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A Solution to the Fokker-Planck Equation for Slowly Driven Brownian Motion: Emergent Geometry and a Formula for the Corresponding Thermodynamic Metric

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Considerable progress has recently been made with geometrical approaches to understanding and controlling small out-of-equilibrium systems, but a mathematically rigorous foundation for these methods has been lacking. Towards this end, we develop a perturbative solution to the Fokker-Planck equation for one-dimensional driven Brownian motion in the overdamped limit enabled by the spectral properties of the corresponding single-particle Schrödinger operator. The perturbation theory is in powers of the inverse characteristic timescale of variation of the fastest varying control parameter, measured in units of the system timescale, which is set by the smallest eigenvalue of the corresponding Schrödinger operator. It applies to any Brownian system for which the Schrödinger operator has a confining potential. We use the theory to rigorously derive a new, exact formula for a Riemannian “thermodynamic” metric in the space of control parameters of the system. We show that up to second order terms in the perturbation theory, optimal dissipation-minimizing driving protocols minimize the length defined by this metric. We also show that a previously proposed metric is calculable from our exact formula with corrections that are exponentially suppressed in a characteristic length scale. We illustrate our formula using the two-dimensional example of a harmonic oscillator with time-dependent spring constant in a time-dependent electric field. Lastly, we demonstrate that the Riemannian geometric structure of the optimal control problem is emergent; it derives from the form of the perturbative expansion for the probability density and persists to all orders of the expansion.

Driven Brownian motion is a paradigmatic model for a certain class of small (micrometer sized and smaller) stochastic machines [1]. The hallmark of these systems is that important quantities such as work and efficiency fluctuate, and are comparable in scale to thermal fluctuations. Their study, stochastic thermodynamics [2], has seen remarkable recent experimental progress [3–23], including the implementation of microscopic single-particle heat engines [24, 25], and much theoretical activity [26–51].

A fundamental problem in stochastic thermodynamics is to understand how small systems do useful work while operating out of equilibrium. A natural framing of this problem is in terms of a notion of optimality out of equilibrium, whereby a system is considered optimal if it minimizes irreversible heat loss to the reservoir on average. Optimal driving protocols can therefore be computed by minimizing the average dissipation over protocols. In general, however, this is a nontrivial optimization problem to solve [52].

The introduction of the thermodynamic metric framework [53, 54] simplified the problem for a restricted class of systems by recasting it in a geometric picture in which the average dissipation is proportional to a measure of length in the space of control parameters of the system. The “length” is defined by a Riemannian metric on this space. An optimal protocol between two points in control space is then given by the minimum of this length, which

is generally easier to compute than solutions to the original optimization problem. This framework is a generalization to mesoscale, out-of equilibrium systems of geometrical approaches originally developed for macroscale, endoreversible systems [55–61].

Since its introduction, the thermodynamic metric framework has found success in predicting optimal protocols for a number of systems both analytically and numerically [62–66], and in illuminating their general characteristics, opening up a window onto the physics of small machines that operate out of equilibrium.

The concept of a thermodynamic geometry at mesoscopic length scales emerges independently from various different assumptions about the dynamics of the stochastic system. All these approximations have in common a notion of closeness to equilibrium. In the original work, the approximations were linear response plus slow driving [54]. Subsequent work derived a thermodynamic metric under approximations of derivative truncation [62], and timescale separation [66]. Slow driving was also assumed in order to extend the thermodynamic metric framework to driven discrete-time systems [67].

In this paper we provide a new and rigorous derivation of a thermodynamic metric within the framework of the Fokker-Planck equation for Brownian motion with time-varying control parameters. We work in a regime in which the control parameters vary on a timescale that is much longer than the intrinsic timescale of the system, which is set by its relaxation time. The solution to the time-dependent Fokker-Planck equation is obtained as an expansion in a small dimensionless parameter ν

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that is the ratio of the relaxation time of the system to the the shortest characteristic timescale of variation among the control parameters. The expansion is enabled by the spectral properties of the corresponding Schrödinger operator. The formula for the thermodynamic metric we derive in this framework is exact and has a generalization to higher dimensions.

In addition, we demonstrate an emergent diffeomorphism symmetry in the space of control parameters arising from the expansion in ν of the probability density. Every term with n indices in the corresponding expansion for the average dissipation is a rank n tensor under the diffeomorphism symmetry.

The harmonic potential is a canonical system to study in stochastic thermodynamics, both experimentally and theoretically [19, 24, 25, 52, 62, 68–73]. For this reason we illustrate our formalism and formulae using the example of a harmonic oscillator with a time-varying spring constant in a time-varying electric field.

I. DRIVEN BROWNIAN MOTION

Consider a small system in contact with a reservoir such as a Brownian particle in a suspension subject to an external potential $V_{\lambda(t)}(x)$ that can depend on a possibly time-dependent control vector $\lambda \in \mathbb{R}^k$. The space \mathcal{C} of all possible values of λ is a subset of \mathbb{R}^k . The position of the particle is given by $x \in \mathbb{R}$ and its probability density $\rho(x; t)$ evolves according to a Fokker-Planck equation [74],

$$\frac{\partial}{\partial t} \rho(x; t) = \hat{\mathcal{L}}_{\lambda(t)}(x) \rho(x; t), \quad (1)$$

where $\hat{\mathcal{L}}_{\lambda(t)}(x)$, the Fokker-Planck operator, is a second-order differential operator involving spatial derivatives of the potential. In the overdamped limit, where inertial effects are neglected, $\hat{\mathcal{L}}_{\lambda(t)}(x)$ takes the form

$$\hat{\mathcal{L}}_{\lambda(t)}(x) = \frac{1}{\gamma} \frac{\partial}{\partial x} \left(V'_{\lambda(t)}(x) + \frac{1}{\beta} \frac{\partial}{\partial x} \right), \quad (2)$$

