Stochastic entropy production for dynamical systems with restricted diffusion

Jonathan Dexter and Ian J. Ford
Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, U.K.

Modelling the evolution of a system using stochastic dynamics typically implies a greater subjective uncertainty in the adopted system coordinates as time progresses, and stochastic entropy production has been developed as a measure of this change. In some situations the evolution of stochastic entropy production can be described using an Itô process, but mathematical difficulties can emerge if diffusion in the system phase space is restricted to a subspace of lower dimension. This can arise if there are constants of the motion, for example, or more generally when there are functions of the coordinates that evolve without noise. We discuss such a case for an open three-level quantum system modelled within a framework of Markovian quantum state diffusion and show how the problem of computing the stochastic entropy production in such a situation can be overcome. We go on to illustrate how a nonequilibrium stationary state of the three-level system, with a constant mean production rate of stochastic entropy, can be established under suitable environmental couplings.

I. INTRODUCTION

Entropy quantifies subjective uncertainty in the configuration of a system when limited information is available. If the evolution of such a system is modelled using stochastic dynamics, representing the effects of coupling to an underspecified environment, then subjective uncertainty in the configuration of the world (the system plus its environment) increases with time, corresponding to a growth in the total entropy. The second law of thermodynamics arises when the world is characterised or perceived at a coarse grained level, but governed by underlying equations of motion with a sufficient degree of deterministic chaos [1].

For system variables that evolve continuously according to a set of Markovian stochastic differential equations (SDEs), or Itô processes, it may be shown that the associated stochastic entropy production can also be described using an SDE, but only if the noise terms satisfy certain requirements [2–4]. Problems arise from constraints imposed on the dynamics, for example the existence of constants of the motion. In such cases, the matrix describing the diffusion of system coordinates in their phase space becomes singular. There are directions in the space in which diffusion does not take place and mathematical difficulties in the evaluation of the stochastic entropy production arise as a consequence.

The central aim of this paper is to show how to take such constraints on diffusion into account when computing the stochastic entropy production. In Section II we briefly discuss how an SDE for stochastic entropy production may be derived from Markovian SDEs for a set of system coordinates. The mathematical treatment of cases where diffusion is restricted is discussed in Section III. In Section IV we consider the stochastic dynamics of the reduced density matrix of an open three-level quantum system, subjected to environmental disturbance manifested as raising and lowering operators associated with transitions between the levels [5, 6]. The diffusion matrix is singular but we demonstrate how the stochastic entropy production can still be evaluated. We go on to compute the environmental component of mean stochastic entropy production numerically in order to characterise equilibrium and nonequilibrium stationary states of the system. Application to classical systems is also possible. Our conclusions are given in Section V.

II. STOCHASTIC ENTROPY PRODUCTION FOR ITÔ PROCESSES

We consider a set of coordinates $\boldsymbol{x} \equiv (x_1, x_2, \cdots, x_N)$ that specify the configuration of a system, and model their evolution using Markovian stochastic differential equations, or Itô processes:

$$dx_i = A_i(\boldsymbol{x}, t)dt + \sum_j B_{ij}(\boldsymbol{x}, t)dW_j, \tag{1}$$

where the dW_j are independent Wiener increments. We define [3]

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

and

$$A_i^{\rm rev}(\boldsymbol{x}, t) = \frac{1}{2}\left[A_i(\boldsymbol{x}, t) - \varepsilon_i A_i(\boldsymbol{\varepsilon x}, t)\right] = -\varepsilon_i A_i^{\rm rev}(\boldsymbol{\varepsilon x}, t), \tag{3}$$

where $\varepsilon_i = 1$ for variables x_i with even parity under time reversal symmetry (for example position) and $\varepsilon_i = -1$ for variables with odd parity (for example velocity). The notation $\boldsymbol{\varepsilon x}$ represents $(\varepsilon_1 x_1, \varepsilon_2 x_2, \cdots)$. Defining an $N \times N$ diffusion matrix $\boldsymbol{D}(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{B}(\boldsymbol{x})\boldsymbol{B}(\boldsymbol{x})^{\mathsf{T}}$, the Fokker-Planck equation for the probability density function (pdf) $p(\boldsymbol{x}, t)$ is

$$\frac{\partial p}{\partial t} = -\sum_i \frac{\partial}{\partial x_i}\left(A_i p\right) + \frac{\partial}{\partial x_i \partial x_j}\left(D_{ij} p\right). \tag{4}$$

The stochastic entropy production of the system and its environment, associated with the stochastic motion described by Eq. (1), is a measure of the difference in probability between pairs of time-reversed sequences of events, and is defined by [7]

$$\Delta s_{\rm tot} = \ln\left(\frac{\text{Prob(forward trajectory)}}{\text{Prob(backward trajectory)}}\right). \tag{5}$$

This is usually separated into system and environmental contributions:

$$d\Delta s_{\rm tot} = d\Delta s_{\rm sys} + d\Delta s_{\rm env}, \tag{6}$$

with $d\Delta s_{\rm sys} = -d\ln p(\boldsymbol{x},t)$. The evolution of the environmental stochastic entropy production is governed by [4]:

$$\begin{aligned}
d\Delta s_{\rm env} = &-\sum_i \frac{\partial A_i^{\rm rev}(\boldsymbol{x})}{\partial x_i}dt + \sum_{i,j}\Bigg\{\frac{D_{ij}^{-1}(\boldsymbol{x})}{2}\left(A_i^{\rm irr}(\boldsymbol{x})dx_j + A_j^{\rm irr}(\boldsymbol{x})dx_i\right) \\
&- \frac{D_{ij}^{-1}(\boldsymbol{x})}{2}\left(\left(\sum_n \frac{\partial D_{jn}(\boldsymbol{x})}{\partial x_n}\right)dx_i + \left(\sum_m \frac{\partial D_{im}(\boldsymbol{x})}{\partial x_m}\right)dx_j\right) - \frac{D_{ij}^{-1}(\boldsymbol{x})}{2}\left(A_i^{\rm rev}(\boldsymbol{x})A_j^{\rm irr}(\boldsymbol{x}) + A_j^{\rm rev}(\boldsymbol{x})A_i^{\rm irr}(\boldsymbol{x})\right)dt \\
&+ \frac{D_{ij}^{-1}(\boldsymbol{x})}{2}\left(A_j^{\rm rev}(\boldsymbol{x})\left(\sum_m \frac{\partial D_{im}(\boldsymbol{x})}{\partial x_m}\right) + A_i^{\rm rev}(\boldsymbol{x})\left(\sum_n \frac{\partial D_{jn}(\boldsymbol{x})}{\partial x_n}\right)\right)dt \\
&+ \frac{1}{2}\sum_k\Bigg[D_{ik}(\boldsymbol{x})\frac{\partial}{\partial x_k}\left(D_{ij}^{-1}(\boldsymbol{x})A_j^{\rm irr}(\boldsymbol{x})\right) + D_{jk}(\boldsymbol{x})\frac{\partial}{\partial x_k}\left(D_{ij}^{-1}(\boldsymbol{x})A_i^{\rm irr}(\boldsymbol{x})\right) \\
&- D_{ik}(\boldsymbol{x})\frac{\partial}{\partial x_k}\left(D_{ij}^{-1}(\boldsymbol{x})\left(\sum_n \frac{\partial D_{jn}(\boldsymbol{x})}{\partial x_n}\right)\right) - D_{jk}(\boldsymbol{x})\frac{\partial}{\partial x_k}\left(D_{ij}^{-1}(\boldsymbol{x})\left(\sum_m \frac{\partial D_{im}(\boldsymbol{x})}{\partial x_m}\right)\right)\Bigg]dt\Bigg\}.
\end{aligned} \tag{7}$$

