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Mesoscopic and Macroscopic Entropy Balance Equations in a Stochastic Dynamics and Its Deterministic Limit

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Abstract

Entropy, its production, and its change in a dynamical system can be understood from either a fully stochastic dynamic description or a deterministic dynamics exhibiting chaotic behaviors. By taking the former approach based on the general diffusion process with diffusion $\alpha^{-1}\boldsymbol{D}(\mathbf{x})$ and drift $\mathbf{b}(\mathbf{x})$, where α represents the "size parameter" of a system, we show that there are two distinctly different entropy balance equations. One reads $\mathrm{d}S^{(\alpha)}/\mathrm{d}t = e_p^{(\alpha)} + Q_{ex}^{(\alpha)}$ for all α. Our key result addresses the asymptotic of the entropy production rate $e_p^{(\alpha)}$ and heat exchange rate $Q_{ex}^{(\alpha)}$ up to $O(\frac{1}{\alpha})$-corrections as system's size $\alpha \to \infty$. It yields in particular that the "extensive", leading α-order terms of $e_p^{(\alpha)}$ and $Q_{ex}^{(\alpha)}$ are exactly canceled out. Therefore in the asymptotic limit of $\alpha \to \infty$, there is a second, local entropy balance equation $\mathrm{d}S/\mathrm{d}t = \nabla \cdot \mathbf{b}(\mathbf{x}(t)) + \left(\boldsymbol{D} : \boldsymbol{\Sigma}^{-1}\right)(\mathbf{x}(t))$ on the order of $O(1)$, where $\alpha^{-1}\boldsymbol{D}(\mathbf{x}(t))$ represents the randomness generated in the dynamics usually represented by metric entropy, $\alpha^{-1}\boldsymbol{\Sigma}(\mathbf{x}(t))$ is the covariance matrix of the local Gaussian description at $\mathbf{x}(t)$ that is a solution to the ordinary differential equation $\dot{\mathbf{x}} = \mathbf{b}(\mathbf{x})$ at time t, and $\boldsymbol{D} : \boldsymbol{\Sigma}^{-1}$ is the Frobenius product of $\boldsymbol{D}$ and $\boldsymbol{\Sigma}^{-1}$. This latter equation is akin to the notions of volume-preserving conservative dynamics and entropy production in the deterministic dynamic approach to irreversible thermodynamics *à la* D. Ruelle [55]. Our study follows the rigorous approach and formalism of [28]; the mathematical details with sufficient care are given in the appendices.

In memory of Professor Min Qian (1927-2019), pioneer in mathematical physics of entropy production

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1 Introduction and Summary

There are currently two rather different mathematical frameworks for establishing the concept of entropy in dynamics: Deterministic dynamics [1, 13, 36, 54] and stochastic processes [28, 50, 59, 60]. It is quite straightforward in the latter to derive the fundamental equation for the balance of entropy, which first appeared in irreversible thermodynamics [12, 41]

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{đ_i S}{đt} + \frac{đ_e S}{đt}. \tag{1}$$

In the present work we shall denote the rate of entropy production $đ_i S/\mathrm{d}t$ as e_p and the rate of entropy exchange $đ_e S/\mathrm{d}t$ as Q_{ex}/T, to emphasize the fact that in general neither quantity on the right hand side of (1) is a time derivative of any time-dependent thermodynamic state function; both are *process dependent* signified by the $đ/đt$ [49]. In the deterministic framework an equation like (1) has been established in the work of D. Ruelle [55] following the measure-theoretic "thermodynamic formalism" [54]. Since Hamiltonian dynamics is Liouvillian volume-preserving, the notion of heat exchange has been widely recognized as the divergence of a vector field in nonlinear dynamics [2, 13, 53]; see [8] and references therein for more extensive literature. The establishment of folding entropy as e_p, even its positivity [33, 34, 68], is mathematically highly specialized and has been out of the reach for the broader statistical physics community. For example one key result known as Pesin's formula states that the sum of all the positive Lyapunov exponents is equal to the metric entropy of a dynamical system [20, 52, 68]. Because of all this, the relationship between these two approaches to Eq. (1) and its related decompositions discovered in recent years in stochastic thermodynamics [14, 22], has remained unclear.

Deterministic dynamics is the limiting behavior of a stochastic process. The macroscopic version of Eq. (1) therefore could be addressed either through (i) deterministic dynamics without "noise" as in [55, 68], or (ii) establishing mesoscopic version of (1) first as in stochastic thermodynamics followed by the zero noise limit. By "mesoscopic" we mean a descrip-

tion of dynamics that includes fluctuations [46], *i.e.*, stochastic noise, in contradistinction to "macroscopic" behavior with deterministic dynamics. The present paper carries out the limit in (ii); the actual work turns out to be careful computations of the higher order terms in the zero-noise limit, from which a set of results consistent with (i) is revealed.

A deterministic dynamics in (i) is a limit of stochastic descriptions; it can be formulated according to two gross categories: "averaging in space" as represented by the α parameter in the present work, or *lifting* [66] the state space to the space of all paths (see below). We call the attention that this second perspective is actually already implied in Kolmogorov's mathematical formulation of a stochastic process. "Averaging in time" only yields time-independent equilibrium without a dynamics. Using finite state discrete time Markov chain as an illustration, we give a brief sketch of this second formulation in Sec. 2.1, taken mainly from [1, 65]. This part is not needed for the main body of the paper, and it could be considered as irrelevant mathematics; but we believe it provides a global understanding of the broader issues on deterministic and stochastic dynamics and their irreversible thermodynamics captured by Eq. (1) and alike.

The main purpose of this paper is to study the asymptotic of e_p, Q_{ex}, and $\mathrm{d}S/\mathrm{d}t$ up to order $O(\frac{1}{\alpha})$ as system's size $\alpha \to \infty$. Our key result indicates that both e_p and Q_{ex} are *extensive quantities*, that is, their leading order is $O(\alpha)$, and moreover, their leading terms are exactly the same except having opposite signs. As a result, the macroscopic rate of entropy change $\mathrm{d}S/\mathrm{d}t$ is determined. It is not an extensive quantity, but on the order $O(1)$.

The paper is organized as follows: In Sec. 2.1, for the sake of completeness, we provide a very brief summary of the current mathematical formulation of a dynamical system using the simplest finite state discrete time notions. The important distinction between deterministic and stochastic, or "path tracking" vs. "state tracking" is outlined. Sec. 2.2 introduces the dynamics represented by the Fokker-Planck equation, which is in fact stochastic dynamics with a continuous state space in continuous time and having continuous path. Our key result regarding the large α asymptotic of e_p and Q_{ex} up to order $O(\frac{1}{\alpha})$ is derived in Sec. 3. They allow us to connect (5) with the asymptotic of $\mathrm{d}S/\mathrm{d}t$ and form a complete understanding of the theory of entropy production. With the mathematical relationship in hand, Sec. 4 further elucidates heuristically the contradistinction between the meaning(s) of entropy production in macroscopic deterministic dynamics and entropy productions in mesoscopic dynamics. Sec. 5 discusses our mathematical results in terms of *time scales*, one of the enduring ideas in statistical physics and applied mathematics. The mathematical formulae are familiar [22, 23, 47]; but the discussion is only possible under Eq. (8): Dissipative and conservative motions are on the entirely different time scales. The paper concludes with Sec. 6 which contains a discussion. All the mathematical details for computations are given in the Appendices A-D.

2 Dynamics: Deterministic and Stochastic Formulations

2.1 Stochastic Formulation of Dynamical Systems and its Implied Topological Determinism

Kolmogorov's axiomatic theory of stochastic processes with discrete time and the modern ergodic theory of nonlinear dynamics share a common foundation [1, 65]. In its simplest form with a finite state space $\mathcal{S} = \{0, 1, \cdots, K-1\}$, one important concept that deserves specific articulation in Kolmogorov's theory is the Ω space of all elementary events defined by $\Omega = \mathcal{S}^{\mathbb{N}}$; each event is a one-sided infinite sequence of states $\omega = (s_1 s_2 s_3 \cdots)$ with

$s_t \in \mathcal{S}$ and $t \in \mathbb{N}$. For a given $\omega_0 = (s_1^o s_2^o s_3^o \cdots) \in \Omega$, there is a *deterministic trajectory in the Ω space*

$$\omega_0, \cdots, \omega_n, \omega_{n+1}, \cdots, \quad \text{where } \omega_n \in \Omega, \tag{2a}$$

that is recursively defined by $\omega_{k+1} = T\omega_k \in \Omega$, where T is called a *shift operator*

$$T\omega \equiv T(s_1 s_2 s_3 \cdots) = (s_2 s_3 s_4 \cdots) \in \Omega. \tag{2b}$$

Moreover, there is a corresponding *stochastic trajectory in the state space $\mathcal{S}$* as a coarse-grained description of (2a)

$$s_1^o, \cdots, s_n^o, s_{n+1}^o, \cdots, \quad \text{where } s_n^o \in \mathcal{S}, \tag{2c}$$

Note the states in (2a) are ω's in Ω and the states in (2c) are s's in $\mathcal{S}$.

To better illustrate the deterministic dynamics defined by T on Ω, we can employ a topological semi-conjugacy between T on Ω and the expanding map E_K on [0, 1] via the representation [65]

$$\omega \equiv (s_1 s_2 s_3, \cdots) \in \Omega \longrightarrow \left(\sum_{n=1}^{\infty} \frac{s_n}{K^n} \right) \in [0, 1], \tag{3}$$

where $E_k : [0, 1] \to [0, 1]$ is defined by

$$E_K x = Kx \pmod 1, \ t \in \mathbb{N}.$$

A deterministic ergodic dynamics means that a single trajectory, consisting of only a countably infinite set of ω values, is sufficient to statistically represent the entire [0, 1] that is a continuum. We emphasize that there are as many as the entire [0, 1] number of different trajectories; all the trajectories corresponding to rational numbers on [0, 1] are not ergodic, but they total a set of zero measure and thus are negligible in a statistical sense.

Heuristically and in a nutshell, each Kolmogorov's elementary event $\omega \in \Omega$ implies an entire trajectory of a deterministic dynamics. Ruelle's thermodynamics [54] is based on representations like in (2a) and trajectories determined by E_K [54], while stochastic thermodynamics is based on the representation in (2c) and one additional necessary supposition: a probability measure $\mathbb{P}$ on $(\Omega, \mathcal{F})$, under which quantities that involve subsets of Ω such as

$$\mathbb{P}\{s_1 = k_1\}, \ \mathbb{P}\{s_1 = k_1, s_2 = k_2\}, \ \text{and } \mathbb{P}\{s_1 = k_1, s_2 = k_2, s_3 = k_3\}$$

become meaningful, where $\mathcal{F}$ is the cylindrical σ-algebra of Ω. Simple counting is no longer applicable to quantifying the sizes of random events like $\{s_1 = k_1\}$ and $\{s_1 = k_1, s_2 = k_2\}$, as they are all non-denumerable.[1] The probability measure $\mathbb{P}$ provides a more refined description of the shift dynamics T on Ω than the probability density function on [0, 1] for the dynamics E_K, which is merely a topological representation of the former: There are many different invariant measures of T on $(\Omega, \mathcal{F})$ corresponding to the uniform density on [0, 1], defining the unique invariant measure of E_K on $([0, 1], \mathcal{B}([0, 1]))$ in the class of invariant measures absolutely continuous with respect to the Lebesgue measure [68], where $\mathcal{B}([0, 1])$ is the Borel σ-algebra of [0, 1].

