

$$\frac{dP_s}{dt} = g_s P_t - g_r P_s, \quad (2.1)$$
$$\frac{dP_t}{dt} = g_r P_s - g_s P_t. \quad (2.2)$$

Here $g_r$ is the transition rate from the strained state S to the relaxed state R and $g_s$ is the rate from R to S. In the stationary state we have

$$P_s = \frac{g_s}{g_s + g_r}, \quad (2.3)$$
$$P_t = \frac{g_r}{g_s + g_r}. \quad (2.4)$$

Simple arguments show that in order to obtain the motor property, i.e., the motion of the motor in the absence of a load, at least two internal coordinates $x$ and $y$ are required, accounting for the conformal changes. The motor, moreover, has to interact with a track. In the Mogilner model the interaction with the track is modeled by a time dependent friction $\zeta(t)$ which is synchronized with the ATP hydrolysis and the associated conformal transitions assume two values. When the active head at coordinate $x$ is in contact with the track during a cycle we assume that $\zeta(t) = \zeta_p$, where $\zeta_p$ is the so-called protein friction. During the phase where the motor is detached from the track we assume that $\zeta(t) = \zeta_v$, where $\zeta_v$ is the friction due to the solvent. This friction is of the order of the Stokes value $6\pi R \eta$; here $R$ is the size of the motor and $\eta$ is the viscosity of the medium. This scenario, discussed in detail in [31], is described by the coupled equations of motion

$$\zeta(t) \frac{dx}{dt} = -\frac{dU}{dx} - f, \quad (2.5)$$
$$\zeta_v \frac{dy}{dt} = -\frac{dU}{dy}. \quad (2.6)$$
where $U$ is the time dependent harmonic potential

$$U(x, y, t) = \frac{k(t)}{4} [y - x - L(t)]^2. \quad (2.7)$$

The time dependence of $k(t)$ and $L(t)$ is given by the stochastic switches of the motor between the internal states, characterized by the master equations (2.1) and (2.2). In (2.5) and (2.6) we are considering the over damped case relevant in biology and, moreover, ignore the thermal noise which takes place on a much faster time scale than the conformational changes in the motor. In (2.5) we have included a load force $f$ acting on the active head at coordinate $x$.

The procedure for solving the motor problem is straightforward. Assuming a general time dependence of $\zeta(t)$, $k(t)$, and $L(t)$ the linear equations (2.5) and (2.6) with potential (2.7) are readily solved analytically. In order to compute distributions and averages the calculation is completed by averaging over $\zeta(t)$, $k(t)$, and $L(t)$ according to the master equations (2.1) and (2.2). Regarding the stationary mean velocity $v$ both with and without load $f$, this calculation using residence time distributions was carried out in [31].

For a concrete realization of the motor parameters $\zeta(t)$, $k(t)$, and $L(t)$, i.e., $\zeta(t) = \{\zeta_p, \zeta_v\}$, $k(t) = \{k_r, k_s\}$, and $L(t) = \{L_r, L_s\}$, and introducing the relative position $\Delta y = y - x$ and the damping parameter $\Gamma = (k/2)(1/\zeta + 1/\zeta_v)$ (note, in [31] this quantity was denoted $\dot{\gamma}$), we have

$$\frac{d\Delta y}{dt} = -\Gamma \Delta y + \Gamma L + \frac{f}{\zeta}, \quad (2.8)$$

with solution

$$\Delta y = L + \frac{f}{\zeta} + \left(\Delta y_0 - L - \frac{f}{\zeta} \Gamma \right) \exp(-\Gamma t); \quad (2.9)$$

here $\Delta y_0$ is the initial value at $t = 0$. At long times $t \gg 1/\Gamma$ we obtain

$$\langle \Delta y \rangle_r = L_r + \frac{2f}{k_r(1 + \zeta_p/\zeta_v)}, \quad (2.10)$$

$$\langle \Delta y \rangle_s = L_s + \frac{f}{k_s}, \quad (2.11)$$

and for the mean separation

$$\langle \Delta y \rangle = P_r \langle \Delta y \rangle_r + P_s \langle \Delta y \rangle_s, \quad (2.12)$$

where $P_r$ and $P_s$ are given by (2.3) and (2.4). Note that since $d\Delta y/dt = 0$ for $t \gg 1/\Gamma$ it follows that $\langle v_x \rangle = \langle v_y \rangle$, i.e., the two heads move together on average. However, as shown in [31], the mean velocity $v = (1/2)(\langle v_x \rangle + \langle v_y \rangle)$ is nonvanishing even for $f = 0$, establishing the motor property. As an illustration in figure 1 we have sketched the behavior of $\Delta y$ as a function of $t$ for $f = 0$. The time instants $t_1$, $t_2$, etc indicate when we have transitions between the relaxed and strained states.

3. Energetics and efficiency

Here we turn to the main issues of this paper, namely the energetics and efficiency of the ATP driven motor model discussed in section 2.

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Figure 1. The relative coordinate $\Delta y$ as a function of time $t$ for a concrete realization of the time dependent parameters. At the time instants $t_n$ there are transitions between the relaxed and strained states driven by the master equations (arbitrary units).

3.1. Energetics

Subject to the ATP hydrolysis, energy is imparted to the motor, temporarily stored in the spring, dissipated owing to the friction, and performs work on the environment. Energy conservation is expressed in (1.2), i.e., $\epsilon_{in} = p + q_{out}$, where $\epsilon_{in}$ is the energy input rate, $q_{out}$ the dissipation rate, and $p$ the rate of work performed on the surroundings. It is instructive to sketch the energy flow. Expressing the over damped equation of motion (2.8) in the form

$$\frac{d\Delta y}{dt} = -\Gamma \frac{d\tilde{U}}{d\Delta y},$$

(3.1)

$$\tilde{U} = \frac{1}{2} \left( \Delta y - L - \frac{f}{2\Gamma} \right)^2.$$  

(3.2)

The main effect is due to the conformational changes of the rest length $L$. At a given time instant a transition with rate $g_r$ excites the motor from the S state to the R state increasing the potential energy. Subsequently, the energy is dissipated by friction until a new transition from state R to state S with rate $g_s$ again increases the potential energy. In figure 2 we have illustrated the decay mechanism for two possible scenarios for $f = 0$. By inspection it is clear that over a cycle the change in potential energy $\Delta \tilde{U} > 0$, i.e., a positive dissipation consistent with the second law of thermodynamics.

