Monotonicity of the dynamical activity

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We prove that the Donsker-Varadhan large deviation functional for the occupations in a finite Markov jump process is monotone under the Master equation evolution. This functional is non-entropic when the system is driven away from detailed balance; it rather measures an excess in time-symmetric dynamical activity. Our proof of monotone behavior works under two conditions: (1) the initial distribution is close enough to stationarity, or equivalently for our context, we look at large times with respect to the relaxation time, and (2) a certain spectral sector–condition equivalent to “normal” linear-response behavior is satisfied.

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I. INTRODUCTION — MAIN FINDING

Large deviation theory for Markov processes was developed by Donsker and Varadhan in 1975, [5]. We recall the main setting.

Consider an ergodic Markov jump process \( P_\rho \) with stationary probability law \( \rho \) and with transition rates \( k(x,y) \) over a finite state space \( K \). The empirical fraction of time that the system spends in state \( x \in K \) over time-interval \([0,T]\) is

\[
p_T(\omega, x) := \frac{1}{T} \int_0^T \delta_{x_s,x} \, ds, \quad x \in K
\]

where \( \omega = (x_s, 0 \leq s < T) \) is the piecewise constant trajectory. By the assumed ergodicity, \( p_T \to \rho \) for \( T \uparrow +\infty \), \( P_\rho \)–almost surely. For the fluctuations around that law of large times,
there is a principle of large deviations, abbreviated as

\[ P_\rho[\rho_T \simeq \mu] \propto e^{-T^2} \mu \]  

(I.2)

for probability distributions \( \mu \) on \( K \), in the usual logarithmic and asymptotic sense \( T \uparrow +\infty \); see e.g. [3, 4]. A lot is known about the large deviation functional \( \mathcal{I} \) in (I.2). There is for example the variational expression

\[ \mathcal{I}(\mu) = \sup_{g > 0} \left\{ -\sum_x \frac{\mu(x)}{g(x)} \sum_y k(x, y) \left[ g(y) - g(x) \right] \right\} \]  

(I.3)

over positive functions \( g \). In the present setting \( \mathcal{I}(\mu) \) is a strictly convex functional and \( \mathcal{I}(\mu) \geq 0 \) with equality only for \( \mu = \rho \). It is therefore natural to ask whether \( \mathcal{I}(\mu_t) \) is also monotonically decaying to zero under the Master equation

\[ \frac{d}{dt} \mu_t(x) = \sum_{y \in K} \left[ k(y, x) \mu_t(y) - k(x, y) \mu_t(x) \right], \quad \mu_0 = \mu \]

at least when \( \mu \) (the initial condition) is sufficiently close to \( \rho \). The present paper answers that question in the affirmative under some further condition. Basically, the monotonicity is verified when the system shows normal linear response, which we explain in Section III. In particular it will be easy to show that the monotonicity holds when the system satisfies the condition of detailed balance, and hence, by a continuity argument, the monotone return to steady nonequilibrium is also valid around detailed balance. Yet, as we will see, the monotonicity often continues to hold even beyond the linear regime around detailed balance. Nevertheless we also present in Section IV counterexamples for systems very far from equilibrium.

Recently, from the point of view of nonequilibrium statistical mechanics, there has been great interest in dynamical fluctuation theory, and in the occupation statistics in particular. It turns out that the functional \( \mathcal{I}(\mu) \) is connected with the notion of dynamical activity (DA), which refers to a combination of properties of a statistical mechanical system that are related to its reactivity and the ability to escape from its present state. DA has been studied in connection with glassy behavior and the glass transitions; kinetically constrained models show a reduced dynamical activity over an extensive number of states which leads to dynamical phase transitions, [2, 6–8]. Finally, DA has appeared in fluctuation and
response theory for steady nonequilibria, [1, 12, 13]. The point is that as a function on trajectories, the dynamical activity is time-symmetric and therefore provides an essential complement to entropic considerations for understanding transport and response beyond the linear regime around equilibrium. In fact, our result mirrors the monotone behavior of the relative entropy which is associated to the \textit{static} fluctuations of the system.

The next section specifies the mathematical set-up and the main definitions. Section III collects the main properties, with our result on monotone behavior. Section IV discusses various specific examples far and close-to-equilibrium. We also give a brief comparison with more standard entropic functionals in Section V. Proofs are collected in Section VI.

\section*{II. SET-UP}

We consider a Markov jump process on a finite state space $K$ with states $x, y, \ldots$ and transition rates $k(x, y)$. Probability distributions on $K$ will be denoted by $\rho, \mu, \nu, \ldots$. The backward generator on functions $f$ is

$$Lf(x) := \sum_{y \in K} k(x, y) [f(y) - f(x)]$$

and its transpose generates the Master equation

$$\frac{d}{dt} \mu_t(x) + \sum_{y \in K} j_{\mu}(x, y) = 0, \quad j_{\nu}(x, y) := k(x, y) \nu(x) - k(y, x) \nu(y)$$

for the evolution on probabilities $\mu_t$ starting from some initial $\mu_0 = \mu$ on $K$. We assume that the Markov process is irreducible with unique stationary probability distribution $\rho$, i.e., $\rho(x) > 0$ solves $\sum_y j_\rho(x, y) = 0$ for all $x \in K$.

