Maximum entropy principle for stationary states underpinned by stochastic thermodynamics

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The selection of an equilibrium state by maximising the entropy of a system, subject to certain constraints, is often powerfully motivated as an exercise in logical inference, a procedure where conclusions are reached on the basis of incomplete information. But such a framework can be more compelling if it is underpinned by dynamical arguments, and we show how this can be provided by stochastic thermodynamics, where an explicit link is made between the production of entropy and the stochastic dynamics of a system coupled to an environment. The separation of entropy production into three components allows us to select a stationary state by maximising the change, averaged over all realisations of the motion, in the principal relaxational or nonadiabatic component, equivalent to requiring that this contribution to the entropy production should become time independent for all realisations. We show that this recovers the usual equilibrium probability density function (pdf) for a conservative system in an isothermal environment, as well as the stationary nonequilibrium pdf for a particle confined to a potential under nonisothermal conditions, and a particle subject to a constant nonconservative force under isothermal conditions. The two remaining components of entropy production account for a recently discussed thermodynamic anomaly between over- and underdamped treatments of the dynamics in the nonisothermal stationary state.

I. INTRODUCTION

The standard distributions in equilibrium statistical mechanics can be derived in an appealingly straightforward fashion using the principle of maximum entropy or MaxEnt. The procedure seems first to have been employed by Gibbs [1], and was vigorously championed by Jaynes [2] as an example of logical inference, namely the optimal determination of a statistical description of an imperfectly specified system.

The essential idea is that a system can possess an informational entropy that measures the uncertainty of an observer's perception, expressed through a probability distribution over all the configurations (microstates) that the system could adopt. In order to represent the situation in as objectively neutral a fashion as possible, so the argument goes, we should select the distribution that has the greatest informational entropy, while enforcing consistency with any known properties of the system, represented as expectation values over the distribution. For various mathematical and physical reasons [3, 4], the informational entropy S_I of a probability distribution $p(i)$ over a set of microstates labelled i is written $S_I = -\sum_i p(i)\ln p(i)$ and if the constraints take the form of fixed expectation values $\langle C_n\rangle = \sum_i C_n(i)p(i)$ of a set of microstate-dependent quantities C_n, then it can be shown by way of the method of Lagrange multipliers that the statistical representation that makes no unwarranted further assumptions about the system is $p(i) \propto \exp[-\sum_n \lambda_n C_n(i)]$ where the λ_n are constants. So if we consider a physical system and employ the constraint that it possesses an identifiable mean energy as a consequence of being coupled to an isothermal reservoir acting as a source and sink of heat, then the optimal representation is canonical: $p(i) \propto \exp(-E(i)/kT_r)$, where $E(i)$ is the system energy in microstate i, the reservoir is characterised by a temperature T_r, and k is the Boltzmann constant. Such a distribution would clearly represent a situation with time independent system properties.

Jaynes argued that similar procedures should be used to select probability density functions (pdfs) in more general situations, particularly for nonequilibrium stationary states [2, 5]. The general strategy would be to introduce constraints relating to the existence of a non-zero flux of energy or particles through or within a system and some progress along these lines has been made, for example in [6]. Principles for selecting the most probable path taken by a system have a long history ([7, 8] also reviewed in [9]) and a similar rationale underlies the nonequilibrium statistical operator method (NESOM) developed by Zubarev and coworkers [10–12]. Variational principles involving the production *rate* of entropy in stationary states have also been proposed [13, 14] as well as the maximisation of *relative* entropy [15].

A puzzling aspect of MaxEnt, however, is that the selection of the prevailing constraints appears to be rather arbitrary. For example, if a system is exposed to a heat reservoir such that an expectation value of energy is identifiable and therefore relevant to the MaxEnt procedure, then why are the expectation values of additional functions of energy not relevant? Why does a term proportional to $[E(i)]^2$ not appear in the exponent of the canonical distribution in addition to $E(i)$? An argument is often made that constraints are placed upon dynamically conserved quantities, which would exclude arbitrary functions of energy, but this strongly suggests that dynamics must underpin the procedure. It is our aim here to demonstrate that the framework of stochastic thermodynamics can provide the underlying dynamics in the derivation of the MaxEnt principle.

In Section II we give a brief overview of stochastic thermodynamics, discussing the way in which (stochastic) entropy production is both a reflection of the mechanical irreversibility of the underlying stochastic dynamics and the basis of a measure of the change in microstate-level uncertainty of a system with time. We describe how the total entropy production may usefully be separated into three components, each with a specific character. In Section III we discuss the dynamics of mean total entropy production for a system subject to a conservative force field and coupled to an isothermal reservoir, arguing that this viewpoint provides a route to the canonical solution to the stochastic dynamics, and showing how this maps onto the traditional MaxEnt variational principle. We see how the constraints on the variational procedure emerge as a result of the dynamical coupling of the system to the reservoir. Only one of the three components of entropy production is non-zero in this case.

In Section IV we consider a nonequilibrium situation where a system is exposed to a background temperature gradient and show that the stationary state may be selected by the maximisation of the mean relaxational or nonadiabatic entropy production, one of the three components, or equivalently by requiring the increment in this component to be zero for all possible dynamical scenarios. We note that the average of the remaining two components accounts for a recently discussed anomaly in entropy production between over- and underdamped treatments [16, 17]. Supporting analysis is provided in Appendix A and a system driven by a nonconservative force under isothermal conditions is discussed in Appendix B. We give our conclusions in Section V.

II. STOCHASTIC DYNAMICS AND THERMODYNAMICS

Stochastic thermodynamics is based on a set of stochastic differential equations (SDEs) that describe the evolution of system dynamical variables [18–20], together with a definition of the entropy production associated with a possible realisation of the motion [21–24].

We focus our discussion on the motion in one spatial dimension of a single particle coupled to a set of heat reservoirs, each corresponding to a given position of the particle. The motion is described by the following Itō-rules SDEs:

$$dx = vdt \tag{1}$$

$$dv = -\gamma v dt + \frac{F(x)}{m}dt + \left(\frac{2kT_r(x)\gamma}{m}\right)^{1/2} dW, \tag{2}$$

where x and v are the particle position and velocity, respectively, t is time, γ is the friction coefficient, $F(x)$ is a spatially dependent force field acting on the particle, assumed for the moment to be related to a potential $\phi(x)$, m is the particle mass, $T_r(x)$ is a spatially dependent reservoir temperature and dW is an increment in a Wiener process. Such a starting point for discussing the stochastic behaviour of a particle in a temperature gradient is often employed, though alternatives can also be imagined. The simplicity of Eqs. (1) and (2) is convenient for our purpose.