The energy conservation is also easily extracted from the equations of motion (2.5) and (2.6). The dissipation force on the active head, i.e., the head in contact with the track, is $-\zeta(t)dx/dt$, whereas the dissipation force on the passive or free head is $-\zeta_v dy/dt$. Consequently, the mean rate of heat dissipation is given by

$$q_{out} = \langle \zeta(t)(dx/dt)^2 \rangle + \langle \zeta_v(dy/dt)^2 \rangle.$$  

(3.3)

Multiplying (2.5) and (2.6) by $dx/dt$ and $dy/dt$, adding, and averaging over the power stroke cycles we obtain $q_{out} = -p - (1/2)\langle k(\Delta y - L) d\Delta y/dt \rangle$. Here the last term is the...
Energetics and efficiency of a molecular motor model

Figure 2. The dissipation mechanism. In state S the motor undergoes a transition to state R with rate $g_r$ and, subsequently, relaxes until a new transition with rate $g_s$ brings the motor back to state S. The momentary gain in potential energy is relaxed due to dissipation as indicated by the arrows. $\Delta y$ is the relative coordinate and $U$ is the potential in (3.2) for $f = 0$ (arbitrary units).

rate of work performed on the head and tail of the motor. Since the motor does not accumulate energy we can identify the input heat flux $\epsilon_{\text{in}} = -(1/2)\langle k(\Delta y - L) d\Delta y/dt \rangle$, in accordance with the energy balance (1.2).

The mean power given by $p = f v$, where $v$ is the mean velocity of the motor, is readily accessible. The mean velocity was computed in [31] and is given by

$$v = v^0 - \mu f,$$

where $v^0$ is the motor velocity in the absence of a load and $\mu$ is the mobility. The velocity $v^0$ can be written in the form

$$v^0 = v_h^0 \frac{\zeta_p - \zeta_v}{\zeta_p + \zeta_v + 1} \frac{1}{1 + g_r + g_s},$$

$$v_h^0 = \frac{g_s g_r}{g_r + g_s} \frac{L_r - L_s}{2} = \frac{L_r - L_s}{2 (\langle t \rangle_r + \langle t \rangle_s)},$$

(3.6)

Here $v_h^0$ is a heuristic expression for the velocity solely based on the conformations $L_r$ and $L_s$ and the residence times $\langle t \rangle_s = 1/g_r$ and $\langle t \rangle_r = 1/g_s$, see [31]. Taking $v^0 = v_h^0$ neglects the internal dynamics of the motor, see [21]. In the correction factor the dimensionless parameters

$$q_s = \frac{g_r}{\Gamma_s},$$

$$q_r = \frac{g_s}{\Gamma_r},$$

where $\Gamma_s = \frac{k_s}{\zeta_v}$, $\Gamma_r = \frac{k_r}{2} \left[ \frac{1}{\zeta_v} + \frac{1}{\zeta_p} \right],$

(3.7)

(3.8)

express the ratios between the spring relaxation times $\Gamma_s^{-1}$ and $\Gamma_r^{-1}$ and the residence times. We note that the coasting velocity $v^0$ vanishes for $L_r = L_s$, corresponding to the absence of conformational changes, and for $\zeta_p = \zeta_v$, i.e., in the absence of a track providing protein friction; for further discussion see [31].

The mobility $\mu$ determines the response of the motor to the load force $f$. In the absence of fluctuations, i.e., the case of constant $k$, constant $L$, and $\zeta(t) = \zeta_p$, we have from (2.5)

$$\epsilon_{\text{in}} = -\left(\frac{1}{2}\langle k \Delta y - L \rangle d\Delta y/dt\right),$$

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and (2.6) $\mu = 1/(\zeta_p + \zeta_v)$, see [21, 31]. In the general case the mobility depends on the model parameters,

$$\mu = \frac{[P_r \zeta_v + P_s \zeta_p][2q_s + (1 + \zeta_v / \zeta_p)q_r] + (1 + P_r)\zeta_v + P_s \zeta_p}{2\zeta_v(\zeta_v + \zeta_p)(1 + q_s + q_r)}.$$  \hfill (3.9)

Finally, for the mean power we have

$$p = (v^0 - \mu f)f,$$ \hfill (3.10)

where $v^0$ and $\mu$ are given by (3.5), (3.6) and (3.9).

The remaining issue in order to establish the energetics of the motor is the evaluation of $\epsilon_{in}$ or, alternatively, $q_{out}$. It turns out to be most convenient to consider the heat dissipation rate $q_{out}$ given by (3.3). Evaluations of $q_{out}$ with or without load can be carried out using the waiting time distribution method employed in [31]. However, in this paper we shall carry out the evaluation using transition probabilities and a more automatic many body scheme. This still rather complex machinery is deferred to the appendix. In the load free case, $f = 0$, we find (see equation (A.45) in the appendix)

$$q_{out}^0 = \frac{(L_r - L_s)^2 g_r g_s}{2(g_r + g_s)} \frac{k_r(1 + q_r) + k_s(1 + q_s)}{(q_r + q_s + 1)(q_r + q_s + 2)}.$$ \hfill (3.11)

In the case of a finite load the output heat rate also depends on $f$ and has a complicated form derived in the appendix. In terms of the appropriate mean values of dynamic variables, i.e., $\langle A \rangle = A_r P_r + A_s P_s$, it reads

$$q_{out} = \frac{a^2}{2} \langle b L^2 \Gamma k \rangle - \frac{fa}{\zeta_v} \langle L k \rangle + \frac{f^2}{\zeta_v} \langle c / (c + \langle \Gamma \rangle) \rangle \left( \langle c b L^2 \Gamma k \rangle + \langle b \Gamma \rangle \langle L \Gamma k \rangle \right)$$

$$+ \frac{fa}{\zeta_v(c + \langle \Gamma \rangle)} \left( \langle c b L k \rangle + \langle b \Gamma \rangle \langle k \rangle \right) + \frac{a^2}{2(c + \langle \Gamma \rangle)(2c + \langle \Gamma \rangle)}$$

$$\times \left[ \langle b \Gamma \rangle^2 \langle \Gamma k \rangle + c \langle b^2 L^2 \Gamma \Gamma k \rangle + 2c \langle b \Gamma \rangle \langle b \Gamma \Gamma k \rangle + 2c^2 \langle b^2 L^2 \Gamma k \rangle \right],$$ \hfill (3.12)

where

$$a = 1 - 2f \frac{k_r - k_s}{k_r k_s(L_r - L_s)},$$ \hfill (3.13)

$$b = 1 - \frac{f}{a \zeta_v} \langle \Gamma \Gamma \rangle^{-1},$$ \hfill (3.14)

$$c = \frac{\Gamma_r \Gamma_s}{g_r + g_s}.$$ \hfill (3.15)