where γ and $\beta = 1/k_B T$ are the friction coefficient and inverse temperature, respectively, and k_B is Boltzmann's constant.¹ Primes denote derivatives with respect to x . Note that $V'_{\lambda(t)}(x) = -F(x; t)$ where F is the force acting on the system. We consider natural boundary conditions, requiring $\rho(x; t) \rightarrow 0$ as $x \rightarrow \pm\infty$. $\rho(x; t)$ satisfies the normalization condition

$$\int dx \rho(x; t) = 1. \quad (3)$$

¹ The action of $\hat{\mathcal{L}}_{\lambda(t)}$ on $\rho(x; t)$ is

$$\frac{1}{\gamma} \frac{\partial}{\partial x} \left(V'_{\lambda(t)}(x) \rho(x; t) + \frac{1}{\beta} \frac{\partial \rho(x; t)}{\partial x} \right).$$

We use the notation $\int dx$ as shorthand for $\int_{-\infty}^{\infty} dx$ throughout the paper.

Eq. (1) can also be written in the form of a continuity equation as

$$\frac{\partial}{\partial t} \rho(x; t) = -\frac{\partial}{\partial x} J(x; t), \quad (4)$$

where J is the probability current:

$$J(x; t) = -\frac{1}{\gamma} \left(V'_{\lambda(t)}(x) + \frac{1}{\beta} \frac{\partial}{\partial x} \right) \rho(x; t). \quad (5)$$

Natural boundary conditions additionally require $J(x; t) \rightarrow 0$ as $x \rightarrow \pm\infty$.

We note that Eq. (1) with $\hat{\mathcal{L}}_{\lambda(t)}$ as given in Eq. (2) is equivalent to the trajectory-level Langevin description

$$\gamma \dot{x} = F(x, t) + \sqrt{\frac{2\gamma}{\beta}} \eta(t), \quad (6)$$

where $\eta(t)$ is mean zero δ -correlated Gaussian noise: $\langle \eta(t) \rangle = 0$, $\langle \eta(t) \eta(t') \rangle = \delta(t - t')$. The dot denotes a derivative with respect to time.

At all times, the state space admits the existence of a unique equilibrium distribution $\rho_{\lambda(t)}^{eq}(x)$ such that

$$\hat{\mathcal{L}}_{\lambda(t)}(x) \rho_{\lambda(t)}^{eq}(x) = 0 \quad (7)$$

and

$$\int dx \rho_{\lambda(t)}^{eq}(x) = 1. \quad (8)$$

$\rho_{\lambda(t)}^{eq}(x)$ is given by

$$\rho_{\lambda(t)}^{eq}(x) = \frac{1}{Z(t)} e^{-\beta V_{\lambda(t)}(x)}, \quad (9)$$

where $Z(t)$ is the partition function

$$Z(t) = \int dx e^{-\beta V_{\lambda(t)}(x)}. \quad (10)$$

All distributions approach $\rho_{\lambda(t)}^{eq}(x)$ asymptotically with time when λ is frozen, and $\rho_{\lambda(t)}^{eq}$ satisfies the detailed balance condition, which requires that the probability current in equilibrium be zero:

$$-\frac{1}{\gamma} \left(V'_{\lambda(t)}(x) + \frac{1}{\beta} \frac{\partial}{\partial x} \right) \rho_{\lambda(t)}^{eq}(x) = 0 \quad \forall x. \quad (11)$$

We note that $\rho_{\lambda(t)}^{eq}$ does not satisfy Eq. (1) except in an approximate sense. While Eq. (7) is exact, the time derivative of $\rho_{\lambda(t)}^{eq}$ is

$$\frac{\partial}{\partial t} \rho_{\lambda(t)}^{eq}(x) = \sum_{i=1}^k \dot{\lambda}_i \frac{\partial}{\partial \lambda_i} \rho_{\lambda(t)}^{eq}(x), \quad (12)$$

which is not zero if $\dot{\lambda}_i \neq 0$. The solution to Eq. (1) we develop in the following is in the limit of small $\dot{\lambda}$. We will show that the ‘smallness’ of $\dot{\lambda}$ is quantified by a parameter ν , defined as the ratio of the relaxation time τ_{α_1} of the system to the driving timescale τ_λ , which must be chosen such that $\nu \ll 1$. In this limit, the timescale of driving is so long that $\rho_{\lambda(t)}^{eq}$ is roughly stationary on the system timescale, which is set by τ_{α_1} . Thus $\rho_{\lambda(t)}^{eq}$ satisfies Eq. (1) to zeroth order in the parameter ν . We return in detail to these ideas in Section ID.

We solve Eq. (1) using the method of Green’s functions. The difficulty in this program is that the Fokker-Planck operator has a zero mode, namely, $\rho_{\lambda(t)}^{eq}$, and is not self-adjoint. We map $\hat{\mathcal{L}}_{\lambda(t)}$ onto its corresponding Schrödinger operator, which is self-adjoint, and leverage the spectral theory of the latter to construct the Green’s function of $\hat{\mathcal{L}}_{\lambda(t)}$.

For the purposes of solving Eq. (1), the partial derivative with respect to time on the left-hand side should be interpreted as acting at fixed λ . We will show in Section ID that this produces a solution that is *consistent*, in the sense that both the left-hand side of Eq. (1) and the time derivative of the solution we find to this equation are $\mathcal{O}(\nu)$.