It may be shown that the average of $d\Delta s_{\rm sys}$ over all possible trajectories is related to the incremental change in Gibbs entropy of the system: $d\langle\Delta s_{\rm sys}\rangle = dS_G$, to which boundary terms should be added in certain circumstances [5]. Computing the environmental stochastic entropy production, on the other hand, presents particular difficulties if the diffusion matrix is singular, since the inverse matrix $\boldsymbol{D}^{-1}$ is required in the above expression. This is the problem we wish to address here..

III. DEFINING DYNAMICAL AND SPECTATOR VARIABLES

A singular diffusion matrix may be regarded as a consequence of having fewer independent noise terms than the number of coupled Itô processes. For example, diffusion might occur on a two dimensional surface within a three dimensional phase space of system coordinates when the motion is described by three Itô processes with only two independent Wiener increments. There is a direction at each point in the phase space in which there is no diffusive current, which makes the 3×3 diffusion matrix singular. These directions lie parallel to spatially dependent eigenvectors of the diffusion matrix with zero eigenvalues, to be referred to as null eigenvectors. The obvious solution is to establish a reduced set of stochastic differential equations that describe the random evolution of, in this example, two coordinates on the surface with the third related deterministically to the other two. We shall denote the stochastically evolving coordinates as ‘dynamical’ and the remaining coordinates as ‘spectators’.

It might be possible in simple cases to identify such a reduced set of coordinates, perhaps by identifying a constant of the motion. However, as we increase the dimensionality of the phase space and hence the size of the diffusion matrix, the difficulties in doing so may become insurmountable. We therefore require a more general treatment of situations with a singular diffusion matrix.

Let us consider a system described by N variables x_i, each of which evolves stochastically according to

$$dx_i = A_i dt + \sum_{j=1}^{M} B_{ij}dW_j, \tag{8}$$

where the dW_j are M independent Wiener increments. According to Itô’s lemma [8], the differential of a function f of these variables can be written

$$df = \sum_{i=1}^{N}\frac{\partial f}{\partial x_i}dx_i + \sum_{i,j=1}^{N}\frac{\partial^2 f}{\partial x_i \partial x_j}D_{ij}dt, \tag{9}$$

where the elements of the $N\times N$ diffusion matrix are $D_{ij} = \frac{1}{2}\sum_{k=1}^{M} B_{ik}B_{jk}$. Consider such a function where the stochastic terms in Eq. (9) vanish, i.e.

$$\sum_{i=1}^{N}\sum_{j=1}^{M}\frac{\partial f}{\partial x_i}B_{ij}dW_j = 0. \tag{10}$$

Taking the square and using $dW_i dW_j = \delta_{ij}dt$ we find that

$$\begin{aligned}\sum_{ijkl}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_k}B_{ij}B_{kl}\delta_{jl}dt &= \sum_{ijk}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_k}B_{ij}B_{kj}dt\\ &= 2\sum_{ik}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_k}D_{ik}dt = 0,\end{aligned} \tag{11}$$

and we therefore have deterministic (noise-free) evolution of f if

$$(\boldsymbol{\nabla} f)^{\mathsf{T}}\boldsymbol{D}\boldsymbol{\nabla} f = 0. \tag{12}$$

Such an outcome can arise if $\boldsymbol{\nabla} f$ is an eigenvector of $\boldsymbol{D}$ with an eigenvalue equal to zero. A matrix is singular if one or more of its eigenvalues are zero, so we have established that $\boldsymbol{D}$ is singular if there exists a function f of the stochastic variables x_i that evolves deterministically. For dynamics evolving in an N dimensional phase space under the influence of M noises where $N > M$, we conjecture that there will be $L = N - M$ such functions, each associated with one of the null eigenvectors of $\boldsymbol{D}$. We shall see that this condition allows us to recast the calculation of the stochastic entropy production to overcome the problematic singularity of $\boldsymbol{D}$.

A. Identifying constants of motion

If the deterministic as well as stochastic terms in Eq. (9) vanish then $df = 0$ and the function f is a constant of the motion: the evolution of variables, or coordinates, is constrained to a contour of constant f. We can therefore write

$$\boldsymbol{\nabla} f \cdot d\boldsymbol{x} = 0, \tag{13}$$

meaning that the infinitesimal vector $d\boldsymbol{x}$ specified by Eq. (8) is tangential to a contour of f. Since $\boldsymbol{\nabla} f$ is also a null eigenvector of the diffusion matrix, this constraint on $d\boldsymbol{x}$ is conveniently identified by evaluating the eigenvectors of $\boldsymbol{D}$.

If there are $L = N - M$ constant functions of the coordinates under the dynamics we can remove L coordinates from the original N dimensional phase space leaving a reduced M dimensional phase space. Without loss of generality, the first M coordinates in the set $\{x_m\}$ with $m = 1, \cdots, M$ will be denoted *dynamical variables* and the remaining L coordinates $\{x_l\}$ with $l = M+1, \cdots, N$ are designated *spectator variables*. The L constants of the motion mean we should be able to write the spectator variables as functions of the dynamical variables, namely $\{x_l(\{x_m\})\}$. The division into dynamical and spectator variables is arbitrary, but, as we shall see, some choices are more convenient for computing stochastic entropy production than others.

In this labelling scheme, the top left $M \times M$ block of the diffusion matrix $\boldsymbol{D}$ remains relevant to the stochastic entropy calculation and will be non-singular, allowing us to use Eq. (7) to compute $\Delta s_{\rm env}$ associated with the evolution, but with i and j ranging only between 1 and M rather than 1 and N. However, if the elements of this matrix block depend on spectator variables, we need to take this into account when performing derivatives with respect to the dynamical variables. To emphasise this point, we write the components of $\boldsymbol{A}, \boldsymbol{D}$ and $\boldsymbol{D}^{-1}$ that appear in Eq. (7) to show their dependence on the dynamical and spectator variables explicitly:

$$\begin{gathered}A_i\left(\{x_m\}, \{x_l(\{x_m\})\}\right)\\ D_{ij}\left(\{x_m\}, \{x_l(\{x_m\})\}\right)\\ D^{-1}_{ij}\left(\{x_m\}, \{x_l(\{x_m\})\}\right),\end{gathered} \tag{14}$$

and Eq. (7) requires us to evaluate derivatives of A_i, D_{ij} and $D^{-1}_{ij}A_j$ with respect to the dynamical variables $\{x_m\}$.

