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Abstract
We propose an efficiency measure for diffusion-mediated transport processes
including molecular-scale engines such as Brownian motors (BMot) moving
in ratchet potentials acting as mechanical 'rectifiers'. The efficiency measure
is based on the concept of 'minimal energy required to complete a task' and is
defined via a class of stochastic optimal control problems. The underlying
objective function depends on both the external force field (i.e. the fluctuation
rectifier in the case of BMot) and the amplitude of the environmental noise.
Ultimately, the efficiency measure can be directly interpreted as the relative
entropy between two probability distributions, namely: the distribution of the
particles in presence of the external rectifying force field and a reference
distribution describing the behaviour in the absence of the rectifier.

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1. Introduction

Despite the already vast available literature, the fact that micro-particles immersed in a noisy
environment can be transported by an *ad hoc* rectification of the fluctuations, continues
to attract attention directed towards applications [1]. The operations of these diffusion-
mediated devices, which essentially act as mechanical diodes, require basically (i) a fluctuating
environment and (ii) a fluctuation rectifier which is driven by an external energy input. This
mechanism is able to generate a net particle current which can be sustained even in the presence
of an opposing force (i.e. an external load). It is therefore possible to extract a net useful work
from these devices, a property appealing for applications in the molecular and microscopic
size ranges. The possibility to extract work allows us to use the word *motors* and also suggests
that a suitable efficiency measure, namely the *motor efficiency* (ME), should be defined for
these devices—this is the goal of the present contribution.

Yet, the issue of efficiency of molecular motors has been and remains an important topic on its own (see e.g., [1] chapter 6.9 and [2, 3]). The main difficulty here is that on the microscopic scale the fluctuations do, simultaneously, favour and hinder the transport process. The external energy injected into the system is indeed dissipated via two mechanisms, (i) the driving energy itself responsible for the transport process and (ii) the heating of the medium which hinders the directed transport thanks to the fluctuation–dissipation relation.

In view of the conjugate actions played by the fluctuations, the study of energetics requires a precise formulation of what the energy output of the system really is. Here we essentially adopt the point of view of Dérenyi *et al* [4] which identifies the energy output with the *minimum energy input* E_{in}^{min} required to accomplish the same task as the molecular motor. Following [4], the generalized efficiency η is defined as

$$\eta = E_{in}^{min} / E_{in}, \tag{1}$$

where E_{in} is the external energy input.

The aim of this paper is to derive a new *systematic method* to characterize the efficiency of the molecular motor. This will be achieved via a stochastic optimal control approach in which the objective function combines the conjugate actions of transport and dissipation.

Formally, assume that a molecular motor operates according to the Langevin dynamics

$$\gamma \, dX_t = (-V'(X_t, t) - F) \, dt + \sigma(X_t, t) \, dB_t, \tag{2}$$

which describes a Brownian particle in an overdamped regime (i.e. inertia is neglected). The stochastic equation is interpreted in the Stratonovich sense (see [5] for an account of Itô–Stratonovich modelling in the context of molecular motors) and models the so-called Brownian motor (BMot). Here dB_t stands for $1D$ standard Brownian motion, $\sigma(x, t) = \sqrt{2\gamma k_B T(x, t)}$ controls the diffusion process with k_B being Boltzmann's constant, $T(x, t)$ the absolute temperature field and γ is the viscous friction coefficient. F is a constant force modelling an external load and $V(x, t)$ is the 'ratchet' potential through which the fluctuations are 'rectified'.

The net effect of the rectifying force given by $-V'(X_t, t)$ is to drive an initial probability distribution δ_{x_0} at time $t = 0$ to a final distribution μ_τ at time $\tau > 0$. In practice, there is a great freedom in choosing rectifying forces able to complete this task. Hence the natural idea behind the efficiency concept is to compare $-V'(x, t)$ to an optimal drift field $u(x, t)$ which operates a similar task (namely transporting δ_{x_0} to μ_τ within a time τ) and simultaneously minimizes the objective functional

$$u \mapsto J_\tau(u) = \frac{1}{2} \mathbb{E}_{x_0} \int_0^\tau \left(\frac{u(X_t^u, t)}{\sigma(X_t^u, t)} \right)^2 \, dt, \tag{3}$$

where X_t^u is evolving as

$$\gamma \, dX_t^u = (u(X_t^u, t) - F) \, dt + \sigma(X_t^u, t) \, dB_t. \tag{4}$$

