Similarities and differences between non-equilibrium steady states and time-periodic driving in diffusive systems

D M Busiello, C Jarzynski and O Raz

1 Dipartimento di Fisica 'G. Galilei', Università di Padova, Via Marzolo 8, I-35131 Padova, Italy
2 Institute for Physical Science and Technology, University of Maryland, College Park, MD 20742, United States of America
3 Department of Chemistry and Biochemistry, University of Maryland, College Park, MD 20742, United States of America
4 Department of Physics, University of Maryland, College Park, MD 20742, United States of America
5 Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot, 76100, Israel

Abstract

A system that violates detailed balance evolves asymptotically into a non-equilibrium steady state (NESS) with non-vanishing currents. Analogously, when detailed balance holds at any instant of time the system is driven through time-periodic variations of external parameters, it evolves toward a time-periodic state, which can also support non-vanishing currents. In both cases the maintenance of currents throughout the system incurs a cost in terms of entropy production. Here we compare these two scenarios for one dimensional diffusive systems with periodic boundary condition, a framework commonly used to model biological and artificial molecular machines. We first show that the entropy production rate in a periodically driven system is necessarily greater than that in a stationary system without detailed balance, when both are described by the same (time-averaged) current and probability distribution. Next, we show how to construct both a NESS and a periodic driving that support a given time averaged probability distribution and current. Lastly, we show that although the entropy production rate of a periodically driven system is higher than that of an equivalent steady state, the difference between the two entropy production rates can be tuned to be arbitrarily small.

1. Introduction

A system that is coupled to a thermal environment generically relaxes to an equilibrium state, in which its interesting properties can be calculated using the standard tools of statistical mechanics and thermodynamics. A similar unifying theory for all non-equilibrium phenomena is still lacking, although systems out of equilibrium have been investigated from various broad perspectives, including linear response theory [1, 2], relaxation towards equilibrium [3], fluctuation theorems [4, 5], non-equilibrium steady states (NESS) [6] and systems with time-periodic driving [7–9]. Many interesting results have been established within each of these frameworks, but much remains to be understood about the similarities and the differences between them.

Systems that are constantly maintained away from equilibrium are of particular interest in biology and nano-science. There are two common ways to maintain a system out of equilibrium for arbitrarily long times: in the first, the system of interest is coupled to multiple environments, e.g. baths with different equilibrium properties such as temperature, chemical potential or voltage. In such cases, the constant fluxes between the baths drive the system into a steady state that is out of equilibrium, as it can only be maintained at the cost of thermodynamic resources (heat, fuel, photons, etc) provided by the baths. These steady states are commonly referred to as NESS, and they are used to model a variety of biological processes, from photosynthesis [10] in which photons are consumed in the carbon fixation process, through the synthesis of ATP by an ATP-synthase where the chemical potential difference of H⁺ ions across membrane is used to convert ADP + P_i into ATP [11, 12], to molecular motors as kinesin [13] that consume ATP molecules and generate directed motion for the transport of molecular cargo.
An alternative method to maintain a system out of equilibrium is to vary, periodically with time, one or more parameters of the system, environment or the coupling between them. This type of driving is often referred to as stochastic pumping or thermal ratcheting. Stochastic pumps (SP) provide simple models of classical and quantum heat engines [14–16] or of the driving mechanism in artificial molecular motors [7, 8, 17–19], where periodic changes in macroscopic parameters such as temperature, pressure and pH keep the motor operating.

Both NESS and SP are characterized by the existence of non-vanishing currents, a non-vanishing entropy production in the environment and a non-equilibrium probability distribution. It is therefore natural and potentially fruitful to ask: are SP and NESS essentially equivalent in terms of currents, probabilities and entropy production? In other words—can any current, probability distribution and entropy production achievable using one type of driving also be achieved with the other type as well? In terms of potential applications, this question can be stated as follows: can an artificial molecular motor driven by periodic changes in the environment exactly mimic a biological molecular motor driven by consuming fuel? For finite-state systems, this question has been recently addressed in [20], where it was shown that SP and NESS are equivalent—both systems can in principle have the same time-averaged probabilities, currents and entropy production rates. Interestingly, however, they are not equivalent in terms of fluctuations [21]: to match the current fluctuations of a NESS, SP must have a higher entropy production. Moreover, it was recently discovered that the average rate of entropy production bounds the fluctuations of any thermodynamic current in a NESS [22, 23]; in contrast, a SP can be designed to achieve arbitrary entropy production rate and current fluctuations [24, 25]. This implies that it is not generally possible to map the current, the cost in terms of entropy production and the precision in terms of current fluctuations between the two scenarios.