[1] There is actually a third representation: $s_1^o, s_1^o s_2^o, s_1^o s_2^o s_3^o, \cdots$, which corresponds to a sequence of subsets of Ω or elements in $\mathcal{F}$, called a *filtration*. In this case, the filtration represents a sequence of increasingly refined sub-σ-algebra while probability decreases with n. This description is complementary to that in (2b): the operator T is represented by a "time mark": $s_0 s_1 \cdots s_{t-1}, s_t\, s_{t+1} \cdots \ \to \ s_1 \cdots s_{t-1}\, s_t, s_{t+1} \cdots$. In terms of the filtration, the decreasing size of the subsets corresponds to the increasing information in the sub-σ-algebra generated by the smaller subsets. In other words, decreasing probability implies decreasing randomness, or fluctuations, and increasing deterministic characteristics.

With a given $\mathbb{P}$ on $(\Omega, \mathcal{F})$ that is invariant under T, Kolmogorov-Sinai (KS) entropy is the Shannon entropy per step for the entire Ω [21]. It can be shown that this KS entropy is never greater than the *topological entropy* of T [1, 54]. The latter being a topological concept, therefore, is intrinsic to the deterministic dynamical system with the path tracking representation in (2). It is independent of the probability $\mathbb{P}$; it is non-random.

2.2 Stochastic Dynamics in Continuous Space and Time with Continuous Path

Shift operators for infinite alphabets (state space) and/or continuous time are highly non-trivial mathematical matters. Heuristically, for a continuous time stochastic process on $\mathbb{R}^N$, the Ω is the space of $\mathbb{R}^N$-valued functions on $[0, \infty)$; each $\omega \in \Omega$ is a function $\mathbf{x}(t) \in \mathbb{R}^N$, $t \geq 0$. The shift operator $T(\tau)$ takes the $\mathbf{x}(t)$ to $T(\tau)\mathbf{x}(t) = \mathbf{x}(t+\tau)$. It is easy to verify that $T(\tau)$ is a linear operator on the function space; it has various *operational calculus representations* [26]. One example first employed by Lagrange for smooth $x(t) \in \mathbb{R}$ is via Taylor expansion:

$$x(t+\tau) = \sum_{k=0}^{\infty} \frac{\tau^k}{k!} \frac{\mathrm{d}^k}{\mathrm{d}t^k} x(t) \equiv \left\{ \exp\left(\tau \frac{\mathrm{d}}{\mathrm{d}t} \right) \right\} x(t).$$

We shall not follow this line of inquiry except noticing that it has a clear connection to functional analysis and theory of Lie groups.

As in Eq. (2c), the stochastic dynamics representation follows the $\mathbf{x}(t)$ in the state space $\mathbb{R}^N$. The given probability measure $\mathbb{P}$ on Ω is the Wiener measure, which is also called a white noise. Under the further assumption that $\mathbf{x}(t)$ is a continuous function of t, the theory of stochastic differential equation is to a K-state Markov chain.

As a mathematical representation of physical movements at such a fundamental level, the very stochastic formulation for $\mathbf{x}(t) \in \mathbb{R}^N$ already embodies the three most important irreversible dissipative phenomena in statistical physics: diffusion process, heat conduction as energy transfer studied by Fourier, and viscosity via momentum transfer is directly related to diffusion through Einstein's relation. In stochastic thermodynamics, therefore, one asks not how irreversibility arises from deterministic reversible dynamics, rather one studies what reversible dynamics is in stochastic processes [28]. In recent years, the theory of stochastic Markov dynamics has provided a coherent narrative of nonequilibrium thermodynamics at a mesoscopic level; see [49, 60] and the references cited within. By "mesoscopic", we mean a mechanistic description of dynamical systems of complex individuals in terms of stochastic processes [45]. At the center of this new development is an entropy balance equation, mathematically derivable, in which the notion of *entropy production* has been firmly established [35, 44, 50, 59, 63]. By introducing a "system's size parameter" α, one can confidently investigate macroscopic thermodynamics as the limit of the mesoscopic description: It has been shown that Gibbs' equilibrium chemical thermodynamics of heterogeneous substances is the emergent large deviations theory of a Delbrück-Gillespie process of chemical kinetics [22–24]. It suggests that "stochastic kinetics or kinematics dictates energetics", a saying imitating C. N. Yang's aphorism *symmetry dictates interaction* [67]. See [37, 47] for more discussion.

Consider the general diffusion process with continuous state space $\mathbb{R}^N$ and in continuous time, with its Fokker-Planck equation [28, 44, 50]

$$\frac{\partial f_\alpha(\mathbf{x}, t)}{\partial t} = \nabla \cdot \left(\tfrac{1}{\alpha} \boldsymbol{D}(\mathbf{x}) \nabla f_\alpha(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}) f_\alpha(\mathbf{x}, t) \right), \tag{4}$$

where α represents the size of a system, $\mathbf{b}(\mathbf{x})$ is the drift field, $\frac{1}{\alpha}\boldsymbol{D}(\mathbf{x})$ denotes the non-degenerate diffusion. It is understood that $f_\alpha(\mathbf{x}, 0) = \delta_{\mathbf{x}_0}$ with $\mathbf{x}_0 \in \mathbb{R}^N$ arbitrarily given. More mathematical details regarding the well-posedness of (4) and basic properties of f_α are given in Appendix A. In addition to many models in physics [27], stochastic formulation of a rapidly stirred nonlinear chemical reaction system follows the *chemical master equation*, in which individual molecules are counted one at a time [45]. In the limit of the system's volume and the number of molecules tend to infinity, their concentrations follow a chemical Langevin equation [25] in which the volume of the chemical reaction vessel is the α.

The Shannon entropy functional $S = S[f_\alpha]$, which is defined by

$$S = -\int_{\mathbb{R}^N} f_\alpha(\mathbf{x}, t) \ln f_\alpha(\mathbf{x}, t) \mathrm{d}\mathbf{x},$$

has an instantaneous rate of change [22, 28, 50, 64]:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = e_p + Q_{ex}, \tag{5a}$$

where the entropy production rate e_p and heat exchange rate Q_{ex}, measured in units of $k_B T$, are given as

$$e_p = \int_{\mathbb{R}^N} \left[\tfrac{1}{\alpha}\boldsymbol{D}(\mathbf{x})\nabla f_\alpha(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}) f_\alpha(\mathbf{x}, t)\right] \cdot \left[\nabla \ln f_\alpha(\mathbf{x}, t) - \alpha \boldsymbol{D}^{-1}(\mathbf{x})\mathbf{b}(\mathbf{x})\right] \mathrm{d}\mathbf{x} \tag{5b}$$

and

$$Q_{ex} = \int_{\mathbb{R}^N} \left[\tfrac{1}{\alpha}\boldsymbol{D}(\mathbf{x})\nabla f_\alpha(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}) f_\alpha(\mathbf{x}, t)\right] \cdot \left[\alpha \boldsymbol{D}^{-1}(\mathbf{x})\mathbf{b}(\mathbf{x})\right] \mathrm{d}\mathbf{x}. \tag{5c}$$

While e_p is positive, Q_{ex} can have either signs.

If the system is non-driven without external work being done, then the drift $\mathbf{b}(\mathbf{x})$ has a potential $U(\mathbf{x})$ such that

$$\mathbf{b}(\mathbf{x}) = -\boldsymbol{D}(\mathbf{x})\nabla U(\mathbf{x}). \tag{6}$$

It follows that

$$\begin{aligned} Q_{ex} &= -\alpha \int_{\mathbb{R}^N} \left[\tfrac{1}{\alpha}\boldsymbol{D}(\mathbf{x})\nabla f_\alpha(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}) f_\alpha(\mathbf{x}, t)\right] \cdot \nabla U(\mathbf{x}) \mathrm{d}\mathbf{x} \\ &= \alpha \frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^N} f_\alpha(\mathbf{x}, t) U(\mathbf{x}) \mathrm{d}\mathbf{x} = \alpha \frac{\mathrm{d}}{\mathrm{d}t} \mathbb{E}_{f_\alpha}[U]. \end{aligned}$$

For this class of systems, one can in fact introduce a new functional $F = \alpha \mathbb{E}_{f_\alpha}[U] - S$, and then $\mathrm{d}F/\mathrm{d}t < 0$. The potential condition implies that Q_{ex} can be expressed asα times the change of the mean energy $\mathbb{E}_{f_\alpha}[U]$. Such a link only exists in equilibrium systems. The stationary state of such a system is an *equilibrium* with zero entropy production and minimal F. Eq. (5a) in fact reminds one of the Clausius inequality in thermal physics, where F is called a Helmholtz free energy [66].

3 Derivation of the Macroscopic Entropy Balance Equation

In the limit of system's size $\alpha \to \infty$, the mathematical theory of large deviations (see Appendix A.1) shows that

$$f_\alpha(\mathbf{x}, t) \sim \left(R_0(\mathbf{x}, t) + \tfrac{1}{\alpha} R_1(\mathbf{x}, t)\right) e^{-\alpha\varphi(\mathbf{x}, t)}, \tag{7}$$

where the rate function $\varphi(\mathbf{x}, t)$ solves the Hamilton-Jacobi equation

$$-\frac{\partial \varphi(\mathbf{x}, t)}{\partial t} = \nabla\varphi(\mathbf{x}, t) \cdot (\boldsymbol{D}(\mathbf{x})\nabla\varphi(\mathbf{x}, t) + \mathbf{b}(\mathbf{x})),$$

$R_0(\mathbf{x}, t)$ solves the linear equation $\mathcal{L}R_0(\mathbf{x}, t) = 0$, and $R_1(\mathbf{x}, t)$ solves the non-homogeneous equation $\mathcal{L}R_1(\mathbf{x}, t) = \nabla \cdot (\boldsymbol{D}(\mathbf{x})\nabla R_0(\mathbf{x}, t))$. In which, the linear operator $\mathcal{L}$ reads

$$\mathcal{L} = \partial_t + (2\boldsymbol{D}(\mathbf{x})\nabla\varphi(\mathbf{x}, t) + \mathbf{b}(\mathbf{x})) \cdot \nabla + \nabla \cdot (\boldsymbol{D}(\mathbf{x})\nabla\varphi(\mathbf{x}, t) + \mathbf{b}(\mathbf{x})).$$

Moreover, $\varphi(\mathbf{x}, t)$ has a global minimum at $\hat{\mathbf{x}}(t)$ for each t, where the function $\hat{\mathbf{x}}(t)$ is the solution to the ordinary differential equation (ODE) $\mathrm{d}\hat{\mathbf{x}}/\mathrm{d}t = \mathbf{b}(\hat{\mathbf{x}})$ with initial value $\hat{\mathbf{x}}(0) = \mathbf{x}_0$.