Note that the objective functional (sometimes called the cost functional) depends on the stochastic dynamics via both the drift u and the diffusion σ fields. Due to the structure of the cost functional, transport with small diffusion is very costly—a property which reflects the diffusion-mediated transport processes where fluctuations directly participate to the driving of particles. Define now the optimal rectifier $u^*(x, t)$ force field to be the one, able to achieve the transporting task, namely $\delta_{x_0} \mapsto \mu_\tau$ while minimizing the global value function $J_\tau(u^*)$ given by equation (3). With such an optimal rectifier at hand, the generalized efficiency of a BMot subject to a potential V satisfying $0 < J_\tau(V') < \infty$, is now simply defined as

$$\eta(\tau) = \frac{J_\tau(u^*)}{J_\tau(V')}. \tag{5}$$

The ME $\eta(\tau)$ compares the expected costs incurred by both the optimal trajectories $X_t^{u^*}$ and the actual motor trajectories X_t and therefore takes fully into account the probabilistic nature of the underlying process. This is, we believe, the conceptual advantage of the present approach over the one proposed in [4] where the minimum energy input is defined via a purely mechanical view not explicitly invoking the underlying stochastic dynamics.

From a mathematical point of view, the efficiency parameter given by equation (5) is well defined. It directly relies on the possibility of assigning a unique Markov process to given initial and final distributions (here δ_{x_0} and μ_τ)—a problem first formulated by Schrödinger in [6]. A mathematically rigorous exposition of this program has been given by Dai Pra [7]. The optimal control interpretation of the stochastic dynamics is thereby realized by the concept of logarithmic transformations introduced by Jamisson [8] and Flemming [9]. Using this approach, the minimal value $J_\tau(u^*)$—entering the definition of $\eta(\tau)$—coincides with the relative entropy $K(\mu_\tau, \overline{\mu}_\tau)$ between the distributions μ_τ and $\overline{\mu}_\tau$ with $\overline{\mu}_\tau$ being the probability distribution at time τ describing the position $\overline{X}_\tau$ of a particle evolving under the control free dynamics

$$\gamma \, d\overline{X}_t = -F \, dt + \sigma(\overline{X}_t, t) \, dB_t, \qquad \overline{X}_0 = x_0 \in \mathbb{R}. \tag{6}$$

The efficiency of the Brownian motor then reads

$$\eta(\tau) = K(\mu_\tau, \overline{\mu}_\tau)/J_\tau(V'). \tag{7}$$

This way of writing the ME, which is equivalent to equation (5), does not explicitly use the underlying control and is therefore intrinsic. Its connection with the control problem relies on the remarkable property that both

 (i) the quasi-free evolution, i.e. the evolution in absence of an external potential given by equation (6) and
 (ii) the evolution under the optimal control u^*

produce identical families of 'most probable paths' [7]. The concept of 'most probable path' is based on a variational principle applicable for Langevin equations driven by White Gaussian Noise. The associated transition probability measures (i.e. the solutions of the relevant Fokker–Planck equations) can be expressed as the weighted sum of random trajectories with given initial and final conditions. The relative weights entering the summation directly depend upon the drift and the diffusion coefficients and are expressed by the Onsager–Machlup functional [10]. Intuition suggests that the more probable a particular trajectory is, the more effectively it will contribute to the global value function. The fact that the most probable path under u^* coincides with the most probable path under the quasi-free dynamics physically shows that the optimal control u^* does in fact interfere as little as possible with the most probable trajectory of the quasi-free dynamics.

The paper is organized as follows. In section 2, we specify the hypothesis of the BM-model, state the optimal control problem and recall its solution. In section 3 we calculate the efficiency for a generic class of examples and indicate how to construct optimal rectifiers.