4. Discussion

Here we proceed to discuss the energetics and efficiency of the motor. First, let us focus on the energy bookkeeping. The motor is driven by the attachment of ATP and the subsequent hydrolysis to ADP and P. This chemical reaction triggers the motor as expressed by the rate $g_s$. During a cycle the system absorbs the energy $\Delta \mu$ arising from the ATP hydrolysis. Consequently, the rate of energy input is $\Delta \mu g_s$, where $g_s$ is the transition rate from the relaxed motor state R to the strained motor state S. The amount of energy
that the motor can absorb per cycle depends on the actual state of the motor at the moment the hydrolysis takes place, see figures 1 and 2. Consequently, we can define the intermediate ATP related efficiency

$$\eta_{\text{ATP}} = \frac{\epsilon_{\text{in}}}{\Delta \mu g_s},$$

(4.1)

where $\epsilon_{\text{in}}$ is the rate of input energy recovered by the motor. The size of $\eta_{\text{ATP}}$, while not exceeding $\eta_{\text{ATP}} = 1$, depends on the frictional energy rate, $\Delta \mu g_s - \epsilon_{\text{in}}$, absorbed by degrees of freedom not included in the present motor model. In that sense $\eta_{\text{ATP}}$ is a ‘fudge’ parameter which can only be estimated qualitatively. The efficiency specifically associated with the motor model is given by

$$\eta_{\text{motor}} = \frac{p}{\epsilon_{\text{in}}},$$

where $p$, as given by equation (3.10), expresses the work exerted on the environment. This efficiency is given by

$$\eta_{\text{motor}} = \frac{(v_0^0 - \mu f)}{q_{\text{out}} + (v_0^0 - \mu f)f}.$$  

(4.2)

The total efficiency, $\eta_2$, relating the power $p$ to the ATP energy input rate, is thus given by the product of the two efficiencies,

$$\eta_2 = \eta_{\text{ATP}} \eta_{\text{motor}}.$$  

(4.3)

In discussing the motor efficiency $\eta_{\text{motor}}$ it is useful to first as a reference use the heuristic expressions by Mogilner et al [21]. Neglecting the internal dynamics of the motor the velocity for $f = 0$ is given by

$$v_h^0 = (L_r - L_s)g_s g_r / (g_r + g_s)$$

in (3.6). In the presence of a load $f$ the velocity is to a first approximation reduced by $f/\zeta_p$, where $\zeta_p$ is the protein friction, i.e., $v_r = v_h^0 - f/\zeta_p$, with mobility $\mu = 1/\zeta_p$. A more detailed analysis based on (2.5) and (2.6), see also [31], yields $\mu = 1/(\zeta_v + \zeta_p)$ in the relaxed state R and $\mu = 1/2\zeta_v$ in the strained state S. Interpolating between the two states we can thus define the effective mobility

$$\mu_h = P_r \frac{1}{\zeta_p + \zeta_v} + P_s \frac{1}{2\zeta_v},$$

(4.4)

which agrees with (3.9) for $g_s = g_r = 0$. Hence, we obtain for $v_h$

$$v_h = v_h^0 - \mu_h f.$$  

(4.5)

For the power $p_h$ neglecting the internal dynamics we thus obtain

$$p_h = (v_h^0 - \mu_h f)f.$$  

(4.6)

On the basis of (3.3) we can make a simple estimate for $q_{\text{out}}$. In state R the friction $\zeta(t) = \zeta_p$ and we have $q_{\text{out}} \sim \zeta_p v_r^2 + \zeta_v v_y^2 = (\zeta_p + \zeta_v)v^2$; in state S we have $\zeta(t) = \zeta_v$ and we obtain $q_{\text{out}} \sim 2\zeta_v v^2$. By the same interpolation as in the case of $\mu_h$ we thus obtain the estimate

$$q_{\text{out}}^h \sim (P_r(\zeta_p + \zeta_v) + 2P_s \zeta_v)v_h^2 = \zeta_h v_h^2,$$

(4.7)

where we have introduced the effective viscosity

$$\zeta_h = P_r(\zeta_p + \zeta_v) + 2P_s \zeta_v.$$  

(4.8)
Energetics and efficiency of a molecular motor model

For the efficiency we thus obtain
\[ \eta_h = \frac{v_h f}{\zeta_h v_h^2 + v_h f}. \tag{4.9} \]
In this simple approximation
\[ \eta_h = \frac{f}{\zeta_h v_h + f}. \tag{4.10} \]
For \( f = 0 \) we have \( p_h = 0 \) and thus \( \eta_h = 0 \). At the stall force \( f_{\text{stall}} = v_0^h/\mu_h \) we have \( v_h = 0 \) and the efficiency \( \eta_h = 1 \). The power \( p_h \) has a maximum for \( f = v_0^h/2\mu_h \) and we obtain the efficiency at maximum power (EMP)
\[ \eta_h^{\text{emp}} = \frac{1}{\mu_h \zeta_h + 1}. \tag{4.11} \]
Inserting biological parameters from Mogilner et al [21], i.e., \( \zeta_p = 50 \times 10^{-6} \text{ pN}^{-1} \text{ s nm}^{-1} \), \( \zeta_v = 10^{-6} \text{ pN}^{-1} \text{ s nm}^{-1} \), \( g_t = 10^3 \text{ s}^{-1} \), \( g_s = 10^3 \text{ s}^{-1} \), \( P_r = 0.5 \), and \( P_s = 0.5 \), we obtain \( \mu_h = 2.6 \times 10^3 \text{ nm pN}^{-1} \text{ s}^{-1} \) and \( \zeta_h = 2.6 \times 10^{-5} \text{ pN}^{-1} \text{ s nm}^{-1} \), yielding the efficiency at maximum power \( \eta_h^{\text{emp}} = 0.13 \).

The next issue is to examine how the above heuristic expression for the motor efficiency depends on the intrinsic motor parameters. For the mobility \( \mu \), entering in the expression for the power and the velocity, we have from (3.9), see also [31],
\[ \mu = \mu_h C_\mu, \tag{4.12} \]
\[ C_\mu = \frac{1 + [2q_s + (1 + \zeta_v/\zeta_p)q_r][P_r \zeta_v + P_s \zeta_p + P_z \zeta_p + \zeta_v]}{1 + q_s + q_r}. \tag{4.13} \]
where the correction factor depends on the motor parameters. Inserting \( k_z = 0.01 \text{ pN nm}^{-1} \), \( k_s = 0.5 \text{ pN nm}^{-1} \), yielding \( q_r = 0.2 \) and \( q_s = 2 \times 10^{-3} \), we obtain \( C_\mu = 0.998 \), i.e., close to 1. Likewise, for the coasting velocity we have from (3.5) and (3.6)
\[ v^0 = v_0^h C_v, \tag{4.14} \]
\[ C_v = \frac{\zeta_p - \zeta_v}{\zeta_p + \zeta_v} \frac{1}{1 + q_s + q_r}. \tag{4.15} \]
Inserting biological parameters we find \( v_0^h = 0.5 \times 10^4 \text{ nm s}^{-1} \) and the correction factor \( C_v = 0.8 \), i.e., close to 1. Since the power \( p = (v^0 - \mu f) f \) attains the maximum value \( p_{\text{max}} = (v^0)^2/4\mu \) for \( f_{\text{max}} = v^0/2\mu \) the central quantity determining \( \eta^{\text{emp}} \) is the dissipation rate \( q_{\text{out}} \) which has a dependence on the load force \( f \). Referring to the heuristic ansatz we set
\[ q_{\text{out}} = \zeta_h v_0^h C_q(f). \tag{4.16} \]
The correction factor \( C_q(f) \) is then determined from \( q_{\text{out}} \) evaluated in the appendix. With these definitions we have
\[ p = (v_0^h C_v - \mu_h C_\mu f) f, \tag{4.17} \]
\[ q_{\text{out}} = \zeta_h v_0^h C_q, \tag{4.18} \]
\[ \eta = \frac{(v_0^h C_v - \mu_h C_\mu f) f}{\zeta_h v_0^h C_q + (v_0^h C_v - \mu_h C_\mu f) f}. \tag{4.19} \]