We say that the dynamics satisfies detailed balance when there is a function $U$ on $K$ for which

$$k_e(x, y) e^{-U(x)} = k_e(y, x) e^{-U(y)}, \quad \rho_e(x) \propto e^{-U(x)}$$

Here and below we decorate the rates and the stationary law in that detailed balance case with the subscript ‘e’. Then, the free energy functional

$$\mathcal{F}(\mu) := \sum_x \mu(x) U(x) + \sum_x \mu(x) \log \mu(x) \geq \mathcal{F}(\rho_e) = - \log \sum_x \exp \left[ -U(x) \right]$$
satisfies the monotonicity $\mathcal{F}(\mu_t) \downarrow \mathcal{F}(\rho_e)$ as a function of time $t$. That is just a standard consequence of the general monotonicity of the relative entropy under stochastic transformations. However, the relation between the Shannon entropy $-\sum_x \mu(x) \log \mu(x)$ and physical notions as work or heat is mostly lost when far away from detailed balance. A physically relevant alternative when moving away from detailed balance, is to consider the instantaneous entropy production $E(\mu)$, which for the given context is

$$E(\mu) := \sum_{x,y} \mu(x) k(x,y) \log \frac{\mu(x) k(x,y)}{\mu(y) k(y,x)} = \frac{1}{2} \sum_{x,y} j(\mu)(x,y) A(\mu)(x,y), \quad A(\mu)(x,y) := \log \frac{\mu(x) k(x,y)}{\mu(y) k(y,x)}$$

as the product of “fluxes” $j(\mu)(x,y)$ and “forces” $A(\mu)(x,y)$ when the system’s distribution is $\mu$, reminiscent of irreversible thermodynamics — see e.g. [15] for more details. We come back to these entropic functionals and their temporal behavior in the relaxation to nonequilibrium in Section V.

We now introduce our main object. We embed the original dynamics into a larger family of processes with transition rates,

$$k_W(x,y) := k(x,y) \exp \frac{W(y) - W(x)}{2}$$

parameterized by functions $W$ on $K$. These functions $W$ are also called potentials. Here we consider potentials that are directly connected with a probability distribution. For that we need a solution of the inverse stationary problem. What follows should be a rather standard observation within the theory of large deviations. Yet we do not find in the literature a direct proof of both existence and uniqueness for continuous-time processes. For completeness therefore, we give a full proof in Section VI A.

**Proposition II.1.** For an arbitrary probability distribution $\mu > 0$ there exists a potential $V = V_\mu$ on $K$ such that $\mu$ is invariant under the modified dynamics with transition rates $k_V(x,y)$. The potential $V_\mu$ is unique up to an additive constant when the dynamics is irreducible.

In other words, for arbitrary $\mu > 0$ we can always find a function $V$ so that

$$\sum_{y \in K} \left[ k_V(x,y) \mu(x) - k_V(y,x) \mu(y) \right] = 0, \quad x \in K$$
We can compare this with (I.3). Indeed, the Donsker–Varadhan large deviation functional can be written in terms of a potential $W$: taking $g = e^W$ in (I.3),

$$ I(\mu) = \sup_W \sum_{x,y \in K} \mu(x) [k(x,y) - kW(x,y)] \quad \text{(II.6)} $$

When the process is irreducible, cf. Proposition II.1 and its proof in Section VIA, we then have

$$ I(\mu) = \sum_{x,y \in K} \mu(x) [k(x,y) - V(x,y)] \quad \text{with } V = V_\mu \quad \text{(II.7)} $$

It is worth noting that $I(\mu)$ is an excess or difference between the expected escape rates $\sum_x \mu(x) \sum_y k(x,y)$ and $\sum_x \mu(x) \sum_y kV(x,y)$. Such an expected escape rate estimates the dynamical activity, i.e., the number of transitions per unit time in the process. We refer to the physics literature for further discussion, [1, 2, 6–8, 13].

**III. MAIN RESULT**

For simplicity in the sequel we always assume the irreducibility of continuous time Markov processes with finite state space. Our main finding is that $I(\mu_t)$ is monotone under the evolution (II.1) when close enough to stationarity, i.e., for large enough times $t$ compared to the relaxation time, at least under some further and physically interpretable condition.

Define the real–space scalar product $(f, g) := \sum_x f(x)g(x) \rho(x)$ so that $(f, Lg) = (L^*f, g)$. Here, we have introduced the generator $L^*$ of the time-reversed process,

$$ L^* f(x) := \sum_{y \in K} \frac{\rho(y)k(y,x)}{\rho(x)} [f(y) - f(x)] $$

We write $L_s$ for the symmetric part of the generator: $L_s := \frac{1}{2}(L + L^*)$, and

$$ \|\|f\|\| := \max_{x,y} |f(x) - f(y)| $$

for the variation of a function $f$ on $K$.