We consider derivatives of D_{ij} in the following, but the argument is easily extend to other expressions. We begin by noting that Eq. (13) can be separated according to dynamical and spectator variables such that

$$\sum_{m=1}^{M}\alpha_{km}dx_m + \sum_{l=M+1}^{N}\alpha_{kl}dx_l = 0, \tag{15}$$

where α_{km} and α_{kl} are the dynamical and spectator components, respectively, of the kth null eigenvector of $\boldsymbol{D}$, with $k = 1, \cdots, L$. Therefore

$$\sum_{l=M+1}^{N}\alpha_{kl}dx_l = -\sum_{m=1}^{M}\alpha_{km}dx_m. \tag{16}$$

Arranging the α_{km} as elements of a rectangular $L \times M$ matrix Q_{km} and the α_{kl} as elements of a square $L \times L$ matrix P_{kl} we have

$$dx_l = -\sum_{k,m}P^{-1}_{lk}Q_{km}dx_m = \sum_{m=1}^{M}R_{lm}dx_m, \tag{17}$$

where R_{lm} is an element of the $L \times M$ matrix $\boldsymbol{R} = \boldsymbol{P}^{-1}\boldsymbol{Q}$. Next we write

$$dD_{ij} = \sum_{m=1}^{M}\frac{\partial D_{ij}}{\partial x_m}dx_m + \sum_{l=M+1}^{N}\frac{\partial D_{ij}}{\partial x_l}dx_l, \tag{18}$$

and by substituting dx_l from Eq. (17) into Eq. (18), we arrive at the following expression for the derivative of D_{ij} with respect to the dynamical coordinate x_m:

$$\frac{dD_{ij}}{dx_m} = \frac{\partial D_{ij}}{\partial x_m} + \sum_{l=M+1}^{N} \frac{\partial D_{ij}}{\partial x_l} R_{lm}. \tag{19}$$

We were seeking and have identified an additional term on the right hand side.

To summarise, the described framework allows the computation of entropy production in cases where the diffusion matrix is singular as a result of constraints on the dynamics through L constants of motion. The method employs these constants of motion to reduce the dimensionality of the phase space across which the system evolves such that the appropriately reduced diffusion matrix is non-singular. Having carried out this transformation, Eq. (7) can be used to compute entropy production with derivatives determined according to Eq. (19).

B. Identifying deterministically evolving functions

We have considered a function f of the stochastic variables $\{x_i\}$ evolving according to

$$df = \sum_i \frac{\partial f}{\partial x_i} dx_i + \sum_{i,j} \frac{\partial^2 f}{\partial x_i \partial x_j} D_{ij} dt, \tag{20}$$

and looked at situations where both the deterministic and stochastic terms in Eq. (20) vanish, making the function f a constant of motion of the dynamics. However, it is only necessary for the stochastic terms to vanish for there to be a restriction on the diffusive motion. We now consider the more general case where

$$df = \left(\sum_i \frac{\partial f}{\partial x_i} A_i + \sum_{i,j} \frac{\partial^2 f}{\partial x_i \partial x_j} D_{ij} \right) dt \tag{21}$$

is nonzero. Following earlier arguments, $\boldsymbol{\nabla} f$ is still a null eigenvector of $\boldsymbol{D}$ and we take each null eigenvector to correspond to a deterministically evolving function. To illustrate this, consider a system evolving stochastically in two dimensions (x_1,x_2) with a diffusion matrix that possesses a single null eigenvector. A function $f(x_1, x_2, t)$ evolving deterministically according to Eq. (21) allows us to reduce the number of variables needed to describe the motion from two to one. The other becomes a spectator variable. To understand this better, imagine that at time t_0 the function f is given by

$$f(x_1, x_2, t_0) = c_0, \tag{22}$$

where c_0 is a constant defining a contour of f in the space. Equation (22) allows us to express spectator variable x_2 as a function of dynamical variable x_1 at time t_0.

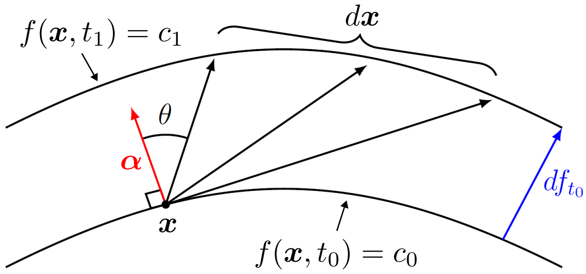

Figure 1. Illustration of the evolution of system coordinates between contours defined by a deterministically evolving function $f(\boldsymbol{x}, t)$, constructed to be normal to a spatially dependent null eigenvector $\boldsymbol{\alpha}$ of the diffusion matrix. There is a limited choice of stochastic increments $d\boldsymbol{x}$, defined by angle θ and the contours visited at the beginning and end of the timestep, which restricts the diffusive evolution and complicates the computation of the stochastic entropy production.

Between times t_0 and $t_1 = t_0 + dt$, f changes deterministically by an amount df_{t_0} to define a new contour

$$f(x_1, x_2, t_1) = c_1, \tag{23}$$

according to which we can again express x_2 as a function of x_1 at the later time. The evolution of the system is confined to a sequence of contours of the deterministically evolving function f such that we can always express x_2 in terms of x_1. We can parametrise the evolution with a single coordinate and thereby employ a reduced diffusion matrix to compute an entropy production. The argument easily generalises to an arbitrary number of dimensions.

As in the previous section we need to consider how derivatives are modified when we reduce the dimensionality of the phase space. We write $\boldsymbol{\nabla} f = g\boldsymbol{\alpha}$ where g is equal to $|\boldsymbol{\nabla} f|$ and $\boldsymbol{\alpha}$ is a normalised null eigenvector of $\boldsymbol{D}$, , with $|\boldsymbol{\alpha}| = 1$, lying perpendicular to the contour of f. Infinitesimal changes in coordinates $\boldsymbol{x}$ within a timestep dt are given by $d\boldsymbol{x}$, and $\boldsymbol{x}$ is constrained to pass between points on specified contours of f at specified times, hence with only certain $d\boldsymbol{x}$ allowed. The situation is illustrated in Fig. 1.