2. Problem formulation

Consider the controlled diffusion process $X^u(t)$ defined on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$ that solves the following Stratonovich stochastic differential equation:

$$\gamma \, dX_t^u = \left(u(X_t^u, t) - F\right) dt + \sigma\left(X_t^u, t\right) dB_t. \tag{8}$$

Formally, the above Langevin equation is obtained by replacing in equation (2) the force field $-V'(x, t)$ by a control $u(x, t)$. The efficiency measure to be constructed relies on the following optimal control problem:

Problem (P). Find an admissible control $u^*(x, t)$ such that

(1) $X_0^{u^*}$ is distributed according to δ_{x_0} and $X_\tau^{u^*}$ according to μ_τ,
(2) between all admissible controls satisfying (1), the control u^* minimizes the energy cost functional

$$u \mapsto J_\tau(u) = \frac{1}{2} \mathbb{E} \int_0^\tau \left(\frac{u\left(X_t^u, t\right)}{\sigma\left(X_t^u, t\right)} \right)^2 \, dt. \tag{9}$$

Remarks

(a) In order for equation (8) to admit a unique, t-continuous strong solution $X^u(t)$, σ and u must satisfy the following classical assumptions: σ and u are linearly bounded in x uniformly for $t \in [0, \tau]$ and satisfy a Lipschitz condition in x for every fixed $t \in [0, \tau]$. These conditions ensure the uniqueness of X_t^u and are supposed to hold from now on. In the autonomous case i.e., when both u and σ do not explicitly depend on time, existence and uniqueness of the solution are already guaranteed for $u, \sigma \in \mathcal{C}^1(\mathbb{R})$ [11].

(b) A control $u(X_t(\cdot), t) : \Omega \to \mathbb{R}$ is admissible if: (i) u satisfies the regularity conditions stated in (a), (ii) u is adapted to the filtration $\mathcal{F}_t = \sigma\{X_t^u\}$ and (iii) $J_\tau(u) < \infty$. The potential V entering equation (2) is supposed to be admissible and non-trivial i.e. $J_\tau(V') > 0$.

(c) A similar approach also holds for non-deterministic initial distributions μ_0. The only restriction on μ_0 is the existence of a finite second moment, i.e. $\int x^2 \mu_0(dx) < \infty$. In this case, the problem (P) does still have a well defined solution.

(d) The Stratonovich stochastic differential equation (8)—commonly encountered in physical modelling where the white Gaussian noise is viewed as the limit of shortly correlated coloured noises—is equivalent to the Itô stochastic differential equation:

$$\gamma \, dX_t^u = \left[u\left(X_t^u, t\right) - F + \tfrac{1}{2}\sigma'\left(X_t^u, t\right)\sigma\left(X_t^u, t\right) \right] dt + \sigma\left(X_t^u, t\right) dB_t, \tag{10}$$

which, due to the fact that the noise term is a martingale, is more frequently used in control theory.

For $0 \leqslant s < t \leqslant \tau$ and $y, x \in \mathbb{R}$, denote by $q(s, y, t, x)$ the fundamental solution to the backward Fokker–Planck equation of the Markov process $\overline{X}_t$ defined in equation (6):

$$\frac{\partial}{\partial t} q(s, y, t, x) = L q(s, y, t, x), \qquad 0 \leqslant s < t \leqslant \tau \tag{11}$$

$$q(s, y, s, x) = \delta_{x,y} \tag{12}$$

where the operator $L(\cdot)$ is

$$L(\cdot) = \left[-F + \frac{1}{2}\sigma'(x, t)\sigma(x, t) \right] \frac{\partial(\cdot)}{\partial x} + \frac{1}{2}\sigma(x, t)^2 \frac{\partial^2(\cdot)}{\partial x \partial x}. \tag{13}$$

For μ and ν, two probability distributions on the real line, write $d\nu/d\mu$ for the Radon–Nykodim derivative of ν with respect to μ (i.e. ν is assumed to be absolutely continuous with respect to μ). Introduce now the relative entropy (also known as the Kullback 'distance' [12]) $K(\mu, \nu)$ which quantifies the 'discrepancy' between μ and ν:

$$K(\mu, \nu) = \int_\mathbb{R} \log\left(\frac{d\mu}{d\nu} \right) d\mu. \tag{14}$$

The 'distance' $K(\cdot, \cdot)$ is commonly used for fitting and classifying statistical models, hypothesis testing and risk minimization. In the context of our minimization problem (P), we have the following central result (theorem 3.1 in [7]):