Given the dynamics, entropy production is defined in the fashion proposed by Seifert [23]. It is fundamentally a measure of the probabilistic mechanical irreversibility of the motion. For a given time interval $0 \leq t \leq \tau$, the dynamics can generate a trajectory $\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}$ (where $\vec{\boldsymbol{x}}$ represents a function $x(t)$ in the specified time interval) according to a probability density function $\mathcal{P}[\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}]$. In the situation under consideration, the latter can be written as a product of the probability density $p(x, v, t)$ of a microstate with $x = x(0)$ and $v = v(0)$ at $t = 0$, and a conditional probability density that the specified trajectory is followed thereafter. The dynamics are also capable of generating an *antitrajectory* after an inversion of the particle velocity at time τ, and under the influence of a reversed time evolution of the force field and reservoir temperature, if relevant [25–27], until a total time 2τ has elapsed. In this period $\tau \leq t \leq 2\tau$ we can identify the probability density $\mathcal{P}^{\mathrm{R}}[\vec{\boldsymbol{x}}^\dagger, \vec{\boldsymbol{v}}^\dagger]$ that an antitrajectory $\vec{\boldsymbol{x}}^\dagger, \vec{\boldsymbol{v}}^\dagger$ starting at $x(\tau), -v(\tau)$ and ending at $x(0), -v(0)$ is generated, with the superscript R reminding us that the potential and reservoir temperature evolve with time in a reverse fashion with respect to the period $0 \leq t \leq \tau$. The antitrajectory $\vec{\boldsymbol{x}}^\dagger, \vec{\boldsymbol{v}}^\dagger$ is the 'time-reversed' partner of $\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}$ [28–30]. The total entropy production associated with the trajectory $\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}$ is then defined by

$$\Delta s_{\mathrm{tot}}[\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}] = \ln \left[\frac{\mathcal{P}[\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}]}{\mathcal{P}^{\mathrm{R}}[\vec{\boldsymbol{x}}^\dagger, \vec{\boldsymbol{v}}^\dagger]} \right], \tag{3}$$

and after multiplication by Boltzmann's constant and averaging over all trajectories, this corresponds to the production of thermodynamic entropy in the process. In a condition of thermal equilibrium, when the dynamics would be expected to generate a trajectory and its time-reversed partner with equal likelihood, the entropy production associated with *all* feasible trajectories will vanish.

The entropy production along a trajectory evolves stochastically, and for the system dynamics considered here an increment in Δs_{tot} is specified by the Itō-rules SDE

$$d\Delta s_{\mathrm{tot}} = -d[\ln p(x, v, t)] - \frac{1}{kT_r(x)} d\left(\frac{mv^2}{2}\right) + \frac{F(x)}{kT_r(x)}dx. \tag{4}$$

The origin of this expression is described in Appendix A and elsewhere [23, 29]. The second term is the negative increment in the kinetic energy of the particle over the time interval dt, and the third term is the negative increment in its potential energy, both divided by the local reservoir temperature. Together, they represent a positive increment in the energy of the local reservoir (which we may regard as a heat transfer dQ_r to that reservoir) divided by the local temperature. This would then correspond to a Clausius-type incremental change

$d\Delta s_{\rm res} = dQ_r/kT_r(x)$ in the entropy of the local reservoir in the interval of time dt. It is then natural to regard the first term in Eq. (4) as the change in the entropy of the system (the particle) over this period. Seifert defined a stochastic system entropy $s_{\rm sys} = -\ln p(x,v,t)$ in terms of the evolving phase space probability density function p generated by the stochastic dynamics [23], such that we can write

$$d\Delta s_{\rm tot} = d\Delta s_{\rm sys} + d\Delta s_{\rm res}. \quad (5)$$

Since velocity evolves in Eq. (2) under the direct influence of a stochastic force, the rules of stochastic calculus apply when we manipulate increments of a function of v. Since we employ Itō rules it would be incorrect to proceed from Eq. (4) by writing $d(v^2) = 2vdv$, which only applies under Stratonovich rules. An additional term proportional to dt would appear [20, 31]. Taking this properly into account removes an apparent anomaly in $d\Delta s_{\rm tot}$ discussed in [32].

The evaluation of $\Delta s_{\rm tot}$ for a specific realisation of the motion requires us to determine the evolution of the pdf as well as the system variables x and v: we need to solve the Fokker-Planck equation [18]

$$\frac{\partial p}{\partial t} = \mathcal{L}p = -\frac{\partial J_v^{\rm ir}}{\partial v} - v\frac{\partial p}{\partial x} - \frac{F}{m}\frac{\partial p}{\partial v}, \quad (6)$$

that corresponds to Eqs. (1) and (2), where $J_v^{\rm ir} = -\gamma v p - \partial(D_v p)/\partial v$ is the irreversible probability current, with $D_v = \gamma k T_r(x)/m$.

In spite of fluctuations in the total entropy production as the particle follows a trajectory, it can be shown that the average of this quantity is non-negative, a property that arises from an integral fluctuation relation [23]. This is regarded as the second law of thermodynamics in this framework, expressed as $d\langle\Delta s_{\rm tot}\rangle = d\langle\Delta s_{\rm sys}\rangle + d\langle\Delta s_{\rm res}\rangle \geq 0$ where the angled brackets denote an expectation over the pdfs of system coordinates at the beginning and end of the incremental time period.

The entropy production can be separated into a specific set of components, each with a particular character. Initial developments in this direction were provided by Van den Broeck and Esposito [33–35] and extended by Spinney and Ford [28–30], working within a framework suggested by Oono and Paniconi [36]. The total entropy production may be written as three terms [28, 29]

$$d\Delta s_{\rm tot} = d\Delta s_1 + d\Delta s_2 + d\Delta s_3, \quad (7)$$

with the Δs_1 and Δs_2 components defined in terms of ratios of probabilities that specific trajectories are taken by the system. We give particular attention to the first component, given by

$$\Delta s_1[\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}] = \ln\left[\frac{\mathcal{P}[\vec{\boldsymbol{x}}, \vec{\boldsymbol{v}}]}{\mathcal{P}^{\rm ad,R}[\vec{\boldsymbol{x}}^R, \vec{\boldsymbol{v}}^R]}\right], \quad (8)$$

where $\vec{\boldsymbol{x}}^R, \vec{\boldsymbol{v}}^R$ represents a reversal of the system trajectory *without* the inversion of velocity coordinates [29], and the superscript 'ad' indicates that 'adjoint' dynamical rules are employed to work out the probability of its generation.

Our key point is that a dynamical underpinning of the MaxEnt principle can be obtained by considering the properties of the Δs_1 component. The approach of the pdf under the dynamics towards stationarity is equivalent to a variational principle for its selection expressed in terms of Δs_1. Such a principle holds irrespective of whether the stationary state is one of equilibrium, in which case Δs_2 and Δs_3 are both zero during the evolution, or nonequilibrium such that Δs_2 and Δs_3 are in general non-zero. In both cases $d\Delta s_1$ vanishes asymptotically and $\langle\Delta s_1\rangle$ reaches a ceiling.

Let us substantiate these claims. It was shown in [28, 29] that the average values of Δs_{1-3} are related to the transient and stationary system pdfs (p and $p_{\rm st}$, respectively) as follows:

$$\begin{aligned}\frac{d\langle\Delta s_1\rangle}{dt} &= -\int dxdv\, \frac{\partial p}{\partial t}\ln\left[\frac{p(x,v,t)}{p_{\rm st}(x,v)}\right] \\ &= \int dxdv\, \frac{p}{D_v}\left(\frac{J_v^{\rm ir}}{p} - \frac{J_v^{\rm ir,st}}{p_{\rm st}}\right)^2 \geq 0, \quad (9)\end{aligned}$$

$$\frac{d\langle\Delta s_2\rangle}{dt} = \int dxdv\, \frac{p}{D_v}\left[\frac{J_v^{\rm ir,st}(x,-v)}{p_{\rm st}(x,-v)}\right]^2 \geq 0, \quad (10)$$

$$\frac{d\langle\Delta s_3\rangle}{dt} = -\int dxdv\, \frac{\partial p}{\partial t}\ln\left[\frac{p_{\rm st}(x,v)}{p_{\rm st}(x,-v)}\right], \quad (11)$$