The component of $d\boldsymbol{x}$ in the direction normal to f is given by

$$d\boldsymbol{x}_\perp = |d\boldsymbol{x}| \cos\theta = |\boldsymbol{\alpha}||d\boldsymbol{x}| \cos\theta = \boldsymbol{\alpha} \cdot d\boldsymbol{x}, \tag{24}$$

where the angle θ is shown in Fig. 1. We can also write

$$df = |\boldsymbol{\nabla} f| d\boldsymbol{x}_\perp = |\boldsymbol{\nabla} f| \boldsymbol{\alpha} \cdot d\boldsymbol{x} = g\boldsymbol{\alpha} \cdot d\boldsymbol{x}, \tag{25}$$

such that

$$g\boldsymbol{\alpha} \cdot d\boldsymbol{x} = \left(\sum_i \frac{\partial f}{\partial x_i} A_i + \sum_{i,j} \frac{\partial^2 f}{\partial x_i \partial x_j} D_{ij} \right) dt. \tag{26}$$

For notational convenience we rewrite the term in brackets on the right hand side as gG so that

$$\boldsymbol{\alpha} \cdot d\boldsymbol{x} = G dt. \tag{27}$$

For a set of null eigenvectors of $\boldsymbol{D}$ labelled by $k = 1, ..., L$ there are several deterministically evolving functions of the coordinates, and we can specify relationships between increments in dynamical and spectator variables such that

$$\sum_{m=1}^{M} \alpha_{km} dx_m + \sum_{l=M+1}^{N} \alpha_{kl} dx_l = G_k dt. \tag{28}$$

Following the reasoning in Eq. (17) we write

$$dx_l = -P_{lk}^{-1} Q_{km} dx_m + P_{lk}^{-1} G_k dt = R_{lm} dx_m + S_l dt, \tag{29}$$

with implied summation over repeated indices, and substituting Eq. (29) into Eq. (18) we obtain

$$dD_{ij} = \sum_{m=1}^{M} \frac{\partial D_{ij}}{\partial x_m} dx_m + \sum_{l=M+1}^{N} \frac{\partial D_{ij}}{\partial x_l} \left(R_{lm} dx_m + S_l dt \right), \tag{30}$$

such that, as before, the required derivatives of the relevant elements of the diffusion matrix are

$$\frac{dD_{ij}}{dx_m} = \frac{\partial D_{ij}}{\partial x_m} + \sum_l \frac{\partial D_{ij}}{\partial x_l} R_{lm}. \tag{31}$$

We therefore find that contributions to derivatives with respect to dynamical variables, where the expression in question also depends on spectator variables, are the same whether f is a constant of the motion or a deterministic function of the dynamics. This is useful since, in general, we are unlikely to be able to determine if the singularity of a diffusion matrix is due to the existence of a constant or a deterministically evolving function.

C. Simple example of restricted diffusive evolution

To illustrate the above reasoning, consider the two SDEs

$$\begin{aligned} dx_1 &= \left(1 - x_1^2\right) dW \\ dx_2 &= -\frac{1}{2} x_2 dt - x_1 x_2 dW, \end{aligned} \tag{32}$$

which present a case of restricted diffusive evolution since there are two Itô processes but only one noise. The 2×2 diffusion matrix for the (x_1, x_2) phase space can be shown to be singular. The reversible deterministic terms $A_{1,2}^{\mathrm{rev}}$ in both SDEs are zero. We proceed first by regarding x_1 as the dynamical variable and x_2 as a spectator and use Eq. (7) to write

$$\begin{aligned} d\Delta s_{\mathrm{tot}} = &-d \ln p_1(x_1, t) + \frac{1}{D_{11}} A_1^{\mathrm{irr}} dx_1 - \frac{1}{D_{11}} \frac{dD_{11}}{dx_1} dx_1 \\ &+ \left[D_{11} \frac{d}{dx_1} \left(\frac{1}{D_{11}} A_1^{\mathrm{irr}} \right) - D_{11} \frac{d}{dx_1} \left(\frac{1}{D_{11}} \frac{dD_{11}}{dx_1} \right) \right] dt, \end{aligned} \tag{33}$$

where $p_1(x_1, t) = \int p(x_1, x_2, t) dx_2$ and $p(x_1, x_2, t)$ satisfies the Fokker-Planck equation associated with Eqs. (32). Since $A_1^{\mathrm{irr}} = 0$ and $D_{11} = \frac{1}{2}(1 - x_1^2)^2$ we can take derivatives unencumbered by implicit dependence on x_1 arising from dependence on x_2.

However, we could just as well decide to compute the stochastic entropy production by regarding x_2 as the dynamical variable and x_1 as the spectator and write

$$\begin{aligned} d\Delta s_{\mathrm{tot}} = &-d \ln p_2(x_2, t) + \frac{1}{D_{22}} A_2^{\mathrm{irr}} dx_2 - \frac{1}{D_{22}} \frac{dD_{22}}{dx_2} dx_2 \\ &+ \left[D_{22} \frac{d}{dx_2} \left(\frac{1}{D_{22}} A_2^{\mathrm{irr}} \right) - D_{22} \frac{d}{dx_2} \left(\frac{1}{D_{22}} \frac{dD_{22}}{dx_2} \right) \right] dt, \end{aligned} \tag{34}$$

with $p_2(x_2, t) = \int p(x_1, x_2, t) dx_1$, $A_2^{\mathrm{irr}} = -\frac{1}{2} x_2$ and $D_{22} = \frac{1}{2} x_1^2 x_2^2$. Since D_{22} depends on the (current) spectator variable x_1 we have to employ derivatives like

$$\frac{dD_{22}}{dx_2} = \frac{\partial D_{22}}{\partial x_2} + R \frac{\partial D_{22}}{\partial x_1}, \tag{35}$$

and identify the coefficient R using the (single) null eigenvector of $\boldsymbol{D}$, which may be shown to be proportional to $(x_1 x_2, (1 - x_1^2))^{\mathsf{T}}$. In this example the dynamics preserve the value of the function $f(t) = x_1^2(t) + K x_2^2(t) - 1$ with arbitrary constant K, as long as $f(0) = 0$ is imposed as an initial condition (namely the motion is confined to an ellipse). We can therefore use Eq. (16) in the form $\alpha_1 dx_1 + \alpha_2 dx_2 = 0$ where α_i is the ith component of the null eigenvector. We then obtain

$$x_1 x_2 dx_1 = -\left(1 - x_1^2\right) dx_2, \tag{36}$$

such that $R = -(1 - x_1^2)/(x_1 x_2)$. The computation of Δs_{env} using Eqs. (34) and 35) can then proceed.

The point we are making is that in cases of restricted diffusive evolution, we can divide the stochastic variables arbitrarily into dynamical and spectator sets. The implication is that some choices of the division might be more convenient than others; in the case just considered it is more sensible to regard x_2 as a spectator variable rather than x_1.