Applying (7), one can determine the following key results of this paper (see Appendix B.2 for details). Both e_p and Q_{ex} are *extensive quantities*, that is, their leading order is $O(\alpha)$:

$$e_p = \alpha\mathbf{b} \cdot \boldsymbol{D}^{-1}\mathbf{b} + \boldsymbol{D} : \nabla\nabla\varphi + 2\nabla \cdot \mathbf{b} + R + O\left(\tfrac{1}{\alpha}\right), \tag{8a}$$

$$Q_{ex} = -\alpha\mathbf{b} \cdot \boldsymbol{D}^{-1}\mathbf{b} - \nabla \cdot \mathbf{b} - R + O\left(\tfrac{1}{\alpha}\right), \tag{8b}$$

where all the terms on the right-hand side of (8) are calculated at $\mathbf{x} = \hat{\mathbf{x}}(t)$, the colon : denotes the Frobenius product of two matrices of the same size, and R is given by

$$R = \frac{1}{2}\nabla\nabla\left(R_0\mathbf{b} \cdot \boldsymbol{D}^{-1}\mathbf{b}\right) : \boldsymbol{\Sigma} - \frac{1}{6}\nabla(R_0\mathbf{b} \cdot \boldsymbol{D}^{-1}\mathbf{b}) \cdot \nabla\nabla\nabla\varphi\Theta + \frac{R_1\mathbf{b} \cdot \boldsymbol{D}^{-1}\mathbf{b}}{\sqrt{\det \nabla\nabla\varphi}}.$$

In which, $\boldsymbol{\Sigma} = (\nabla\nabla\varphi)^{-1}$ and $\nabla\nabla\nabla\varphi\Theta$ is an N-dimensional vector and its i-th component is given by

$$(\nabla\nabla\nabla\varphi\Theta)_i = \sum_{j,k,\ell=1}^{N} \partial^3_{x_j x_k x_\ell}\varphi\Theta_{ijk\ell},$$

where

$$\Theta_{ijk\ell} = \frac{1}{(2\pi)^{N/2}\sqrt{\det \boldsymbol{\Sigma}}} \int_{\mathbb{R}^N} y_i y_j y_k y_\ell e^{-\frac{\mathbf{y}\cdot\nabla\nabla\varphi\mathbf{y}}{2}} \mathrm{d}\mathbf{y}.$$

The leading asymptotics of e_p and Q_{ex} have been studied and applied to a variety of model systems (see e.g. [15]). Our main contribution is the calculation of the $O(1)$ term. We identify a very important fact from (8): The leading order terms of e_p and Q_{ex} are exactly the same except having opposite signs. As a result, the macroscopic rate of entropy change is not an extensive quantity, but it is on the order $O(1)$:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \underbrace{\nabla \cdot \mathbf{b}\left(\hat{\mathbf{x}}(t)\right)}_{\text{local heat exchange}} + \underbrace{\boldsymbol{D}\left(\hat{\mathbf{x}}(t)\right) : \nabla\nabla\varphi\left(\hat{\mathbf{x}}(t), t\right)}_{\text{local entropy production}} + O\left(\tfrac{1}{\alpha}\right). \tag{9}$$

This is expected since $S = -\frac{N}{2}\ln\alpha + O(1)$ (see Appendix B.2) is not a rapidly oscillating function of t in the limit of system's size $\alpha \to \infty$. The natural logarithmic scaling with the system's size α is a result of taking ln of $f_\alpha(\mathbf{x}, t)$ whose normalization constant as shown in (19) is $\left(\frac{\alpha}{2\pi}\right)^{N/2}$ thanks to the non-degeneracy of the rate function $\varphi(\mathbf{x}, t)$ at its minimum $\hat{\mathbf{x}}(t)$.

The prefactor in (7) only appears within the R in (8), as a compensation between e_p and Q_{ex} [43, 48]. While their explicit forms have been difficult to obtain in general (see Appendix B.2), $R_1 = 0$ and $R(\mathbf{x}, t)$ becomes independent of $\mathbf{x}$ for an Ornstein-Uhlenbeck process with linear drift $\mathbf{b}(\mathbf{x}) = \boldsymbol{B}\mathbf{x}$ and constant non-degenerate diffusion $\frac{1}{\alpha}\boldsymbol{D}$. In fact, according to the

precise WKB ansatz (31) in this case, $R_1 = 0$ and $\nabla\nabla\nabla\varphi\Theta = 0$ as φ is quadratic, and therefore,

$$R = \frac{1}{2}\nabla\nabla\left(R_0\mathbf{b}\cdot\boldsymbol{D}^{-1}\mathbf{b}\right) : \boldsymbol{\Sigma} = \frac{\left(\boldsymbol{B}^\top\boldsymbol{D}^{-1}\boldsymbol{B}\right) : \boldsymbol{\Sigma}(t)}{\sqrt{\det\boldsymbol{\Sigma}(t)}},$$

where $\boldsymbol{\Sigma}(t) = 2\int_0^t e^{\boldsymbol{B}(t-s)}\boldsymbol{D}e^{\boldsymbol{B}^\top(t-s)}ds$. The R aside, the emergent macroscopic nonequilibrium thermodynamic structure is completely determined by $\mathbf{b}(\mathbf{x})$, $\boldsymbol{D}(\mathbf{x})$, and most importantly $\varphi(\hat{\mathbf{x}}, t)$ as an irreversible thermodynamic process.

Even though both Eqs. (5) and (9) are equations for entropy balance, their contradistinction suggests subtle but important physics of mesoscopic vs. macroscopic systems.

First, in the macroscopic limit, the entropy production rate e_p and heat exchange rate Q_{ex} become exactly the same; their difference yields zero for $\mathrm{d}S/\mathrm{d}t$ on the order $O(\alpha)$, that is, the rate of entropy change is actually very slow. The macroscopic heat exchange has the familiar Newtonian frictional form of "rate $\mathbf{b}$ times force $\boldsymbol{D}^{-1}\mathbf{b}$"; it is the same as entropy production rate, thus non-negative.

Second, the "very slow" rate of entropy change, however, is a balance between $\nabla\cdot\mathbf{b}\left(\hat{\mathbf{x}}(t)\right)$ and $\boldsymbol{D}\left(\hat{\mathbf{x}}(t)\right) : \nabla\nabla\varphi\left(\hat{\mathbf{x}}(t), t\right)$. In the theory of deterministic dynamical systems, volume preserving dynamics with $\nabla\cdot\mathbf{b}(\mathbf{x}) = 0$ is considered as "conservative". This is completely consistent with identifying $\nabla\cdot\mathbf{b}(\mathbf{x})$ as a system's energy exchange with the environment, i.e., heat [2, 51, 53, 55, 56]. Then in the true stationary state, on the order $O(1)$, there is an exact balance between fluctuations $\boldsymbol{D}\left(\hat{\mathbf{x}}(t)\right) : \nabla\nabla\varphi\left(\hat{\mathbf{x}}(t), t\right)$ and dissipation $-\nabla\cdot\mathbf{b}\left(\hat{\mathbf{x}}(t)\right)$.

Third, Eq. (9) is actually a generalization of a known result: For an Ornstein-Uhlenbeck process with linear drift $\mathbf{b}(\mathbf{x}) = \boldsymbol{B}\mathbf{x}$ and constant non-degenerate diffusion $\frac{1}{\alpha}\boldsymbol{D}$, the covariance matrix $\frac{1}{\alpha}\boldsymbol{\Sigma}(t)$ satisfies $\boldsymbol{\Sigma}'(t) = 2\boldsymbol{D} + \boldsymbol{B}\boldsymbol{\Sigma}(t) + \boldsymbol{\Sigma}(t)\boldsymbol{B}^\top$ [7, 42]. Noting that the entropy of a Gaussian distribution is (see Appendix D)

$$S = -\frac{N}{2}\ln\alpha + \frac{N}{2}\ln(2\pi e) + \frac{1}{2}\ln\Big(\det\boldsymbol{\Sigma}(t)\Big),$$

one finds from Jacobi's formula that

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{1}{2}\mathrm{tr}\left[\boldsymbol{\Sigma}^{-1}(t)\boldsymbol{\Sigma}'(t)\right] = \nabla\cdot\mathbf{b} + \boldsymbol{D} : \boldsymbol{\Sigma}^{-1}(t) = \nabla\cdot\mathbf{b} + \boldsymbol{D} : \nabla\nabla\varphi,$$

where $\varphi(\mathbf{x}, t) = \frac{1}{2}\left(\mathbf{x} - e^{\boldsymbol{B}t}\mathbf{x}_0\right)\cdot\boldsymbol{\Sigma}^{-1}(t)\left(\mathbf{x} - e^{\boldsymbol{B}t}\mathbf{x}_0\right)$ is the rate function in this case. The present work establishes a connection between this equation for the variance of a time-dependent Gaussian process, a form of the central limit theory [31], and the general entropy balance equation in the asymptotic limit of $\alpha \to \infty$. It shows that the trace of the covariance equation can be interpreted as "entropy balance".

Fourth, the local entropy production rate in (9) deserves further elaboration, given in Sec. 4.

4 Local Entropy Production and Entropy Change

To illustrate several ideas in stochastic dynamics, let us first consider a Markov chain with a probability distribution $\{p_i(t) : 1 \le i \le N\}$ at time $t \in \mathbb{N}$ and an one-step transition probability $\left\{P_{ij} : 1 \le i, j \le N\right\}$. According to the representation in (2a), which we call "path tracking", the entropy associated with the probability measure $\mathbb{P}$ for all ω's, each being a function of time $t \in [0, \infty)$, grows to infinite as $t \to \infty$. Therefore one defines the rate as $t \to \infty$, also known as entropy per step in the case of discrete time [21]: $-\sum_{i,j=1}^N p_i(t)P_{ij}\ln P_{ij}$.

This expression has also been interpreted as the *entropy produced in the dynamic process*, over a single step transition from state i to j being $-\ln P_{ij}$, thus $-\sum_{i,j=1}^{N} p_i(t)P_{ij}\ln P_{ij}$ being the mean value.

The representation in (2c) which we call "state tracking", however, only focuses on the probability distribution among different states at a time t, $p_i(t)$. Therefore it is reasonable to say that not all the "amount" of entropy generated from $\omega_t \to \omega_{t+1}$ is being kept in the $p_i(t+1)$: In fact the *change in the entropy* associated with $s_t \to s_{t+1}$ is

$$-\ln\left(\sum_{k=1}^{N} p_k(t)P_{kj}\right) + \ln p_i(t), \tag{10}$$

with the mean value

$$\begin{aligned} &-\sum_{i,j=1}^{N} p_i(t)P_{ij}\left[\ln\left(\sum_{k=1}^{N} p_k(t)P_{kj}\right) - \ln p_i(t)\right] \\ &= -\sum_{j=1}^{N} p_j(t+1)\ln p_j(t+1) + \sum_{i=1}^{N} p_i(t)\ln p_i(t). \end{aligned}$$

Therefore the difference between these two differently formulated entropy is [21]

$$\begin{aligned} &\underbrace{\{-\ln P_{ij}\}}_{\text{total entropy generated}} - \underbrace{\left\{-\ln\left(\sum_{k=1}^{N} p_k(t)P_{kj}\right) + \ln p_i(t)\right\}}_{\text{entropy change in the system}} = -\ln\left(\frac{p_i(t)P_{ij}}{\sum_{k=1}^{N} p_k(t)P_{kj}}\right) \\ &= \underbrace{-\ln\left(\Pr\left\{X(t)=i \middle| X(t+1)=j\right\}\right)}_{\text{entropy discarded is associated with uncertainty in the past}} \geq 0. \end{aligned} \tag{11}$$

The quantity $-\ln P_{ij}$ is the entropy change in a path tracking representation of a Markov chain (2a), Eq. (10) is the entropy change in the state tracking representation (2c) of the same Markov chain. The latter representation is a projection of the former. The difference given in (11) is indeed related to the folding entropy in [33, 34, 55]. Its interpretation is intimately related to A. Ben-Naim's notion of entropy of assimilation [3]. *The difference between the uncertainty in the future and the uncertainty in the past is the entropy change in the system*: One verifies a connection between the entropy change in a system according to the state tracking and past-future asymmetry in the path tracking.