**Theorem III.1.** Suppose that there is a constant $c > 0$, so that $(L_s f, Lf) \geq c \|\|f\|\|^2$ for all functions $f$ on $K$. Then, there is a time $t_o > 0$ so that for all initial probability distributions $\mu$ on $K$,

$$ \frac{d}{dt} I(\mu_t) \leq 0 \quad \text{for all times } t \geq t_o $$
At the end of the proof, the time $t_o$ after which monotonicity sets in will be shown to be of the order of the relaxation time (inverse of the exponential rate of convergence).

Since $L$ and $L_s$ have a bounded inverse on the functions $f$ that have zero mean $\sum_x \rho(x)f(x) = 0$, the condition of Theorem III.1 in essence means to require that $(L_s f, L f) > 0$ for non-constant $f$. A sufficient condition for $(L_s f, L f) > 0$ is

$$(f, L^2 f) > 0$$  \tag{III.1}$$

Obviously, if the rates $k(x, y)$ satisfy detailed balance (II.2), $L_e = L_e^*$ and (III.1) holds true; see under the section IVB for further discussion. A comparison with the behavior of the relative entropy and of the entropy production is waiting in Section V.

The inequality (III.1) is a sector condition on the eigenvalues of the generator $L$; their imaginary part should not be too big when their (negative) real part is small. It is satisfied under and close to the detailed balance condition (II.2).

A physical interpretation of the hypothesis for Theorem III.1 is in terms of the generalized susceptibility for the linear response around the stationary probability $\rho$. For a function $B$ on $K$ consider perturbed transition rates

$$k(\tau; x, y) := k(x, y) e^{h_{\tau}[B(y)-B(x)]}, \quad \tau \geq 0$$  \tag{III.2}$$

with small time-dependent amplitude $h_{\tau}$, $|h_{\tau}| \leq \varepsilon$. That new time-dependent process is started from time zero in the distribution $\rho$ which is stationary for $h \equiv 0$. At a later time $t > 0$, in the process with rates (III.2), when taking the expectation of a function $G$, we see the difference

$$\langle G(x_t) \rangle^h - \sum_x G(x)\rho(x) = \int_0^t d\tau h_{t-\tau} \chi_{GB}(\tau) + O(\varepsilon^2)$$

which defines the generalized susceptibility $\chi_{GB}$. There is an explicit formula for that functional derivative, extending the standard fluctuation–dissipation theorem, see e.g. [1]:

$$\chi_{GB}(t) := \frac{\delta}{\delta h_0} \langle G(x_t) \rangle^h \bigg|_{h=0} = -\frac{1}{2} \left[ \frac{d}{dt} \left\langle B(x_0) G(x_t) \right\rangle_{\rho} + \left\langle L B(x_0) G(x_t) \right\rangle_{\rho} \right]$$  \tag{III.3}$$

with right-hand expectations in the original stationary process $P_{\rho}$. It is then a simple computation, that we do in (VI.9), to conclude that for $t \downarrow 0$,

$$\frac{d}{dt} \chi_{ff}(t = 0) = \chi_{L_f,f}(t = 0) = -(L_s f, L f)$$  \tag{III.4}$$
The right-hand side of (III.4) exactly figures in the condition to Theorem III.1. Heuristically therefore, the Donsker-Varadhan functional $\mathcal{I}(\mu_t)$ is certainly monotone for large times $t$ whenever the linear response $\chi_{ff}(t)$ starts out by decaying right after the perturbation, for all functions $f$.

IV. EXAMPLES AND COUNTEREXAMPLES

We make the statements of the previous section more explicit by providing some examples and counterexamples.