Theorem. *Suppose that $K(\mu_\tau, \overline{\mu}_\tau) < \infty$ and define $h : \mathbb{R} \times [0, \tau] \to \mathbb{R}$ by*

$$h(x, t) = \int_\mathbb{R} q(t, x, \tau, z) \frac{\mathrm{d}\mu_\tau}{\mathrm{d}\overline{\mu}_\tau}(z) \, \mathrm{d}z.$$

Then

(a) $u^*(x, t) = \sigma^2(x, t) \frac{\partial}{\partial x} \log(h(x, t))$ solves the control problem (P) and
(b) $J_\tau(u^*) = K(\mu_\tau, \overline{\mu}_\tau)$.

This result has three implications of practical relevance for the transport processes under study, namely:

(1) It establishes that the ME $\eta(\tau)$ takes values between 0 and 1 (remember that $J_\tau(u)$ is positive). Moreover, $\eta(\tau)$ takes its maximum value 1 exactly if the motor realizes its task $(\delta_{x_0} \to \mu_\tau)$ in the energetically most favourable way.
(2) It allows an intrinsic (i.e. control free) definition of the efficiency:

$$\eta(\tau) = K(\mu_\tau, \overline{\mu}_\tau)/J_\tau(V'), \tag{15}$$

which relates the relative entropy between the distribution of the particle subject to V and the distribution of the quasi-free particle with the expected cumulated costs $J_\tau(V')$.
(3) It furnishes an explicit formula for u^* which can be used as a theoretical guideline to physically realize *optimal* motors.

3. Applications for a class of pulsating potentials

In the couple of examples which follow, we suppose that the Brownian particle is released at time $t = 0$ from $X_0 = 0$ and evolves under the isothermal dynamics:

$$\gamma \, \mathrm{d}X_t = [-V'(X_t, \varphi(t)) - F] \, \mathrm{d}t + \sqrt{2\gamma^2 D_0} \, \mathrm{d}B_t, \tag{16}$$

with $D_0 = \frac{k_B T}{\gamma}$ constant. The next example 3.1 deals with a pulsating potential $V(x, \varphi(t))$ which is space periodic with period L and where $\varphi(t)$ is either a periodic or a stochastic function of time. We calculate η in the central limit regime. In 3.2. we impose the optimal efficiency $\eta = 1$ (i.e. the BMot operates under optimal conditions) and derive the associated optimal force field.

3.1. The efficiency for a pulsating potential in the central limit regime

Consider a Brownian particle evolving according to the working model for pulsating ratchets given by equation (16) (see e.g., [1] chapter 3.3 for a classification scheme for BMot). We make the simplifying assumption that $\varphi(t)$ is either periodic in t with a unique periodic long-time behaviour or a stationary stochastic process independent of the Brownian motion $\mathrm{d}B_t$. This allows us, on a sufficiently coarse grained space-scale ($\gg L$), to approximately view the evolution as the succession of single, independent and identically distributed hopping events ([1] p 88). Invoking the central limit theorem, the particle distribution for large τ approaches a Gaussian measure μ_τ with the density

$$f(x, \tau) = \frac{1}{\sqrt{4\pi D_{\mathrm{eff}}\tau}} \exp\left(-\frac{[(a\tau - x)^2]}{4D_{\mathrm{eff}}\tau}\right), \tag{17}$$

where $a = \lim_{t \to \infty} X_t/t$ is the average particle current and $D_{eff} = \lim_{t \to \infty} (\langle X_t^2 \rangle - \langle X_t \rangle^2)/(2t)$ is the effective diffusion coefficient—both quantities can be measured in actual applications [13].