IV. AN OPEN THREE-LEVEL QUANTUM SYSTEM WITH RESTRICTED DIFFUSION

A. SDEs and selection of spectator variables

We have developed the present framework for computing stochastic entropy production because there are physical systems of interest where some of the stochastically evolving variables are spectators. Specifically, we consider the dynamics of an open quantum system characterised by the stochastic evolution of its (reduced) density matrix ρ. The stochasticity is brought about by coupling to the environment, as described elsewhere [5, 6, 9]. In Appendix A it is shown how a Markovian stochastic Lindblad equation for the evolution of the reduced density matrix of an open system can be derived starting from the so-called Lindblad operators that specify the dynamical effect of the environment on the system. Using this formalism we consider a three-level bosonic system with environmental coupling characterised by the three raising (c_{1-3}) and three lowering (c_{4-6}) Lindblad operators given by

$$c_1 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad c_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad c_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$c_4 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad c_5 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad c_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \tag{37}$$

in a basis of kets $|1\rangle, |2\rangle$ and $|3\rangle$ corresponding to the three levels. The SDE describing the dynamics of the system is given by

$$d\rho = \sum_{i=1}^{6} \Bigg[\left(c_i \rho c_i^\dagger - \frac{1}{2} \rho c_i^\dagger c_i - \frac{1}{2} c_i^\dagger c_i \rho \right) dt + \left(\rho c_i^\dagger + c_i \rho - \mathrm{Tr}\left[\rho \left(c_i + c_i^\dagger \right) \right] \rho \right) dW_i \Bigg] . \tag{38}$$

A sketch of the inter-level transitions brought about by the c_i is given in Fig. 2.

The reduced density matrix ρ for the open quantum system is a complex, 3×3 Hermitian matrix with a unit trace, corresponding to eight degrees of freedom. We therefore parametrise ρ in terms of an eight dimensional vector $\boldsymbol{x}$ evolving as

$$d\boldsymbol{x} = \boldsymbol{A} dt + \boldsymbol{B} d\boldsymbol{W}, \tag{39}$$

where $\boldsymbol{A}$ is an eight dimensional vector, $\boldsymbol{B}$ is an 8×6 matrix and $d\boldsymbol{W}$ is a six dimensional vector of independent Wiener increments. It is clear that with fewer noise terms than SDEs, the diffusive motion will be restricted in some way.

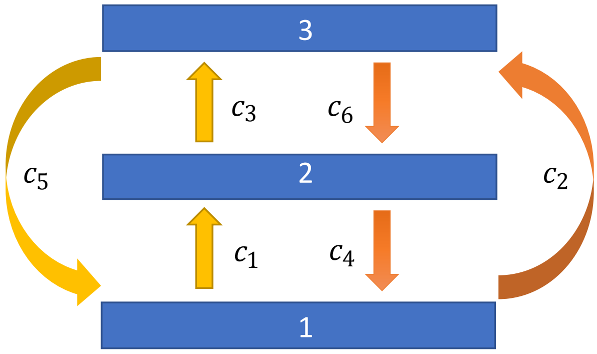

Figure 2. A sketch of the dynamics of an open three-level quantum system with system-environment coupling characterised by the set of six raising (c_{1-3}) and lowering (c_{4-6}) operators. By reducing the probabilities of the transitions shown in yellow, through multiplying the Lindblad operators $c_{1,3,5}$ in the stochastic Lindblad equation (38) by a weighting factor $w < 1$, a probability current through states $1 \to 3 \to 2 \to 1$ characterised by positive mean stochastic entropy production can be generated. For $w = 1$ the system would otherwise adopt an equilibrium state with zero current and zero stochastic entropy production.

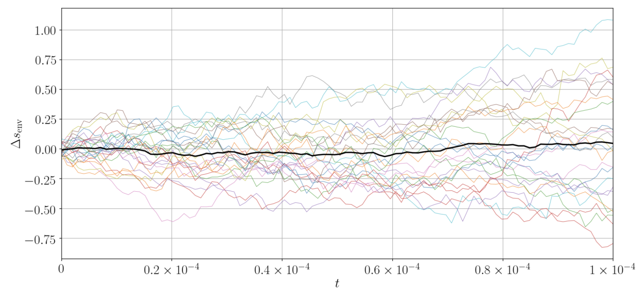

Figure 3. Environmental component of stochastic entropy production as a function of time in the three-level quantum system, computed for 25 trajectories with equally weighted Lindblads. The black line represents the ensemble mean.

In order to proceed we employ the eight Gell-Mann matrices given by

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} . \tag{40}$$

It is convenient to work with eight real variables

s, t, u, v, w, x, y and z, defined by $\mathrm{Tr}\,(\lambda_1 \rho) = s$, $\mathrm{Tr}\,(\lambda_2 \rho) = t$, $\mathrm{Tr}\,(\lambda_3 \rho) = u$ etc, corresponding to the eight components of $\boldsymbol{x}$. We can then write ρ as

$$\rho = \begin{pmatrix} \frac{u}{2} + \frac{\sqrt{3}z}{6} + \frac{1}{3} & \frac{s}{2} - \frac{it}{2} & \frac{v}{2} - \frac{iw}{2} \\ \frac{s}{2} + \frac{it}{2} & -\frac{u}{2} + \frac{\sqrt{3}z}{6} + \frac{1}{3} & \frac{x}{2} - \frac{iy}{2} \\ \frac{v}{2} + \frac{iw}{2} & \frac{x}{2} + \frac{iy}{2} & -\frac{\sqrt{3}z}{3} + \frac{1}{3} \end{pmatrix}.$$

The SDEs now take the form

$$\begin{pmatrix} ds \\ dt \\ du \\ dv \\ dw \\ dx \\ dy \\ dz \end{pmatrix} = \begin{pmatrix} -2s \\ -2t \\ -3u \\ -2v \\ -2w \\ -2x \\ -2y \\ -3z \end{pmatrix} dt + \begin{pmatrix} -sv+x & -s^2-u+\frac{\sqrt{3}z}{3}+\frac{2}{3} & -sx+v & -sv & -s^2+u+\frac{\sqrt{3}z}{3}+\frac{2}{3} & -sx \\ -tv-y & -st & -tx+w & -tv & -st & -tx \\ v(1-u) & s(1-u) & -x(u+1) & -uv & -s(u+1) & -ux \\ -v^2-\frac{2\sqrt{3}z}{3}+\frac{2}{3} & -sv+x & -vx & u-v^2+\frac{\sqrt{3}z}{3}+\frac{2}{3} & -sv & s-vx \\ -vw & -sw+y & -wx & -vw & -sw & t-wx \\ -vx & -sx & -x^2-\frac{2\sqrt{3}z}{3}+\frac{2}{3} & s-vx & -sx+v & -u-x^2+\frac{\sqrt{3}z}{3}+\frac{2}{3} \\ -vy & -sy & -xy & -t-vy & -sy+w & -xy \\ \frac{v(-3z+\sqrt{3})}{3} & \frac{s(-3z+\sqrt{3})}{3} & \frac{x(-3z+\sqrt{3})}{3} & -\frac{v(3z+2\sqrt{3})}{3} & \frac{s(-3z+\sqrt{3})}{3} & -\frac{x(3z+2\sqrt{3})}{3} \end{pmatrix} \begin{pmatrix} dW_1 \\ dW_2 \\ dW_3 \\ dW_4 \\ dW_5 \\ dW_6 \end{pmatrix}. \tag{41}$$