A. Asymmetric diffusion on the ring

Consider a ring consisting of $N > 2$ sites, labelled $x = 1, 2, \ldots, N + 1 \equiv 1$. For a totally asymmetric random walker the only non-zero transition rates are of the form $k(x, x + 1) > 0$ with Master equation (II.1) simplified to
\[
\frac{d\mu_t}{dt}(x) = \mu_t(x - 1)k(x - 1, x) - \mu_t(x)k(x, x + 1)
\]
The stationary distribution is
\[
\rho(x) = \frac{C}{k(x, x + 1)}, \quad C^{-1} = \sum_x \frac{1}{k(x, x + 1)}
\]
The corresponding generators of Theorem III.1 are
\[
Lf(x) = k(x, x + 1)[f(x + 1) - f(x)], \quad L_s f(x) = \frac{1}{2}k(x, x + 1)[f(x + 1) + f(x - 1) - 2f(x)]
\]
so that the hypothesis of Theorem III.1 concerns
\[
(L_s f, L f) = \frac{C^2}{2} \sum_x \frac{1}{\rho(x)} \left[f(x + 1) - f(x)\right] \left[f(x + 1) + f(x - 1) - 2f(x)\right] \tag{IV.1}
\]
To begin let us take $k(x, x + 1) \equiv p$ for some given $p > 0$. In that homogeneous case, (IV.1) is bounded from below by the variation of $f$ because, with $g(x) = f(x + 1) - f(x)$,
\[
\sum_x g(x)[g(x) - g(x - 1)] = \frac{1}{2} \sum_x [g(x) - g(x - 1)]^2 \geq 0 \text{ on the ring.}
\]
But we can also show that $\mathcal{I}(\mu_t)$ is monotone for all times $t$ and starting from all possible $\mu > 0$. For this we find the potential $V_\mu$ solving
\[
0 = \mu(x)pe^{[V(x+1)-V(x)]/2} - \mu(x - 1)pe^{[V(x)-V(x-1)]/2}
\]
or
\[
\frac{V(x+1) - V(x)}{2} = -\log \mu(x) + \tilde{C}, \quad \tilde{C} = \frac{1}{N} \sum_x \log \mu(x)
\]
Therefore the Donsker-Varadhan functional (II.7) equals
\[
\mathcal{I}(\mu) = \sum_x p\mu(x) \left[ 1 - e^{\frac{V(x+1) - V(x)}{2}} \right]
= p - pN \left[ \prod_{y=1}^N \mu(y) \right]^{\frac{1}{N}}
\]
with time derivative at \( \mu_t = \mu \) computed to be
\[
\frac{d}{dt} \mathcal{I}(\mu_t) = -p^2 \left[ \prod_{y=1}^N \mu(y) \right] \sum_{x=1}^N \left\{ \frac{\mu(x-1)}{\mu(x)} - 1 \right\}
\]
which is non-positive by applying Jensen’s inequality as
\[
\log \left( \frac{1}{N} \sum_{x=1}^N \frac{\mu(x-1)}{\mu(x)} \right) \geq \frac{1}{N} \sum_{x=1}^N \log \frac{\mu(x-1)}{\mu(x)} = 0
\]
In fact, by the same argument, the time-derivative is strictly negative whenever \( \mu \neq \rho \).
Therefore, for homogeneous totally asymmetric walkers on a ring, we always have monoton-icity of the dynamical activity. We next continue by breaking the translation invariance.

We look back at (IV.1) which is now of the form \( \sum_x \frac{1}{\rho(x)} g(x)[g(x) - g(x-1)] \). In fact a simple computation shows that for \( \mu_t = \mu \)
\[
\frac{d}{dt} \mathcal{I}(\mu_t) = 2\epsilon^2 C^2 \sum_x \frac{V(x)}{\rho(x)} [V(x-1) - V(x)] + o(\epsilon^2) \quad (IV.2)
\]
for \( V(x) := -h(x) + \frac{1}{N} \sum_x h(x) \) when \( \mu(x) = \rho(x)[1 + \epsilon h(x)] \). We thus see how the condition in Theorem III.1 appears. Without further condition and depending on the shape of the stationary distribution \( \rho \), this time-derivative (IV.2) can be either positive or negative. For a counterexample making \( \mathcal{I}(\mu_t) \) non-montone, we take \( N = 4 \) with
\[
g(1) = 1, g(2) = -3, g(3) = 0, g(4) = 2 \quad (IV.3)
\]
Then the time-derivative (IV.2) is positive whenever
\[
\frac{1}{\rho(1)} > \frac{12}{\rho(2)} + \frac{4}{\rho(4)}
\]
FIG. 1: The functional $\mathcal{I}(\mu_t)$ as a function of time. The curve with open circles shows the evolution of $\mathcal{I}(\mu_t)$ for the case of a homogeneous stationary distribution. The black curve (closed smaller circles) represent the case where the stationary distribution is inhomogeneous: $\rho(1) = 1/91, \rho(2) = \rho(3) = \rho(4) = 30/91$.

To visualize this example we show in Fig. 1 the result of a numerical computation of $\mathcal{I}(\mu_t)$ for this initial condition (IV.3) with $\epsilon = 0.02$ and rates $k(1, 2) = 30, k(2, 3) = k(3, 4) = k(4, 1) = 1$. Observe however, even in this counterexample, that after a short while $\mathcal{I}(\mu_t)$ starts decreasing monotonically. In other words, while for all $\epsilon > 0$ there is a probability $\mu$ in the neighborhood of the stationary law $\rho$ with variational distance $d(\mu, \rho) \leq \epsilon$, so that $\mathcal{I}(\mu_t)$ is not monotone at $\mu_t = \mu$, still $\mathcal{I}(\mu_t)$ decays monotonically to zero eventually (after a long enough time $t$). This also indicates that the hypothesis in Theorem III.1 is not at all necessary.