According to equation (6), the quasi-free particle evolves under the dynamics

$$\overline{X}_t = -\frac{F}{\gamma}t + \sqrt{2D_0}B_t. \tag{18}$$

Its distribution $\overline{\mu}_\tau$ at τ is therefore a Gaussian measure with the density

$$\overline{f}(x, \tau) = \frac{1}{\sqrt{4\pi D_0 \tau}} \exp\left(-\frac{[x - \frac{F}{\gamma}\tau]^2}{4D_0 \tau}\right). \tag{19}$$

The relative entropy of the two Gaussian measure equations (17) and (19) reads

$$\begin{aligned} K(\mu_\tau, \overline{\mu}_\tau) &= \int_{\mathbb{R}} \ln(f(x, \tau)/\overline{f}(x, \tau)) f(x, \tau)\, dx \\ &= \frac{(F/\gamma - a)^2}{4D_0}\tau + \left\{\frac{1}{2}\ln\left(\frac{D_0}{D_{eff}}\right) + \frac{D_{eff} - D_0}{2D_0}\right\}. \end{aligned} \tag{20}$$

This expression, valid for large τ, enables us to separately appreciate the influence of the potential V on the particles current and on the rectifying process. The first term describes the external energy input necessary to maintain the particles current a. The symmetry in the difference $F/\gamma - a$ shows that exceeding or undergoing the quasi-free current F/γ by the amount $|F/\gamma - a|$ requires the same energy input. The second contribution—non-negative as the former one—is related to the part of the energy input required to get an effective diffusion D_{eff}. In contrast to the current difference $F/\gamma - a$, the diffusion difference $D_0 - D_{eff}$ contributes non-symmetrically to the relative entropy. Setting

$$H(D_{eff}) := \ln\left(\frac{D_0}{D_{eff}}\right) + \frac{D_{eff} - D_0}{D_0}, \tag{21}$$

we indeed have

$$H(D_0 - \Delta) > H(D_0 + \Delta), \qquad \Delta \in (0, D_0). \tag{22}$$

Hence, rectifying the diffusion to ensure that $D_{eff} = D_0 - \Delta$ with $\Delta \geqslant 0$ costs more than to let it increase by the same amount (i.e. $D_{eff} = D_0 + \Delta$). In the limiting case where V 'ties down' the effective diffusion to zero, we have $H(0) = \infty$ and consequently, the relative entropy $K(\mu_\tau, \overline{\mu}_\tau)$ becomes infinite.

On the other hand, the cost functional for the given potential is

$$\begin{aligned} J_\tau(V') &= \frac{1}{4\gamma k_B T_0}\mathbb{E}\int_0^\tau V'(X_t)^2\, dt \\ &= \frac{\tau}{4\gamma^2 D_0}\mathbb{E}\frac{1}{\tau}\int_0^\tau V'(X_t)^2\, dt, \end{aligned} \tag{23}$$

which due to ergodicity behaves asymptotically as

$$J_\tau(V') \simeq \frac{\tau}{4\gamma^2 D_0}\langle V'^2 \rangle, \tag{24}$$

where the ensemble mean $\langle V'^2 \rangle$ is taken over one space period of V. Using equations (20) and (24), we have

$$\eta(\tau) = \frac{K(\mu_\tau, \overline{\mu}_\tau)}{J_\tau(V')} = \frac{(F - \gamma a)^2}{\langle V'^2 \rangle} + \mathcal{O}\left(\frac{1}{\tau}\right) \tag{25}$$

where explicitly the $\mathcal{O}\left(\frac{1}{\tau}\right)$ term is given by

$$\mathcal{O}\left(\frac{1}{\tau}\right) = \frac{1}{\tau}\frac{2\gamma^2 D_{\text{eff}}}{\langle V'^2\rangle}\left(1 + \frac{D_0}{D_{\text{eff}}}\left[\ln\left(\frac{D_0}{D_{\text{eff}}}\right) - 1\right]\right). \tag{26}$$

In the central limit regime, reached for $\tau \to \infty$, only the part contributing to the transport process influences the efficiency measure, namely:

$$\eta(\tau) = \frac{(F - \gamma a)^2}{\langle V'^2\rangle}, \qquad \text{for} \quad \tau \to \infty. \tag{27}$$

Remarks.

(a) The efficiency $\eta(\tau)$ compares an effective driving force, namely the difference between the load and the drag force with the external force field.

(b) The parameters F, γ, V', D_0, a and D_{eff} entering equations (26) and (27) are experimentally measurable as it is discussed in [13]. Hence, the efficiency $\eta(\tau)$ can be calculated for actual applications. Note in addition that the time series of motor positions, measurable with the current bioengineering technology, allow us to solve a reverse problem, namely to reconstruct the rectifying potential V [14].