where $\mathcal{L}p_{\rm st} = 0$, and $J_v^{\rm ir,st} = -\gamma v p_{\rm st} - \partial(D_v p_{\rm st})/\partial v$ is the irreversible probability current in the stationary state. The positivity of the rate of change of $\langle\Delta s_1\rangle$ and $\langle\Delta s_2\rangle$ is here explicit, but is also a consequence of integral fluctuation relations for these two components of entropy production [28, 33, 37]. Furthermore, the unaveraged increments $d\Delta s_1$ and $d\Delta s_3$ take the form

$$d\Delta s_1 = -d[\ln p(x,v,t)] + d[\ln p_{\rm st}(x,v)], \quad (12)$$

and

$$d\Delta s_3 = -d[\ln p_{\rm st}(x,v)] + d[\ln p_{\rm st}(x,-v)], \quad (13)$$

making clear the conditions for which they vanish ($p(x,v,t) = p_{\rm st}(x,v)$ and $p_{\rm st}(x,v)] = p_{\rm st}(x,-v)$, respectively), while $d\Delta s_2 = d\Delta s_{\rm res} - d[\ln p_{\rm st}(x,-v)]$. The SDEs that govern the evolution of Δs_{1-3} for a general Markovian dynamical framework are given in Appendix A.

The three contributions to the total entropy production can be interpreted as follows. Δs_1 is the principal relaxational entropy production associated with the approach of a system towards a stationary state. Once a system is in a stationary state, with $p = p_{\rm st}$, no further increments in Δs_1 take place. This component of entropy production, averaged over all possible realisations of the motion initiated at $t = 0$, namely $\langle\Delta s_1\rangle$, increases monotonically towards a positive constant, since Eq. (9) indicates that $d\langle\Delta s_1\rangle/dt \to 0$ as $p \to p_{\rm st}$. The Δs_1 contribution was denoted the nonadiabatic entropy production by

Esposito and Van den Broeck [33–35] and its properties were given particular attention by Hatano and Sasa [37].

Δs_3 is also associated with relaxation towards the stationary state, but in contrast to Δs_1, its average value does not necessarily evolve monotonically with time; there is no definite sign attached to $d\langle \Delta s_3\rangle/dt$ in Eq. (11). If the stationary pdf is velocity symmetric, however, Eq. (13) shows that $d\Delta s_3$ is identically zero. Since a velocity asymmetric stationary pdf is typically associated with a non-zero mean flux of some kind, and also with an underlying breakage of the principle of detailed balance in the stochastic dynamics [33–35], this component arises in situations where there is a nonequilibrium stationary state. It was designated the transient housekeeping entropy production by Spinney and Ford [28].

Δs_2 is also associated with a nonequilibrium stationary state, since a non-zero rate of change of its average over all possible realisations of the dynamics requires there to be a non-zero current $J_v^{\rm ir,st}$ in the stationary state. The rate of change of the average Δs_2 is non-negative [38], but is non-zero in a nonequilibrium stationary state, in contrast to the rate of change of the average Δs_1 which would then be zero. This is the most distinctive difference between these two components of entropy production. Esposito and Van den Broeck referred to Δs_2 as the adiabatic entropy production (and they considered it only in the context of the dynamics of even coordinates such as position), and Spinney and Ford, who considered odd coordinates such as velocity as well, denoted it the generalised housekeeping entropy production.

Other separations of total entropy production into three components are possible [39], but the choice employed here has the advantage that the Δs_3 component vanishes in the absence of velocity variables in the dynamics, and on average its rate of change in a stationary state is also zero.

As a system approaches stationarity, all three kinds of entropy production take place, but in the stationary state only Δs_2 and Δs_3 can potentially receive increments. The mean total entropy production rate in the stationary state is represented by $d\langle \Delta s_2\rangle/dt$ alone. If detailed balance holds, both Δs_2 and Δs_3 would be zero. Our proposal is that the monotonic increase in $\langle \Delta s_1\rangle$ towards a ceiling, or equivalently the vanishing of $d\Delta s_1$ in the stationary state, underpins MaxEnt for equilibrium situations, and offers an extension of the procedure to nonequilibrium circumstances. We now explore the implications of this viewpoint for isothermal and then nonisothermal situations.

III. SELECTION OF AN EQUILIBRIUM STATE

If the reservoirs were isothermal ($T_r(x) = T_0$), then irrespective of the initial conditions, the system under consideration should relax under the stochastic dynamics to an equilibrium state with zero irreversible probability current and canonical statistics. Let us examine how this works out dynamically and thermodynamically.

We presume that the contributions $d\Delta s_2$ and $d\Delta s_3$ are zero throughout as a consequence of the associated condition of detailed balance in the dynamics, as suggested by the velocity symmetry of the expected canonical pdf. This can be checked later. If the change in total entropy production is indeed entirely given by $d\Delta s_1$ then the total entropy production satisfies not only the incremental representation in terms of system and reservoir contributions in Eqs. (4) and (5), but also the mean behaviour represented by Eq. (9).

We are therefore in a position to write

$$\frac{d\langle \Delta s_{\rm tot}\rangle}{dt} \geq 0 \quad \text{and} \quad \lim_{t\to\infty} \frac{d\langle \Delta s_{\rm tot}\rangle}{dt} = 0. \qquad (14)$$

The mean total change in entropy of system plus reservoir will increase monotonically until it reaches a ceiling. The equilibrium state will be achieved when $\langle \Delta s_{\rm tot}\rangle$ becomes time-independent.

We argue that Eqs. (14) are equivalent to the maximisation of a constrained Gibbs system entropy over the range of possible pdfs, namely a MaxEnt procedure. The maximisation would have its origin in the dynamics, and would not arise merely from considerations of logical inference.

To support this viewpoint, we note that the incremental transfer of energy dQ_r to the reservoir, that specifies the entropy production $d\Delta s_{\rm res}$ in Eq. (5), is equal to $-d\Delta E$, the negative of the increment in the change (with respect to $t = 0$) in the energy of the system as it evolves over the time interval dt. Since $d\Delta s_{\rm res} = dQ_r/kT_0$, we can rewrite Eq. (5) as

$$\frac{d\langle \Delta s_{\rm tot}\rangle}{dt} = \frac{d\langle \Delta s_{\rm sys}\rangle}{dt} - \frac{1}{kT_0}\frac{d\langle \Delta E\rangle}{dt}. \qquad (15)$$

Next, we recognise that since $s_{\rm sys} = -\ln p$ is a function of system coordinates at a specified time t rather than a function of a trajectory of coordinates, the average $\langle \Delta s_{\rm sys}\rangle$ over realisations of the dynamics is a difference in the expectation of $s_{\rm sys}$ between the final and initial states. That is $\langle \Delta s_{\rm sys}\rangle = \overline{s_{\rm sys}}(t) - \overline{s_{\rm sys}}(0)$ where the expectations (indicated by overbars) are averages over the system pdf; thus $\overline{s_{\rm sys}}(t) = \int dxdv\, p(x,v,t)[-\ln p(x,v,t)] = S_G(t)$, the Gibbs informational entropy. For similar reasons, $\langle \Delta E\rangle = \overline{E}(t) - \overline{E}(0)$. Equations (14) and (15) tell us that the quantity $\overline{s_{\rm sys}}(t) - \overline{E}(t)/kT_0$ increases with time and reaches a ceiling as a consequence of the exploration of system phase space represented by the stochastic dynamics and the evolution of the pdf of the system.