The dynamics of ρ are expressed in terms of $N = 8$ Itô processes with $M = 6$ noise terms. We therefore expect the diffusion matrix to be singular (this has been checked using Mathematica) and for there to exist $L = N - M = 2$ deterministically evolving functions of the stochastic variables $s, \cdots, z$. We choose to assign y and z as spectator variables allowing us to focus instead on the six SDEs:

$$\begin{pmatrix} ds \\ dt \\ du \\ dv \\ dw \\ dx \end{pmatrix} = \begin{pmatrix} -2s \\ -2t \\ -3u \\ -2v \\ -2w \\ -2x \end{pmatrix} dt + \begin{pmatrix} -sv+x & -s^2-u+\frac{\sqrt{3}z}{3}+\frac{2}{3} & -sx+v & -sv & -s^2+u+\frac{\sqrt{3}z}{3}+\frac{2}{3} & -sx \\ -tv-y & -st & -tx+w & -tv & -st & -tx \\ v(1-u) & s(1-u) & -x(u+1) & -uv & -s(u+1) & -ux \\ -v^2-\frac{2\sqrt{3}z}{3}+\frac{2}{3} & -sv+x & -vx & u-v^2+\frac{\sqrt{3}z}{3}+\frac{2}{3} & -sv & s-vx \\ -vw & -sw+y & -wx & -vw & -sw & t-wx \\ -vx & -sx & -x^2-\frac{2\sqrt{3}z}{3}+\frac{2}{3} & s-vx & -sx+v & -u-x^2+\frac{\sqrt{3}z}{3}+\frac{2}{3} \end{pmatrix} \begin{pmatrix} dW_1 \\ dW_2 \\ dW_3 \\ dW_4 \\ dW_5 \\ dW_6 \end{pmatrix}. \tag{42}$$

The diffusion matrix formed from Eq. (42) via $\boldsymbol{D} = \frac{1}{2}\boldsymbol{B}\boldsymbol{B}^{\mathsf{T}}$ is too elaborate to obtain an analytical expression for its inverse. It is possible, however, to compute an inverse numerically, remembering to append terms to any derivatives in the matrix elements according to the procedure described in the previous section. In actual fact, with this choice of spectator variables, *no* such additional terms are required, making this route very convenient.

B. Equilibrium and nonequilibrium stationary states

Codes have been written to solve the SDEs for the dynamics of the reduced density matrix and the evolution of the environmental component of the stochastic entropy production. Calculating the system component Δs_{sys} requires solution of a Fokker-Planck equation, which is computationally demanding, but which does not add to the understanding we develop regarding the *stationary* states of the system. We comment further on this point later.

The computational demands of solving Eq. (7) are considerable for the system under investigation, so only limited ensembles of trajectories were generated. Runs for environmental stochastic entropy production were typically executed with a timestep of $dt = 10^{-6}$, and the reduced density matrix was initiated in the condition $s = t = u = v = w = x = y = z = 0.1$ throughout.

Figure 3 illustrates the range of environmental stochastic entropy production for 25 runs. The average environmental entropy production is nearly always within one standard deviation of zero, which, given the limited statistics, provides a strong indication that a zero mean rate of environmental stochastic entropy production has been established in the stationary state. This is precisely what is to be expected of an equilibrium state, and the mean rate of system stochastic entropy production ought to be zero as well since it corresponds in typical situations to the rate of change of Gibbs entropy [5].

We now investigate a nonequilibrium stationary state with a probability current passing through the system phase space. Our interest in the three-level system arises precisely because it is the simplest quantum system in which such a state might be possible. We create a non-

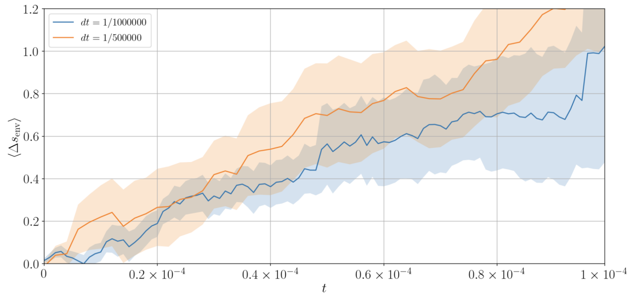

Figure 4. Comparison of the environmental stochastic entropy production computed with timesteps $dt = 1/1000000$ and $1/500000$ for a weighting of $w = 0.2$. Averages were taken over 50 runs for each value of timestep. Bands represent the standard error and solid lines the average.

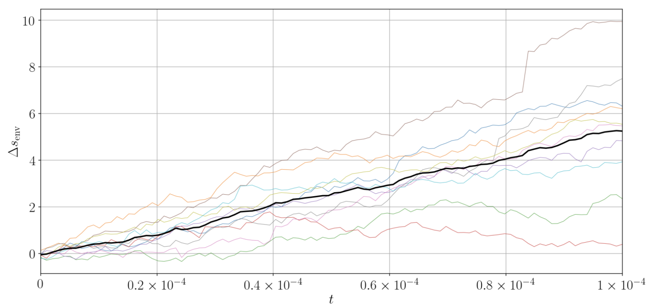

Figure 5. Environmental stochastic entropy production computed for 10 trajectories with $w = 0.1$ and $dt = 10^{-6}$. The black line represents the ensemble mean.

equilibrium stationary state by breaking detailed balance and favouring a pattern of transitions $|3\rangle \to |2\rangle \to |1\rangle \to |3\rangle$ around the system. We do this by reducing the coupling strength associated with the Lindblad operators linked to the opposite pattern. Specifically, we multiply Lindblads c_1, c_2 and c_5 in (37) by a weighting factor $w < 1$ and derive a modified set of dynamical equations. Such a non-equilibrium stationary state is expected to be associated with a positive mean rate of stochastic entropy production. Moreover, we expect the strength with which the system is weighted towards such a non-equilibrium stationary state to be related to the irreversibility of its behaviour and to the degree of mean stochastic entropy production.

We indeed observe a mean positive rate of environmental stochastic entropy production, within statistical errors. In Fig. 4 we check the accuracy of the calculations for $w = 0.2$ by comparing the production for two values of the timestep and find them to be consistent. Figure 5 shows the environmental stochastic entropy production for an ensemble of 10 runs with a weighting of $w = 0.1$.

In line with expectations, we see a constant mean rate of environmental stochastic entropy production which we associate with the system being in a nonequilibrium stationary state. The mean system stochastic entropy production is not expected to make a contribution in a stationary state since the Gibbs entropy of the system is then constant in time. Figure 6 shows the mean rate of environmental stochastic entropy production for a selection of weightings. There is clear indication of a relationship between the breakage of detailed balance and the mean rate of environmental stochastic entropy production. For the points $w = 0.4$ and $w = 0$ we have $\langle \Delta s_{\rm env} \rangle / \Delta t < 0$, a result at odds with second law, but we attribute this to statistical error, which could be achieved by, for example, increasing the number of runs used to generate each point. Figure 6 provides strong support that our approach is a means by which to quantify the irreversibility of open quantum systems.