In this manuscript we extend the NESS-SP comparison to overdamped systems that evolve diffusively in one dimension, whose dynamics are described by a Fokker–Planck equation on a ring. For artificial molecular motors, this model is typically more accurate than the discrete state case, which can be viewed as a coarse-grained version of a diffusive system. In the context of ‘no pumping theorems’, a similar extension from discrete state models [26–32] to diffusive systems [33] revealed a complete analogy between the two models.

As we show below, in the context of controllability, diffusive systems are quite different from the discrete systems studied in [20]. In discrete systems one can achieve full control of the system in the following sense: given a desired set of currents, entropy production, and probability distribution (which are time independent in the case of NESS, or time-averaged over one period of driving in the case of SP), one can determine the parameters of the model required to achieve these targets. By contrast, in diffusive systems full control of averaged currents and probability is possible, but these set a minimal bound on the corresponding entropy production rate, or even uniquely determine it for a NESS. Moreover, diffusive SP always generate more entropy production than NESS, when both drive the same averaged current and probability distribution. This suggests a natural optimization problem: finding the SP that achieves a target current and probability, with minimal averaged entropy production rate.

This manuscript is organized as follows: in section 2 we introduce the mathematical framework to model diffusive SP and NESS systems. In section 3 the entropy production inequality is derived. In section 4 we show full controllability of NESS in terms of current and probability distribution. This is done constructively, by obtaining the potential and velocity that generate a given target current and probability distribution. In section 5 we solve the analogous problem for SP; our construction requires several preliminary steps that illustrate crucial points of the analysis. In section 6 we consider the optimization problem of minimizing the entropy production for a given target current and probability distribution. The general case of this problem is discussed in the appendix. We conclude in section 7 with discussions and proposals for further investigations.

2. Mathematical framework

We aim to compare two types of driving in diffusive systems: the first is performed by the breakage of detailed balance in a time-independent system, and the second concerns the time-periodic variations of parameters of a detailed balanced system. To this end, let us first consider a diffusion process on a ring for which detailed balance holds instantaneously. The state of the system at time t is denoted by x(t) ∈ [0, 1], using units such that the length along the ring is 1, and we identify x = 1 with x = 0 (periodic boundary conditions). The time-dependent probability density P(x, t) obeys the Fokker–Planck equation

$$\partial_t P = \gamma^{-1} \partial_x \left( (\partial_x U) P \right) + D \partial_{xx} P,$$

where $U(x, t)$ is the time-periodic potential in which the system diffuses, and $\gamma$ and $D$ are the damping coefficient and diffusion constant, respectively. Motivated by the modeling of molecular motors, we assume that the diffusion constant $D$ does not depend on position, $x$. We also assume that $\gamma$ and $D$ satisfy the fluctuation-dissipation relation $\beta D = 1/\gamma$, where $\beta$ is the inverse temperature.
For the system to satisfy the detailed balance condition at all times, the potential must be periodic in $x$, namely $U(0, t) = U(1, t)$ for each $t$. Indeed, if the potential were suddenly frozen, the system would relax to an equilibrium state described by the Boltzmann distribution, with vanishing probability currents. We denote the period of the driving by $T$, i.e. $U(x, t) = U(x, t + T)$. Equation (1) sets the basic model for a diffusive system driven by periodic variations of external parameters, commonly referred to as a SP or a thermal ratchet [34, 35]. In this model, the time dependence of the driving is encoded in the temporal variations of the potential $U(x, t)$. By Floquet theory, the probability distribution $P(x, t)$ of such a system converges with time to a unique solution that is periodic in both $x$ and $t$. We denote this periodic solution by $P^p(x, t)$.

A probability distribution $P(x, t)$ evolving under equation (1) can be associated with a probability current

$$J(x, t) = -D \left[ \partial_x P(x, t) + \beta P(x, t) \partial_x U(x, t) \right],$$

such that the probability obeys a continuity equation,

$$\partial_t P(x, t) + \partial_x J(x, t) = 0.$$  

The current associated with the periodic solution is

$$J^p(x, t) = -D \left[ \partial_x P^p(x, t) + \beta P^p(x, t) \partial_x U(x, t) \right].$$

Integrating both sides of equation (3) over one period of driving, at fixed $x$, gives

$$\langle P^p(x, T) \rangle = P^p(x, 0) + T \partial_x \int_{0}^{T} J^p(x, t) \, dt = 0,$$

where the overbar denotes temporal averaging over one cycle. By the temporal periodicity of $P^p$, the first two terms cancel out, hence $\langle P^p(x, t) \rangle$ must be independent of $x$. This agrees with the intuitive expectation that, over one cycle, the same total probability flux flows across any point $x$.