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The maximum power \( p_{\text{max}} = (v_h^0 C_v)^2 / 4 \mu_h C_\mu \) is attained for \( f_{\text{max}} = v_h^0 C_v / 2 \mu_h C_\mu \), and we obtain the efficiency at maximum power

\[
\eta^{\text{emp}} = \frac{(v_h^0 C_v)^2 / 4 \mu_h C_\mu}{\zeta_h v_h^2 C_q + (v_h^0 C_v)^2 / 4 \mu_h C_\mu}.
\] (4.20)

Choosing the biological parameters \( L_r = 40 \text{ nm} \), \( L_s = 20 \text{ nm} \), we obtain \( p_{\text{max}} = 24 \text{ pN nm s}^{-1} \) and \( f_{\text{max}} = 9.6 \times 10^{-3} \text{ pN} \). Moreover, from (4.7) \( q_{\text{out}}^h = \zeta_h v_h^2 = 1.6 \times 10^2 \text{ pN nm s}^{-1} \). From equation (3.12) we obtain for \( f = f_{\text{max}} \) the dissipation rate \( q_{\text{out}} = 1.94 \times 10^4 \text{ pN nm s}^{-1} \), i.e., \( C_q = 1.2 \times 10^2 \), and the maximum efficiency drops to \( \eta^{\text{emp}} = 1.2 \times 10^{-3} \), i.e. about a per mille. Thus, we find that including the internal dynamics of the motor \( \eta^{\text{emp}} \) is reduced from about 10% in the heuristic Mogilner case to about 1 per mille in the full motor case. The dissipation associated with the motor activity acts as a bottle neck reducing \( \eta^{\text{emp}} \). Based on the expressions in the appendix we have in figure 3 presented a 3D plot of \( \eta^{\text{emp}} \) as a function of the dimensionless parameters \( q_s \) and \( q_r \) characterizing the motor dynamics. We note that for \( q_s \) of order 100 and \( q_r \) of order 1000 \( \eta^{\text{emp}} \) reaches a plateau at around an \( \eta^{\text{emp}} \) of about 10%. In figure 4 we have depicted the corresponding contour plot of \( \eta^{\text{emp}} \) as a function of \( q_r \) and \( q_s \). Here the plateau in \( \eta^{\text{emp}} \) attained for large \( q_r \) and \( q_s \) is clearly discernible.

In the limit of large \( q_{r,s} = (\Gamma_{r,s} \langle t \rangle_{r,s})^{-1} \) we have \( \langle t \rangle_{r,s} \ll \Gamma_{r,s}^{-1} \), where \( \langle t \rangle_{r,s} \) are the residence times and \( \Gamma_{r,s}^{-1} \) are the spring relaxation times. Consequently, the motor switches rapidly between its internal states and the fluctuations about the internal length \( L(t) \) are small. Based on this approximation one can derive approximate expressions for \( q_{\text{out}} \) and \( \eta^{\text{emp}} \). The expressions are lengthy and the analysis is therefore deferred to the appendix. Among other results we find that scaling the residence times by a common factor yields invariant expressions for \( p_{\text{max}} \) and \( q_{\text{out}} \). This scaling behavior accounts for the approximately linear contours of constant \( \eta^{\text{emp}} \) at large \( q_r \) and \( q_s \), depicted in figure 4.

In figure 5 we depict in a 3D plot the EMP, denoted \( \eta^{\text{app}} \), showing strong agreement with the exact result in figure 3. The fact that the EMP is as low as a few per mille at physical motor parameters reflects the opposite limit where the residence times are larger than the spring relaxation times. In this case the motor spends a long time in the passive mode, where the internal spring is fully relaxed, waiting for the next conformational change to
Figure 4. Contour plot of the exact expression for the EMP, $\eta^{\text{emp}}$ given by (3.12), versus $q_r$ and $q_s$. The white dashed line corresponds to the condition $q_r = 13q_s$. The maximum efficiency $\eta^{\text{emp}} = 0.12$ is attained along this line for large values of $q$.

Figure 5. 3D plot of the approximate (large-$q$) expression for the EMP, $\eta^{\text{app}}$, versus $q_r$ and $q_s$, derived in section A.3.

occur. In this situation all that happens is that the load force pulls the motor backwards contributing negatively to $\eta^{\text{emp}}$.

Since the efficiency evaluated here applies to the motor per se it is instructive to consider the efficiency relative to the burning of ATP, $\eta_2$, defined by (4.3). In figure 6 we have depicted $\eta_2$ at maximum power.

5. Summary

In this paper we have discussed the efficiency of the Mogilner motor model based on protein friction in some detail [21], extending the previous analytical findings in [31] to include the energetics and efficiency. In the process we have developed a many body scheme for the evaluation of dissipation rates applied to the interplay between two coupled overdamped equations of motion and a two-step Markov process described by coupled master equations. Due to the strong dissipation concurrent with the motor operation we find in
Figure 6. 3D plot of the efficiency at maximum power relative to the ATP burning (given by $g_s\Delta \mu$ with $\Delta \mu = 15k_B T$, see (4.3)) versus $q_r$ and $q_s$. The maximum of $\eta_2 = 1.1\%$ is attained for $(q_r, q_s) = (0.7, 0.4)$.

In the biological regime an $\eta^{\text{emp}}$ of the order of 1 per mille. The dissipation associated with the medium and the protein friction acts as an effective bottle neck in the transfer of energy from the ATP hydrolysis to the power exerted on the environment. We stress that our analysis applies to the efficiency of the motor model per se and not the assembly including the attachment and hydrolysis of ATP. Including this feature would require an extension of the model; this has not been attempted in the present context.