A. The associated Schrödinger operator and Green’s function

The Fokker-Planck operator $\hat{\mathcal{L}}_{\lambda(t)}$ is not self-adjoint. However, we can construct a self-adjoint operator $\hat{\mathcal{H}}$ from $\hat{\mathcal{L}}_{\lambda(t)}$ by making the similarity transformation

$$\hat{\mathcal{H}} = e^{\beta V_{\lambda(t)}/2} \hat{\mathcal{L}}_{\lambda(t)} e^{-\beta V_{\lambda(t)}/2}. \quad (13)$$

We have suppressed the x -dependence of the potential and the operators for notational convenience. $\hat{\mathcal{H}}$ and $\hat{\mathcal{L}}_{\lambda(t)}$ share eigenvalues, and their eigenfunctions are related by a simple transformation that we will discuss shortly. $\hat{\mathcal{H}}$ takes the form

$$\hat{\mathcal{H}}(x) = \frac{1}{\gamma\beta} \left(\frac{\beta}{2} V_{\lambda(t)}''(x) - \left(\frac{\beta}{2} V_{\lambda(t)}'(x) \right)^2 + \frac{\partial^2}{\partial x^2} \right). \quad (14)$$

It is related to the one-dimensional single-particle Schrödinger operator $\hat{\mathcal{H}}_{\mathcal{S}}$ as follows:

$$\hat{\mathcal{H}}_{\mathcal{S}} = -\frac{1}{2} \hat{\mathcal{H}}. \quad (15)$$

We have

$$\hat{\mathcal{H}}_{\mathcal{S}} = -\frac{1}{2\gamma\beta} \frac{\partial^2}{\partial x^2} + U_{\lambda(t)}(x), \quad (16)$$

where the potential $U_{\lambda(t)}$ is given by

$$U_{\lambda(t)}(x) = \frac{1}{2\gamma\beta} \left(\left(\frac{\beta}{2} V_{\lambda(t)}'(x) \right)^2 - \frac{\beta}{2} V_{\lambda(t)}''(x) \right). \quad (17)$$

The map we have described between Fokker-Planck operators and Schrödinger operators is well-known [75, 76]. We use it here to apply the spectral theory of the Schrödinger operator to driven Brownian motion. Any potential for which the spectral decomposition of the Schrödinger operator is known and possesses certain properties then becomes accessible to us for the purposes of solving Eq. (1).

As mentioned, the requirements for this approach to be viable involve conditions on the spectrum of $\hat{\mathcal{H}}_{\mathcal{S}}$. Natural boundary conditions on Eq. (1) already require $V_{\lambda(t)}(x) \rightarrow \infty$ as $x \rightarrow \pm\infty$. We additionally require $V_{\lambda(t)}$ to be such that $U_{\lambda(t)}$ is also confining. That is, $U_{\lambda(t)}(x) \rightarrow \infty$ as $x \rightarrow \pm\infty$. This is satisfied, for example, if $V_{\lambda(t)}$ is harmonic, and not satisfied if it is logarithmic in $|x|$ at large x .

We use E_n and ψ_n to denote the eigenvalues and eigenfunctions of $\hat{\mathcal{H}}_{\mathcal{S}}$. The eigenvalue equation is

$$\hat{\mathcal{H}}_{\mathcal{S}}(x)\psi_n(x) = E_n\psi_n(x), \quad n = 0, 1, \dots \quad (18)$$

For $x \in \mathbb{R}$, with the stated boundary condition on $U_{\lambda(t)}$, we are guaranteed that the spectrum of $\hat{\mathcal{H}}_{\mathcal{S}}$ is discrete, non-degenerate ($E_m \neq E_n$ for $m \neq n$), and ordered ($E_n < E_{n+1} \forall n$). The fact that a confining potential confers a discrete non-degenerate spectrum can be proved rigorously (see theorem 10.7 in [77]). From a physical point of view this is reasonable to expect because in one spatial dimension a confining potential has bounded closed orbits which are quantized to give a discrete non-degenerate spectrum. (Tunneling effects can split degenerate energy levels separated by a potential barrier.) The discreteness of the spectrum crucially enables a simple definition of the Green’s function of $\hat{\mathcal{H}}_{\mathcal{S}}$. See [78] for a proof of non-degeneracy.

It is simple to check² that $E_0 = 0$ and that the zeroth eigenfunction of $\hat{\mathcal{H}}_{\mathcal{S}}$ is given by

$$\psi_0(x) = \frac{1}{\sqrt{\mathcal{Z}}} e^{-\beta V_{\lambda(t)}(x)/2}. \quad (19)$$

Note that $\rho_{\lambda(t)}^{eq} = \psi_0^2$. The ψ_n are real, and form a complete orthonormal basis [78]:

$$\int dx \psi_n(x)\psi_m(x) = \delta_{nm}, \quad (20)$$

where δ_{nm} is the Kronecker delta. This guarantees the representation

$$\delta(x-y) = \sum_n \psi_n(x)\psi_n(y) \quad (21)$$

² Schrödinger operators customarily have nonzero zero-point energies. Here, $E_0 = 0$ due to the specific construction of $U_{\lambda(t)}$, which is “shifted” downward by a factor of $V_{\lambda(t)}''/4\gamma$ such that the usual zero-point energy of Eq. (16) is exactly removed.

for the delta function.

For $n > 0$, the eigenvalues of $\hat{\mathcal{H}}_S$ satisfy $E_n > 0$. The proof of this claim is as follows. Left-multiplying Eq. (18) by ψ_n and integrating with respect to x , we have

$$E_n = \int dx \left(\frac{1}{2\gamma\beta} \left(\frac{\partial\psi_n}{\partial x} \right)^2 + U_{\lambda(t)}\psi_n^2 \right). \quad (22)$$

Writing $\psi_n(x) = \rho_{l,n}(x)\psi_0(x)$ where $\rho_{l,n}$ is a smooth function with n nodes, this is

$$E_n = \int dx \frac{1}{2\gamma\beta} \psi_0^2 \left(\frac{\partial\rho_{l,n}}{\partial x} \right)^2 \geq 0, \quad (23)$$

with equality holding only for $n = 0$ since $\rho_{l,0} = 1$. The subscript l notation will become clear in the next section.