In addition to the probability densities and currents which we consider as the desired outcome of the driving, we are interested in the cost of the driving, given by the environment’s entropy production rate [36],

$$\dot{S}^p(t) = \int_{0}^{1} dx \frac{J^p(x, t)^2}{Dp^p(x, t)}.$$  

In order to compare the time-periodic scenario described above with time-independent systems driven by an external force that violates detailed balance, we now introduce a description for the latter. Let us consider the Fokker–Planck equation

$$\partial_t P = \gamma^{-1} \left[ (\partial_x U(x)) P \right] + D \partial_{xx} P - \nu \partial_x P,$$

where $U(x)$ is spatially periodic, $U(0) = U(1)$, as before, but time independent. The term $\nu \partial_x P$ violates the detailed balance condition for any $\nu \neq 0$. The constant $\nu$ can be interpreted as a characteristic velocity of the probability flow, or alternatively as arising from an additional linear potential that breaks the spatial periodicity of $U(x)$, generating a non-conservative force.

For any $P(x, t)$ evolving under equation (7) the instantaneous probability current is given by

$$J(x, t) = -D \left[ \partial_x P + \beta P \partial_x \left( U(x) - \frac{\nu}{\beta D} x \right) \right]$$

such that $J$ and $P$ satisfy the continuity equation equation (3). Note that equation (8) reduces to equation (2) when $\nu = 0$.

For finite $\nu$ and bounded $U(x)$, equation (7) has a unique steady state solution, denoted by $P^s(x)$, with an associated probability current

$$J^s = -D \left[ \partial_x P^s + \beta P^s \partial_x \left( U(x) - \frac{\nu}{\beta D} x \right) \right] = -D e^{-\beta U} \partial_x (e^{\beta U} P^s) + \nu P^s$$

which is independent of $x$ since $\partial_x P^s = -\partial_x P^s = 0$.

The entropy production rate of a NESS is given by an expression similar to equation (6), which simplifies because $J^s$ does not depend on $x$:

$$\dot{S}^s = (J^s)^2 \int_{0}^{1} dx \frac{1}{DP^s(x)}.$$  

Our main interest in what follows is the controllability of NESS and SP in terms of probability distribution, current and entropy production. As we have just shown, in contrast with discrete state models, for diffusive systems in NESS the current and probability distribution uniquely define the entropy production, equation (10). We next establish that if a given NESS and SP support the same probability and current (after time-averaging in
the case of the SP), then the entropy production in the SP is no less than that in the NESS. This implies a lower bound, equation (13), for the time-averaged entropy production of a SP.

### 3. Entropy production inequality

To show that the entropic cost of a SP is at least as high as that of a NESS supporting the same averaged current and probability distribution, we first note that given \( J^p(x), P^p(x), J^{ss}(x, t) \) and \( P^{ss}(x, t) \) the values of the entropy production rates \( \dot{S}^{ss} \) and \( \dot{S}^{ps} \) (t) are fully determined by equations (6) and (10). Therefore, in diffusive systems with a uniform diffusion constant we cannot impose the entropy production as an independent condition, as was done for discrete state systems [20]. This constitutes a fundamental difference between continuous and discrete state systems: there is a minimal cost, in terms of entropy production, for driving a current through a diffusive system, whereas in discrete state systems currents can have arbitrary small cost. We note that if the diffusion constant \( D \) can be varied as a function of position and time, then the analysis in [33] implies that diffusive systems would have the same behavior as discrete state systems. However, in contrast to the effective diffusion constant at the nano-scale is experimentally challenging, therefore we limit our discussion to systems in which it is constant.

Let us suppose, for the moment, full controllability of both NESS and SP in terms of their currents and probability distribution. Under this assumption, we can compare the entropy production of the two different scenarios, both supporting the same current and probability distribution. To this aim, consider the integral

\[
\mathcal{I} = \int \frac{dt}{D} \int dx \left[ \frac{J^p(x, t)}{P^{ps}(x, t)} - \frac{J^{ss}}{P^{ss}(x)} \right] P^{ss}(x, t) \geq 0. \tag{11}
\]

Expanding the square in the integrand and rewriting each term, using equations (6) and (10) along with simple manipulations, the following inequality can be derived:

\[
\mathcal{I} = \frac{1}{T} \int dt \dot{S}^{ps}(x, t) - \dot{S}^{as} = \int dx \frac{dy}{D P^{ps}(x)} \geq 0. \tag{12}
\]