In recent works an efficiency at maximum power, $\eta^{\text{emp}}$, approaching 100% has been reported, in marked contrast to the present results where $\eta^{\text{emp}}$ is of the order of 10% by a heuristic estimate and furthermore reduced to about 1 per mille when the motor mechanics is included properly. Refraining from a detailed discussion, see incidentally [31], it is common to all the studies cited above that the motor dynamics is not treated explicitly. The motor molecule driven by ATP hydrolysis and interacting with a track is described schematically either by a power stroke model or by a Brownian ratchet model. These studies throw light on the fundamental energy transfer in a molecular motor and can, due to their schematic nature, yield large $\eta^{\text{emp}}$. In this study the motor is modeled explicitly; the price paid, however, is a low $\eta^{\text{emp}}$ due to dissipation and an energy ‘bottle neck’ effect.

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Appendix. Evaluation of $q_{\text{out}}$

Unlike the method used in [31] where the evaluations of the mean velocity $v^0$ and the mobility $\mu$ are based on waiting time distributions, we here develop a technique directly based on transition probabilities given by the master equations (2.1) and (2.2). To ease the notation we set $s = 1$ and $r = 2$. Denoting in the following a time derivative by a dot, the master equations (2.1) and (2.2) then read $\dot{P}_1 = g_1 P_2 - g_2 P_1$ and $\dot{P}_2 = g_2 P_1 - g_1 P_2$. 

\begin{align*}
\dot{P}_1 &= g_1 P_2 - g_2 P_1 \\
\dot{P}_2 &= g_2 P_1 - g_1 P_2
\end{align*}
with stationary solutions
\begin{align}
P_1 &= \frac{g_1}{g}, \tag{A.1} \\
P_2 &= \frac{g_2}{g}, \tag{A.2} \\
g &= g_1 + g_2. \tag{A.3}
\end{align}

The conditional transition probabilities $P_{nm}(t)$ from state $n = 1, 2$ to state $m = 1, 2$ satisfy the master equations [30]
\begin{align}
\dot{P}_{11} &= g_1 P_{12} - g_2 P_{11}, \\
\dot{P}_{22} &= g_2 P_{21} - g_1 P_{22}, \\
\dot{P}_{12} &= g_2 P_{11} - g_1 P_{12},
\end{align}
and
\begin{align*}
\dot{P}_{21} &= g_1 P_{22} - g_2 P_{21}.
\end{align*}

Imposing the boundary conditions $P_{nm}(0) = \delta_{nm}$ and normalization condition $\sum_m P_{nm}(t) = 1$ we infer the solution
\begin{align}
P_{nm}(t) &= A_{nm} + B_{nm} \exp(-gt), \tag{A.4}
\end{align}
where we have introduced the matrices
\begin{align}
A &= \begin{pmatrix} P_1 & P_2 \\ P_1 & P_2 \end{pmatrix}, \\
B &= \begin{pmatrix} P_2 & -P_2 \\ -P_1 & P_1 \end{pmatrix}; \tag{A.5}
\end{align}

note that (A.4) satisfies the Chapman–Enskog equation [30]
\begin{align}
P_{nm}(t_3 - t_1) = \sum_k P_{nk}(t_2 - t_1) P_{km}(t_3 - t_2), \quad \text{for } t_1 < t_2 < t_3. \tag{A.6}
\end{align}

We also require the diagonal matrix characterizing the initial stationary distribution,
\begin{align}
P^0 &= \begin{pmatrix} P_1 & 0 \\ 0 & P_2 \end{pmatrix}. \tag{A.7}
\end{align}

Introducing the Fourier transform
\begin{align}
P_\omega &= \int_0^\infty dt \ \exp(i\omega t)(A + B \exp(-gt)), \tag{A.8}
\end{align}
we have
\begin{align}
P_\omega &= - \left( \frac{A}{i\omega} + \frac{B}{i\omega - g} \right); \tag{A.9}
\end{align}

note that with this definition $\omega$ lies in the upper half plane above the real axis and a contour integration is performed by closing the contour in the lower half plane. Also, $P_\omega$ has poles at $\omega = 0$ and $ig$.

By quadrature the equations of motion (2.5) and (2.6) with potential (2.7) yield for $f = 0$, for details see [31],
\begin{align}
v_x^0(t) &= -\frac{k(t)}{2\zeta(t)} \int_0^t dt' \ \dot{L}(t') A(t, t'), \tag{A.10} \\
v_y^0(t) &= \frac{k(t)}{2\zeta_\nu} \int_0^t dt' \ \dot{L}(t') A(t, t'), \tag{A.11} \\
A(t, t') &= \exp \left( - \int_{t'}^t d\tau \ \Gamma(\tau) \right), \tag{A.12}
\end{align}
doi:10.1088/1742-5468/2013/12/P12001
\[ \Gamma(t) = \frac{k(t)}{2} \left( \frac{1}{\zeta(t)} + \frac{1}{\zeta_v} \right). \] (A.13)

Correspondingly, in the presence of a load \( f \) we have

\[ v_x(t) = -\frac{k(t)}{2\zeta(t)\zeta_v} \int_0^t \, dt' \left( \tilde{f}(t') + \zeta_v \tilde{L}(t') \right) A(t, t'), \] (A.14)

\[ v_y(t) = \frac{k(t)}{2\zeta_v^2} \int_0^t \, dt' \left( \tilde{f}(t') + \zeta_v \tilde{L}(t') \right) A(t, t') - \frac{f}{\zeta_v}, \] (A.15)

\[ \tilde{f}(t) = f \left( 1 - 2\zeta_v \frac{k(t)}{k(t)^2} \right). \] (A.16)

**A.1. The mean heat for \( f = 0 \)**

We first turn to the evaluation of the average heat \( q_{\text{out}}^0 \) for \( f = 0 \) using the above scheme. Inserting (A.10) and (A.11) in (3.3) we obtain using (A.13)

\[ q_{\text{out}}^0(t) = \frac{1}{2} \int_0^t \, dt' \int_0^t \, dt'' \langle \tilde{L}(t') \tilde{L}(t'') A(t, t') \tilde{L}(t'') A(t, t'') \Gamma(t) k(t) \rangle. \] (A.17)

First, carrying out a partial integration, noting that the initial value \( L(0) \) will not contribute in the long time limit, we have, using \( dA(t, t')/dt' = \Gamma(t') A(t, t') \),

\[ q_{\text{out}}^0(t) = \frac{1}{2} \left( \left( L(t) - \int_0^t \, dt' \, L(t') \Gamma(t') A(t, t') \right)^2 \Gamma(t) k(t) \right). \] (A.18)

Expanding we have

\[ q_{\text{out}}^0(t) = A(t) + B(t) + C(t), \] (A.19)

where

\[ A(t) = \frac{1}{2} \langle L(t)^2 \Gamma(t) k(t) \rangle, \] (A.20)

\[ B(t) = -\int_0^t \, dt' \langle L(t') \Gamma(t') A(t, t') L(t) \Gamma(t) k(t) \rangle, \] (A.21)

\[ C(t) = \frac{1}{2} \int_0^t \, dt' \int_0^t \, dt'' \langle L(t') \Gamma(t') A(t, t') L(t'') \Gamma(t'') A(t, t'') \Gamma(t) k(t) \rangle. \] (A.22)

Inserting (A.7) and (A.9) we obtain in Fourier space

\[ A_\omega = \frac{1}{2} \sum_{nm} [P^0 P_n L^2 \Gamma k]_{nm}; \] (A.23)

we note that \( L, \Gamma, \) and \( k \) are diagonal matrices and that the sum is performed over all matrix elements.