Parallel to the above discussion on a discrete-time and discrete-space Markov chain, for a continuous-time and continuous-space Gaussian process with variance σ^2 at time t and a Brownian step from t to $t+\tau$ with a diffusion coefficient D, the probability distribution at $t+\tau$ is again Gaussian with variance $\sigma^2 + 2D\tau$. The instantaneous rate of entropy change in the continuous system, corresponding to (10), then is

$$\lim_{\tau\to 0} \frac{\ln\sqrt{2\pi e(\sigma^2+2D\tau)} - \ln\sqrt{2\pi e\sigma^2}}{\tau} = \frac{D}{\sigma^2}. \tag{12}$$

Applying the result in (12) to the local entropy production rate in (9), $\nabla\nabla\varphi\left(\hat{\mathbf{x}}(t), t\right)$ is the inverse of the local Gaussian variance at $\hat{\mathbf{x}}(t)$ at time t. Therefore, $\boldsymbol{D}(\hat{\mathbf{x}}(t)) : \nabla\nabla\varphi\left(\hat{\mathbf{x}}(t), t\right)$ is the local entropy production at time t that is kept by the system, due to the randomness in the dynamics. See [47] for a more thorough mathematical analysis of the diffusion process in the limit of $\alpha \to \infty$.

The local entropy production is no longer a characterization of the violation of detailed balance or time irreversibility, two essential concerns in stochastic thermodynamics. Rather, it is a characterization of the randomness generated by the dynamics, $\boldsymbol{D}$, and the uncertainties in the system, $\boldsymbol{\Sigma}^{-1} = \nabla\nabla\varphi$.

We use the term "local" to signify the following fact: The mean value of stochastic thermodynamic quantities such as e_p, Q_{ex}, as well as F and Q_{hk} below, are all integrals of the distribution function $f_\alpha(\mathbf{x}, t)$ over the entire state space $\mathbb{R}^N$. However in the limit of $\alpha \to \infty$ the $f_\alpha(\mathbf{x}, t) \to \delta\big(\mathbf{x} - \hat{\mathbf{x}}(t)\big)$. The corresponding macroscopic thermodynamic quantities are now functions of $\hat{\mathbf{x}}(t)$ which is a single point in $\mathbb{R}^N$ at a time. Therefore in contrast to the former, the latter is defined locally in the state space.

5 Time Scales in the Nonequilibrium Thermodynamic Description of Stochastic Dynamics

5.1 Free Energy Balance Equation

For stochastic mechanical systems in contact with a heat bath, entropy is not the appropriate equilibrium thermodynamic potential, free energy is. In classical thermodynamics, the difference between entropy and free energy is the mean internal energy. This is reflected in the generalized free energy (also called non-adiabatic entropy [60], Kullback–Leibler divergence or relative entropy [4, 9]) $F = F[f_\alpha]$ defined by

$$F = \int_{\mathbb{R}^N} f_\alpha(\mathbf{x}, t) \ln \frac{f_\alpha(\mathbf{x}, t)}{\pi_\alpha(\mathbf{x})} \mathrm{d}\mathbf{x},$$

where $\pi_\alpha(\mathbf{x})$ is the positive stationary solution to the Fokker-Planck equation (4) and satisfies $\int_{\mathbb{R}^N} \pi_\alpha(\mathbf{x})\mathrm{d}\mathbf{x} = 1$. For fixed system's size α, $F \to 0$ as $t \to \infty$, and therefore, it describes the relaxation of $f_\alpha(\mathbf{x}, t)$ to the steady state $\pi_\alpha(\mathbf{x})$ as $t \to \infty$.

For equilibrium systems, that is, $\mathbf{b}(\mathbf{x})$ satisfies (6), we have $\pi_\alpha(\mathbf{x}) = \frac{1}{K_\alpha} e^{-\alpha U(\mathbf{x})}$ with $K_\alpha = \int_{\mathbb{R}^N} e^{-\alpha U(\mathbf{x})}\mathrm{d}\mathbf{x}$. As a result, $F = \alpha \mathbb{E}_{f_\alpha}[U] - S + \ln K_\alpha$. Introducing $\widetilde{U} = \alpha^{-1} \ln K_\alpha$ yields $F = \alpha \mathbb{E}_{f_\alpha}[\widetilde{U}] - S$, which is analogous to the Helmholtz free energy [14].

The functional F also has a balance equation of its own [14, 22, 27]:

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -e_p + Q_{hk}, \tag{13}$$

where the house-keeping heat rate Q_{hk} (also known as the adiabatic entropy production rate) is

$$Q_{hk} = \int_{\mathbb{R}^N} \left[\tfrac{1}{\alpha}\boldsymbol{D}(\mathbf{x})\nabla f_\alpha(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}) f_\alpha(\mathbf{x}, t)\right] \cdot \left[\nabla \ln \pi_\alpha(\mathbf{x}) - \alpha \boldsymbol{D}^{-1}(\mathbf{x})\mathbf{b}(\mathbf{x})\right] \mathrm{d}\mathbf{x}.$$

It is also a non-negative quantity, and is actually positive unless $\mathbf{b}(\mathbf{x})$ is a gradient field (6) (see Appendix C.1). The non-negativity of both e_p and Q_{hk} suggests that they can be identified as "sink" and "source" of the generalized free energy F in a nonlinear stochastic dynamical system. Moreover, the "sink" is stronger than the "source", resulting in the nice Lyapunov property $\mathrm{d}F/\mathrm{d}t < 0$. This is a well-known fact; we provide the details in Appendix C.1 for completeness.

In the limit of size parameter $\alpha \to \infty$, both F and Q_{hk} are extensive quantities on the order of $O(\alpha)$ (see Appendix C.2 for details):

$$F = \alpha\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big) + \mathcal{C}_\alpha + O(1), \tag{14a}$$

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -\alpha\left[\nabla\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big)\cdot \boldsymbol{D}\big(\hat{\mathbf{x}}(t)\big)\nabla\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big)\right] + O(1), \tag{14b}$$

$$Q_{hk} = \alpha\left[\boldsymbol{\gamma}\big(\hat{\mathbf{x}}(t)\big)\cdot \boldsymbol{D}^{-1}\big(\hat{\mathbf{x}}(t)\big)\boldsymbol{\gamma}\big(\hat{\mathbf{x}}(t)\big)\right] + O(1), \tag{14c}$$

where $\varphi^{ss}(\mathbf{x})$ is the leading-order exponent of $\pi_\alpha(\mathbf{x}) \sim e^{-\alpha\varphi^{ss}(\mathbf{x})}$, $\mathcal{C}_\alpha$ is a constant satisfying $\lim_{\alpha\to\infty}\frac{1}{\alpha}\ln\left(|\mathcal{C}_\alpha|+1\right) = 0$, and $\boldsymbol{\gamma}(\mathbf{x}) = \mathbf{b}(\mathbf{x}) + \boldsymbol{D}(\mathbf{x})\nabla\varphi^{ss}(\mathbf{x})$. In the case that the ODE $\dot{\mathbf{x}} = \mathbf{b}(\mathbf{x})$ admit a globally asymptotically stable and non-degenerate equilibrium, there holds $\mathcal{C}_\alpha = 0$. The leading terms in the asymptotic (14) have been discussed in [16, 47] with applications to the emergent second law of thermodynamics. They are also used in [57] to bound asymptotic escape rates from metastable states.

One of important results from the theory of large deviations [17] is that

$$\boldsymbol{\gamma}(\mathbf{x})\cdot\nabla\varphi^{ss}(\mathbf{x}) = 0. \tag{15}$$

In fact, Eq. (13), on the macroscopic scale, becomes a Pythagorean triangle equality:

$$\left\|\boldsymbol{D}\big(\hat{\mathbf{x}}(t)\big)\nabla\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big)\right\|^2_{\boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))} + \left\|\boldsymbol{\gamma}\big(\hat{\mathbf{x}}(t)\big)\right\|^2_{\boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))} = \left\|\mathbf{b}\big(\hat{\mathbf{x}}(t)\big)\right\|^2_{\boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))},$$

where the norm of a vector $\mathbf{v}$ is defined as $\|\mathbf{v}\|_{\boldsymbol{D}^{-1}(\mathbf{x})} = \sqrt{\mathbf{v}\cdot\boldsymbol{D}^{-1}(\mathbf{x})\mathbf{v}}$ [47].

5.2 Time Scales, Short-Time and Long-Time Perspectives

Among all the thermodynamic quantities we discussed above, macroscopic F, Q_{hk}, and $\mathrm{d}F/\mathrm{d}t$ are defined via $\varphi^{ss}(\mathbf{x})$, while macroscopic e_p and Q_{ex}, and local heat exchange rate are functions of $\mathbf{x}$ via $\boldsymbol{D}(\mathbf{x})$ and $\mathbf{b}(\mathbf{x})$. $\mathrm{d}S/\mathrm{d}t$ and its corresponding local entropy production rate, however, are defined via $\varphi(\mathbf{x}, t)$, which is dependent upon the choice of $\varphi(\mathbf{x}, 0)$, e.g., initial fluctuations. The $\varphi^{ss}(\mathbf{x})$ plays the role of a macroscopic potential energy function. In the macroscopic, deterministic limit, free energy and its rate of change are dominated by this energy function $\varphi^{ss}(\mathbf{x})$.

The fact that $\mathrm{d}F/\mathrm{d}t \sim O(\alpha)$ and $\mathrm{d}S/\mathrm{d}t \sim O(1)$ tells us that in time-dependent nonequilibrium thermodynamics, free energy relaxation is fast, while entropy change is slow. This is a point that has escaped general attention in the past discussion on nonequilibrium thermodynamics. Through $\varphi^{ss}(\mathbf{x})$, free energy is a "global" characterization of the nonlinear stochastic dynamics, while entropy dynamics is only local.

The physical meaning of $\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big)$ and $\varphi\big(\hat{\mathbf{x}}(t), t\big)$, where $\hat{\mathbf{x}}(t)$ being the solution to the deterministic motion as the solution to $\mathrm{d}\hat{\mathbf{x}}/\mathrm{d}t = \mathbf{b}(\hat{\mathbf{x}})$, deserves further discussion: $\nabla\varphi\big(\hat{\mathbf{x}}(t), t\big) = 0$ for all time t. The matrix $\boldsymbol{\Sigma}\left(\hat{\mathbf{x}}(t), t\right) = (\nabla\nabla\varphi)^{-1}\left(\hat{\mathbf{x}}(t), t\right)$, as a function of $\hat{\mathbf{x}}(t)$, is the local fluctuation in the asymptotic limit of α being very large but not infinite. It is usually called time-dependent *fluctuations*. There is a time-dependent Gaussian process that describes this regime, following the theory of van Kampen's system-size expansion, or Keizer's nonequilibrium statistical thermodynamics [29]. $\nabla\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big)$, on the other hand, tells eventually in a very long time scale, the local probability and its gradient at $\hat{\mathbf{x}}(t)$. It also provide a definitive statement that $\mathrm{d}\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big)/\mathrm{d}t = \mathbf{b}\big(\hat{\mathbf{x}}(t)\big)\cdot\nabla\varphi^{ss}\big(\hat{\mathbf{x}}(t)\big) \le 0$ is never positive, thanks to Eq. (15). $\varphi^{ss}(\mathbf{x})$ is a landscape for the dynamics with permanence, irrespective of the initial $\varphi(\mathbf{x}, 0)$.

All this discussion reflects a "competition" between the two limits $\alpha \to \infty$ and $t \to \infty$ in an ergodic system, as first understood in the theory of equilibrium phase transition: With larger and larger α, a trajectory with less stochasticity will take longer and longer time to visit and re-visit all the space states. When $\alpha = \infty$, ergodicity is broken in nonlinear deterministic dynamics with multiple attractors. However, no matter how large α is, as long as $\alpha < \infty$, there will be enough time for the dynamics to cover the whole state space as $t \to \infty$. See [46] for an extensive discussion on this issue.

6 Discussion

In current textbooks on equilibrium statistical mechanics, thermodynamic limit is rigorously defined as a system's size, α, tending to infinity. There is no statement on the time scales of the rate of changes in thermodynamic quantities, particularly their dependency upon the system's size α. Time scale(s), however, is certainly central to physics. We discover that there is a deep relation between the $\alpha \to \infty$ and time scales of an entropy balance and for a free energy balance: The former is on the order of $O(1)$ but the latter is on the order $O(\alpha)$.