The function $\rho_{l,n}$ satisfies the eigenvalue equation

$$\frac{1}{\gamma} \left(-V'_{\lambda(t)}(x) + \frac{1}{\beta} \frac{\partial}{\partial x} \right) \frac{\partial\rho_{l,n}}{\partial x} = \hat{\mathcal{L}}_{\lambda(t)}^\dagger \rho_{l,n} = -2E_n \rho_{l,n}, \quad (24)$$

where $\hat{\mathcal{L}}_{\lambda(t)}^\dagger$ is the Kolmogorov backward operator.³ $\hat{\mathcal{L}}_{\lambda(t)}^\dagger$ satisfies the symmetrization relation

$$\hat{\mathcal{H}} = e^{-\beta V_{\lambda(t)}/2} \hat{\mathcal{L}}_{\lambda(t)}^\dagger e^{\beta V_{\lambda(t)}/2}. \quad (25)$$

Given the structure of the spectrum of $\hat{\mathcal{H}}_S$, its Green's function $G_S(x; y)$ is given by the following standard definition:

$$G_S(x; y) = \sum_{n \neq 0} \frac{1}{E_n} \psi_n(x) \psi_n(y). \quad (26)$$

The action of $\hat{\mathcal{H}}_S$ on G_S is

$$\hat{\mathcal{H}}_S(x) G_S(x; y) = \delta(x - y) - \psi_0(x) \psi_0(y). \quad (27)$$

Note that the right-hand side of Eq. (26) has the form of a projection. It indicates that $\hat{\mathcal{H}}_S$ is only invertible in the space of functions orthogonal to ψ_0 .

$\hat{\mathcal{H}}$ and $\hat{\mathcal{H}}_S$ share eigenfunctions ψ_n . Writing α_n for the eigenvalues of $\hat{\mathcal{H}}$, these are given by

$$\alpha_n = -2E_n, \quad (28)$$

where $\alpha_0 = 0$ and $\alpha_{n>0} < 0$. The eigenvalue equation for $\hat{\mathcal{H}}$ is

$$\hat{\mathcal{H}}(x) \psi_n(x) = \alpha_n \psi_n(x). \quad (29)$$

The Green's function $G_{\mathcal{H}}$ of $\hat{\mathcal{H}}$ is given by Eq. (26) with the replacement $E_n \rightarrow \alpha_n$:

$$G_{\mathcal{H}}(x; y) = \sum_{n \neq 0} \frac{1}{\alpha_n} \psi_n(x) \psi_n(y). \quad (30)$$

The action of $\hat{\mathcal{H}}$ on $G_{\mathcal{H}}$ is

$$\hat{\mathcal{H}}(x) G_{\mathcal{H}}(x; y) = \delta(x - y) - \psi_0(x) \psi_0(y). \quad (31)$$

³ This operator is self-adjoint under the measure $dm(x)$ defined by $dm(x) = \left(\rho_{\lambda(t)}^{eq}(x) \right)^{-1} dx$.

B. The Green's function of $\hat{\mathcal{L}}_{\lambda(t)}$

We use the discussion of the previous section to write down the eigenfunctions of $\hat{\mathcal{L}}_{\lambda(t)}$ and $\hat{\mathcal{L}}_{\lambda(t)}^\dagger$, and the Green's function of $\hat{\mathcal{L}}_{\lambda(t)}$.

From Eqs. (13), (25), and (29), we immediately have the relations

$$\hat{\mathcal{L}}(x) \rho_{r,n}(x) = \alpha_n \rho_{r,n}(x), \quad (32a)$$

$$\hat{\mathcal{L}}^\dagger(x) \rho_{l,n}(x) = \alpha_n \rho_{l,n}(x), \quad (32b)$$

where

$$\rho_{r,n}(x) = \psi_0(x) \psi_n(x), \quad (33a)$$

$$\rho_{l,n}(x) = (\psi_0(x))^{-1} \psi_n(x). \quad (33b)$$

$\rho_{r,n}$ and $\rho_{l,n}$ are called the right and left eigenfunctions, respectively. Together, they form a biorthogonal system that diagonalizes $\hat{\mathcal{L}}_{\lambda(t)}$. They are complete:

$$\delta(x - y) = \sum_n \rho_{r,n}(x) \rho_{l,n}(y), \quad (34)$$

and orthonormal:

$$\int dx \rho_{r,n}(x) \rho_{l,m}(x) = \delta_{nm}. \quad (35)$$

Eq. (34) follows from Eq. (21) and Eq. (35) follows from Eqs. (20) and (34). The zeroth right eigenfunction is the equilibrium distribution of $\hat{\mathcal{L}}_{\lambda(t)}$ corresponding to the specific value of λ at time t , and the zeroth left eigenfunction is a constant:

$$\rho_{r,0}(x) = \psi_0^2(x) = \rho_{\lambda(t)}^{eq}(x), \quad \rho_{l,0}(x) = 1. \quad (36)$$

Due to these last two facts, the right and left eigenfunctions share the simple relationship

$$\rho_{r,n} = \rho_{r,0} \rho_{l,n}. \quad (37)$$

We can now write down the Green's function $G_{\lambda(t)}$ of $\hat{\mathcal{L}}_{\lambda(t)}$. Using the representation Eq. (13) for $\hat{\mathcal{H}}$, and suppressing the subscript $\lambda(t)$ for visual clarity, from Eq. (31) we have

$$e^{\beta V(x)/2} \hat{\mathcal{L}}(x) e^{-\beta V(x)/2} G_{\mathcal{H}}(x; y) = \sum_{n \neq 0} \psi_n(x) \psi_n(y). \quad (38)$$