(c) When $\varphi(t) \equiv 0$, equation (16) models a so-called tilted pulsating potential. In this case the asymptotic analysis can be pushed further. Indeed in this case both a and D_{eff} are analytically related to the modelling parameters entering equation (16) through [15]:

$$a = \frac{1 - e^{-LF/k_B T}}{\frac{1}{L}\int_0^L dx\, I_+(x)}, \tag{28}$$

$$D_{\text{eff}} = D_0 \frac{\frac{1}{L}\int_0^L dx\, I_+(x)^2 I_-(x)}{\left(\frac{1}{L}\int_0^L dx\, I_+(x)\right)^3} \tag{29}$$

with

$$I_\pm(x) = \frac{1}{D_0}\int_0^L dy \exp(\pm V(x) \mp V(x \mp y) - yF)/(k_B T). \tag{30}$$

From equation (28) we directly see that for a vanishing load $F \to 0$, the efficiency consistently vanishes. Indeed no work can be done in the absence of load.

3.2. Conceiving efficient Brownian motors

As stated by Derényi *et al* [4], it is only a matter of time before molecular motors will be currently manufactured. One therefore is potentially interested in building highly efficient transport motors. Starting from the quasi-free dynamics

$$d\overline{X}_t = -\frac{F}{\gamma}dt + \sqrt{2D_0}\,dB_t \tag{31}$$

with F, γ and D_0 constant, let us construct an optimal force field $u^*(x, t)$ realizing $\eta(\tau) = 1$. The fundamental solution to the associated backward evolution equation (11) is

$$q(s, y, t, x) = \frac{1}{\sqrt{4\pi D_0(t - s)}}\exp\left(-\frac{\left[((x - y) - \frac{F}{\gamma}(t - s))^2\right]}{2D_0(t - s)}\right) \tag{32}$$

and $\overline{\mu}_\tau$ is Gaussian with density $\overline{f}(x,\tau) = \int_{\mathbb{R}} q(0,y,\tau,x)\delta_0(\mathrm{d}y) = q(0,0,\tau,x)$. The minimum energy control $u^*(x,t)$ is now

$$u^*(x,t) = 2D_0 \frac{\partial}{\partial x} \ln\left(\int_{\mathbb{R}} q(t,x,\tau,z) \frac{f(z,\tau)}{q(0,0,\tau,z)} \,\mathrm{d}z \right), \tag{33}$$

which after lengthy but elementary calculations yields

$$u^*(x,t) = \frac{D_0\left(\frac{F}{\gamma}t - x - \tau\left(a - \frac{F}{\gamma}\right)\right)}{D_0(\tau - t) + D_{\mathrm{eff}}\tau}. \tag{34}$$

Setting $\frac{F}{\gamma} = a$ and $D_{\mathrm{eff}} = D_0$ and prolonging $u(x,t)$ periodically in x resp. t with period L resp. τ to $\mathbb{R} \times \mathbb{R}_+$, we find the optimal drift field

$$u^*(x,t) = \frac{at - x}{2\tau - t}, \qquad 0 \leqslant x \leqslant L, \quad 0 \leqslant t \leqslant \tau$$

$$u^*(x+L,t) = u^*(x,t), \qquad u^*(x,t+\tau) = u^*(x,t).$$

As it stands, $u^*(x,t)$ is linear in x and depends explicitly on time. Note that the space-linearity is expected from the fact that in this case the initial and final measures are both Gaussian. The time-dependent drift field $u^*(x,t)$ defines an evolution belonging to the class of travelling ratchets (according to the classification in [1]) and might serve as a simple guideline in the attempts to actually realize isothermal molecular motors.

4. Conclusions

The stochastic optimal control formalism is well suited to define an efficiency measure for diffusion-mediated transport processes governed by the Langevin dynamics. The objective function to be minimized combines, in a single functional, the competing effects of the drift and diffusion forces responsible for the transport process. The explicit construction of the optimal force field that minimizes the objective functional, offers a rigorous and systematic way to conceive efficient diffusion-mediated transport devices.

Acknowledgments

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