There have been two approaches to statistical thermodynamics, one based on classical mechanics originated by L. Boltzmann, and one based on probability originated by J. W. Gibbs [32]. Development in nonlinear dynamical systems based on chaotic hypothesis [19] and Sinai-Ruelle-Bowen measure [10, 52, 68] is the continuation of the former [13, 56], while the stochastic thermodynamics [49, 60] and in-depth explorations of the theory of probability were the further development of the latter [6, 22, 23, 28, 66]. The present result provides a natural logic bridge between the entropy balance equations, as the fundamental of nonequilibrium thermodynamics, that emerge in these two approaches. If one identifies $\alpha = \epsilon^{-1}$ where ϵ being the size of a Markov partition for a deterministic dynamical system, then taking the limit of $\alpha \to \infty$ is consistent with the modern treatment in terms of a generating partition which gives rise to Kolmogorov-Sinai metric entropy and the nonequilibrium thermodynamics *à la* D. Ruelle [13].

Our present result might also have implications to equilibrium thermodynamic analysis in which researchers are routinely partitioning the energetic and entropic contributions to total free energy change via van't Hoff method [58]. A compensation between the entropy and energy changes has been extensively discussed in the past [43, 48]. With $\Delta S = 0$ on $O(\alpha)$ in Δt time, it is tempting to interpret $e_p \Delta t$ and $Q_{ex} \Delta t$ as entropy change and energy change in a quasi-stationary process.

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Declarations

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A Fokker-Planck Equation and WKB Ansatz

Consider the following Fokker-Planck equation

$$\partial_t f_\alpha = \nabla \cdot \left(\tfrac{1}{\alpha} \boldsymbol{D} \nabla f_\alpha - \mathbf{b} f_\alpha\right) \quad \text{in} \quad \mathbb{R}^N, \tag{16a}$$

$$f_\alpha(\cdot, 0) = \delta_{\mathbf{x}_0} \tag{16b}$$

where α represents the size of a system, $\mathbf{x}_0 \in \mathbb{R}^N$, $\delta_{\mathbf{x}_0}$ denotes the Dirac measure at $\mathbf{x}_0$, the diffusion matrix $\boldsymbol{D} = \boldsymbol{D}(\mathbf{x})$ is symmetric positive definite and sufficiently smooth, and the vector/drift field $\mathbf{b} = \mathbf{b}(\mathbf{x})$ is sufficiently smooth. Mild growth conditions on $\boldsymbol{D}(\mathbf{x})$ and $\mathbf{b}(\mathbf{x})$ as $|\mathbf{x}| \to \infty$ can be imposed to guarantee that Eq. (16) is well-posed and admits a classical solution f_α in $\mathbb{R}^N \times (0, \infty)$. Moreover, the solution satisfies $f_\alpha > 0$ in $\mathbb{R}^N \times (0, \infty)$, $\int_{\mathbb{R}^N} f_\alpha(\mathbf{x}, t) \mathrm{d}\mathbf{x} = 1$ for all $t > 0$, and, together with its derivatives, decays to 0 sufficiently fast as $|\mathbf{x}| \to \infty$ [28, 40].

In addition, if $\mathbf{x}_\alpha(t)$ is the solution to the SDE associated with Eq. (16a) with initial condition $\mathbf{x}_\alpha(0) = \mathbf{x}_0$, then for any $t > 0$, $f_\alpha(\mathbf{x}, t)$ is the density of the distribution of $\mathbf{x}_\alpha(t)$.

Under dissipative conditions (e.g., Lyapunov conditions), Eq. (16a) admits a unique positive stationary solution π_α satisfying $\int_{\mathbb{R}^N} \pi_\alpha \mathrm{d}\mathbf{x} = 1$ [30]. Setting

$$\mathbf{J}_\alpha = \tfrac{1}{\alpha} \boldsymbol{D} \nabla \ln \pi_\alpha - \mathbf{b}, \tag{17}$$

then π_α satisfies

$$\nabla \cdot (\pi_\alpha \mathbf{J}_\alpha) = 0. \tag{18}$$

Below, we state the Wentzel–Kramers–Brillouin (WKB) ansatz of f_α and π_α for large α.

A.1 WKB Ansatz of f_α

For each $t > 0$, the WKB ansatz of $f_\alpha(\mathbf{x}, t)$ in $\mathbf{x}$ for large α reads (see e.g. [17, 18, 61])

$$f_\alpha = \left(\frac{\alpha}{2\pi}\right)^{N/2} R_\alpha e^{-\alpha\varphi} = \left(\frac{\alpha}{2\pi}\right)^{N/2} \left[R_0 + \tfrac{1}{\alpha} R_1 + O(\tfrac{1}{\alpha^2})\right] e^{-\alpha\varphi}, \tag{19}$$

where $\varphi = \varphi(\mathbf{x}, t)$ is the rate function and $R_\alpha = R_\alpha(\mathbf{x}, t)$ is the prefactor. The regularity of φ, R_α, $R_0 = R_0(\mathbf{x}, t)$, and $R_1 = R_1(\mathbf{x}, t)$ is not automatic, but can be achieved under technical assumptions (see [61, Section 3]).

The rate function φ solves the Hamilton-Jacobi equation

$$-\partial_t \varphi = \nabla\varphi \cdot (\boldsymbol{D}\nabla\varphi + \mathbf{b}).$$

Moreover, if $\hat{\mathbf{x}}(t)$ denotes the solution to the ODE $\dot{\mathbf{x}} = \mathbf{b}(\mathbf{x})$ with initial condition $\hat{\mathbf{x}}(0) = \mathbf{x}_0$, then for any $t > 0$, the following hold:

- $\varphi(\hat{\mathbf{x}}(t), t) = 0 < \varphi(\mathbf{x}, t)$ for all $\mathbf{x} \in \mathbb{R}^N \setminus \{\hat{\mathbf{x}}(t)\}$; in particular, $\nabla\varphi(\hat{\mathbf{x}}(t), t) = 0$;
- $\nabla\nabla\varphi(\hat{\mathbf{x}}(t), t)$ is positive definite, where $\nabla\nabla\varphi$ denotes the Hessian matrix of φ.

The leading term R_0 of the prefactor R_α solves the following linear equation

$$-\partial_t R_0 = (2\boldsymbol{D}\nabla\varphi + \mathbf{b}) \cdot \nabla R_0 + \nabla \cdot (\boldsymbol{D}\nabla\varphi + \mathbf{b}) R_0,$$

while R_1 solves the following non-homogeneous equation

$$-\partial_t R_1 = -\nabla \cdot (\boldsymbol{D}\nabla R_0) + (2\boldsymbol{D}\nabla\varphi + \mathbf{b}) \cdot \nabla R_1 + \nabla \cdot (\boldsymbol{D}\nabla\varphi + \mathbf{b}) R_1. \tag{20}$$

Since $\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = \int_{\mathbb{R}^N} f_\alpha \mathrm{d}\mathbf{x} = 1$, Laplace's method yields

$$\frac{R_0(\hat{\mathbf{x}}(t),t)}{\sqrt{\det \nabla\nabla\varphi(\hat{\mathbf{x}}(t),t)}} = 1.$$

A.2 WKB Ansatz of π_α

The WKB ansatz of π_α reads

$$\pi_\alpha = \frac{R_\alpha^{ss}}{C_\alpha} e^{-\alpha\varphi^{ss}}, \tag{21}$$

where C_α is the sub-exponential (i.e., $\lim_{\alpha\to\infty}\frac{1}{\alpha}\ln C_\alpha = 0$) normalizing constant, the rate function φ^{ss} satisfies $\min\varphi^{ss} = 0$ and solves the stationary Hamilton-Jacobi equation

$$\nabla\varphi^{ss}\cdot\left(\boldsymbol{D}\nabla\varphi^{ss} + \mathbf{b}\right) = 0, \tag{22}$$

and the prefactor R_α^{ss} satisfies

$$R_\alpha^{ss} = R_0^{ss} + O\left(\frac{1}{\alpha}\right),$$

in which R_0^{ss} solves

$$\left(2\boldsymbol{D}\nabla\varphi^{ss} + \mathbf{b}\right)\cdot\nabla R_0^{ss} + \left[\nabla\cdot\left(\boldsymbol{D}\nabla\varphi^{ss}\right) + \nabla\cdot\mathbf{b}\right]R_0^{ss} = 0.$$

When $\mathbf{b}$ admits a potential U, namely, $\mathbf{b} = -\boldsymbol{D}\nabla U$, then $\varphi = U$ and $R_\alpha^{ss} \equiv 1$. This is the only trivial case. In general, the WKB ansatz of π_α relies heavily on the dynamical structure of the ODE

$$\dot{\mathbf{x}} = \mathbf{b}(\mathbf{x}). \tag{23}$$

The existence of the rate function φ^{ss} has been justified under different dynamical assumptions on (23) by examining the limit of $-\frac{1}{\alpha}\ln\pi_\alpha$ as $\alpha\to\infty$. The asymptotic properties of R_α^{ss} are only known when (23) admit a globally asymptotically stable and non-degenerate equilibrium. See [5, 11, 38, 62].

B Entropy

We present the entropy balance equation and study related large α asymptotics.

B.1 Entropy Balance Equation

The entropy $S = S[f_\alpha]$, entropy production rate $e_p = e_p[f_\alpha]$, and heat exchange rate $Q_{ex} = Q_{ex}[f_\alpha]$ are defined by

$$\begin{aligned} S &= -\int_{\mathbb{R}^N} f_\alpha \ln f_\alpha \mathrm{d}\mathbf{x}, \\ e_p &= \int_{\mathbb{R}^N}\left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b}f_\alpha\right)\cdot\left(\nabla\ln f_\alpha - \alpha\boldsymbol{D}^{-1}\mathbf{b}\right)\mathrm{d}\mathbf{x}, \quad \text{and} \\ Q_{ex} &= \alpha\int_{\mathbb{R}^N}\left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b}f_\alpha\right)\cdot\left(\boldsymbol{D}^{-1}\mathbf{b}\right)\mathrm{d}\mathbf{x}, \end{aligned}$$

respectively. Whenever f_α is fixed, they are just functions of the time variable t.

Clearly, e_p can be written as

$$e_p = \alpha \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla \ln f_\alpha - \mathbf{b}\right) \cdot \boldsymbol{D}^{-1} \left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla \ln f_\alpha - \mathbf{b}\right) f_\alpha \mathrm{d}\mathbf{x}. \tag{24}$$

The positive definiteness of $\boldsymbol{D}^{-1}$ ensures that $e_p > 0$.