Since Eq. (15) may be written $d\langle \Delta s_{\rm tot}\rangle/dt = dS_G(t)/dt - (kT_0)^{-1} d\overline{E}(t)/dt$, the dynamical increase and saturation of $\langle \Delta s_{\rm tot}\rangle$, irrespective of the initial pdf, is, we argue, equivalent to the functional maximisation of the quantity $S_G - \overline{E}/kT_0$ with respect to the pdf. In other words, the equilibrium pdf can also result from implementing the condition

$$\frac{\delta}{\delta p_{\rm st}}\left[-\int p_{\rm st}\ln p_{\rm st}\, dxdv - \lambda \int p_{\rm st} E\, dxdv\right] = 0, \qquad (16)$$

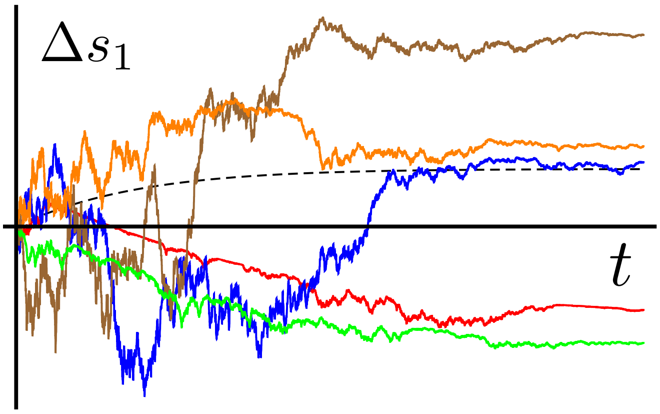

Figure 1. Examples of the time evolution of Δs_1 (continuous lines) associated with phase space trajectories taken by a system as it relaxes towards a stationary state for a particular stochastic process. The dashed line is the average of Δs_1 over all possible trajectories, satisfying $\langle \Delta s_1 \rangle \geq 0$. The stationary state is approached as $t \to \infty$ and is characterised by the condition $d\langle \Delta s_1 \rangle/dt = 0$ or equivalently the property $d\Delta s_1 = 0$ for all possible realisations, both of which are evident.

with Lagrange multiplier $\lambda = 1/kT_0$, leading to $p_{\rm st}(x,v) = p_{\rm eq} \propto \exp(-E/kT_0)$ with $E = mv^2/2 + \phi(x)$. The canonical distribution can be identified by a constrained maximisation of the informational entropy of the system. It is significant to observe that the only constraint that has to be taken into account involves the average of the energy, and that this has its origin in the production of entropy in the reservoir brought about by the dynamics of energy exchange between reservoir and the system. No constraints on other functions of energy should be included in the procedure. Furthermore, the Lagrange multiplier need not be deduced later on to make the result conform to the canonical distribution; its value had been fixed when writing down the original stochastic dynamical equations. Finally, it is easy to check using Eq. (13) that $d\Delta s_3 = 0$ since $p_{\rm eq}(x,v) = p_{\rm eq}(x,-v)$, and because $J_v^{\rm ir,st} = -\gamma v p_{\rm eq} - (\gamma kT_0/m)\partial p_{\rm eq}/\partial v = 0$, we can deduce from Eq. (10) that $d\langle \Delta s_2 \rangle/dt = 0$. Moreover, consideration of Eq. (A6) leads to the stronger conclusion $d\Delta s_2 = 0$, to be shown explicitly in the next section.

An equivalent demonstration of the emergence of a canonical pdf from the dynamics of stochastic entropy production is to note that $d\Delta s_{\rm tot} = d\Delta s_1 = 0$ for all possible incremental paths taken by the system when in the equilibrium state, from which we conclude that $-d\ln p_{\rm eq} - dE/kT_0 = 0$ with the equilibrium pdf following by integration. The association of $d\Delta s_1 = 0$ with the property $d\langle \Delta s_1 \rangle/dt = 0$ is illustrated in Figure 1.

Intuitively, the saturation of $S_G(t) - \overline{E}(t)/kT_0$ is equivalent to the maximisation of the uncertainty in the joint microstate adopted by the system and reservoir, brought about by the stochastic dynamics as $t \to \infty$. This is a reflection of the progressive loss of knowledge of microstate, as time elapses, in models where a system is coupled dynamically to a coarsely specified environment instead of one where the microscopic detail is retained [25].

IV. SELECTION OF A NONISOTHERMAL STATIONARY STATE

A. Underdamped dynamics

It is apparent that Eq. (4), together with the dynamics of Eqs. (1) and (2), can provide a framework for the time evolution of the total entropy production for a system exposed to an environment with a spatially dependent temperature. We have up to now regarded F as a conservative force, and this could be generalised to include a nonconservative component that drives a steady spatial flow. We investigate the latter in Appendix B but in this section we shall restrict the discussion to a conservative force field in order to make contact with a previous study of a particle in a nonisothermal environment [40]. The system will adopt a stationary nonequilibrium state where non-zero mean energy flows take place between the reservoirs at each spatial position, by way of the system, such that there will be a non-zero irreversible current $J_v^{\rm ir,st}$ in the stationary state, bringing about a steady rate of mean total entropy production. In the absence of a nonconservative force we would expect the mean velocity in the stationary state to vanish for all x.

We could identify the stationary pdf of such a system by solving the appropriate Fokker-Planck equation, but there is an alternative entropy-based approach. The dynamics generate a stationary pdf that embodies maximum uncertainty at the microstate level consistent with the nonisothermal constraints. The physical interpretation is that the component of mean entropy production associated with relaxation evolves to become as large as possible.

Our strategy is to establish an expression for $d\Delta s_1$ and set it equal to zero for all dynamical scenarios, a condition equivalent to $p = p_{\rm st}$ and hence through Eq. (9) to the reaching of a ceiling in the mean value of Δs_1. Using the general results in Appendix A for the dynamics under consideration, we can write

$$d\Delta s_2 = \frac{kT_r\gamma}{m}\left(\frac{\partial \ln[1+\psi(x,-v)]}{\partial v}\right)^2 dt - \frac{\partial \ln[1+\psi(x,-v)]}{\partial v}\left(\frac{2kT_r\gamma}{m}\right)^{1/2} dW, \quad (17)$$

where ψ is a component of a convenient, but still general, specification of the stationary pdf, namely $p_{\rm st}(x,v) = P_{\rm st}(x)[1+\psi(x,v)]f(x,v)$ where $f(x,v) = (m/2\pi kT_r)^{1/2}\exp(-mv^2/2kT_r)$ is a local canonical distribution, and $P_{\rm st} = \int dv\, p_{\rm st}$. Note that if $\psi = 0$ we have a canonical distribution over velocity and $d\Delta s_2$ vanishes as claimed in the previous section.

We also write

$$d\Delta s_3 = -d\ln[1+\psi(x,v)] + d\ln[1+\psi(x,-v)], \quad (18)$$

and using $d\Delta s_1 = d\Delta s_{\rm tot} - d\Delta s_2 - d\Delta s_3$ we have

$$d\Delta s_1 = -d\ln P_{\rm st} - d\ln f - \frac{1}{kT_r} d\left(\frac{mv^2}{2}\right) + \frac{F}{kT_r}dx - d\Delta s_2 - d\ln[1+\psi(x,-v)], \quad (19)$$

and this reduces to

$$\begin{aligned} d\Delta s_1 = &-d\ln P_{\rm st} + \left(1 - \frac{mv^2}{kT_r}\right)\frac{T_r'}{2T_r}dx + \frac{F}{kT_r}dx \\ &- \frac{kT_r\gamma}{m}\left(\frac{\partial \ln[1+\psi(x,-v)]}{\partial v}\right)^2 dt \\ &- \frac{\partial \ln[1+\psi(x,-v)]}{\partial x}dx \\ &- \frac{\partial \ln[1+\psi(x,-v)]}{\partial v}\left(-\gamma v + \frac{F}{m}\right)dt \\ &- \frac{\partial^2 \ln[1+\psi(x,-v)]}{\partial v^2}\frac{kT_r\gamma}{m}dt. \end{aligned} \quad (20)$$

where $T_r' = dT_r/dx$.