Thus the entropy production rate of a NESS supporting a given steady state current \( J^{ss} \) and probability distribution \( P^{ss}(x) \) sets a lower bound on the average entropy production rate of a SP supporting the same (after time-averaging) current \( \mathcal{I}^{ps} \) and probability distribution \( P^{ps}(x) \). Using equation (10) we obtain, explicitly,

\[
\dot{S}^{ps}(t) \geq \mathcal{I}^{ps} \int_0^1 \frac{dy}{D P^{ps}(x)}. \tag{13}
\]

In what follows we will show that for any non-singular \( P^{ps}(x, t) \), equation (12) is a strict inequality. However, the entropy production under periodic driving can be arbitrarily close to the bound set by the NESS.\(^6\)

### 4. Non-equilibrium steady state

#### 4.1. Current and probability distribution controllability

We first show that NESS can support any target probability distribution \( P(x) \) and current \( J \) as its steady state values. To this end, we aim at finding the velocity \( v \) and potential \( U(x) \) for which \( P^{ps}(x) \) and \( J^{ps} \), defined in equation (9), are equal to the target values. This is achieved by inverting equation (9), which can be viewed as a linear equation for \( U(x) \). This gives, up to an additive constant:

\[
U(x) = -\frac{J^{ss}}{\beta D} \int_0^x \frac{dy}{P^{ss}(y)} - \beta^{-1} \log P^{ss}(x) + \frac{v x}{\beta D}. \tag{14}
\]

To determine \( v \) we impose periodicity on \( U(x) \). Using the periodicity of \( P^{ps}(x) \) this gives:

\[
v = J^{ps} \int_0^1 \frac{dy}{P^{ps}(y)}. \tag{15}
\]

These equations show how to build a NESS with desired \( P^{ps}(x) \) and \( J^{ps} \).

#### 4.2. Minimal entropy production in NESS

As we have just seen, the steady state current and probability distribution of a NESS can be chosen independently—the value of one of them does not constrain the value of the other. It is therefore natural to ask: given \( J^{ss} \), what choice of probability distribution \( P^{ps} \) minimizes the entropy production? The dual question, namely given \( P^{ps} \)

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\(^6\) It can be shown that inequality (11) is valid in higher-dimensional systems with non-isotropic positively defined diffusion matrix.
what \( J^a \) minimizes the entropy production, is trivial: when \( J^a = 0 \) (equilibrium conditions) there is no entropy production. The above question can be written as a simple minimization problem:

\[
\min_{P^s(x)} \left( \frac{J^a}{D} \int_0^1 \left[ \frac{1}{P^s(x)} + \lambda P^s(x) \right] dx \right)
\]

where \( \lambda \) is a Lagrange multiplier associated with the normalization of \( P^s(x) \). In principle, there is additional constraint in the problem, the positivity of \( P^s(x) \), however, this is a non-holonomic constraint, and as we next show the optimal solution satisfies this constraint without having to impose it. The Euler–Lagrange equation for the above optimization problem is given by:

\[
-(P^s(x))^2 + \lambda = 0,
\]

which combines with normalization to give \( P^s(x) = 1 \). Thus the minimal entropy production required to drive a steady current \( J^a \), is by equation (10),

\[
S_{\text{min}}^s = \frac{(J^a)^2}{D},
\]

which is achieved with a flat potential \( U(x) = 0 \) and \( v = J^a \).

5. Current and probability controllability in SPs

In the previous section we showed how to construct a NESS with a target current and probability distribution. This task was simple, since the NESS has an explicit solution for the current (equation (8)) in terms of the potential \( U(x) \), the steady state distribution \( P^s(x) \) and the parameters, \( v, D \) and \( \beta \). In the current section, we consider the problem of controlling the time-averaged current and probability distribution in a system driven by a time-periodic potential, in which detailed balance holds instantaneously. Unfortunately, there is no simple explicit solution for \( P^s(x, t) \) in terms of \( U(x, t) \) which can be inverted as in section 4. However, we have considerable freedom in choosing the potential \( U(x, t) \); as shown below, there are many choices that result in the same averaged probability distribution and current. An example of such a protocol can be constructed once the constraints set by detailed balance are taken into account.

To frame this discussion, it will be useful to imagine that we have already constructed a NESS with a desired current \( J^a \) and probability distribution \( P^s(x) \), and we want to design a SP that matches these values after time averaging, i.e. we aim to satisfy the conditions

\[
\mathcal{T}^p \equiv \frac{1}{T} \int_0^T J^a(x, t) \, dt = J^a
\]

\[
\mathcal{P}^s(x) \equiv \frac{1}{T} \int_0^T P^s(x, t) \, dt = P^s(x).
\]

(Recall from section 2 that \( \mathcal{T}^p \) does not depend on \( x \).)