Note that

$$\begin{aligned}
\frac{\mathrm{d}S}{\mathrm{d}t} &= -\int_{\mathbb{R}^N} \partial_t f_\alpha \left(\ln f_\alpha + 1\right) \mathrm{d}\mathbf{x} \\
&= -\int_{\mathbb{R}^N} \nabla \cdot \left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \left(\ln f_\alpha + 1\right) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \cdot \nabla \ln f_\alpha \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \cdot \left(\nabla \ln f_\alpha - \alpha \boldsymbol{D}^{-1}\mathbf{b} + \alpha \boldsymbol{D}^{-1}\mathbf{b}\right) \mathrm{d}\mathbf{x}.
\end{aligned}$$

Hence, the following entropy balance equation holds:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = e_p + Q_{ex}. \tag{25}$$

B.2 Asymptotics

The large α asymptotics of S, Q_{ex}, e_p, and $\frac{dS}{dt}$ are given as follows.

$$\begin{aligned}
S &= -\frac{N}{2}\ln\alpha + O(1), \\
Q_{ex} &= -\alpha \mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) \\
&\quad - C(\hat{\mathbf{x}}(t), t) - \frac{R_1(\hat{\mathbf{x}}(t), t)}{\sqrt{\det \nabla\nabla\varphi(\hat{\mathbf{x}}(t), t)}} \mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) - \nabla \cdot \mathbf{b}(\hat{\mathbf{x}}(t)) + O(\tfrac{1}{\alpha}), \\
e_p &= \alpha \mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) \\
&\quad + C(\hat{\mathbf{x}}(t), t) + \frac{R_1(\hat{\mathbf{x}}(t), t)}{\sqrt{\det \nabla\nabla\varphi(\hat{\mathbf{x}}(t), t)}} \mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) + 2\nabla \cdot \mathbf{b}(\hat{\mathbf{x}}(t)) \\
&\quad + \boldsymbol{D}(\hat{\mathbf{x}}(t)) : \nabla\nabla\varphi(\hat{\mathbf{x}}(t), t) + O(\tfrac{1}{\alpha}), \\
\frac{\mathrm{d}S}{\mathrm{d}t} &= \boldsymbol{D}(\hat{\mathbf{x}}(t)) : \nabla\nabla\varphi(\hat{\mathbf{x}}(t), t) + \nabla \cdot \mathbf{b}(\hat{\mathbf{x}}(t)) + O\left(\tfrac{1}{\alpha}\right),
\end{aligned}$$

where the colon : denotes the Frobenius product of two matrices of the same size, and

$$C(\hat{\mathbf{x}}(t), t) = \left[\frac{1}{2}\nabla\nabla(R_0\mathbf{b} \cdot \boldsymbol{D}^{-1}\mathbf{b}) : \nabla\nabla\varphi - \frac{1}{6}\nabla(R_0\mathbf{b} \cdot \boldsymbol{D}^{-1}\mathbf{b}) \cdot (\nabla\nabla\nabla\varphi\Theta)\right]\Bigg|_{\mathbf{x}=\hat{\mathbf{x}}(t)}. \tag{26}$$

In which, $\nabla\nabla\nabla\varphi\Theta$ is an N-dimensional vector and its i-th component is given by

$$(\nabla\nabla\nabla\varphi\Theta)_i = \sum_{j,k,\ell=1}^{N} \partial^3_{x_j x_k x_\ell}\varphi\Theta_{ijk\ell},$$

where

$$\Theta_{ijk\ell} = \frac{1}{(2\pi)^{N/2}\sqrt{\det(\nabla\nabla\varphi)^{-1}}} \int_{\mathbb{R}^N} y_i y_j y_k y_\ell e^{-\frac{\mathbf{y}\cdot\nabla\nabla\varphi\mathbf{y}}{2}} \mathrm{d}\mathbf{y}.$$

Below, we provide the detailed derivation of these asymptotics.

Asymptotic of S. Clearly,

$$\begin{aligned} S &= -\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \left(\frac{N}{2}\ln\frac{\alpha}{2\pi} + \ln R_\alpha - \alpha\varphi\right) R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &= -\frac{N}{2}\ln\frac{\alpha}{2\pi} - \ln R_0(\hat{\mathbf{x}}(t), t) + O\left(\tfrac{1}{\alpha}\right) + \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \varphi R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \end{aligned}$$

The asymptotic of S follows from the following:

$$\begin{aligned} \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \varphi R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x} &= -\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \frac{\varphi\nabla\varphi}{|\nabla\varphi|^2} R_\alpha \cdot \nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &= \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \nabla\cdot\left(\frac{\varphi\nabla\varphi}{|\nabla\varphi|^2} R_\alpha\right) e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = O(1). \end{aligned}$$

Asymptotic of Q_{ex}. Since

$$\left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right)\cdot\left(\boldsymbol{D}^{-1}\mathbf{b}\right) = \left(\frac{\alpha}{2\pi}\right)^{N/2}\left[\tfrac{1}{\alpha}\mathbf{b}\cdot\nabla R_\alpha - \left(\mathbf{b}\cdot\nabla\varphi + \mathbf{b}\cdot\boldsymbol{D}^{-1}\mathbf{b}\right) R_\alpha\right] e^{-\alpha\varphi},$$

we find

$$\begin{aligned} Q_{ex} &= -\alpha\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \mathbf{b}\cdot\nabla\varphi e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &\quad - \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \mathbf{b}\cdot\boldsymbol{D}^{-1}\mathbf{b} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &\quad + \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \mathbf{b}\cdot\nabla R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &= I_1(\alpha) + I_2(\alpha) + I_3(\alpha). \end{aligned}$$

Note that

$$I_1(\alpha) = \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \mathbf{b}\cdot\nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = -\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \left(\nabla R_\alpha\cdot\mathbf{b} + R_\alpha\nabla\cdot\mathbf{b}\right) e^{-\alpha\varphi}\mathrm{d}\mathbf{x}.$$

Then,

$$I_1(\alpha) + I_3(\alpha) = -\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \nabla\cdot\mathbf{b} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = -\nabla\cdot\mathbf{b}(\hat{\mathbf{x}}(t)) + O\left(\tfrac{1}{\alpha}\right)$$

For $I_2(\alpha)$, we see that

$$\begin{aligned} -\tfrac{1}{\alpha} I_2(\alpha) &= \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \left(R_0 + \tfrac{1}{\alpha}R_1 + O(\tfrac{1}{\alpha^2})\right) \mathbf{b}\cdot\boldsymbol{D}^{-1}\mathbf{b} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &= \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_0 \mathbf{b}\cdot\boldsymbol{D}^{-1}\mathbf{b} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &\quad + \tfrac{1}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_1 \mathbf{b}\cdot\boldsymbol{D}^{-1}\mathbf{b} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} + O(\tfrac{1}{\alpha^2}) \\ &= I_{21}(\alpha) + \tfrac{1}{\alpha} I_{22}(\alpha) + O(\tfrac{1}{\alpha^2}). \end{aligned}$$

Since

$$I_{21}(\alpha) = \mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) + \tfrac{1}{\alpha}C(\hat{\mathbf{x}}(t), t) + O(\tfrac{1}{\alpha^2}),$$
$$I_{22}(\alpha) = \frac{R_1(\hat{\mathbf{x}}(t), t)}{\sqrt{\det \nabla\nabla\varphi(\hat{\mathbf{x}}(t), t)}}\mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) + O(\tfrac{1}{\alpha}),$$

where $C(\hat{\mathbf{x}}(t), t)$ is given in (26), we arrive at

$$\begin{aligned} I_2(\alpha) = &-\alpha\mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) \\ &- C(\hat{\mathbf{x}}(t), t) - \frac{R_1(\hat{\mathbf{x}}(t), t)}{\sqrt{\det \nabla\nabla\varphi(\hat{\mathbf{x}}(t), t)}}\mathbf{b}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\mathbf{b}(\hat{\mathbf{x}}(t)) + O(\tfrac{1}{\alpha}). \end{aligned}$$

The asymptotic of Q_{ex} follows.

Asymptotic of e_p. Note that

$$e_p = -Q_{ex} + \underbrace{\int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \cdot \nabla \ln f_\alpha \mathrm{d}\mathbf{x}}_{I(\alpha)}.$$

Given the asymptotic of Q_{ex}, we only need to treat $I(\alpha)$. Straightforward calculations yield

$$\begin{aligned} &\left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \cdot \nabla \ln f_\alpha \\ &\quad = \left(\frac{\alpha}{2\pi}\right)^{N/2} \left[\tfrac{1}{\alpha}\frac{\nabla R_\alpha \cdot \boldsymbol{D}\nabla R_\alpha}{R_\alpha} - (2\boldsymbol{D}\nabla\varphi + \mathbf{b}) \cdot \nabla R_\alpha + \alpha\left(\boldsymbol{D}\nabla\varphi + \mathbf{b}\right) R_\alpha \cdot \nabla\varphi\right] e^{-\alpha\varphi}. \end{aligned}$$

Then,

$$\begin{aligned} I(\alpha) = &\tfrac{1}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \frac{\nabla R_\alpha \cdot \boldsymbol{D}\nabla R_\alpha}{R_\alpha} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} - \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} (2\boldsymbol{D}\nabla\varphi + \mathbf{b}) \cdot \nabla R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &+ \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \nabla\varphi \cdot \boldsymbol{D}\nabla\varphi e^{-\alpha\varphi}\mathrm{d}\mathbf{x} + \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \mathbf{b} \cdot \nabla\varphi e^{-\alpha\varphi}\mathrm{d}\mathbf{x}. \end{aligned}$$

Note that the fourth term on the RHS of the above equality can be written as

$$-\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \mathbf{b} \cdot \nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \left(\nabla R_\alpha \cdot \mathbf{b} + R_\alpha \nabla \cdot \mathbf{b}\right) e^{-\alpha\varphi}\mathrm{d}\mathbf{x}.$$

Hence,

$$\begin{aligned} I(\alpha) = &\tfrac{1}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \frac{\nabla R_\alpha \cdot \boldsymbol{D}\nabla R_\alpha}{R_\alpha} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} - 2\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \boldsymbol{D}\nabla\varphi \cdot \nabla R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &+ \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \nabla\varphi \cdot \boldsymbol{D}\nabla\varphi e^{-\alpha\varphi}\mathrm{d}\mathbf{x} + \left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} R_\alpha \nabla \cdot \mathbf{b} e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ = &\, I_4(\alpha) + I_5(\alpha) + I_6(\alpha) + I_7(\alpha). \end{aligned}$$

Clearly, $I_4(\alpha) = O\left(\frac{1}{\alpha}\right)$ and $I_7(\alpha) = \nabla \cdot \mathbf{b}(\hat{\mathbf{x}}(t)) + O\left(\frac{1}{\alpha}\right)$. For $I_5(\alpha)$,

$$\begin{aligned} I_5(\alpha) &= \tfrac{2}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \boldsymbol{D}\nabla R_\alpha \cdot \nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x} \\ &= -\tfrac{2}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2} \int_{\mathbb{R}^N} \nabla \cdot \left(\boldsymbol{D}\nabla R_\alpha\right) e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = O\left(\tfrac{1}{\alpha}\right). \end{aligned}$$

For $I_6(\alpha)$,

$$\begin{aligned}
I_6(\alpha) &= -\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} R_\alpha \boldsymbol{D}\nabla\varphi\cdot\nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= \left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} \nabla\cdot\left(R_\alpha \boldsymbol{D}\nabla\varphi\right)e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= \left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} \left[\nabla R_\alpha\cdot\boldsymbol{D}\nabla\varphi + R_\alpha\left(\nabla\cdot\boldsymbol{D}\right)\cdot\nabla\varphi + R_\alpha\boldsymbol{D}:\nabla\nabla\varphi\right]e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= -\tfrac{1}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} \left[\boldsymbol{D}\nabla R_\alpha + R_\alpha\left(\nabla\cdot\boldsymbol{D}\right)\right]\cdot\nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&+ \left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} R_\alpha\boldsymbol{D}:\nabla\nabla\varphi e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= \tfrac{1}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} \nabla\cdot\left[\boldsymbol{D}\nabla R_\alpha + R_\alpha\left(\nabla\cdot\boldsymbol{D}\right)\right]e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&+ \left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N} R_\alpha\boldsymbol{D}:\nabla\nabla\varphi e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= O\left(\tfrac{1}{\alpha}\right) + \boldsymbol{D}(\hat{\mathbf{x}}(t)):\nabla\nabla\varphi(\hat{\mathbf{x}}(t),t).
\end{aligned}$$

Hence,

$$I(\alpha) = \boldsymbol{D}(\hat{\mathbf{x}}(t)):\nabla\nabla\varphi(\hat{\mathbf{x}}(t),t) + \nabla\cdot\mathbf{b}(\hat{\mathbf{x}}(t)) + O\left(\tfrac{1}{\alpha}\right).$$

The asymptotic of e_p then follows.