The evaluation of \( B \) and \( C \) requires more analysis. In order to invoke the causal structure of the calculation we time order the expansion of \( A(t, t') \), i.e.,

\[ A(t, t') = \sum_{p=0} \frac{(-1)^p}{p!} \left( \int_0^t \, d\tau \, \Gamma(\tau) \right)^p = \sum_{p=0} (-1)^p T \left( \int_0^t \, d\tau \, \Gamma(\tau) \right)^p, \] (A.24)
where the time ordering $T$ is defined according to, see [32],

$$ T \left( \int_{t'}^t d\tau \Gamma(\tau) \right)^p = \int_{t'}^t dt_1 \int_{t_1}^t dt_2 \cdots \int_{t_{p-1}}^t dt_p \Gamma(t_1) \Gamma(t_2) \cdots \Gamma(t_p). \quad (A.25) $$

Considering first $B(t)$ we have

$$ B(t) = -\int_t^t dt' \sum_{p=0} (-1)^p \langle L(t') \Gamma(t') \rangle T \left( \int_{t'}^t d\tau \Gamma(\tau) \right)^p L(t) \Gamma(t)k(t), \quad (A.26) $$

and in Fourier space, noting that the time ordering corresponds to a convolution,

$$ B_\omega = -\sum_{p=0} (-1)^p \sum_{nm} \langle P^0 P_\omega L \Gamma(P_\omega \Gamma)^p P_\omega \Gamma Lk \rangle_{nm}. \quad (A.27) $$

In the case of $C(t)$ we must first time order the $t'$ and $t''$ integrations, noting that the integrand is symmetric in $t'$ and $t''$, and subsequently break up $A(t, t')$ according to $A(t, t') = A(t, t'')A(t'', t')$ in order to achieve the complete causal time ordering of the expression. We obtain in Fourier space

$$ C_\omega = \sum_{p=0} (-1)^p \sum_{q=0} (-2)^q \sum_{nm} \langle P^0 P_\omega L \Gamma(P_\omega \Gamma)^p P_\omega \Gamma L \langle P_\omega \Gamma \rangle^q P_\omega \Gamma Lk \rangle_{nm}. \quad (A.28) $$

Rearranging (A.27) and (A.28) and carrying out the binomial sums we have

$$ B_\omega = -\sum_{nm} \langle P^0 P_\omega L \Gamma P_\omega (1 + \Gamma P_\omega)^{-1} L \Gamma k \rangle_{nm}, \quad (A.29) $$

$$ C_\omega = \sum_{nm} \langle P^0 P_\omega L \Gamma P_\omega (1 + \Gamma P_\omega)^{-1} L \Gamma P_\omega (1 + 2\Gamma P_\omega)^{-1} \Gamma k \rangle_{nm}. \quad (A.30) $$

The long time behavior of $q_{\text{out}}$ is determined by the pole at $\omega = 0$. Evaluating $(1 + \Gamma P_\omega)^{-1}$ and $(1 + 2\Gamma P_\omega)^{-1}$ using the diagonal matrix $\Gamma$ with matrix elements $\Gamma_1$ and $\Gamma_2$ and $P_\omega$ given by (A.9) it is easily seen that these factors are constant for $\omega = 0$. Consequently, setting $\Gamma P_\omega (1 + \Gamma P_\omega)^{-1} = 1 - (1 + \Gamma P_\omega)^{-1}$ and $\Gamma P_\omega (1 + 2\Gamma P_\omega)^{-1} = (1/2) (1 - (1 + 2\Gamma P_\omega)^{-1})$ the factor $P_\omega$ possessing a pole at $\omega = 0$, $P_\omega \sim -A/i\omega$, governs the long time behavior. At $\omega = 0$ we obtain

$$ (1 + \Gamma P_\omega)^{-1} |_{\omega=0} = F_1 C, \quad \text{(A.31)} $$

$$ (1 + 2\Gamma P_\omega)^{-1} |_{\omega=0} = F_2 C, \quad \text{(A.32)} $$

$$ F_1 = \frac{1}{(P_1 \Gamma_1 + P_2 \Gamma_2) + \Gamma_1 \Gamma_2 / g}, \quad \text{(A.33)} $$

$$ F_2 = \frac{1}{(P_1 \Gamma_1 + P_2 \Gamma_2) + 2\Gamma_1 \Gamma_2 / g}, \quad \text{(A.34)} $$

$$ C = \begin{pmatrix} \Gamma_2 P_2 & -\Gamma_1 P_2 \\ -\Gamma_2 P_1 & \Gamma_1 P_1 \end{pmatrix}. \quad \text{(A.35)} $$

For $A_\omega$, $B_\omega$, and $C_\omega$ we then obtain the pole contributions

$$ A_\omega = -\frac{1}{2i\omega} \sum_{nm} \langle P^0 A L^2 \Gamma k \rangle_{nm}, \quad \text{(A.36)} $$

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Energetics and efficiency of a molecular motor model

\[ B_\omega = \frac{1}{i\omega} \sum_{nm} [P^0 A L (1 - F_1 C) L \Gamma k]_{nm}, \quad (A.37) \]

\[ C_\omega = -\frac{1}{2i\omega} \sum_{nm} [P^0 A L (1 - F_1 C) L (1 - F_2 C) \Gamma k]_{nm}. \quad (A.38) \]