5.1. Current loop

In discrete systems, a useful constraint on periodic driving is set by the ‘no current loops’ condition, which states that if a system satisfies the detailed balance condition at a given instant in time, then there can be no instantaneous current loops, regardless of the instantaneous probability distribution (see [20] for details). We now show that a similar constraint holds for 1D diffusive systems.

Given instantaneous values of \( P(x, t) \) and \( J(x, t) \), a simple condition shows whether or not detailed balance is satisfied. Consider the integral

\[
\mathcal{J}(t) = \int_0^1 \frac{J(x, t)}{P(x, t)} \, dx,
\]

which has a natural physical interpretation: writing the current density as the probability density times a mean local velocity, \( J(x, t) = P(x, t) u(x, t) \) \[4\], \( \mathcal{J}(t) \) is the instantaneous spatial average of this local velocity\(^7\). Using the spatial periodicity of \( P(x, t) \) and \( U(x, t) \) along with equation (8), we obtain

\[
\mathcal{J} = -D \int_0^1 \partial_x \left[ \log P + \beta U - \frac{v}{D} \right] \, dx = v
\]

hence detailed balance is satisfied if and only if \( \mathcal{J} = 0 \).

For the periodically driven SP that we consider here, detailed balance is satisfied at all times by assumption, hence \( \mathcal{J}(t) = 0 \). As \( P^s(x, t) \) is necessarily positive, this condition implies that \( J^a(x, t) \) changes its sign as

\(^7\) A similar idea was recently discussed in [39].
function of $x$—this is the no-current-loops condition analogous to the one derived in [20]. Thus we cannot satisfy equation (19a) by demanding that $J^P(x, t) = J^s$; rather, $J^P(x, t)$ must depend non-trivially on both $x$ and $t$.

An additional consequence of the condition $\mathcal{J}(t) = 0$ is that the entropy production inequality, equation (12), is a strict inequality. By equation (11), $\mathcal{I} = 0$ only when

$$ \frac{J^P(x, t)}{P^P(x, t)} = \frac{J^s}{P^s(x)} $$

for all $x$ and $t$, which in turn implies that the sign of $J^P(x, t)$ is the same as that of $J^s$. This, however, is inconsistent with the requirement that $J^P(x, t)$ change sign as a function of $x$. We conclude that $\mathcal{I} > 0$, hence $\overline{S}^P > S^s$.

Given an instantaneous probability distribution $P(x, t)$ and current density $J(x, t)$ satisfying $\mathcal{J}(t) = 0$, we can use equation (2) to obtain, up to an additive constant,

$$ U(x, t) = -\frac{1}{\beta D} \int_0^x \frac{J(y, t)}{P(y, t)} dy - \beta^{-1} \log P(x, t) $$

which satisfies the condition $U(1, t) = U(0, t)$. Equation (23) gives the time-dependent potential $U(x, t)$ that generates the current pattern $J(x, t)$ for the probability distribution $P(x, t)$.

### 5.2. Compatibility of $P(x, t)$ with detailed balance

So far we have discussed the constraint between $P(x, t)$ and $J(x, t)$ imposed by the condition of detailed balance, namely $\mathcal{J}(t) = 0$, and we have shown how to construct $U(x, t)$ from $P(x, t)$ and $J(x, t)$, at any instant in time (equation (23)). It is natural to ask next: given a smooth, normalized $P(x, t)$, does there always exist a time-dependent potential $U(x, t)$ such that $P(x, t)$ is a solution of equation (1)? In other words, is any well-behaved $P(x, t)$ compatible with detailed balance? Naively, one might expect the answer to be negative, as the detailed balance condition sets a constraint on $J(x, t)$ and therefore on the time derivative of $P(x, t)$. Fortunately, this is not the case. It can be shown that an arbitrary well-behaved (smooth and normalized) $P(x, t)$ can be driven by a time-dependent detailed balance periodic potential.

To establish this result we first construct, given $P(x, t)$, the corresponding current $J(x, t)$ that is compatible with detailed balance. From the continuity equation (equation (3)) we have:

$$ J(x, t) = J(0, t) - \int_0^x \partial_t P(x', t) \, dx' $$

which necessarily satisfies the periodicity condition $J(0, t) = J(1, t)$ as $\partial_t \int_0^1 P(x', t) \, dx' = 0$ for normalized probabilities. Thus the continuity equation dictates $J(x, t)$ up to a time-dependent function, $J(0, t)$.