Leaving the total asymmetry and allowing two-way traffic, we consider the diffusion limit of our random walker as described by the Itô-stochastic dynamics

$$\text{d}x_t = \chi(x_t) \left[ F - U'(x_t) \right] \text{d}t + \chi'(x_t) \text{d}t + \sqrt{2\chi(x_t)} \text{d}B_t \quad \text{(IV.4)}$$

for $x_t \in S^1$ on the circle, where $U$ is a potential and $F \neq 0$ is a constant making the total force $F - U'$ nonconservative. The noise $\text{d}B_t$ is standard Gaussian white noise, and
we have chosen a possibly inhomogeneous mobility \( \chi(x) > 0 \). Detailed balance (II.2) here corresponds to \( F = 0 \) for which the stationary density is \( \rho_e(x) \propto \exp[-U(x)] \). However also for \( F \neq 0 \) (the nonequilibrium case) we can calculate the analogue of (II.5)–(II.7), [10]. At least for \( \mu > 0 \), the Donsker–Varadhan fluctuation functional is explicitly given as

\[
4\mathcal{I}(\mu) = \int \left[ F - U'(x) - (\log \mu)'(x) \right] j_\mu(x) \, dx - \frac{F^2}{\int (\mu \chi)^{-1}(x) \, dx}, \quad j_\mu := \chi \mu[F - U'] - \chi \mu'
\]

So here again we can investigate quite explicitly the time-dependence of \( \mathcal{I}(\mu_t) \) under \( \dot{\mu}_t = (\chi \mu')' - (\chi \mu[F - U'])' \). A numerically obtained picture can be found as Fig. 1 in [11] where we see that \( \mathcal{I}(\mu_t) \) keeps decaying monotonically while the entropy production \( \mathcal{E}(\mu_t) \), the continuum version of (II.3), oscillates in time.

### B. At detailed balance

Under detailed balance (II.2), we can take \( g = \sqrt{\rho_e/\mu} \) in (I.3) to find equality with the Dirichlet form

\[
\mathcal{I}_c(\mu) = -\sum_x \rho_e(x) \sqrt{\frac{\mu(x)}{\rho_e(x)}} (L_c \sqrt{\frac{\mu}{\rho_e}})(x) = -\left( \sqrt{\frac{\mu}{\rho_e}}, L_c \sqrt{\frac{\mu}{\rho_e}} \right)
\]

Furthermore, for \( \mu_t = \mu \) at time \( t \)

\[
\dot{\mu}_t = \rho_e \frac{\mu}{\rho_e}
\]

so that we get the time derivative

\[
\frac{d}{dt} \mathcal{I}_c(\mu_t) = -\sum_x \rho_e(x) \frac{1}{f(x)} (L_c f^2)(x) (L_c f)(x)
\]

(IV.5)

where we have abbreviated \( f = \sqrt{\mu/\rho_e} \). Obviously, that time-derivative is negative whenever \( f - 1 \) is sufficiently small (close-to-stationarity): with \( f(x) = 1 + \epsilon h(x) \),

\[
\frac{d}{dt} \mathcal{I}_c(\mu_t) = -2\epsilon^2 \sum_x \rho_e(x) ((L_c h)(x))^2 + o(\epsilon^2)
\]

That is equivalent to what was mentioned before under Theorem III.1: the hypothesis there is always satisfied under detailed balance, and we see that the time \( t_0 \) will be of the order of the relaxation time, characterizing the uniform exponentially fast convergence to equilibrium. More explicit calculations reveal also that the derivative (IV.5) is strictly negative for all \( f > 0 \) when \(|K| \leq 3\).
However, (IV.5) is not always negative. To sketch a counterexample we consider the case of a diffusion process where the forward generator takes the form of the differential operator, say on $\mathbb{R}$,

$$L_{e}g = \frac{1}{\rho e} \frac{d}{dx} (\rho e \frac{d}{dx} g)$$

for smooth functions $g$. Let us take $\mu(x) = a/\rho e(x)$ inside the interval $[1, \ell]$, where $\ell > 1$ and $a$ is a normalization, and $\mu(x) \simeq \rho e(x)$ very rapidly decaying to zero outside that same interval. Then, at that $\mu$, (IV.5) becomes

$$\frac{d}{dt} I_{e}(\mu_{t}) \simeq -2 \int_{1}^{\ell} dx f''(x) (\log f)'(x)$$

which will be positive e.g. when $f$ is convex while $\log f$ is concave. For example, with $\rho e(x) = c \ell / x^2$ on $[1, \ell]$, we have $f(x) \sim x^2$, $\log f(x) \sim \log x$ on that same interval.

## V. COMPARISON WITH ENTROPIC FUNCTIONALS

We start with the relative entropies.