Asymptotic of $\frac{\mathrm{d}S}{\mathrm{d}t}$. It follows from the entropy balance equation Eq. (25) and the asymptotics of e_p and Q_{ex}. Alternatively, the asymptotic of $\frac{\mathrm{d}S}{\mathrm{d}t}$ follows from the fact that $\frac{\mathrm{d}S}{\mathrm{d}t} = I(\alpha)$.

C Free Energy

We present the free energy balance equation and study related large α asymptotics.

C.1 Free Energy Balance Equation

The free energy $F = F[f_\alpha]$ and house-keeping heat rate $Q_{hk} = Q_{hk}[f_\alpha]$ are defined by

$$\begin{aligned}
F &= \int_{\mathbb{R}^N} f_\alpha \ln\frac{f_\alpha}{\pi_\alpha}\mathrm{d}\mathbf{x} \quad \text{and}\\
Q_{hk} &= \int_{\mathbb{R}^N}\left(\tfrac{1}{\alpha}\boldsymbol{D}\nabla f_\alpha - \mathbf{b}f_\alpha\right)\cdot\left(\nabla\ln\pi_\alpha - \alpha\boldsymbol{D}^{-1}\mathbf{b}\right)\mathrm{d}\mathbf{x},
\end{aligned}$$

respectively. It is known that $F > 0$ and $Q_{hk} \geq 0$, and the following free energy balance equation holds:

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -e_p + Q_{hk}. \tag{27}$$

Below, we provide the details.

Positivity of F. Note that

$$F = -\int_{\mathbb{R}^N} f_\alpha \ln \frac{\pi_\alpha}{f_\alpha} \mathrm{d}\mathbf{x} \geq -\ln \int_{\mathbb{R}^N} \frac{\pi_\alpha}{f_\alpha} f_\alpha \mathrm{d}\mathbf{x} = 0,$$

where we used Jensen's inequality. Moreover, since the function $x \mapsto -\ln x$ is strictly convex, the above inequality is strict unless $f_\alpha \equiv \pi_\alpha$. As $f_\alpha \neq \pi_\alpha$, one concludes $F > 0$.

Non-negativity of Q_{hk}. We show

$$Q_{hk} = \alpha \int_{\mathbb{R}^N} \mathbf{J}_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha f_\alpha \mathrm{d}\mathbf{x} \geq 0, \tag{28}$$

where $\mathbf{J}_\alpha$ is defined in (17). Note that $\mathbf{J}_\alpha = \mathbf{0}$ so that $Q_{hk} = 0$ when $\mathbf{b}$ admits a potential U, namely, $\mathbf{b} = -\boldsymbol{D}\nabla U$. Otherwise, $Q_{hk} > 0$.

Indeed, we calculate

$$\begin{aligned}
Q_{hk} &= \alpha \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha} \boldsymbol{D}\nabla \ln f_\alpha - \mathbf{b}\right) f_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha \mathrm{d}\mathbf{x} \\
&= \alpha \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha} \boldsymbol{D}\nabla \ln f_\alpha - \tfrac{1}{\alpha} \boldsymbol{D}\nabla \ln \pi_\alpha + \mathbf{J}_\alpha\right) f_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha \mathrm{d}\mathbf{x} \\
&= \alpha \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha} \boldsymbol{D}\nabla \ln f_\alpha - \tfrac{1}{\alpha} \boldsymbol{D}\nabla \ln \pi_\alpha\right) f_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha \mathrm{d}\mathbf{x} + \alpha \int_{\mathbb{R}^N} \mathbf{J}_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha f_\alpha \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^N} \boldsymbol{D}\nabla \ln \frac{f_\alpha}{\pi_\alpha} f_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha \mathrm{d}\mathbf{x} + \alpha \int_{\mathbb{R}^N} \mathbf{J}_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha f_\alpha \mathrm{d}\mathbf{x}.
\end{aligned}$$

The expected result follows readily from

$$\int_{\mathbb{R}^N} \boldsymbol{D}\nabla \ln \frac{f_\alpha}{\pi_\alpha} f_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^N} \nabla \frac{f_\alpha}{\pi_\alpha} \cdot (\pi_\alpha \mathbf{J}_\alpha)\, \mathrm{d}\mathbf{x} = -\int_{\mathbb{R}^N} \frac{f_\alpha}{\pi_\alpha} \nabla \cdot (\pi_\alpha \mathbf{J}_\alpha)\, \mathrm{d}\mathbf{x} = 0, \tag{29}$$

where we used Eq. (18) in the last equality.

Free energy balance equation. We show

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -e_p + Q_{hk} = -\tfrac{1}{\alpha} \int_{\mathbb{R}^N} \left(\nabla \ln \frac{f_\alpha}{\pi_\alpha}\right) \cdot \boldsymbol{D} \left(\nabla \ln \frac{f_\alpha}{\pi_\alpha}\right) f_\alpha \mathrm{d}\mathbf{x} < 0.$$

The strict inequality is a result of the fact that $f_\alpha \neq \pi_\alpha$.

The first equality follows readily.

$$\begin{aligned}
\frac{\mathrm{d}F}{\mathrm{d}t} &= \int_{\mathbb{R}^N} \partial_t f_\alpha \left(\ln \frac{f_\alpha}{\pi_\alpha} + 1\right) \mathrm{d}\mathbf{x} \\
&= \int_{\mathbb{R}^N} \nabla \cdot \left(\tfrac{1}{\alpha} \boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \left(\ln \frac{f_\alpha}{\pi_\alpha} + 1\right) \mathrm{d}\mathbf{x} \\
&= -\int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha} \boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \cdot (\nabla \ln f_\alpha - \nabla \ln \pi_\alpha)\, \mathrm{d}\mathbf{x} \\
&= -\int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha} \boldsymbol{D}\nabla f_\alpha - \mathbf{b} f_\alpha\right) \cdot \left(\nabla \ln f_\alpha - \alpha \boldsymbol{D}^{-1} \mathbf{b} + \alpha \boldsymbol{D}^{-1} \mathbf{b} - \nabla \ln \pi_\alpha\right) \mathrm{d}\mathbf{x} \\
&= -e_p + Q_{hk}.
\end{aligned}$$

Now, we treat the second equality. From (24), one deduces

$$\begin{aligned} e_p &= \alpha \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha} \boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} + \mathbf{J}_\alpha \right) \cdot \boldsymbol{D}^{-1} \left(\tfrac{1}{\alpha} \boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} + \mathbf{J}_\alpha \right) f_\alpha \mathrm{d}\mathbf{x} \\ &= \tfrac{1}{\alpha} \int_{\mathbb{R}^N} \left(\boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} \right) \cdot \boldsymbol{D}^{-1} \left(\boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} \right) f_\alpha \mathrm{d}\mathbf{x} \\ &\quad + 2 \int_{\mathbb{R}^N} \left(\boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} \right) \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha f_\alpha \mathrm{d}\mathbf{x} + \alpha \int_{\mathbb{R}^N} \mathbf{J}_\alpha \cdot \boldsymbol{D}^{-1} \mathbf{J}_\alpha f_\alpha \mathrm{d}\mathbf{x} \\ &= \tfrac{1}{\alpha} \int_{\mathbb{R}^N} \left(\nabla \ln \frac{f_\alpha}{\pi_\alpha} \right) \cdot \boldsymbol{D} \left(\nabla \ln \frac{f_\alpha}{\pi_\alpha} \right) f_\alpha \mathrm{d}\mathbf{x} + Q_{hk}, \end{aligned}$$

where we used Eq. (28) and Eq. (29) in the last equality. The free energy balance equation follows.

Rewriting

$$\frac{\mathrm{d}F}{\mathrm{d}t} = -\alpha \int_{\mathbb{R}^N} \left(\tfrac{1}{\alpha} \boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} \right) \cdot \boldsymbol{D}^{-1} \left(\tfrac{1}{\alpha} \boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} \right) f_\alpha \mathrm{d}\mathbf{x}$$

and introducing the inner product and the associated norm

$$\langle \mathbf{V}_1, \mathbf{V}_2 \rangle_{\boldsymbol{D}^{-1}, f_\alpha} = \int_{\mathbb{R}^N} \mathbf{V}_1 \cdot \boldsymbol{D}^{-1} \mathbf{V}_2 f_\alpha \mathrm{d}\mathbf{x} \quad \text{and} \quad \|\mathbf{V}\|_{\boldsymbol{D}^{-1}, f_\alpha} = \sqrt{\langle \mathbf{V}, \mathbf{V} \rangle_{\boldsymbol{D}^{-1}, f_\alpha}}$$

for vector fields $\mathbf{V}_1$, $\mathbf{V}_2$ and $\mathbf{V}$ on $\mathbb{R}^N$, the free energy balance equation can be rewritten as

$$\left\| \tfrac{1}{\alpha} \boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} \right\|^2_{\boldsymbol{D}^{-1}, f_\alpha} + \|\mathbf{J}_\alpha\|^2_{\boldsymbol{D}^{-1}, f_\alpha} = \left\| \tfrac{1}{\alpha} \boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha} + \mathbf{J}_\alpha \right\|^2_{\boldsymbol{D}^{-1}, f_\alpha}, \tag{30}$$

which is equivalent to the orthogonality between $\boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha}$ and $\mathbf{J}_\alpha$ w.r.t. the inner product, that is,

$$\left\langle \boldsymbol{D} \nabla \ln \frac{f_\alpha}{\pi_\alpha}, \mathbf{J}_\alpha \right\rangle_{\boldsymbol{D}^{-1}, f_\alpha} = 0.$$

This is just Eq. (29).

C.2 Asymptotics

The asymptotics of F, Q_{hk}, and $\frac{\mathrm{d}F}{\mathrm{d}t}$ are given as follows:

$$\begin{aligned} F &= \alpha \varphi^{ss}(\hat{\mathbf{x}}(t)) + \frac{N}{2} \ln \alpha - \ln C_\alpha + O(1), \\ Q_{hk} &= \alpha \boldsymbol{\gamma}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t)) \boldsymbol{\gamma}(\hat{\mathbf{x}}(t)) + O(1), \\ \frac{\mathrm{d}F}{\mathrm{d}t} &= -\alpha \nabla \varphi^{ss}(\hat{\mathbf{x}}(t)) \cdot \boldsymbol{D}(\hat{\mathbf{x}}(t)) \nabla \varphi^{ss}(\hat{\mathbf{x}}(t)) + O(1), \end{aligned}$$

where C_α is given in (21) and $\boldsymbol{\gamma} = \boldsymbol{D} \nabla \varphi^{ss} + \mathbf{b}$. If (23) admit a globally asymptotically stable and non-degenerate equilibrium, then $C_\alpha = \left(\frac{\alpha}{2\pi} \right)^{-N/2}$, resulting in $F = \alpha \varphi^{ss}(\hat{\mathbf{x}}(t)) + O(1)$.