Next, we impose the constraint of detailed balance, $\mathcal{J}(t) = 0$. Substituting equation (24) into (20) gives:

$$ \mathcal{J}(t) = \int_0^1 J(0, t) - \int_0^x \partial_t P(x', t) \, dx' = 0 $$

and by setting the right side to zero we arrive at

$$ J(0, t) = \frac{\int_0^1 \left( \int_0^1 \frac{\partial_t P(x', t)}{P(x, t)} \, dx' \right) dx}{\left( \int_0^1 \frac{1}{P(x, t)} \, dx \right)} $$

In other words, under the assumption of detailed balance $P(x, t)$ uniquely determines $J(x, t)$, and then the two together determine the potential $U(x, t)$, by equation (25).

The next challenge is to choose a periodic $P^P(x, t)$ such that (i) its time average is equal to $P^s(x)$ (equation (19b)), and (ii) the corresponding time-averaged current is equal to $J^s$ (equation (19a)). An explicit construction with these properties is shown in the next subsection.

### 5.3. Constructing $U(x, t)$ to generate a desired $\overline{P^P}(x)$ and $\overline{J^P}$

We begin by defining a dimensionless time $\tau = \nu T$, and we consider how both $\overline{P^P}(x)$ and $\overline{J^P}$ scale with the total period of cycling, $T$, for a given choice of $P^P(x, s)$. We obtain:

$$ \overline{P^P}(x) = \int_0^1 P^P(x, s) \, ds $$

$$ \overline{J^P} = \frac{1}{T} \int_0^1 J^P(x, s) \, ds $$

using equations (24) and (26) to construct $J^P$ from $P^P$. Thus $\overline{P^P}(x)$ does not vary with $T$, while $\overline{J^P}$ scales as $1/T$. Similarly, the time reversal of $P^P(x, s)$ defined by $P^T(x, s) = P^P(x, 1-s)$ has the same temporal average as...
$P^p(x, s)$, but the corresponding averaged current has opposite sign: $\overline{P^p}(x) = \overline{P^e}(x)$ and $\overline{P^o} = -\overline{P^e}$.

Therefore, to satisfy equations (19a) and (19b), we can choose a probability distribution $P^p(x, t)$ with the desired temporal average and with a non-vanishing averaged current, and then match the averaged current by the rescaling of $T$ and its sign by time reversal. Lastly, given $P^o(x, t)$ and $J^o(x, t)$, we can use equation (23) to construct $U(x, t)$.

Importantly, the construction above has a lot of freedom: the only constraints on $P^o(x, s)$ are its time average, positivity, smoothness and a non-vanishing average current. This freedom implies that there exist many periodic potentials generating the same time-averaged current and probability distribution. We now illustrate this procedure with a simple example.

5.3.1. An example for a protocol
Let us construct $U(x, t)$ that drives a time-averaged current and probability distribution

$$\overline{P^e} = 1, \quad \overline{P^o}(x) = 1 + 0.5 \sin(2\pi x).$$

(29)

As discussed above, $P^p(x, s)$ can be chosen arbitrarily, provided it is positive, normalized and has the correct time average and non-vanishing current. The specific choice

$$P^o(x, s) = 1 + 0.5 \sin(2\pi x) + 0.1 \sin(2\pi (s - x)),$$

(30)

gives the desired time averaging $\overline{P^o}(x)$. Equation (24) implies in this case

$$J^p(x, s) = \frac{1}{T} \left( J^o(0, s) + 0.1 \sin(2\pi (s - x)) \right),$$

where the expression for $J^o(0, s)$, although analytical, is cumbersome and is not given explicitly. To match the target $\overline{P^e}$, we further set $T \approx 0.58$. Figure 1 shows $P^o(x, s)$ for this example, as well as the corresponding $J^p(x, s)$ and $U(x, s)$; the latter was calculated numerically using equation (23) with $\beta = 1$ and $D = 1$.

6. Optimal driving protocol
As we have seen, there is considerable freedom in constructing a protocol $U(x, t)$ that drives a target $\overline{P^o}(x)$ and $\overline{J^e}$. Moreover, in section 3 it was shown that the entropy production rate of a SP always exceeds that of a NESS, when both share the same time averaged probability distribution and current; see equation (12). It is therefore natural to look for the protocol $U(x, t)$ that drives the target averages at the minimal entropy production cost. In other words, we would like to solve the following minimization problem:

$$\min_{U(x, t)} \left[ \frac{1}{T} \int_0^T S^o[U(x, t)] \, dt \right]$$

(31)

under the constraints:

$$\overline{P^o}[U(x, t)](x) = p_{\text{target}}(x)$$

(32)

$$\overline{J^o}[U(x, t)] = J_{\text{target}}.$$  

(33)

Solving the optimization problem directly is challenging, but unnecessary: it is possible to construct a specific protocol that asymptotically approaches the bound in equation (13). The construction of this protocol for generic $\overline{P^o}(x)$ is given in the appendix. In this section a simple example of this construction is demonstrated.