**Proposition V.1.** Suppose that $(L_{s}f, L^{*}f) \geq c \|f\|^{2}$ for all functions $f$ on $K$, for some constant $c > 0$. For all large enough times $t$, the relative entropies

$$s(\mu_{t} \mid \rho) := \sum_{x} \mu_{t}(x) \log \frac{\mu_{t}(x)}{\rho(x)}, \text{ and also } s(\rho \mid \mu_{t})$$

are convex non-increasing in time $t$ whatever the starting distribution $\mu_{0}$:

$$\frac{d^2}{dt^2} s(\mu_{t} \mid \rho) \geq 0, \quad \frac{d^2}{dt^2} s(\rho \mid \mu_{t}) \geq 0 \quad (V.1)$$

The fact that these relative entropies are non-increasing for all times $t$ is well known. What is interesting is that their convexity (for large times) follows from exactly the same condition as in Theorem III.1 for the monotonicity of the Donsker-Varadhan functional, but with $L$ replaced by $L^{*}$ (generator of the time-reversed process).

The relative entropy $s(\rho \mid \mu_{t})$ was recently considered in [14] because its time-derivative equals

$$\frac{d}{dt} s(\rho \mid \mu_{t}) = \sum_{x} \rho(x) \frac{1}{\mu_{t}(x)} H_{\mu_{t}}(x) \geq 0$$

with $H_{\mu_{t}}(x) := \sum_{y \in K} j_{\mu_{t}}(x, y)$, cf. (II.1). The right-hand side is a stationary expectation, always non-negative and which vanishes only when $\mu_{t} = \rho$. 
Secondly, we consider the entropy production (II.3). Under detailed balance this entropy production functional \(E\) has the same monotonicity as the relative entropy, \(E(\mu_t) \downarrow E(\rho_e)\). Its advantage compared to the relative entropies above is that \(E\) does keep a more direct physical meaning also when moving away from the detailed balance condition. Yet, \(E(\mu_t)\) fails to be monotone then (and it becomes even ill-defined for totally asymmetric rates as in the first examples of Section IV A). To understand the situation, let us take \(\mu = \rho(1+\epsilon h)\) for some function \(h\) with mean \(\sum \rho(x) h(x) = 0\), and consider the first terms in the expansion of \(E(\mu)\) around \(\epsilon = 0\). We get

\[
E(\mu) - E(\rho) = \epsilon \sum_x \rho(x) h(x) \sum_y k(x,y) A_\mu(x,y) - \epsilon^2 (h,Lh) + O(\epsilon^3) \quad (V.2)
\]

We see that the first order (linear in \(\epsilon\)) contributes with stationary “force” \(A_\mu(x,y) = \log [\rho(x)k(x,y)/\rho(y)k(y,x)]\). There is no reason why that term should have a definite sign, and when \(h\) becomes time-dependent (from the time-dependence of \(\mu\)) we expect oscillations in time in the approach to the nonequilibrium stationary distribution. Indeed, see Fig. 1 in [11] for an example. The reason is mainly that the stationary distribution \(\rho\) does not need to minimize the entropy production functional when well away from detailed balance. On the other hand, in detailed balance \(A_{\rho_e}(x,y) = 0, E(\rho_e) = 0\) and \(E(\mu_t) = -\frac{d}{dt} s(\mu_t|\rho_e) \geq 0\).

VI. PROOFS

A. Proof of Proposition II.1

For arbitrary \(\mu > 0\) we consider the auxiliary functional

\[
Y_\mu(W) := \sum_{x,y \in K} \mu(x) k_W(x,y) = \sum_{x,y \in K} \mu(x) k(x,y) \exp \left[ \frac{W(y) - W(x)}{2} \right] \quad (VI.1)
\]

defined on all functions on \(K\). Of course, since the value only depends on the differences \(W(y) - W(x)\) we can as well take \(W \in C_0(K)\), the collection of all functions that are equal to zero on a fixed “root” \(x_0 \in K\). This functional \(Y_\mu\) is nonnegative and convex,

\[
Y_\mu(\lambda W_1 + (1 - \lambda)W_2) \leq \lambda Y_\mu(W_1) + (1 - \lambda)Y_\mu(W_2) \quad (VI.2)
\]

by convexity of each contribution \(\mu(x) k_W(x,y)\). Below in Lemma VI.1 we prove that under the irreducibility assumption, \(Y_\mu\) is actually strictly convex and that it attains inside \(C_0(K)\)
a unique minimum at some $W = W_\mu$. Hence, $W_\mu$ is also a minimizer (unique up to an additive constant) on the unconstrained space of all functions on $K$, implying that for all $x \in K$,

$$0 = \frac{\partial Y_\mu}{\partial W(x)}|_{W=W_\mu} = \frac{1}{2} \sum_{y \in K} [\mu(y) k_W(y, x) - \mu(x) k_W(x, y)]$$  \hspace{1cm} (VI.3)

which is just the stationarity of $\mu$ for the dynamics with rates $k_W(x, y)$, i.e., $V = V_\mu$ of Proposition II.1 does exist and equals $W_\mu$. This also proves formula (II.6) as

$$I(\mu) = \sum_{x,y \in K} \mu(x) k(x, y) - Y_\mu(W_\mu) = \sup_V \sum_{x,y \in K} \mu(x) [k(x, y) - k_V(x, y)]$$ \hspace{1cm} (VI.4)

A general reducible dynamics can be decomposed into irreducible components (including isolated sites) and for each of them the above argument holds true, i.e., the supremum on the right-hand side of (II.6) is attained on a function $V_\mu$, which is also a solution of the inverse stationarity problem and which is unique up to a constant within each component.