Left-multiplying by $e^{-\beta V(x)/2}$, right-multiplying by $e^{\beta V(y)/2}$, and using Eq. (33), we arrive at

$$\hat{\mathcal{L}}(x) e^{-\beta V(x)/2} G_{\mathcal{H}}(x; y) e^{-\beta V(y)/2} = \sum_{n \neq 0} \rho_{r,n}(x) \rho_{l,n}(y), \quad (39)$$

from which we identify $G_{\lambda(t)}$:

$$\begin{aligned} G_{\lambda(t)}(x; y) &= e^{-\beta V_{\lambda(t)}(x)/2} G_{\mathcal{H}}(x; y) e^{\beta V_{\lambda(t)}(y)/2} \\ &= \sum_{n \neq 0} \frac{1}{\alpha_n} \rho_{r,n}(x) \rho_{l,n}(y). \end{aligned} \quad (40)$$

The action of $\hat{\mathcal{L}}_{\lambda(t)}$ on $G_{\lambda(t)}$ is given by Eq. (39). Using Eqs. (34) and (36), this can be rewritten as

$$\hat{\mathcal{L}}_{\lambda(t)}(x)G_{\lambda(t)}(x; y) = \delta(x - y) - \rho_{\lambda(t)}^{eq}(x). \quad (41)$$

C. Solution to the Fokker-Planck equation

We can decompose the probability distribution in Eq. (1) into the sum of $\rho_{\lambda(t)}^{eq}(x)$ and a correction $\delta\rho(x; t)$:

$$\rho(x; t) = \rho_{\lambda(t)}^{eq}(x) + \delta\rho(x; t). \quad (42)$$

We must have $\int dx \delta\rho(x; t) = 0$ to preserve normalization. Using this representation for $\rho(x; t)$ in Eq. (1), we

obtain the dynamics of $\delta\rho(x; t)$:

$$\hat{\mathcal{L}}_{\lambda(t)}(x)\delta\rho(x; t) = \frac{\partial}{\partial t}\rho(x; t). \quad (43)$$

In order to apply the method of Green's functions, we interpret the right-hand side of Eq. (43) as a source term. From this follows the solution

$$\delta\rho(x; t) = \int dy G_{\lambda(t)}(x; y) \frac{\partial}{\partial t}\rho(y; t). \quad (44)$$

Eq. (44) contains the quantity $\delta\rho$ on both sides and can be solved iteratively. Thus we arrive at the solution

$$\rho(x; t) = \rho_{\lambda(t)}^{eq}(x) + \int dx' G_{\lambda(t)}(x; x') \frac{\partial}{\partial t}\rho_{\lambda(t)}^{eq}(x') + \int dx'' G_{\lambda(t)}(x; x'') \frac{\partial}{\partial t} \int dx' G_{\lambda(t)}(x''; x') \frac{\partial}{\partial t}\rho_{\lambda(t)}^{eq}(x') + \dots, \quad (45)$$

with the partial time derivative of $\rho_{\lambda(t)}^{eq}$ given by Eq. (12).

The form of Eq. (45) is $\rho(x; t) = \rho_{\lambda(t)}^{eq}(x) + \sum_{n=1}^{\infty} \delta\rho^{(n)}(x; t)$, where the quantities $\delta\rho^{(n)}$ are corrections to $\rho_{\lambda(t)}^{eq}$. We observe that the corrections have a recursive structure, and integrate to zero:

$$\delta\rho^{(n+1)}(x; t) = \int dx' G_{\lambda(t)}(x; x') \frac{\partial}{\partial t}\delta\rho^{(n)}(x'; t), \quad (46a)$$

$$\int dx \delta\rho^{(n+1)}(x; t) = 0, \quad n \geq 0. \quad (46b)$$

In the above, we have notated $\rho_{\lambda(t)}^{eq}(x)$ as $\delta\rho^{(0)}(x; t)$. The form of Eq. (46a) indicates that $\delta\rho^{(n+1)}(x; t)$ contains precisely $n + 1$ derivatives with respect to time. This motif will be important in Section II A, where we will see that it introduces geometric structure to the average dissipation.

D. The expansion parameter ν

Eq. (45) is a derivative expansion. In this section, we justify this claim.

There are two sources of timescales in this problem: the eigenvalues of the Fokker-Planck operator, and the time variation of the control parameters.

The eigenvalues α_n of $\hat{\mathcal{L}}_{\lambda(t)}$ have the physical units of inverse time, and their absolute values set the various natural timescales of the system. Calling these timescales τ_{α_n} , we have $\tau_{\alpha_n} = 1/|\alpha_n|$. Due to the ordering of the α_n , the τ_{α_n} are also ordered. The longest natural timescale in the system is τ_{α_1} , known as the relaxation time.

Each external parameter λ_i has a characteristic timescale τ_{λ_i} associated with its time evolution. We denote the shortest of these timescales as $\tau_{\lambda} = \min_i \tau_{\lambda_i}$.

Now let us examine the total time variation of $\rho(x; t)$:

$$\frac{d}{dt}\rho(x; t) = \frac{\partial}{\partial t}\rho(x; t) + \sum_i \dot{\lambda}_i \frac{\partial}{\partial \lambda_i}\rho(x; t). \quad (47)$$

In the first term on the right-hand side of Eq. (47), the time derivative acts at fixed λ and the time evolution is generated by the Fokker-Planck operator, i.e., by Eq. (1). The second term describes the time variation resulting from the time dependence of the external control parameters, which is not determined by the Fokker-Planck operator.⁴ Note that if we replace $\rho(x; t)$ by $\rho_{\lambda(t)}^{eq}(x)$ in Eq. (47), the first term on the right-hand side evaluates to zero, exactly consistent with Eq. (12).