Let us consider driving a given current, $\overline{P^o} = J_0$, with $\overline{P^o} = 1$. This example is of special interest since for a current $J_0$, the bound on $\overline{S^o}$, given by $\overline{S^o}$ of a NESS with the same averaged probability and current, is minimal for a uniform probability distribution $P^u(x) = 1$, as discussed in section 4.2. To construct the driving, we consider a probability distribution of the form $P(x, t) = f(x - ut)$ for a positive, normalized, non-uniform function $f(x)$. In other words, we consider a probability distribution with a fixed shape that moves at a constant velocity $u$. The cycle time for this driving is $T = u^{-1}$, and the spatial symmetry implies that the temporal average of $P^u(x, t)$ is $\overline{P^o}(x) = P^u = 1$. In this case, the continuity condition in equation (24) implies that

$$J^o(x, t) = J^o(0, t) + u \left( f(x - ut) - f(-ut) \right),$$

(34)

where $J^o(0, t)$ is set by the detailed balance condition $J^o = 0$, equation (26), to be

$$J^o(0, t) = -u(\alpha - f(-ut)), \quad \alpha \equiv \left[ \int_0^1 \frac{dx}{f(x)} \right]^{-1} \in (0, 1).$$

(35)
The averaged current is therefore given by
\[ \langle J^{\bar{u}} \rangle = u(1 - \alpha). \] (36)

The target current is set to be \( \langle J^{\bar{u}} \rangle = J_0 \), which gives us
\[ u = \frac{J_0}{1 - \alpha}. \] (37)

Figure 1. The example in equation (30). Upper panel: \( P(x, s) \), given in equation (30). Middle panel: the corresponding \( J(x, s) \) for which the driving is assured to be detailed balance. Lower panel: the corresponding driving \( U(x, u) \), given by equation (23).
Substituting the above results into equation (6), we get after some trivial algebra:

$$
\dot{S}^{\text{ps}} = \frac{J_0^2}{D(1 - \alpha)},
$$

which—as one might have guessed by translation symmetry—does not depend on time. We see that $\dot{S}^{\text{ps}}$ is minimal when $\alpha^{-1} = \int_0^L f(x)^{-1}dx$ is maximal. But this integral is not bounded from above: for example, in the limit $P(x, t) \to \delta(x - ut)$ the integral $\int_0^L f(x)^{-1}dx$ diverges, and we then get $\alpha \to 0$ hence $\dot{S}^{\text{ps}} \to \mathcal{P}^2/D$.

Comparing with equation (18) we see that, in this limit, the entropy production of the periodically driven state approaches the bound set by the corresponding steady state value.

7. Discussion

In this work we have discussed similarities and differences between two types of driving that maintain a diffusive system on a ring out of equilibrium: periodic variations of a potential along the ring, and static driving by breaking the detailed balance condition. We have shown that the two scenarios can drive any averaged current and probability distribution, but in contrast to discrete state Markovian systems there is no full control in terms of the averaged entropy production. Moreover, it was shown that the averaged entropy production of a steady state driving is smaller than that of a system driven by periodic changes in the potential that achieves the same averaged current and probability distribution. In terms of applications, this implies that the common driving in biological molecular motors—burning fuel and reaching a steady state—has a lower thermodynamic cost, i.e. the depletion of a thermodynamic resource, than the common driving of artificial molecular motors, namely periodic variation of external parameters. This result is different than what was obtained in a coarse-grained description of the same system—discrete state Markovian modeling—since a diffusive description reduces the number of controllable parameters (i.e. energy barriers).

Many important aspects were not discussed in this work and they could be subjects to future investigations. These include mapping between NESS and SP that matches other features (e.g. heat or work in heat engines [37, 38], current fluctuations [21] or entropy production fluctuations [9]), as well as comparison of these two types of driving to other non-equilibrium scenarios.

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Appendix. Minimizing entropy production for non-uniform $\mathcal{P}^{\text{ps}}(x)$

In section 6 we analyzed a specific example where the entropy production rate of a SP can get arbitrarily close to that of a NESS with the same time averaged current and probability distribution. In this appendix we generalize this construction for arbitrary target $\mathcal{P}^{\text{ps}}(x)$ and $\mathcal{P}^n$.