Setting $d\Delta s_1 = 0$ corresponds to a general condition for the structure of ψ and hence the pdf in the stationary state. For illustration, however, we proceed with an assumption that ψ is small and inversely proportional to γ, which is the commonly used perturbative Chapman-Enskog representation [41, 42], a well-established approach to solving problems in kinetic theory [43] to first order in inverse friction coefficient. This is not the same as making an assumption of overdamped dynamics, which would involve a different specification of the underlying stochastic dynamics. We shall consider such an approach in Section IV B. We identify the leading contributions to $d\Delta s_1$, namely those of order γ^0 and write

$$\begin{aligned} d\Delta s_1 = &-d\ln P_{\rm st} + \left(1 - \frac{mv^2}{kT_r}\right)\frac{T_r'}{2T_r}dx + \frac{F}{kT_r}dx \\ &+ \frac{\partial\psi(x,-v)}{\partial v}\gamma dx - \frac{\partial^2\psi(x,-v)}{\partial v^2}\frac{kT_r\gamma}{m}dt + O(\gamma^{-1}). \end{aligned} \quad (21)$$

For the right hand side to vanish term by term we deduce that a polynomial representation of $\psi(x,-v)$ can only contain linear and cubic terms in v. We write $\psi(x,v) = av + cv^3$ and require contributions to $d\Delta s_1$ proportional to $v^2 dx$ to vanish by demanding that

$$-\frac{mv^2}{kT_r}\frac{T_r'}{2T_r}dx - 3cv^2\gamma dx = 0. \quad (22)$$

so that $c = -mT_r'/(6\gamma kT_r^2)$.

We consider a situation where the particle is spatially confined by the potential, in the sense that the pdf vanishes as $x \to \pm\infty$. This implies the physical requirement that the mean velocity $\int_{-\infty}^{\infty} vp_{\rm st}(x,v)dv$ at a given x is zero in the stationary state, equivalent to the condition $\int_{-\infty}^{\infty} vf(x,v)\psi(x,v)dv = 0$. This means that $a + 3ckT_r/m = 0$ and hence to lowest order in γ^{-1},

$$\psi(x,v) = \frac{T_r'}{2\gamma T_r}\left(v - \frac{m}{3kT_r}v^3\right), \quad (23)$$

from which we conclude that

$$\frac{\partial\psi(x,-v)}{\partial v} = -\frac{T_r'}{2\gamma T_r}\left(1 - \frac{m}{kT_r}v^2\right), \quad (24)$$

and

$$\frac{\partial^2\psi(x,-v)}{\partial v^2} = \frac{mT_r'}{\gamma kT_r^2}v, \quad (25)$$

giving

$$d\Delta s_1 = -d\ln P_{\rm st} + \frac{F}{kT_r}dx - \frac{T_r'}{T_r}dx + O(\gamma^{-1}). \quad (26)$$

We deduce that the spatial part of the stationary pdf, to lowest order in γ^{-1}, is

$$P_{\rm st} \propto T_r^{-1}\exp\left(\int \frac{F}{kT_r}dx\right), \quad (27)$$

and the selection procedure is complete, with the result

$$\begin{aligned} p_{\rm st} \propto\ & T_r^{-3/2}\exp\left(-\frac{mv^2}{2kT_r} + \int\frac{F}{kT_r}dx\right) \\ &\times\left[1 + \frac{T_r'}{2\gamma T_r}\left(v - \frac{m}{3kT_r}v^3\right)\right]. \end{aligned} \quad (28)$$

The solution of the appropriate Fokker-Planck equation to first order in γ^{-1} should, of course, produce the same outcome [40], but our purpose here is to demonstrate that it can emerge also from considerations of entropy production.

We now examine the mean production of Δs_2, writing

$$\frac{J_v^{\rm ir,st}}{p_{\rm st}} = -\gamma v - \frac{kT_r\gamma}{mp_{\rm st}}\frac{\partial p_{\rm st}}{\partial v} = -\frac{kT_r\gamma}{m}\frac{\partial\ln(1+\psi)}{\partial v}, \quad (29)$$

and employing Eq. (10) we obtain

$$\frac{d\langle\Delta s_2\rangle}{dt} = \int dxdv\, p\frac{kT_r\gamma}{m}\left(\frac{\partial\ln[1+\psi(x,-v)]}{\partial v}\right)^2, \quad (30)$$

which is consistent with a direct averaging of Eq. (17). Inserting Eq. (23) we find that

$$\frac{d\langle\Delta s_2\rangle}{dt} = \int dxdv\, p\frac{kT_r\gamma}{m}\left(\frac{T_r'}{2\gamma T_r}\right)^2\left[1 - \frac{m}{kT_r}v^2\right]^2, \quad (31)$$

to lowest order in γ^{-1} and in the stationary state we therefore have

$$\frac{d\langle\Delta s_2\rangle_{\rm st}}{dt} = \int dx\, P_{\rm st}\frac{kT_r'^2}{2m\gamma T_r} + O(\gamma^{-2}). \quad (32)$$

Similarly, Eq. (11) gives

$$\frac{d\langle\Delta s_3\rangle}{dt} = -\int dxdv\,\frac{\partial p}{\partial t}\ln\left[\frac{1+\psi(x,v)}{1+\psi(x,-v)}\right], \quad (33)$$

which leads to

$$\frac{d\langle\Delta s_3\rangle}{dt} \approx -\int dxdv\,\frac{\partial p}{\partial t}\left[\frac{T_r'}{\gamma T_r}\left(v - \frac{m}{3kT_r}v^3\right)\right]. \quad (34)$$

This clearly vanishes in the stationary state, and for p close to stationarity in the velocity coordinate (in the sense that $p/P = f + O(\gamma^{-1})$, where $P(x,t) = \int p\, dv$), the mean rate of production $d\langle \Delta s_3 \rangle/dt$ is of order γ^{-2}.

Note that the stationary solution to the dynamics (28) satisfies a local equipartition condition $\int dv\, v^2 p_{\rm st} = P_{\rm st} kT_r/m$ but that this relationship is valid only to first order in γ^{-1}, in contrast to the approach of [44] where such a condition is taken to be a requirement to all orders. Under the dynamics assumed here, the system is maintained away from exact local equipartition through the flows of heat between the various local reservoirs.

B. Overdamped dynamics

It is instructive to consider next the variational identification of the stationary state under nonisothermal conditions within a framework of *overdamped* dynamics, and to contrast the outcome with the analysis in Section IV A for underdamped dynamics. The revised dynamics will affect the form of each component of entropy production, although it remains the case that the principal relaxational component will increase on average until the stationary state is reached.