Rewriting \( 1 - F_1 C \) and \( 1 - F_2 C \) in the form

\[ 1 - F_1 C = \frac{cI + \Gamma A}{c + \langle \Gamma \rangle}, \quad (A.39) \]

\[ 1 - F_2 C = \frac{2cI + \Gamma A}{2c + \langle \Gamma \rangle}, \quad (A.40) \]

\[ c = \frac{\Gamma_1 \Gamma_2}{g}, \quad (A.41) \]

using the identities

\[ AdA = A \langle d \rangle, \quad (A.42) \]

\[ \sum_{nm} [P^0 Ad]_{nm} = \langle d \rangle, \quad (A.43) \]

where \( d \) is a diagonal matrix, and extracting \( q^0_{\text{out}} \) from \( q^0_{\text{out}} = \int (d\omega/2\pi) \exp(-i\omega t) (A_\omega + B_\omega + C_\omega) \) by closing the contour in the lower half plane, picking up the residue from the pole at \( \omega = 0 \), we obtain after further reduction

\[ q^0_{\text{out}} = \frac{1}{2(2c + \langle \Gamma \rangle)} [(L^2 \Gamma k) - 2 \langle L \Gamma \rangle \langle L \Gamma k \rangle] \]

\[ + \frac{1}{2(c + \langle \Gamma \rangle)(2c + \langle \Gamma \rangle)} [c \langle L^2 \Gamma \rangle \langle \Gamma k \rangle + \langle L \Gamma \rangle^2 \langle \Gamma k \rangle], \quad (A.44) \]

or insertion

\[ q^0_{\text{out}} = (L_1 - L_2)^2 \frac{g_1 g_2 \Gamma_1 \Gamma_2 (k_1 \Gamma_2 (g_2 + \Gamma_1) + k_2 \Gamma_1 (g_1 + \Gamma_2))}{2(g_1 + g_2)(g(P_1 \Gamma_1 + P_2 \Gamma_2) + \Gamma_1 \Gamma_2)(g(P_1 \Gamma_1 + P_2 \Gamma_2) + 2 \Gamma_1 \Gamma_2)}. \quad (A.45) \]

**A.2. The mean heat for \( f \neq 0 \)**

We proceed to evaluate \( q_{\text{out}} \) in the presence of a load following the method above. First noting that \( \dot{\Gamma} \) is synchronized with \( \dot{L} \) we can express (A.16) in the form

\[ \frac{\dot{f}}{\zeta_v} + \dot{L} = \frac{f}{\zeta_v} + a \dot{L}, \quad (A.46) \]

\[ a = 1 - 2f \frac{k_1 - k_2}{k_1 k_2 (L_1 - L_2)}, \quad (A.47) \]

and we have performing a partial integration

\[ v_x(t) = -a \left[ L(t) + \int_0^t dt' \left( \frac{f}{a \zeta_v} - L(t) \Gamma(t) \right) A(t, t') \right] \frac{k(t)}{2 \zeta(t)}, \quad (A.48) \]

\[ v_y(t) = +a \left[ L(t) + \int_0^t dt' \left( \frac{f}{a \zeta_v} - L(t) \Gamma(t) \right) A(t, t') \right] \frac{k(t)}{2 \zeta(t)} - \frac{f}{\zeta_v}. \quad (A.49) \]

doi:10.1088/1742-5468/2013/12/P12001 17
Inserting in (3.3) and setting

\[ b = 1 - \frac{f}{a \zeta_v} (L \Gamma)^{-1}, \]  

we obtain

\[ q_{\text{out}}(t) = \tilde{A}(t) + \tilde{B}_1(t) + \tilde{B}_2(t) + \tilde{C}(t), \]  

where

\[ \begin{align*}
\tilde{A}(t) &= (a^2/2) \langle L(t)^2 \Gamma(t)k(t) \rangle - (f a / \zeta_v) \langle L(t)k(t) \rangle + (f^2 / \zeta_v), \\
\tilde{B}_1(t) &= -a^2 \int_0^t dt' \langle b(t') L(t') \Gamma(t') A(t, t') L(t) \Gamma(t) k(t) \rangle, \\
\tilde{B}_2(t) &= (fa / \zeta_v) \int_0^t dt' \langle b(t') L(t') \Gamma(t') A(t, t') k(t) \rangle, \\
\tilde{C}(t) &= (a^2 / 2) \int_0^t dt' \int_0^t dt'' \langle b(t') L(t') \Gamma(t') A(t, t') b(t'') L(t'') \Gamma(t'') A(t, t'') \Gamma(t) k(t) \rangle. 
\end{align*} \]  

We note that for \( f = 0 \) we have \( a = 1 \) and \( b = 1 \) and we recover the case for \( q_{\text{out}}^0 \). In Fourier space we obtain as above

\[ \begin{align*}
\tilde{A}_\omega &= (-1/\omega) \left( (a^2/2) \sum_{nm} [P^0 AL^2 \Gamma k]_{nm} - (fa / \zeta_v) \sum_{nm} [P^0 ALk]_{nm} + f^2 / \zeta_v \right), \\
\tilde{B}_{1\omega} &= (-1/\omega) \left( -a^2 \sum_{nm} [P^0 AbL(1 - F_1 C) \Gamma k]_{nm} \right), \\
\tilde{B}_{2\omega} &= (-1/\omega) \left( (fa / \zeta_v) \sum_{nm} [P^0 AbL(1 - F_1 C) k]_{nm} \right), \\
\tilde{C}_\omega &= (-1/\omega) \left( (a^2/2) \sum_{nm} [P^0 AbL(1 - F_1 C) bL(1 - F_2 C) \Gamma k]_{nm} \right),
\end{align*} \]  

and for \( q_{\text{out}} \)

\[ \begin{align*}
q_{\text{out}} &= (a^2/2) \sum_{nm} [P^0 AL^2 \Gamma k]_{nm} - (fa / \zeta_v) \sum_{nm} [P^0 ALk]_{nm} + f^2 / \zeta_v \\
&\quad - a^2 \sum_{nm} [P^0 AbL(1 - F_1 C) \Gamma k]_{nm} + (fa / \zeta_v) \sum_{nm} [P^0 AbL(1 - F_1 C) k]_{nm} \\
&\quad + (a^2/2) \sum_{nm} [P^0 AbL(1 - F_1 C) bL(1 - F_2 C) \Gamma k]_{nm}.
\end{align*} \]  

The final reduction proceeds as in the case above for \( q_{\text{out}}^0 \). We obtain

\[ q_{\text{out}} = \frac{a^2}{2} \langle bL^2 \Gamma k \rangle - \frac{fa}{\zeta_v} \langle Lk \rangle + \frac{f^2}{\zeta_v} - \frac{a^2}{c + \langle \Gamma \rangle} (c \langle bL^2 \Gamma k \rangle + \langle bL \Gamma \rangle \langle L \Gamma k \rangle) \\
+ \frac{fa}{\zeta_v (c + \langle \Gamma \rangle)} (c \langle bLk \rangle + \langle bL \Gamma \rangle \langle k \rangle) + \frac{a^2}{2(c + \langle \Gamma \rangle)(2c + \langle \Gamma \rangle)} \\
\times \left[ \langle bL \Gamma \rangle^2 \langle \Gamma k \rangle + c \langle b^2 L^2 \Gamma \rangle \langle \Gamma k \rangle + 2c \langle bL \Gamma \rangle \langle bL \Gamma k \rangle + 2c^2 \langle b^2 L^2 \Gamma k \rangle \right]. \]  

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A.3. The large $q$ limit, $q_r \gg 1$, $q_s \gg 1$