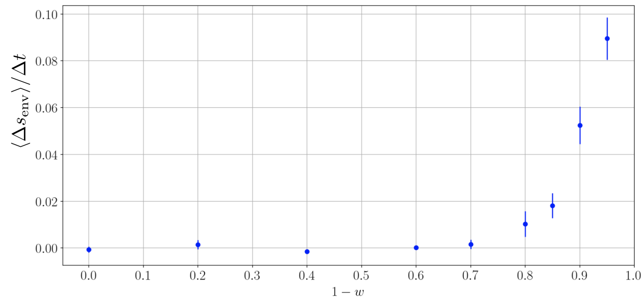

Figure 6. Mean rate of environmental stochastic entropy production against $1 - w$. The latter characterises the degree to which detailed balance is broken: a value $w = 1$ corresponds to no breakage and the equilibrium state. Each average was computed by using linear regression to produce best fit lines for 10 trajectories and then an average was performed over the gradient of these lines, for a time interval $\Delta t = 10^{-4}$. The error bars show the standard error of these averages.

V. CONCLUSIONS

We have employed Itô processes to model the dynamics and thermodynamics of a system interacting with an environment in the absence of detailed information about the exact configuration of either. Such an approach has frequently been used in situations described by classical dynamics [10], and recently this has been extended to quantum systems [5]. In both cases, difficulties arise when there are fewer independent sources of noise than dimensions of the system phase space. Diffusion is restricted and the diffusion matrix becomes singular, which complicates the calculation of stochastic entropy production.

The solution to the problem is simply to eliminate degrees of freedom (spectator coordinates) from the entropy calculation to account for the existence of functions of the coordinates that evolve without noise. We have described a general method for doing so and illustrated it for a particle occupying a three-level quantum system, thermalised by an environment that brings about transitions between the levels. The dynamics take place in an eight dimensional phase space with only six noise terms, and the 8×8 diffusion matrix is singular.

We have shown that a stationary equilibrium state of the system may be established, corresponding to a zero mean rate of environmental stochastic entropy production (and implicitly by a zero mean rate of system stochastic entropy production as well). More interestingly, we have adjusted the probabilities of the transitions induced by the environment to create a nonequilibrium stationary state as well, where the particle is made to cycle through the levels in a particular order. This state is characterised by nonzero mean environmental stochastic entropy production.

Stochastic entropy production realises Boltzmann's programme of linking thermodynamics, and specifically entropy production, to the dynamical evolution of system coordinates [11]. Calculating entropy production quantifies the irreversibility of open system behaviour, addressing how unlikely it is that reversals of sequences of events might be observed. Refining this framework to accommodate special cases such as restricted diffusion adds confidence that such an approach is the most appropriate tool for quantifying irreversibility in open classical and quantum systems.

[1] I. J. Ford, *Statistical Physics: an Entropic Approach* (Wiley, 2013).

[2] R. E. Spinney and I. J. Ford, Nonequilibrium thermodynamics of stochastic systems with odd and even variables, Physical Review Letters **108**, 170603 (2012).

[3] R. E. Spinney and I. J. Ford, Entropy production in full phase space for continuous stochastic dynamics, Physical Review E **85**, 051113 (2012).

[4] R. E. Spinney, *The use of stochastic methods to explore the thermal equilibrium distribution and define entropy production out of equilibrium*, Ph.D. thesis, UCL (University College London) (2012).

[5] D. Matos, L. Kantorovich, and I. J. Ford, Stochastic entropy production for continuous measurements of an open quantum system, Journal of Physics Communications **6**, 125003 (2022).

[6] C. L. Clarke and I. J. Ford, Stochastic entropy production associated with quantum measurement in a framework of Markovian quantum state diffusion, arXiv:2301.08197 [quant-ph] (2023).

[7] U. Seifert, Entropy production along a stochastic trajectory and an integral fluctuation theorem, Physical Review Letters **95**, 040602 (2005).

[8] C. Gardiner, *Handbook of Stochastic Methods*, Vol. 4 (Springer Berlin, 2009).

[9] C. L. Clarke, *Irreversibility Measures in a Quantum Setting*, Ph.D. thesis, UCL (University College London) (2021).

[10] U. Seifert, Stochastic thermodynamics: principles and perspectives, European Physical Journal B **64**, 423 (2008).

[11] C. Cercignani, *Ludwig Boltzmann: the man who trusted atoms* (Oxford, 1998).

[12] K. Jacobs, *Quantum Measurement Theory and its Applications* (Cambridge University Press, 2014).

[13] S. M. Walls, J. M. Schachter, H. Qian, and I. J. Ford, Stochastic quantum trajectories demonstrate the Quantum Zeno Effect in an open spin system, arXiv:2209.10626 [quant-ph] (2022).

[14] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, 2002).

Appendix A: SDEs for quantum state diffusion

The reduced density matrix ρ describing an open quantum system is considered to evolve stochastically in a timestep dt according to quantum maps specified by Kraus operators [12], the details of which are provided here.

We consider i pairs of Kraus operators:

$$M_{i\pm} = \sqrt{\frac{P_i}{2}} \left(\mathbb{I} - \frac{1}{2P_i} c_i^\dagger c_i dt \pm \frac{1}{\sqrt{P_i}} c_i \sqrt{dt} \right), \qquad \text{(A1)}$$

where c_i are the Lindblad operators that specify the mode of coupling between the system and environment. The meaning of the P_i will become clear shortly. A similar scheme has been outlined elsewhere [5, 6, 9, 13], in which the P_i do not appear.

The Kraus operators satisfy

$$M_{i\pm}^\dagger M_{i\pm} = \frac{P_i}{2} \left(\mathbb{I} \pm \frac{1}{\sqrt{P_i}} (c_i + c_i^\dagger) \sqrt{dt} \right), \qquad \text{(A2)}$$

so that $M_{i+}^\dagger M_{i+} + M_{i-}^\dagger M_{i-} = P_i \mathbb{I}$ and the completeness relation [14]

$$\sum_i \left(M_{i+}^\dagger M_{i+} + M_{i-}^\dagger M_{i-} \right) = \mathbb{I}, \qquad \text{(A3)}$$

holds if $\sum_i P_i = 1$.