Analogously to the construction in section 6, we choose the probability distribution to be a translating profile, $\mathcal{P}^{\text{ps}}(x, t) = f(x - x_0(t))$, where $x_0(t)$ changes monotonically from 0 to 1 over the interval $0 \leq t \leq T$. We first show that by appropriately choosing $x_0(t)$ we can construct the target time averaged probability:

$$
\mathcal{P}^{\text{ps}}(x) = \frac{1}{T} \int_0^T f(x - x_0(t)) dt = \frac{1}{T} f^* \frac{1}{x_0},
$$

(A.1)

where $f^* (1/x_0)$ denotes the convolution of the functions $f(x)$ and $1/x_0(x)$, and \( x_0(x) \) is the velocity $dx_0(t)/dt$ expressed as a function of position, $x_0(t) = x$. To gain some intuition, consider the example $f = \delta(x - x_0(t))$. By controlling the speed at which this delta function moves across each point we can manipulate the time averaged probability at this point. Specifically, for this example equation (A.1) gives us $\dot{x}_0(x) = 1/\{T \mathcal{P}^{\text{ps}}(x)\}$. More generally, applying the Fourier theorem of Fourier transforms to equation (A.1), we obtain

$$
\frac{1}{x_0(x)} = T \sum_n e^{i2\pi nx_0} \mathcal{P}^n f_n, \quad (A.2)
$$

where $\mathcal{P}^n$ and $f_n$ are the $n$'th discrete Fourier coefficients of $\mathcal{P}^{\text{ps}}(x)$ and $f(x)$. Note that the above equation shows that not any $f(x)$ can serve for our construction—for example, if the right hand side of the above equation vanishes for some $x$ then the corresponding $\dot{x}_0(x)$ diverges. This can be intuitively understood by considering
the extreme scenario: if \( f(x) = 1 \), then one cannot match any probability distribution by averaging over \( f(x - x_0(t)) \), namely over translated versions of \( f(x) \). Nevertheless, given any \( \overline{P}_P(x) \), one can always choose appropriate \( f(x) > 0 \) which is narrow enough such that the expression in the right hand side of equation (A.2) is strictly positive, as is evident from the delta-function example above.

From the function \( x_0(x) \), we construct \( t(x_0) = \int_0^{x_0} \frac{dx}{f(x)} \), and then invert \( t(x_0) \) to obtain \( x_0(t) \).

Next, let us consider the current. By equation (24),

\[
J_P(x, t) = J_P(0, t) + \dot{x}_0(t) [f(x - x_0(t)) - f(-x_0(t))].
\]

(A.3)

For the detailed balance condition to hold, equation (26) implies that

\[
J_P(0, t) = \dot{x}_0(t) [f(-x_0(t)) - \alpha],
\]

(A.4)

where, as in equation (35),

\[
\alpha \equiv \left[ \int_0^1 \frac{dx}{f(x)} \right]^{-1}.
\]

(A.5)

Equations (A.3) and (A.4) then give us

\[
J_P(x, t) = \dot{x}_0(t) [f(x - x_0(t)) - \alpha].
\]

(A.6)

Let us set the target time averaged current to be \( \overline{J}_P = J_0 \) for arbitrary \( J_0 > 0 \). With this choice the cycle time \( T \) solves the equation

\[
J_0 = \frac{1}{T} \int_0^T J_P(x, t) dt = \frac{1 - \alpha}{T},
\]

(A.7)

where in the last equality we changed the variable of integration from \( t \) to \( x_0 \).

Lastly, substituting equation (A.6) into (6), it can be shown that the entropy production rate at each instant is given by

\[
\overline{S}_P(t) = \frac{\dot{x}_0^2}{D} (1 - \alpha).
\]

(A.8)

The time averaged total entropy production is therefore given by

\[
\overline{S}_P = \frac{1 - \alpha}{TD} \int_0^T \dot{x}_0^2 dt = \frac{J_0}{D} \int_0^1 \dot{x}_0(x_0) dx_0,
\]

(A.9)

using equation (A.7). In the limit \( f(x) \to \delta(t) \) equations (A.1) and (A.5) give us

\[
\dot{x}_0(x) \to \{T \overline{P}_P(x) \}^{-1}, \quad \alpha \to 0
\]

(A.10)

hence \( J_0 \to 1/T \) and

\[
\overline{S}_P \to \frac{J_0}{DT} \int_0^1 \{T \overline{P}_P(x) \}^{-1} dx \to \frac{T \overline{J}_P^2}{D} \int_0^1 \{T \overline{P}_P(x) \}^{-1} dx
\]

(A.11)

which is the bound on the entropy production rate of periodic driving with the corresponding time averaged current and probability (equation (13)).

**ORCID iDs**

D M Busiello https://orcid.org/0000-0002-6754-5019

C Jarzynski https://orcid.org/0000-0002-3464-2920

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