In this work we consider the scenario in which the dynamics of λ is very slow compared to the dynamics generated by the Fokker-Planck operator. This means the longest natural timescale τ_{α_1} must be shorter than the shortest control timescale τ_{λ} :

$$\tau_{\lambda} \gg \tau_{\alpha_1}. \quad (48)$$

Eq. (48) naturally gives rise to a dimensionless small parameter ν , defined as follows: $\nu = \tau_{\alpha_1}/\tau_{\lambda} \ll 1$. It is the smallness of this parameter that justifies our usage

⁴ We will see in a later section that this time variation is determined by another principle, namely, the minimization of the average heat produced in the reservoir over the course of driving.

of Eq. (1) to approximate the true dynamics of $\rho(x; t)$, which is given by the left-hand side of Eq. (47).

In Eq. (45), derivatives with respect to time act (through $G_{\lambda(t)}$ and $\rho_{\lambda(t)}^{eq}$) only on $\lambda(t)$, and so we can

$$\rho(x; \tilde{t}) = \rho_{\lambda(\tilde{t})}^{eq}(x) + \nu \int dx' G_{\lambda(\tilde{t})}(x; x') \frac{\partial \rho_{\lambda(\tilde{t})}^{eq}(x')}{\partial \tilde{t}} + \nu^2 \int dx'' G_{\lambda(\tilde{t})}(x; x'') \frac{\partial}{\partial \tilde{t}} \int dx' G_{\lambda(\tilde{t})}(x''; x') \frac{\partial \rho_{\lambda(\tilde{t})}^{eq}(x')}{\partial \tilde{t}} + \dots \quad (49)$$

What is happening here is that there is a separation of timescales between the laboratory and the control space. In the latter, time must be measured in units of τ_λ . However, the overall timescale of the problem is set by τ_{α_1} , which is fixed by the shape of the potential. Therefore when expanding the density $\rho(x; t)$, it is necessary to measure τ_λ in units of τ_{α_1} . This is why time in control space is scaled by ν .

The condition Eq. (48) imposes a constraint on the dynamics of the spectrum of $\hat{\mathcal{L}}_{\lambda(t)}$, which we now discuss. In general, the α_n are functions of all the control parameters λ_i due to the fact that the spectrum of $\hat{\mathcal{L}}_{\lambda(t)}$ depends on $V_{\lambda(t)}$, which is a function of λ . The time derivative of α_n is

$$\frac{d\alpha_n}{dt} = \sum_i \dot{\lambda}_i \frac{\partial \alpha_n}{\partial \lambda_i}, \quad (50)$$

where the variation of α_n with respect to λ_i is given by the Hellmann-Feynman theorem [79]

$$\frac{\partial \alpha_n}{\partial \lambda_i} = \int dx \psi_n^2(x) \frac{\partial \hat{\mathcal{H}}(x)}{\partial \lambda_i} = -2 \int dx \psi_n^2(x) \frac{\partial U_{\lambda(t)}(x)}{\partial \lambda_i}. \quad (51)$$

For every $i \in (1, \dots, k)$, Eq. (51) is finite and fully determined by the form of the potential $U_{\lambda(t)}$. Therefore Eq. (48), which can equivalently be written as $\max_i |\dot{\lambda}_i| \ll |\alpha_1|$, together with Eq. (50), implies that the quantities $|\dot{\alpha}_n|$ must be small $\forall n$. We can explicitly check that this condition holds. Note that

$$\dot{\lambda}_i = \frac{d\tilde{t}}{dt} \frac{d\lambda}{d\tilde{t}} = \nu \frac{d\lambda}{d\tilde{t}} = \mathcal{O}(\nu), \quad (52)$$

and so $\dot{\lambda}_i$ is of order ν . Together with Eq. (52), Eq. (50) implies that $|\dot{\alpha}_n|$ is also $\mathcal{O}(\nu)$. That is, the condition Eq. (48) forces the spectrum of $\hat{\mathcal{L}}_{\lambda(t)}$ to change slowly over the course of driving.

Due to fact that derivatives with respect to time in Eq. (49) act only on $\lambda(t)$, Eq. (52) also implies that the time derivative of Eq. (49) is $\mathcal{O}(\nu)$, which is consistent with the time-dependence of Eq. (47) on λ .

The last point we must address in this timescale analysis is the fact that ν itself is a function of time. Clearly, in order for the expansion in Eq. (49) to be stable, we

rescale time in λ -space by ν by defining the variable $\tilde{t} = \nu t$. Making the reparameterization $t \rightarrow \tilde{t}$ in Eq. (45), we arrive at an expansion for $\rho(x; t)$ in the manifestly dimensionless small parameter ν :

require the time variation of ν to be small. We can check that Eq. (48) indeed enforces this. Using Eq. (52), we find that

$$\frac{d\nu}{dt} = \mathcal{O}(\nu^2). \quad (53)$$

In fact, the n^{th} time derivative of ν for $n \geq 1$ is of order ν^{n+1} .

Thus as long as the control timescale is chosen such that the slowness condition Eq. (48) is satisfied, the procedure we have presented for solving Eq. (1) is consistent, and Eq. (49) describes the time evolution of $\rho(x; t)$.

In the next section we derive a formula for the thermodynamic metric using Eq. (45). We note that all previous work [54, 62, 66] in which the thermodynamic metric has been derived it is assumed that the timescale of driving is slow with respect to the longest natural timescale of the system. The analysis just given explains why this assumption is necessary: without it, the Fokker-Planck equation is not a good descriptor of the driven Brownian system.

Lastly, we note that other authors have previously made use of eigenfunction expansions of $\rho(x; t)$ to calculate the average dissipation for driven Brownian systems with a single slowly varying control parameter [80, 81]. We will calculate average dissipation in the next section. The authors recognized that their methods must correspond to a perturbative approach to solving Eq. (1) as we have presented here, but this idea was not fully developed. In particular, the precise conditions under which the spectral structure of $\hat{\mathcal{L}}_{\lambda(t)}$ permits a perturbative expansion of $\rho(x; t)$ in ν and the relative importance of the various time scales in the problem were not studied, and τ_λ was not identified.