The $q$ factors are defined by

$$
q_r = \frac{g_r}{\Gamma_r} = \frac{1}{\Gamma_r \langle t \rangle_r},
$$

(A.62)

$$
q_s = \frac{g_r}{\Gamma_s} = \frac{1}{\Gamma_s \langle t \rangle_s},
$$

(A.63)

where $\Gamma_r^{-1}$ and $\Gamma_s^{-1}$ are the spring relaxation times in the R and S states, while $\langle t \rangle_r$ and $\langle t \rangle_s$ are the residence times in R and S. In this subsection we consider the case where $\langle t \rangle_r \ll \Gamma_r^{-1}$ and $\langle t \rangle_s \ll \Gamma_s^{-1}$. The motor then switches rapidly between its internal states and reaches a steady state, where the spring has an almost fixed length $L$, which is pulled a little longer during the R-stage and retracts by a corresponding amount during the S-stage. From (2.8) it follows that the equations of motion for the relative coordinates have the form

$$
\dot{y} - \dot{x} = -\Gamma_r (y - x - L_r) + \frac{f}{\zeta_p} \text{ in the R state,}
$$

(A.64)

$$
\dot{y} - \dot{x} = -\Gamma_s (y - x - L_s) + \frac{f}{\zeta_v} \text{ in the S state.}
$$

(A.65)

The condition that the spring length does not change during a full R + S cycle is

$$
\left( \Gamma_r (L_r - L) + \frac{f}{\zeta_p} \langle t \rangle_r \right) \langle t \rangle_r + \left( -\Gamma_s (L - L_s) + \frac{f}{\zeta_v} \langle t \rangle_s \right) \langle t \rangle_s = 0,
$$

(A.66)

yielding the effective spring length $L$,

$$
L = \frac{q_s L_r + q_r L_s + c f}{q_r + q_s},
$$

(A.67)

where

$$
c = q_s q_r \left( \frac{\langle t \rangle_r}{\zeta_p} + \frac{\langle t \rangle_s}{\zeta_v} \right). \tag{A.68}
$$

The work done during a cycle is given as the force $f$ times the distance traveled by the center of mass. Since $x$ and $y$ move in unison we insert the equation of motion for $y$ in (2.6),

$$
(\langle t \rangle_r + \langle t \rangle_s) p = f \left( -\langle t \rangle_r \frac{k_r}{2\zeta_v} (L - L_r) - \langle t \rangle_s \frac{k_s}{2\zeta_v} (L - L_s) \right)
$$

$$
= \frac{f}{2\zeta_v (q_r + q_s)} (a - bf), \tag{A.69}
$$

where the parameters $a$ and $b$ are given by

$$
a = (k_r \langle t \rangle_r q_r - k_s \langle t \rangle_s q_s)(L_r - L_s) = \tilde{\zeta}_v (L_r - L_s), \tag{A.70}
$$

$$
b = c(k_r \langle t \rangle_r + k_s \langle t \rangle_s) = \frac{c \zeta_v}{q_r q_s} (2\tilde{q}_s + q_r) \tag{A.71}
$$

$$
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$$
\[
\tilde{\zeta}_v = \zeta_v \frac{\zeta_p - \zeta_v}{\zeta_p + \zeta_v}, \tag{A.72}
\]
\[
\tilde{q}_s = q_s \frac{\zeta_p}{\zeta_p + \zeta_v}. \tag{A.73}
\]

For the maximum power \(p_{\text{max}}\) at force \(f_{\text{max}}\) we then have
\[
f_{\text{max}} = \frac{a}{2b}, \tag{A.74}
\]
\[
(\langle t \rangle_r + \langle t \rangle_s)p_{\text{max}} = \frac{a^2}{8b(q_t + q_s)} = \frac{\tilde{\zeta}_v^2}{\zeta_v} \frac{q_t q_s (L_r - L_s)^2}{8c(q_t + q_s)(2\tilde{q}_s + q_t)}. \tag{A.75}
\]

The dissipated energy is given by
\[
(\langle t \rangle_r + \langle t \rangle_s)q_{\text{out}} = \langle t \rangle_t \left[ \frac{1}{\zeta_p} \left( \frac{k_r}{2} (L - L_r) - f \right)^2 + \frac{1}{\zeta_v} \left( \frac{k_v}{2} (L - L_v) \right)^2 \right] + \langle t \rangle_s \frac{1}{\zeta_v} \left[ \left( \frac{k_r}{2} (L - L_r) - f \right)^2 + \left( \frac{k_s}{2} (L - L_s) \right)^2 \right]. \tag{A.76}
\]

Inserting the relations
\[
L - L_r = -(L_r - L_s)q_t \frac{1 - \phi_1}{q_t + q_s}, \tag{A.77}
\]
\[
L - L_r - 2f_{\text{max}}/k_r = -(L_r - L_s)q_t \frac{1 - \phi_2}{q_t + q_s}, \tag{A.78}
\]
\[
L - L_s = (L_r - L_s)q_s \frac{1 + \phi_3}{q_t + q_s}, \tag{A.79}
\]
\[
L - L_s - 2f_{\text{max}}/k_s = (L_r - L_s)q_s \frac{1 + \phi_4}{q_t + q_s}, \tag{A.80}
\]
where
\[
\phi_1 = \frac{\tilde{\zeta}_v q_s}{2\zeta_v (2\tilde{q}_s + q_t)}, \tag{A.81}
\]
\[
\phi_2 = \phi_1 \left( 1 - 2\frac{q_t + q_s}{ck_r} \right), \tag{A.82}
\]
\[
\phi_3 = \frac{\tilde{\zeta}_v q_t}{2\zeta_v (2\tilde{q}_s + q_t)}, \tag{A.83}
\]
\[
\phi_4 = \phi_3 \left( 1 - 2\frac{q_t + q_s}{ck_s} \right). \tag{A.84}
\]
we finally arrive at
\[
(p_{\text{max}})_{\text{out}} = \left( \frac{L_r - L_s}{4(q_r + q_s)} \right)^2 \left[ \frac{2q_r k_r}{1 + \zeta_p / \zeta_r} \left( \frac{\zeta_r}{\zeta_p} (1 - \phi_2) + (1 - \phi_1)^2 \right) \right. \\
\left. + q_s k_s ((1 - \phi_4) + (1 - \phi_3)^2) \right]. \tag{A.85}
\]

It follows from this expression that scaling the residence times by the same factor leads to invariant expressions for \(p_{\text{max}}\) and \(q_{\text{out}}\) which explains the linear contours of constant EMP seen at large \(q_s\) in figure 4. In figure 5 the approximate EMP (=1/(1 + \(q_{\text{out}}/p_{\text{max}}\))) corresponding to equations (A.75) and (A.85) is plotted. The similarity with figure 3 is striking.

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