It is well known [19, 20, 45] that Eqs. (1) and (2) reduce for large γ to the Itō-rules SDE for the position coordinate:

$$dx = \frac{F(x)}{m\gamma} dt + \left(\frac{2kT_r(x)}{m\gamma} \right)^{1/2} dW, \tag{35}$$

together with an associated Fokker-Planck equation for the positional pdf $P^{\rm od}(x,t)$. We investigate the entropy production implied by these dynamics, focussing attention on $\Delta s_1^{\rm od}$ where the superscript 'od' indicates that it is associated with the overdamped dynamics.

For an Itō-rules SDE $dx = A_x^{\rm od}(x)dt + [2D_x^{\rm od}(x)]^{1/2} dW$, Eq. (A4) in Appendix A implies total entropy production given by

$$d\Delta s_{\rm tot}^{\rm od} = -d\ln P^{\rm od} + \frac{A_x^{\rm od}}{D_x^{\rm od}} dx + \frac{dA_x^{\rm od}}{dx} dt - \frac{1}{D_x^{\rm od}} \frac{dD_x^{\rm od}}{dx} dx$$
$$- \frac{A_x^{\rm od}}{D_x^{\rm od}} \frac{dD_x^{\rm od}}{dx} dt - \frac{d^2 D_x^{\rm od}}{dx^2} dt + \frac{1}{D_x^{\rm od}} \left[\frac{dD_x^{\rm od}}{dx} \right]^2 dt, \tag{36}$$

recognising that the rules of stochastic calculus now associated with the variable x differ from those that hold for the full dynamics of Eqs. (1) and (2) since x evolves in Eq. (35) under the direct influence of a stochastic term. Inserting $A_x^{\rm od} = A_x^{\rm od,ir} = F/m\gamma$ and $D_x^{\rm od} = kT_r/m\gamma$ we find that

$$d\Delta s_{\rm tot}^{\rm od} = -d\ln P^{\rm od} + \frac{F}{kT_r} dx + \frac{F'}{m\gamma} dt - \frac{T_r'}{T_r} dx$$
$$- \frac{FT_r'}{m\gamma T_r} dt - \frac{kT_r''}{m\gamma} dt + \frac{kT'^2}{m\gamma T} dt, \tag{37}$$

where $F' = dF/dx$ and $T'' = d^2 T_r/dx^2$. Since under Itō rules we have $d\left[\int FT_r^{-1} dx\right] = FT_r^{-1} dx + D_x^{\rm od} \left(F'T_r^{-1} - FT_r^{-2}T_r' \right) dt$ and $d\ln T_r = T_r^{-1}T_r' dx + D_x^{\rm od}(d[T_r^{-1}T_r']/dx)dt$ this reduces to

$$d\Delta s_{\rm tot}^{\rm od} = -d\ln P^{\rm od} - d\ln T_r + \frac{1}{k} d\left[\int FT_r^{-1} dx \right]. \tag{38}$$

Since velocity coordinates are absent in the overdamped dynamics there are no $d\Delta s_3^{\rm od}$ contributions and the confinement of the particle to a potential such that there is no spatial current in the stationary state would suggest that $d\Delta s_2^{\rm od}$ is zero as well. The observation that the overdamped dynamics miss out the housekeeping entropy production in the stationary state is the origin of an entropy anomaly [16, 17] between treatments based on over- and underdamped dynamics, to be discussed shortly.

If the only non-zero contribution to $d\Delta s_{\rm tot}^{\rm od}$ is $d\Delta s_1^{\rm od}$, then the stationary state is specified by $d\Delta s_{\rm tot}^{\rm od} = 0$. From Eq. (38) we can therefore deduce the form of $P_{\rm st}^{\rm od}$ to be

$$P_{\rm st}^{\rm od}(x) \propto T_r^{-1} \exp \int (F/kT_r) dx, \tag{39}$$

which may be confirmed as the stationary solution to the Fokker-Planck equation

$$\frac{\partial P^{\rm od}}{\partial t} = -\frac{\partial}{\partial x} \left(\frac{FP^{\rm od}}{m\gamma} \right) + \frac{\partial^2}{\partial x^2} \left(\frac{kT_r P^{\rm od}}{m\gamma} \right) \tag{40}$$

for the overdamped dynamics (35). We note that $P_{\rm st}^{\rm od}$ is consistent with the pdf in Eq. (28) obtained to $O(\gamma^{-1})$ using underdamped dynamics, when integrated over v.

This result allows us to check the assertion that $d\Delta s_2^{\rm od}$ vanishes. According to Eq. (A6) we write

$$d\Delta s_2^{\rm od} = \frac{A_x^{\rm od}}{D_x^{\rm od}} dx + \frac{d\varphi^{\rm od}}{dx} dx$$
$$- \frac{1}{D_x^{\rm od}} \frac{dD_x^{\rm od}}{dx} dx + \frac{1}{D_x^{\rm od}} \left(\frac{dD_x^{\rm od}}{dx} \right)^2 dt + D_x^{\rm od} \left(\frac{d\varphi^{\rm od}}{dx} \right)^2 dt$$
$$-2 \frac{d\varphi^{\rm od}}{dx} \frac{dD_x^{\rm od}}{dx} dt + A_x^{\rm od} \frac{d\varphi^{\rm od}}{dx} dt - \frac{A_x^{\rm od}}{D_x^{\rm od}} \frac{dD_x^{\rm od}}{dx} dt, \tag{41}$$

where $\varphi^{\rm od} = -\ln P_{\rm st}^{\rm od}$. Clearly we have $d\varphi^{\rm od}/dx = T_r'/T_r - F/kT_r$ and by inserting the appropriate $A_x^{\rm od}$ and $D_x^{\rm od}$ it follows that $d\Delta s_2^{\rm od} = 0$.

It is possible to construct a MaxEnt principle for the selection of $P_{\rm st}^{\rm od}$, in the form of a functional maximisation, from Eq. (38) together with $d\Delta s_{\rm tot}^{\rm od} = d\Delta s_1^{\rm od}$ and $d\langle \Delta s_1^{\rm od} \rangle/dt \geq 0$, namely

$$\frac{\delta}{\delta P_{\rm st}^{\rm od}} \left[-\int P_{\rm st}^{\rm od} \ln P_{\rm st}^{\rm od}\, dx - \int P_{\rm st}^{\rm od} \ln T_r\, dx \right.$$
$$\left. + \int P_{\rm st}^{\rm od}(x) \left(\int^x dx' \frac{F(x')}{kT_r(x')} \right) dx \right] = 0, \tag{42}$$

which is equivalent to the requirement that $S_G^{\rm od} - \overline{\ln T_r} + \overline{\int dx\, F(x)/kT_r(x)}$ should be maximised. The system informational entropy $S_G^{\rm od}$ is a functional of $P^{\rm od}$, in contrast to the more general form S_G given in terms of p.

The second and third terms in Eq. (42) are effective constraints on the maximisation of system entropy for the selection of the stationary $P_{\rm st}^{\rm od}$ within a framework of overdamped dynamics, and they are unambiguous, if more elaborate than the constraint that appears in the corresponding isothermal case. They have their origin in contributions to the total entropy production in the reservoirs. While demonstrating a connection with the MaxEnt approach employed under isothermal conditions, such a functional maximisation would perhaps not be the most natural approach to use to select the pdf under nonisothermal conditions. Furthermore, it has been derived only for overdamped dynamics. The better strategy would be to focus on the condition for zero increment in Δs_1, namely Eq. (20).