Again turning to irreducible dynamics, we have

**Lemma VI.1.** For any $\mu > 0$, $Y_\mu|_{C_0(K)}$ is strictly convex and has a unique minimum.

**Proof.** By irreducibility, there exists a cyclic sequence of states $(x_0, x_1, \ldots, x_n = x_0)$ that covers the whole space $K$ and such that for all consecutive pairs of states, $\mu(x_{i-1}) k(x_{i-1}, x_i) \geq \delta$ with some $\delta > 0$. If $W_1$ and $W_2$ are such that the relation (VI.2) becomes an equality, then, for all $i = 1, \ldots, n$, $W_1(x_i) - W_1(x_{i-1}) = W_2(x_i) - W_2(x_{i-1})$, by using that the exponential is strictly convex. From $W_1(x_0) = W_2(x_0) = 0$ then follows $W_1 = W_2$, identically. This proves the strict convexity and hence the uniqueness of the minimum for $Y_\mu|_{C_0(K)}$.

To prove that the minimum exists, we consider the compact sets

$$C^n_0(K) := \{W \in C_0(K); |W(x)| \leq a \text{ for all } x\}, \quad a > 0$$

and define $M_\mu := Y_\mu(0) = \sum_{x,y \in K} \mu(x) k(x, y)$. By construction, for any $W \in C_0(K) \setminus C^n_0(K)$ there exists $i$ such that $W(x_i) - W(x_{i-1}) > a/n$ and hence $Y_\mu(W) > \delta e^{a/(2n)}$. Fix now some $a$ so that $\delta e^{a/(2n)} > M_\mu$. By compactness, $Y_\mu$ on the set $C^n_0(K)$ attains the minimum, which then coincides with the minimum of $Y_\mu|_{C_0(K)}$. \hfill \square
B. The map $\mu \mapsto V_\mu$

Most importantly, from the previous section, the map $\mu \mapsto V_\mu$ is a bijection when we think of the potential modulo a constant. Moreover $V_\mu$ depends smoothly on $\mu$, and *vice versa*. In other words, the map $\mu \mapsto V_\mu$ is a diffeomorphism with variational distance $d(\mu, \rho)$ of the same order as $V$:

$$c_0 d(\mu, \rho) \leq |||V_\mu||| \leq c_1 d(\mu, \rho)$$

for constants $c_0, c_1 > 0$. That is really a consequence of the irreducibility of the finite Markov process, or see chapter two in [9].

Heuristically it suffices to understand the linearized map around $\mu = \rho, V_\rho = 0$ since the modified rates $k_{V_1+V_2}(x, y) = k_{V_1}(x, y) \exp\{V_2(y) - V_2(x)\}/2$ each time define an irreducible Markov process for each $V_1$. Writing $\mu = \rho(1 + \varepsilon h)$ for some function $h$ with mean $\sum_x \rho(x)h(x) = 0$ and for small $\varepsilon$, we easily find $V_\mu = \varepsilon v + O(\varepsilon^2)$ with

$$L_\mu v = L^*h$$

(VI.5)

Note here that $\rho$ is also invariant under the time-reversed process and under the (detailed balanced) process generated by $L_\mu$. Hence, $\sum_x \rho(x)L^*h(x) = 0$ and $L^*h$ is in the domain of the (Drazin) pseudo-inverse $(L_\mu)^{-1}$, so that (VI.5) has a unique solution (again up to a constant); in fact $h = 0$ if and only if $v = 0$.

The computation leading to (VI.5) goes as follows. For all $x \in K$,

$$0 = \sum_y \{\mu(y)k(y, x)e^{V(x) - V(y)}/2 - \mu(x)k(x, y)e^{V(y) - V(x)}/2\}$$

which by expanding the exponential directly yields the identity

$$L^*(\frac{\mu}{\rho} - 1)(x) - L_\mu V_\mu(x) = w(x, \mu)$$

(VI.6)

where (with $V = V_\mu$)

$$w(x, \mu) :=$$

$$\sum_y \{\frac{\mu(y)}{\rho(y)} - 1\} \frac{\rho(y)k(y, x) V(x) - V(y)}{2} + \frac{\mu(x)}{\rho(x)} - 1\} k(x, y) \frac{V(x) - V(y)}{2}$$

$$+ \sum_y \left[\frac{\mu(y)}{\rho(y)} k(y, x) - \frac{\mu(x)}{\rho(x)} k(x, y)\right] \delta_V(x, y)$$

(VI.7)
for \( \delta_V(x, y) := \sum_{n=2}^{\infty} \left[ \frac{V(x) - V(y)}{2^n} \right] n \frac{1}{n!} \). Each difference

\[
\frac{\mu(x)}{\rho(x)} - 1 \leq C_0 \|||V_{\mu}|||, \quad x \in K
\]

so that \(|w(x, \mu)| \leq C_1 \|||V_{\mu}|||^2\) for some constant \(C_1\) when \(|||V_{\mu}|||\) is sufficiently small.