II. THE THERMODYNAMIC METRIC

Writing down a driving protocol for a system involves specifying a functional form for the time dependence of the control vector λ . We say a driving protocol Λ is optimal if it minimizes the functional for the average heat $\langle \Delta Q \rangle [\Lambda]$ produced in the reservoir over the course of

driving [54]:

$$\Lambda^{\text{opt}} = \arg \min_{\Lambda} \langle \Delta Q \rangle [\Lambda]. \quad (54)$$

We are interested in the scenario where the system is driven between two fixed values of λ over a fixed time period Ω . Note that we must have $\Omega \gg \tau_{\lambda}$.

The average heat transferred to the reservoir over the course of driving is given by the formula [82]

$$\begin{aligned} \langle \Delta Q \rangle [\Lambda] &= - \int_0^{\Omega} dt \int dx V'_{\lambda(t)}(x) J(x; t) \\ &= \int_0^{\Omega} dt \int dx \rho(x; t) \left(\frac{V'_{\lambda(t)}(x)}{\gamma} - \frac{V''_{\lambda(t)}(x)}{\gamma\beta} \right). \end{aligned} \quad (55)$$

In the second equality, we have replaced $J(x; t)$ with the right-hand side of Eq. (5) and integrated by parts. Note that the quantity in parentheses in Eq. (55) is, up to a constant factor $4/\beta$, the Schrödinger potential $U_{\lambda(t)}$ at inverse temperature 2β .

In the following, we calculate $\langle \Delta Q \rangle$ using the approximation

$$\rho(x; t) = \rho_{\lambda(t)}^{\text{eq}}(x) + \delta\rho^{(1)}(x; t) + \delta\rho^{(2)}(x; t), \quad (56)$$

with the corrections $\delta\rho^{(1)}(x; t)$ and $\delta\rho^{(2)}(x; t)$ given by the second and third terms on the right-hand side of Eq. (45), respectively:

$$\delta\rho^{(1)}(x; t) = \int dx' G_{\lambda(t)}(x; x') \frac{\partial}{\partial t} \rho_{\lambda(t)}^{\text{eq}}(x'), \quad (57a)$$

$$\delta\rho^{(2)}(x; t) = \int dx' G_{\lambda(t)}(x; x') \frac{\partial}{\partial t} \delta\rho^{(1)}(x'; t). \quad (57b)$$

We show that one of the contributions to $\langle \Delta Q \rangle$ coming from $\delta\rho^{(2)}$ contains an integral over a symmetric positive definite matrix in the space of control parameters \mathcal{C} , and we identify this as the thermodynamic metric for systems described by Eq. (1) with the stated conditions on $V_{\lambda(t)}$ and $U_{\lambda(t)}$. We discuss the emergence of this geometric structure in $\langle \Delta Q \rangle$ and show that it persists to all orders in the expansion of $\rho(x; t)$ (Eq. (45)).

A. Calculation of $\langle \Delta Q \rangle$ and derivation of thermodynamic metric

We drop the subscript $\lambda(t)$ for visual clarity.

It is useful to rewrite Eq. (55) in the equivalent form

$$\langle \Delta Q \rangle [\Lambda] = \frac{1}{\gamma\beta^2} \int_0^{\Omega} dt \int dx \rho(x; t) e^{\beta V(x)} \partial_x^2 e^{-\beta V(x)}. \quad (58)$$

The first contribution to $\langle \Delta Q \rangle$ from Eq. (56) corresponds to approximating $\rho(x; t)$ by $\rho^{\text{eq}}(x)$, and it evaluates to zero:

$$\langle \Delta Q \rangle_0 = \frac{1}{\gamma\beta^2} \int_0^{\Omega} dt \int dx \rho^{\text{eq}}(x) e^{\beta V(x)} \partial_x^2 e^{-\beta V(x)} = 0. \quad (59)$$

This is easily seen by using Eq. (9) to replace $e^{-\beta V(x)}$ and applying the normalization condition Eq. (8).

To calculate the next two terms of $\langle \Delta Q \rangle$, we will make use of the following identity:

$$\begin{aligned} \int dx G(x; x') e^{\beta V(x)} \partial_x^2 e^{-\beta V(x)} \\ = \gamma\beta \int dx (1 - \beta V(x)) \hat{\mathcal{L}}(x) G(x; x'). \end{aligned} \quad (60)$$

This is derived by integrating the left-hand side by parts twice, evaluating the resulting double derivative over the product $G(x; x') e^{\beta V(x)}$, and integrating by parts again. The boundary terms in Eq. (60) vanish.

The second contribution to $\langle \Delta Q \rangle$ is

$$\langle \Delta Q \rangle_1 = \frac{1}{\gamma\beta^2} \int_0^{\Omega} dt \int dx \delta\rho^{(1)}(x; t) e^{\beta V(x)} \partial_x^2 e^{-\beta V(x)}. \quad (61)$$

Replacing $\delta\rho^{(1)}$ with Eq. (57a), applying Eq. (60) and then Eq. (41), we have

$$\begin{aligned} \langle \Delta Q \rangle_1 &= \frac{1}{\beta} \int_0^{\Omega} dt \int dx' \partial_t \rho^{\text{eq}}(x') \int dx \\ &\quad (1 - \beta V(x)) \hat{\mathcal{L}}(x) G(x; x') \\ &= -\frac{1}{\beta} \int_0^{\Omega} dt \int dx' \partial_t \rho^{\text{eq}}(x') \beta V(x') \\ &\quad + \frac{1}{\beta} \int_0^{\Omega} dt \int dx' \partial_t \rho^{\text{eq}}(x') \int dx \beta V(x) \rho^{\text{eq}}(x). \end{aligned} \quad (62)$$