A set of $2i$ reduced density matrices, all of which are positive definite and of unit trace, are reachable in the timestep starting from ρ, namely

$$\rho'^{i\pm} = \frac{M_{i\pm} \rho M_{i\pm}^\dagger}{\mathrm{Tr}\left(M_{i\pm} \rho M_{i\pm}^\dagger \right)}. \qquad \text{(A4)}$$

The probabilities of making the transitions to these targets are given by

$$\begin{aligned} p_{i\pm} &= \mathrm{Tr}\left(M_{i\pm} \rho M_{i\pm}^\dagger \right) \\ &= \frac{P_i}{2} \left(1 \pm \sqrt{\frac{dt}{P_i}} \mathrm{Tr}\left[(c_i + c_i^\dagger) \rho \right] \right), \end{aligned} \qquad \text{(A5)}$$

which satisfy $p_{i+} + p_{i-} = P_i$ and $p_{i+} - p_{i-} = P_i\sqrt{\frac{dt}{P_i}}\mathrm{Tr}\left[(c_i + c_i^\dagger)\rho\right]$. P_i is therefore the probability that one of the ith pair of Kraus operators is selected for the map: it is the probability that the environment disturbs the system in such a way as to transform ρ into either ρ'^{i+} or ρ'^{i-}. As a consequence of these dynamical rules, the reduced density matrix is driven along a Brownian trajectory under the influence of the environment. Since the Kraus operators reduce to a multiple of the identity as $dt \to 0$, the Brownian path is continuous. No quantum jumps are allowed (and neither are they necessary [5]).

The statistically averaged form of the new reduced density matrix is

$$\langle\rho'\rangle = \sum_i \left(p_{i+}\frac{M_{i+}\rho M_{i+}^\dagger}{\mathrm{Tr}\left(M_{i+}\rho M_{i+}^\dagger\right)} + p_{i-}\frac{M_{i-}\rho M_{i-}^\dagger}{\mathrm{Tr}\left(M_{i-}\rho M_{i-}^\dagger\right)}\right)$$
$$= \sum_i \left(M_{i+}\rho M_{i+}^\dagger + M_{i-}\rho M_{i-}^\dagger\right), \tag{A6}$$

which corresponds in notation with the standard Kraus map [12].

The average evolution having been established, we now derive an SDE that describes the stochastic evolution of the reduced density matrix. The possible increments in the timestep are $d\rho^{i\pm} = \rho'^{i\pm} - \rho$ where

$$d\rho^{i\pm} = \frac{1}{P_i}\left(c_i\rho c_i^\dagger - \frac{1}{2}\rho c_i^\dagger c_i - \frac{1}{2}c_i^\dagger c_i\rho\right)dt$$
$$-\frac{1}{P_i}\left(\rho c_i^\dagger + c_i\rho - \mathrm{Tr}\left[\rho\left(c_i + c_i^\dagger\right)\right]\rho\right)\mathrm{Tr}\left[\rho\left(c_i + c_i^\dagger\right)\right]dt$$
$$\pm\frac{1}{\sqrt{P_i}}\left(\rho c_i^\dagger + c_i\rho - \mathrm{Tr}\left[\rho\left(c_i + c_i^\dagger\right)\right]\rho\right)\sqrt{dt}. \tag{A7}$$

The average increment in the reduced density matrix is then

$$\langle d\rho\rangle = \sum_i \left(p_{i+}d\rho^{i+} + p_{i-}d\rho^{i-}\right), \tag{A8}$$

which leads after some manipulation to

$$\langle d\rho\rangle = \sum_i \left(c_i\rho c_i^\dagger - \frac{1}{2}\rho c_i^\dagger c_i - \frac{1}{2}c_i^\dagger c_i\rho\right)dt. \tag{A9}$$

The terms in the sum are the dissipators associated with each Lindblad operator, in the form in which they appear in the standard Lindblad equation [12].

Next we compute the variance of $d\rho$. For clarity, we write

$$d\rho^{i\pm} = \frac{1}{P_i}A_i dt \pm \frac{1}{\sqrt{P_i}}B_i\sqrt{dt}, \tag{A10}$$

where

$$A_i = c_i\rho c_i^\dagger - \frac{1}{2}\rho c_i^\dagger c_i - \frac{1}{2}c_i^\dagger c_i\rho$$
$$-\left(\rho c_i^\dagger + c_i\rho - \mathrm{Tr}\left[\rho\left(c_i + c_i^\dagger\right)\right]\rho\right)\mathrm{Tr}\left[\rho\left(c_i + c_i^\dagger\right)\right], \tag{A11}$$

and $B_i = \rho c_i^\dagger + c_i\rho - \mathrm{Tr}\left[\rho\left(c_i + c_i^\dagger\right)\right]\rho$. We then construct the average of $\left(d\rho^{i\pm} - \langle d\rho\rangle\right)^2$ to lowest order in dt. The A_i and $\langle d\rho\rangle$ terms do not contribute because they are already of order dt and we get

$$\sum_i \left(p_{i+}\left(d\rho^{i+} - \langle d\rho\rangle\right)^2 + p_{i-}\left(d\rho^{i-} - \langle d\rho\rangle\right)^2\right)$$
$$= \sum_i \left(p_{i+}\frac{1}{P_i}B_i^2 dt + p_{i-}\frac{1}{P_i}B_i^2 dt\right) = \sum_i B_i^2 dt, \tag{A12}$$

suggesting that the Itô process governing the evolution of ρ is

$$d\rho = \langle d\rho\rangle + \sum_i B_i dW_i$$
$$= \sum_i \Big[\left(c_i\rho c_i^\dagger - \frac{1}{2}\rho c_i^\dagger c_i - \frac{1}{2}c_i^\dagger c_i\rho\right)dt$$
$$+\left(\rho c_i^\dagger + c_i\rho - \mathrm{Tr}\left[\rho\left(c_i + c_i^\dagger\right)\right]\rho\right)dW_i\Big], \tag{A13}$$

and this is the form employed in Eq. (38).

The Kraus operators in Eq. (A1) that underpin our framework are specified in terms of P_i parameters that are to be interpreted as the probabilities of selection of one of the ith pair of Kraus operators for the transformation of the reduced density matrix. By design, these parameters do not appear in the SDE, but it is worth discussing how they might be chosen for use in a Monte Carlo simulation, for example. If there are N Lindblads, a possible choice could be $P_i = 1/N$. This is not completely satisfactory, however, since it would give equal selection weight to the Kraus operators irrespective of the degree of coupling between the system and its environment through each Lindblad operator. It would be better if we ascribe a zero probability of selection to a Lindblad with zero coupling strength.

A solution would be to make P_i dependent on the norm of the matrix representing the Lindblad operator. We could use the Frobenius norm $||\,c_i\,||_{\mathrm{F}} = \sqrt{\mathrm{Tr}(c_i^\dagger c_i)}$, for example, and employ probabilities of selection

$$P_i = \frac{||\,c_i\,||_{\mathrm{F}}}{\sum_i ||\,c_i\,||_{\mathrm{F}}}. \tag{A14}$$

Adding a null Lindblad $c_i = 0$ to the set would not change the Kraus operators representing the other Lindblads, and furthermore such a null Lindblad would have zero probability of being selected. The matter is somewhat academic since the P_i do not affect the derived form of the stochastic dynamics, by design, but it does have impact on the elegance of the framework that emerges for modelling the quantum state diffusion.