**C. Proof of Theorem III.1**

We must take the time-derivative of \(I(\mu_t)\),

\[
\frac{d}{dt} I(\mu_t) = -\frac{1}{2} \sum_{x,y} \mu_t(x) k(x,y) \left[ V_t(y) - V_t(x) + 2\delta_V(y, x) \right]
+ \frac{1}{2} \sum_{x,y} \mu_t(x) k_{V_t}(x,y) \left[ V_t(x) - V_t(y) \right]
\]

(VI.8)

where \(V_t(x) := \frac{d}{dt} V_{\mu_t}(x)\). The second line in (VI.8) equals zero because per fixed time \(t\), \(\mu_t\) is stationary for the dynamics with rates \(k_{V_t}(x,y)\). We thus have

\[
\frac{d}{dt} I(\mu_t) = -\frac{1}{2} \sum_{x} \mu_t(x) \left[ LV_t(x) + 2 \sum_{y} k(x,y) \delta_V(y, x) \right]
\]

Looking at the first term, we use that

\[
\dot{\mu}_t(x) = \rho(x) L^* (\frac{\mu_t}{\rho} - 1)(x) = \rho(x) Ls V_t(x) + \rho(x) w(x, \mu_t)
\]

as introduced in (VI.6). In other words, we have obtained

\[
\frac{d}{dt} I(\mu_t) = -\frac{1}{2} Q(V_t) - \frac{1}{2} \sum_{x} \rho(x) w(x, \mu_t) LV_t(x) - \sum_{x} \dot{\mu}_t(x) k(x,y) \delta_V(y, x)
\]

for the quadratic form \(Q(f) := (Lf, Ls f) = (f, L^*Ls f) = (Ls L f, f)\) which, from the hypothesis of Theorem III.1, is bounded from below by \(c \|||f|||^2\). Since \(|||V_t||| \leq K \exp[-\gamma t]\) for some \(K < \infty, \gamma > 0\), it suffices finally to realize that, at least for large enough times \(t\),

\[
-\frac{1}{2} \sum_{x} \rho(x) w(x, \mu_t) LV_t(x) - \sum_{x} \dot{\mu}_t(x) k(x,y) \delta_V(y, x) \leq C \|||V_t|||^3
\]

for some \(C < \infty\). That easily follows by applying uniform bounds such as \(||LV(x)|| \leq C_2 |||V|||\) and \(||\delta_V(x,y)|| \leq C_3 |||V|||^2\) for small enough \(V\), combined with the previous estimate \(|w(x, \mu)| \leq C_1 |||V_{\mu}|||^2\) making also \(|\dot{\mu}_t(x)| \leq C_4 |||V_t|||\). That concludes the proof of Theorem III.1.
The proof above obviously gives an estimate of the time $t_0$ after which monotonicity surely sets in. Since $|||V_t|||$ is of the order $\exp(-\gamma t)$, $Q(V_t) > 0$ dominates the time-derivative of the Donsker-Varadhan functional when $\gamma t \gg 1$, i.e., for times beyond the relaxation time to the nonequilibrium steady regime.

D. Proof of Proposition V.1

The proof of Proposition V.1 follows by exactly the same computations as the above proof of Theorem III.1. The main remarkable point indeed is that we need to replace there $L$ by $L^*$.

E. Relation with linear response

We still verify (III.4), in computing

$$
\chi_{f,f}(t) = -\frac{1}{2} \left[ \frac{d}{dt} \left\langle f(x_0)f(x_t) \right\rangle_{\rho} + \left\langle Lf(x_0)f(x_t) \right\rangle_{\rho} \right]
$$

$$
= -\frac{1}{2} \left\langle (L + L^*)f(x_0)f(x_t) \right\rangle_{\rho}, \quad t \geq 0
$$

$$
\frac{d}{dt} \chi_{f,f}(t) \bigg|_{t=0} = -(Ls f, Lf)
$$

(VI.9)

or

$$
\frac{d}{dt} \chi_{f,f}(t) \bigg|_{t=0} = -Q(f)
$$

(VI.10)

Similarly, we look at the response of the observable $Lf$ to find

$$
\chi_{L,f,f}(t) = -\frac{1}{2} \left[ \frac{d}{dt} \left\langle f(x_0)Lf(x_t) \right\rangle_{\rho} + \left\langle Lf(x_0)Lf(x_t) \right\rangle_{\rho} \right]
$$

$$
= -\frac{1}{2} \left\langle (L^* + L)f(x_0)Lf(x_t) \right\rangle_{\rho}
$$

$$
\chi_{L,f,f}(0) = -(Ls f, Lf)
$$

(VI.11)

The equality (VI.9) = (VI.11) indicates that we can commute the time-derivative and the derivative with respect to the perturbation.

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