Multiplying the free energy balance equation Eq. (27) by $\frac{1}{\alpha}$ and then letting $\alpha \to \infty$, we derive from the asymptotics of $\frac{dF}{dt}$, e_p, and Q_{hk} the following free energy balance equation on the macroscopic scale:

$$-\nabla \varphi^{ss}(\mathbf{x}) \cdot \boldsymbol{D}(\mathbf{x}) \nabla \varphi^{ss}(\mathbf{x}) = -\mathbf{b}(\mathbf{x}) \cdot \boldsymbol{D}^{-1}(\mathbf{x}) \mathbf{b}(\mathbf{x}) + \boldsymbol{\gamma}(\mathbf{x}) \cdot \boldsymbol{D}^{-1}(\mathbf{x}) \boldsymbol{\gamma}(\mathbf{x}) \quad \text{at} \quad \mathbf{x} = \hat{\mathbf{x}}(t).$$

Introducing the norm $\|\mathbf{v}\|_{\boldsymbol{D}^{-1}(\mathbf{x})} = \sqrt{\mathbf{v}\cdot\boldsymbol{D}^{-1}(\mathbf{x})\mathbf{v}}$ for $\mathbf{v}\in\mathbb{R}^N$, we arrive at the Pythagorean equality

$$\|\boldsymbol{D}(\mathbf{x})\nabla\varphi^{ss}(\mathbf{x})\|^2_{\boldsymbol{D}^{-1}(\mathbf{x})} + \|\boldsymbol{\gamma}(\mathbf{x})\|^2_{\boldsymbol{D}^{-1}(\mathbf{x})} = \|\mathbf{b}(\mathbf{x})\|^2_{\boldsymbol{D}^{-1}(\mathbf{x})} \quad \text{at} \quad \mathbf{x}=\hat{\mathbf{x}}(t),$$

which is equivalent to Eq. (22) (or $\nabla\varphi^{ss}\cdot\gamma = 0$) at $\hat{\mathbf{x}}(t)$. Of course, it is just the leading asymptotic of Eq. (30).

Below, we justify the asymptotics of F, Q_{hk}, and $\frac{dF}{dt}$.

Asymptotic of F. Clearly,

$$\begin{aligned}
F &= S - \int_{\mathbb{R}^N} f_\alpha \ln\pi_\alpha \mathrm{d}\mathbf{x}\\
&= \frac{N}{2}\ln\alpha + O(1) - \left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\left(\ln C_\alpha + \ln R^{ss}_\alpha - \alpha\varphi^{ss}\right)R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= \alpha\varphi^{ss}(\hat{\mathbf{x}}(t)) + \frac{N}{2}\ln\alpha - \ln C_\alpha + O(1).
\end{aligned}$$

Asymptotic of Q_{hk}. Since

$$\mathbf{J}_\alpha = \tfrac{1}{\alpha}\frac{\boldsymbol{D}\nabla R^{ss}_\alpha}{R^{ss}_\alpha} - \boldsymbol{D}\nabla\varphi^{ss} - \mathbf{b} = \tfrac{1}{\alpha}\frac{\boldsymbol{D}\nabla R^{ss}_\alpha}{R^{ss}_\alpha} - \boldsymbol{\gamma},$$

we find

$$\begin{aligned}
Q_{hk} &= \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\left(\tfrac{1}{\alpha}\frac{\boldsymbol{D}\nabla R^{ss}_\alpha}{R^{ss}_\alpha} - \boldsymbol{\gamma}\right)\\
&\qquad\cdot\boldsymbol{D}^{-1}\left(\tfrac{1}{\alpha}\frac{\boldsymbol{D}\nabla R^{ss}_\alpha}{R^{ss}_\alpha} - \boldsymbol{\gamma}\right)R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= \tfrac{1}{\alpha}\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\frac{\nabla R^{ss}_\alpha\cdot\boldsymbol{D}\nabla R^{ss}_\alpha}{(R^{ss}_\alpha)^2}R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&\quad + 2\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\frac{\nabla R^{ss}_\alpha\cdot\boldsymbol{\gamma}}{R^{ss}_\alpha}R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&\quad + \alpha\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\gamma\cdot\boldsymbol{D}^{-1}\boldsymbol{\gamma}R_\alpha e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\
&= \alpha\boldsymbol{\gamma}(\hat{\mathbf{x}}(t))\cdot\boldsymbol{D}^{-1}(\hat{\mathbf{x}}(t))\boldsymbol{\gamma}(\hat{\mathbf{x}}(t)) + O(1).
\end{aligned}$$

Asymptotic of $\frac{\mathrm{d}F}{\mathrm{d}t}$. Since

$$\nabla\ln\frac{f_\alpha}{\pi_\alpha} = \frac{\nabla R_\alpha}{R_\alpha} - \frac{\nabla R^{ss}_\alpha}{R^{ss}_\alpha} - \alpha\left(\nabla\varphi - \nabla\varphi^{ss}\right),$$

we find

$$\begin{aligned}\frac{\mathrm{d}F}{\mathrm{d}t} &= -\tfrac{1}{\alpha}\int_{\mathbb{R}^N}\left(\frac{\nabla R_\alpha}{R_\alpha}-\frac{\nabla R_\alpha^{ss}}{R_\alpha^{ss}}\right)\cdot \boldsymbol{D}\left(\frac{\nabla R_\alpha}{R_\alpha}-\frac{\nabla R_\alpha^{ss}}{R_\alpha^{ss}}\right) f_\alpha \mathrm{d}\mathbf{x}\\ &\quad + 2\int_{\mathbb{R}^N}\left(\nabla\varphi-\nabla\varphi^{ss}\right)\cdot \boldsymbol{D}\left(\frac{\nabla R_\alpha}{R_\alpha}-\frac{\nabla R_\alpha^{ss}}{R_\alpha^{ss}}\right) f_\alpha \mathrm{d}\mathbf{x}\\ &\quad - \alpha\int_{\mathbb{R}^N}\left(\nabla\varphi-\nabla\varphi^{ss}\right)\cdot \boldsymbol{D}\left(\nabla\varphi-\nabla\varphi^{ss}\right) f_\alpha \mathrm{d}\mathbf{x}\\ &= O(1)-\alpha\int_{\mathbb{R}^N}\nabla\varphi\cdot\boldsymbol{D}\nabla\varphi f_\alpha \mathrm{d}\mathbf{x}\\ &\quad + 2\alpha\int_{\mathbb{R}^N}\nabla\varphi\cdot\boldsymbol{D}\nabla\varphi^{ss} f_\alpha \mathrm{d}\mathbf{x} - \alpha\int_{\mathbb{R}^N}\nabla\varphi^{ss}\cdot\boldsymbol{D}\nabla\varphi^{ss} f_\alpha \mathrm{d}\mathbf{x}\\ &= O(1)+I_8(\alpha)+I_9(\alpha)+I_{10}(\alpha).\end{aligned}$$

Clearly,

$$I_{10}(\alpha) = -\alpha\nabla\varphi^{ss}(\hat{\mathbf{x}}(t))\cdot\boldsymbol{D}(\hat{\mathbf{x}}(t))\nabla\varphi^{ss}(\hat{\mathbf{x}}(t)) + O(1).$$

For $I_9(\alpha)$,

$$\begin{aligned}I_9(\alpha) &= -2\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\boldsymbol{D}\nabla\varphi^{ss}R_\alpha\cdot\nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\ &= 2\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\nabla\cdot\left(\boldsymbol{D}\nabla\varphi^{ss}R_\alpha\right)e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = O(1).\end{aligned}$$

For $I_8(\alpha)$,

$$\begin{aligned}I_8(\alpha) &= \left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\boldsymbol{D}\nabla\varphi R_\alpha\cdot\nabla e^{-\alpha\varphi}\mathrm{d}\mathbf{x}\\ &= -\left(\frac{\alpha}{2\pi}\right)^{N/2}\int_{\mathbb{R}^N}\nabla\cdot\left(\boldsymbol{D}\nabla\varphi R_\alpha\right)e^{-\alpha\varphi}\mathrm{d}\mathbf{x} = O(1).\end{aligned}$$

Hence, the expected asymptotic of $\frac{\mathrm{d}F}{\mathrm{d}t}$ follows.

D Ornstein-Uhlenbeck Process

Consider the Ornstein-Uhlenbeck process with linear drift $\mathbf{b}(\mathbf{x}) = \boldsymbol{B}\mathbf{x}$ and constant diffusion matrix $\frac{1}{\alpha}\boldsymbol{D}$ (symmetric and positive definite), where $\boldsymbol{B}$ is a $N\times N$ matrix. Then,

$$f_\alpha(\mathbf{x},t) = \frac{1}{(2\pi)^{N/2}}\frac{1}{\sqrt{\det\boldsymbol{\Sigma}_\alpha(t)}}\exp\left\{-\tfrac{1}{2}\left(\mathbf{x}-e^{\boldsymbol{B}t}\mathbf{x}_0\right)\cdot\boldsymbol{\Sigma}_\alpha^{-1}(t)\left(\mathbf{x}-e^{\boldsymbol{B}t}\mathbf{x}_0\right)\right\},$$

where the covariance matrix $\boldsymbol{\Sigma}_\alpha(t)$ is given by

$$\boldsymbol{\Sigma}_\alpha(t) = \frac{2}{\alpha}\int_0^t e^{\boldsymbol{B}(t-s)}\boldsymbol{D}e^{\boldsymbol{B}^\top(t-s)}ds.$$

Introducing

$$\boldsymbol{\Sigma}(t) = 2\int_0^t e^{\boldsymbol{B}(t-s)}\boldsymbol{D}e^{\boldsymbol{B}^\top(t-s)}ds,$$

one can rewrite f_α as

$$f_\alpha(\mathbf{x},t) = \left(\frac{\alpha}{2\pi}\right)^{N/2}\frac{1}{\sqrt{\det\boldsymbol{\Sigma}(t)}}\exp\left\{-\tfrac{\alpha}{2}\left(\mathbf{x}-e^{\boldsymbol{B}t}\mathbf{x}_0\right)\cdot\boldsymbol{\Sigma}^{-1}(t)\left(\mathbf{x}-e^{\boldsymbol{B}t}\mathbf{x}_0\right)\right\}.$$

The WKB ansatz (19) holds precisely in this case:

$$f_\alpha(\mathbf{x}, t) = \left(\frac{\alpha}{2\pi}\right)^{N/2} R_0(\mathbf{x}, t) e^{-\alpha\varphi(\mathbf{x},t)}, \tag{31}$$

where $R_0(\mathbf{x}, t) = \frac{1}{\sqrt{\det \boldsymbol{\Sigma}(t)}}$ is independent of $\mathbf{x}$ and

$$\varphi(\mathbf{x}, t) = \tfrac{1}{2}\left(\mathbf{x} - e^{\boldsymbol{B}t}\mathbf{x}_0\right) \cdot \boldsymbol{\Sigma}^{-1}(t)\left(\mathbf{x} - e^{\boldsymbol{B}t}\mathbf{x}_0\right).$$

It is well-known that

$$S = \frac{N}{2}\ln(2\pi e) + \frac{1}{2}\ln(\det \boldsymbol{\Sigma}_\alpha(t)) = \frac{N}{2}\ln(2\pi e) + \frac{1}{2}\ln(\det \boldsymbol{\Sigma}(t)) - \frac{N}{2}\ln\alpha.$$

It follows from Jacobi's formula and the formula $\boldsymbol{\Sigma}'(t) = 2\boldsymbol{D} + \boldsymbol{B}\boldsymbol{\Sigma}(t) + \boldsymbol{\Sigma}(t)\boldsymbol{B}^\top$ [42] that

$$\begin{aligned}
\frac{\mathrm{d}S}{\mathrm{d}t} &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\ln(\det \boldsymbol{\Sigma}(t)) \\
&= \frac{1}{2}\mathrm{tr}\left[\boldsymbol{\Sigma}^{-1}(t)\boldsymbol{\Sigma}'(t)\right] \\
&= \mathrm{tr}\left[\boldsymbol{D}\boldsymbol{\Sigma}^{-1}(t)\right] + \mathrm{tr}\boldsymbol{B} \\
&= \boldsymbol{D} : \nabla\nabla\varphi + \nabla\cdot\mathbf{b}.
\end{aligned}$$

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