Let us now reflect on the differences in the thermodynamics that emerge when we use overdamped rather than underdamped dynamics. As already mentioned, a treatment using overdamped dynamics fails to capture the housekeeping entropy production that is expected to take place in a nonisothermal stationary state. For a system with an approximately stationary velocity distribution, such that $p/P \approx f(1+\psi) = p_{\rm st}/P_{\rm st}$ we have seen that the mean contribution $d\langle\Delta s_3\rangle/dt$ is second order in γ^{-1}, and in the same circumstances we can combine Eqs. (7), (9) and (31) to write

$$\frac{d\langle\Delta s_{\rm tot}\rangle}{dt} = -\!\int\! dx \frac{\partial P}{\partial t}\ln\left[\frac{P(x,t)}{P_{\rm st}(x)}\right] + \!\int\! dx P \frac{kT_r'^2}{2m\gamma T_r} + O(\gamma^{-2}). \tag{43}$$

Replacing P in the second term by $P_{\rm st}$, an approximation valid if the system is close to stationarity, and inserting $\Delta s_{\rm tot}^{\rm od} = \Delta s_1^{\rm od}$, we arrive at

$$\frac{d\langle\Delta s_{\rm tot}\rangle}{dt} = \frac{d\langle\Delta s_{\rm tot}^{\rm od}\rangle}{dt} + \int dx\, P_{\rm st}(x) \frac{kT_r'^2}{2m\gamma T_r} + O(\gamma^{-2}). \tag{44}$$

This is the one dimensional version of a similar result in [16] that highlighted an anomaly in mean entropy production between over- and underdamped treatments of the dynamics of a system. It is clear from our analysis that the additional term on the right hand side of Eq. (44) is an approximate form of the mean housekeeping entropy production that is captured by the underdamped treatment but neglected when an overdamped dynamical model is adopted. A rational basis for the difference is to be found in recognising that entropy production is a consequence of the dynamics, and that modifications in the construction of the equations of motion will introduce changes in the form of the entropy production. The identification of the anomaly as a mean housekeeping entropy production (to lowest order in γ^{-1}) using the analysis presented here gives it a clear physical interpretation.

V. CONCLUSIONS

A framework of stochastic thermodynamics [24] provides a direct connection between entropy production and a stochastic model of the trajectory-level dynamics of a system. This dynamical connection has brought clarity to the concept of entropy production in statistical physics, enabling it to be extended to individual realisations of the evolution of a system and situations where fluctuations are important. A description of the mean entropy production can emerge from a treatment of the dynamics at the level of a Fokker-Planck equation, namely the behaviour of the system probability density function, but stochastic thermodynamics adds a crucial specification of the entropy production in terms of the probabilities that certain trajectories might be generated. We can separate the total production of entropy into three components within this framework.

The MaxEnt procedure for selecting equilibrium probability density functions has strong credentials as an exercise in logical inference, but we argue that it is made more compelling by demonstrating that it can arise naturally as a result of the underlying stochastic dynamics. The central question of how to constrain the maximisation of the system informational entropy is resolved by noting that the constraint terms employed in the derivation of the canonical pdf can be related to the mean entropy production in the environment. Constraints are therefore associated with the dynamical couplings of the system to the environment, and these often arise through the exchange of dynamically conserved quantities. The underlying principle of MaxEnt is to maximise the uncertainty in our perception of the microscopic state of the world. This is underpinned by the monotonic increase and saturation of the mean total entropy production at equilibrium according to the dynamics.

Such a framework can be extended to the selection of stationary pdfs for nonequilibrium systems. It is a thermodynamic alternative to seeking a time-independent solution to the appropriate Fokker-Planck equation describing the dynamics. The average of the principal relaxational, or nonadiabatic component of entropy production Δs_1 [28, 33, 37] increases to a ceiling when the stationary state is reached, and increments in this component thereafter vanish. By exploiting the latter property the nonequilibrium pdf can be identified. We have implemented such a strategy in a simple one dimensional system of trapped Brownian motion in a thermal gradient using both under- and overdamped dynamics. In doing so we recover the 'anomaly' between the entropy production obtained under the two treatments [16] and show that it corresponds to housekeeping entropy production. We have also used the strategy, in Appendix B, to recover the known stationary pdf for a particle subjected to a constant nonconservative force and isothermal conditions.

In summary, the principal insight presented in this paper is that the stochastic dynamics of a system generate stationary statistics in a fashion that maximises the mean of a certain component of entropy production, Δs_1, and that this can map onto the procedure of constrained maximisation of system informational entropy based on logical inference. The procedure is equivalent to demanding that the increment $d\Delta s_1$ brought about by the dynamics should vanish for all possible trajectories. We have employed this approach to select an equilibrium state of a system in an isothermal environment and a nonequilibrium state under nonisothermal conditions. We also consider an isothermal system subject to a nonconservative force. The $d\Delta s_1 = 0$ condition is equivalent through Eq. (12) merely to the requirement that the pdf is stationary, but since we can associate the evolution of Δs_1 with energy exchange with an environment and associated system change during relaxation, it has a physical interpretation [37]. Δs_1 is defined in Eq. (8) in terms of probabilities of system evolution at the level of trajectories, one of the foundational statements of stochastic thermodynamics, from which the property $\langle \Delta s_1 \rangle \geq 0$ follows, and an algorithm for the maximisation of $\langle \Delta s_1 \rangle$ is provided by the underlying system dynamics. We suggest that the procedure provides a natural extension of canonical MaxEnt to nonequilibrium situations, at least for systems governed by Markovian stochastic dynamics.

Acknowledgements

I am grateful for support from the Engineering and Physical Sciences Research Council (EPSRC) Network Plus on Emergence and Physics far from Equilibrium.

Appendix A: Components of stochastic entropy production

We summarise the main results concerning the dynamics of components of stochastic entropy production that are derived in more detail in Spinney and Ford [29]. For a system governed by Itō-rules Markovian stochastic differential equations (SDEs)

$$d\mathrm{x}_i = A_i(\mathbf{x}, t)dt + B_i(\mathbf{x}, t)dW_i, \tag{A1}$$

where $\mathbf{x}$ represents a set of dynamical variables $(\mathrm{x}_1, \mathrm{x}_2, \cdots)$ such as (x, v), we define

$$A_i^{\mathrm{ir}}(\mathbf{x}, t) = \frac{1}{2}\left[A_i(\mathbf{x}, t) + \varepsilon_i A_i(\boldsymbol{\varepsilon}\mathbf{x}, t)\right] = \varepsilon_i A_i^{\mathrm{ir}}(\boldsymbol{\varepsilon}\mathbf{x}, t), \tag{A2}$$

$$A_i^{\mathrm{rev}}(\mathbf{x}, t) = \frac{1}{2}\left[A_i(\mathbf{x}, t) - \varepsilon_i A_i(\boldsymbol{\varepsilon}\mathbf{x}, t)\right] = -\varepsilon_i A_i^{\mathrm{rev}}(\boldsymbol{\varepsilon}\mathbf{x}, t), \tag{A3}$$

where $\varepsilon_i = 1$ for variables x_i with even parity under time reversal symmetry (for example position x) and $\varepsilon_i = -1$ for variables with odd parity (for example velocity v), and $\boldsymbol{\varepsilon}\mathbf{x}$ represents $(\varepsilon_1\mathrm{x}_1, \varepsilon_2\mathrm{x}_2, \cdots)$. Defining also $D_i(\mathbf{x}, t) = \frac{1}{2}B_i(\mathbf{x}, t)^2$, it may be shown that the following Itō-rules SDE for the total entropy production emerges:

$$\begin{aligned} d\Delta s_{\mathrm{tot}} = -d\ln p + \sum_i \Bigg[&\frac{A_i^{\mathrm{ir}}}{D_i}d\mathrm{x}_i - \frac{A_i^{\mathrm{rev}}A_i^{\mathrm{ir}}}{D_i}dt + \frac{\partial A_i^{\mathrm{ir}}}{\partial \mathrm{x}_i}dt \\ &- \frac{\partial A_i^{\mathrm{rev}}}{\partial \mathrm{x}_i}dt - \frac{1}{D_i}\frac{\partial D_i}{\partial \mathrm{x}_i}d\mathrm{x}_i + \frac{(A_i^{\mathrm{rev}} - A_i^{\mathrm{ir}})}{D_i}\frac{\partial D_i}{\partial \mathrm{x}_i}dt \\ &- \frac{\partial^2 D_i}{\partial \mathrm{x}_i^2}dt + \frac{1}{D_i}\left(\frac{\partial D_i}{\partial \mathrm{x}_i}\right)^2 dt \Bigg], \end{aligned} \tag{A4}$$

where p is the time dependent pdf of variables $\mathbf{x}$. The corresponding Itō SDE for the principal relaxational entropy production is

$$d\Delta s_1 = -d\ln p + \sum_i \left[-\frac{\partial \varphi}{\partial \mathrm{x}_i}d\mathrm{x}_i - D_i\frac{\partial^2 \varphi}{\partial \mathrm{x}_i^2}dt \right], \tag{A5}$$

where $\varphi = -\ln p_{\mathrm{st}}$ and p_{st} is the stationary pdf. Also

$$\begin{aligned} d\Delta s_2 = \sum_i \Bigg[&-\frac{A_i^{\mathrm{ir}}A_i^{\mathrm{rev}}}{D_i}dt + \frac{A_i^{\mathrm{ir}}}{D_i}d\mathrm{x}_i + \varepsilon_i\varphi_i'(\boldsymbol{\varepsilon}\mathbf{x})d\mathrm{x}_i \\ &- \frac{1}{D_i}\frac{\partial D_i}{\partial \mathrm{x}_i}d\mathrm{x}_i + \frac{1}{D_i}\left(\frac{\partial D_i}{\partial \mathrm{x}_i}\right)^2 dt + D_i(\varphi_i'(\boldsymbol{\varepsilon}\mathbf{x}))^2 dt \\ &- 2\varepsilon_i\varphi_i'(\boldsymbol{\varepsilon}\mathbf{x})\frac{\partial D_i}{\partial \mathrm{x}_i}dt + \varepsilon_i(A_i^{\mathrm{ir}} - A_i^{\mathrm{rev}})\varphi_i'(\boldsymbol{\varepsilon}\mathbf{x})dt \\ &- \frac{(A_i^{\mathrm{ir}} - A_i^{\mathrm{rev}})}{D_i}\frac{\partial D_i}{\partial \mathrm{x}_i}dt \Bigg], \end{aligned} \tag{A6}$$

specifies an increment in Δs_2, using notation $\varphi_i'(\boldsymbol{\varepsilon}\mathbf{x}) = \varepsilon_i \partial\varphi(\boldsymbol{\varepsilon}\mathbf{x})/\partial \mathrm{x}_i$ and

$$\begin{aligned} d\Delta s_3 &= -d\ln p_{\mathrm{st}}(\mathbf{x}) + d\ln p_{\mathrm{st}}(\boldsymbol{\varepsilon}\mathbf{x}) \\ &= \sum_i [\varphi_i'(\mathbf{x}) \circ d\mathrm{x}_i - \varepsilon_i\varphi_i'(\boldsymbol{\varepsilon}\mathbf{x}) \circ d\mathrm{x}_i], \end{aligned} \tag{A7}$$

defines the third component. Stratonovich notation is used in the second line for reasons of compactness, but a more elaborate Itō-rules version can be constructed.

For the dynamics specified by Eqs. (1) and (2) we have $A_x^{\mathrm{ir}} = 0$, $A_x^{\mathrm{rev}} = v$, $A_v^{\mathrm{ir}} = -\gamma v$, $A_v^{\mathrm{rev}} = F/m$, $D_x = 0$ and $D_v = kT_r\gamma/m$ and using Eq. (A4) we recover Eq. (4).

Appendix B: Particle in a nonconservative force field

We consider how the stationary pdf of a particle evolving according to Eqs. (1) and (2) with a nonconservative constant force field $F(x) = F_0$ and an isothermal environment $T_r(x) = T_0$ can be selected according to the condition that $\langle \Delta s_1 \rangle$ should be maximised. As before, we regard this as synonymous with $d\Delta s_1 = 0$.

By adapting Eq. (20), while demanding on physical grounds that the pdf should be spatially independent, we replace $\ln[1 + \psi(x, v)]$ by $h(-v)$ and write $p_{\mathrm{st}}(v) = P_{\mathrm{st}}\exp[h(-v)]f(v)$ with $f(v) =$

$[m/(2\pi kT_0)]^{1/2}\exp[-mv^2/(2kT_0)]$. The function h is specified by

$$d\Delta s_1 = \frac{F_0}{kT_0}dx - \frac{kT_0\gamma}{m}\left(\frac{dh}{dv}\right)^2 dt$$
$$-\frac{dh}{dv}\left(-\gamma v + \frac{F_0}{m}\right)dt - \frac{d^2h}{dv^2}\frac{kT_0\gamma}{m}dt = 0, \quad \text{(B1)}$$

and the normalisation $\int dv\exp[h(-v)]f(v) = 1$. It is apparent that a quadratic in v is the highest finite polynomial form that h can take (the exponent N in the leading term v^N must be even to preserve the normalisation but $N > 2$ would produce a non-vanishing term proportional to $v^{2(N-1)}$), and hence we write $h(v) = a_0 + a_1 v + a_2 v^2$. The condition that terms in Eq. (B1) proportional to $v^2 dt$ vanish is

$$-(kT_0\gamma/m)4a_2^2 + 2a_2\gamma = 0, \quad \text{(B2)}$$

with solutions $a_2 = 0$ or $m/(2kT_r)$, but the normalisation condition eliminates the second option. The condition for terms in both vdt and dt to vanish is found to be $a_1 = -F_0/(\gamma kT_0)$, and the normalised pdf is therefore specified by

$$h(v) = \frac{F_0^2}{2m\gamma^2 kT_0} - \frac{F_0 v}{\gamma kT_0}, \quad \text{(B3)}$$

corresponding to

$$p_{\rm st}(v) \propto \exp\left(-\frac{m[v - F_0/(m\gamma)]^2}{2kT_0}\right), \quad \text{(B4)}$$

which is the known stationary state for such a system [29]. Adapting Eqs. (17) and (18) we identify the increments in the remaining components of entropy production to be

$$d\Delta s_2 = \frac{kT_0\gamma}{m}\left(\frac{\partial h}{\partial v}\right)^2 dt - \frac{\partial h}{\partial v}\left(\frac{2kT_0\gamma}{m}\right)^{1/2} dW$$
$$= \frac{F_0^2}{\gamma mkT_0}dt + \left(\frac{2F_0^2}{\gamma mkT_0}\right)^{1/2} dW, \quad \text{(B5)}$$

and

$$d\Delta s_3 = -dh(-v) + dh(v) = -\frac{2F_0}{\gamma mkT_0}dv, \quad \text{(B6)}$$

which do not vanish, even in the stationary state, unless $F_0 = 0$. Distributions of the components of entropy production in a relaxation process for this system were examined in [29].

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