The second term in Eq. (62) is zero due to Eq. (8), which implies $\partial_t \int dx \rho^{\text{eq}}(x) = \partial_t 1 = 0$. The first term can be written in terms of the difference in entropy ΔS^{eq} between $\rho_{\lambda(0)}^{\text{eq}}(x)$ and $\rho_{\lambda(\Omega)}^{\text{eq}}(x)$. We recall the definition of the entropy S^{eq} of an equilibrium distribution:

$$S_{\lambda(t)}^{\text{eq}} = - \int dx \rho_{\lambda(t)}^{\text{eq}}(x) \log \rho_{\lambda(t)}^{\text{eq}}(x), \quad (63)$$

the time derivative of which is $\int dx \beta V(x) \partial_t \rho^{\text{eq}}(x)$. Thus we have

$$\langle \Delta Q \rangle_1 = -\frac{1}{\beta} \int_0^{\Omega} dt \partial_t S_{\lambda(t)}^{\text{eq}} = -\frac{1}{\beta} \Delta S^{\text{eq}}. \quad (64)$$

If we truncate the approximation of $\rho(x; t)$ at $\delta\rho^{(1)}(x; t)$, we reproduce the quasistatic Clausius equality for diffusive systems [28, 67, 83]:

$$\beta \langle \Delta Q \rangle [\Lambda] + \Delta S^{\text{eq}} = 0. \quad (65)$$

The third contribution to $\langle \Delta Q \rangle$ is

$$\langle \Delta Q \rangle_2 = \frac{1}{\gamma\beta^2} \int_0^{\Omega} dt \int dx \delta\rho^{(2)}(x; t) e^{\beta V(x)} \partial_x^2 e^{-\beta V(x)}. \quad (66)$$

Similar to the calculation of $\langle \Delta Q \rangle_1$, we use Eq. (57b) to replace $\delta\rho^{(2)}$, apply Eq. (60), and then Eq. (41). This gives

$$\begin{aligned} \langle \Delta Q \rangle_2 = & -\frac{1}{\beta} \int_0^\Omega dt \left(\int dx'' \partial_t \delta\rho^{(1)}(x''; t) \beta V(x'') \right. \\ & \left. - \int dx'' \partial_t \delta\rho^{(1)}(x''; t) \int dx \rho^{eq}(x) \beta V(x) \right). \end{aligned} \quad (67)$$

The second term in Eq. (67) is zero due to Eq. (46b). Writing $-\beta V(x'') = \log \rho^{eq}(x'') + \log Z$, the first term can be rewritten as

$$\begin{aligned} \langle \Delta Q \rangle_2 = & -\frac{1}{\beta} \int_0^\Omega dt \int dx'' \delta\rho^{(1)}(x''; t) \partial_t \log \rho^{eq}(x'') \\ & - \frac{1}{\beta} \int_0^\Omega dt (\partial_t \log Z) \int dx'' \delta\rho^{(1)}(x''; t) \\ & - \int_0^\Omega dt \int dx'' \partial_t \left(\delta\rho^{(1)}(x''; t) V(x'') \right). \end{aligned} \quad (68)$$

We evaluate the three terms in Eq. (68) in reverse order.

The third term is the integral of a total time derivative, and depends only on the initial and final values of λ and $\dot{\lambda}$. It can be written as

$$A(\lambda(\Omega), \dot{\lambda}(\Omega)) - A(\lambda(0), \dot{\lambda}(0)) \equiv \Delta A, \quad (69)$$

where the function A is given by

$$A = - \sum_i \dot{\lambda}_i \int \int dx dx' V_{\lambda(t)}(x) G_{\lambda(t)}(x; x') \frac{\partial \rho_{\lambda(t)}^{eq}}{\partial \lambda_i}(x'). \quad (70)$$

The second term in Eq. (68) evaluates to zero due to Eq. (46b).

Lastly, the integral with respect to x'' in the first term in Eq. (68) can be rewritten as a quadratic form:

$$- \int dx'' \delta\rho^{(1)}(x''; t) \partial_t \log \rho_{\lambda(t)}^{eq}(x'') = \dot{\lambda}^\top \zeta \dot{\lambda}, \quad (71)$$

where the elements of the matrix $\zeta(\lambda)$ are given by the formula

$$\zeta_{ij} = - \int dx' dx'' \rho_{\lambda(t)}^{eq}(x'') \left(\frac{\partial}{\partial \lambda_i} \log \rho_{\lambda(t)}^{eq}(x'') \right) G_{\lambda(t)}(x'; x'') \left(\frac{\partial}{\partial \lambda_j} \log \rho_{\lambda(t)}^{eq}(x') \right). \quad (72)$$

$\zeta(\lambda)$ is clearly symmetric. We now prove that it is also positive definite. In terms of ψ_0 and G_S , Eq. (72) takes the following simple form:

$$\zeta_{ij} = 2 \int dx' dx'' \frac{\partial \psi_0(x'')}{\partial \lambda_i} G_S(x'; x'') \frac{\partial \psi_0(x')}{\partial \lambda_j}. \quad (73)$$

Consider the quadratic form $\dot{\lambda}^\top \zeta \dot{\lambda}$. Using Eqs. (26) and (28) in Eq. (73), we have

$$\dot{\lambda}^\top \zeta \dot{\lambda} = - \sum_{n \neq 0} \frac{1}{\alpha_n} \left(2 \sum_{i=1}^k \int dx \dot{\lambda}_i \psi_n(x) \frac{\partial \psi_0(x)}{\partial \lambda_i} \right)^2 > 0. \quad (74)$$

The last inequality is due to the fact that $-\alpha_{n \neq 0} > 0$. Thus, the eigenvalues of $\zeta(\lambda)$ are positive. $\zeta(\lambda)$ therefore induces a Riemannian metric on the space \mathcal{C} , and can be identified as the thermodynamic metric [54] for driven Brownian systems described by Eq. (1) with confining Schrödinger potentials. We note that Eq. (72) contains all the time scales in the problem, since $G_{\lambda(t)}$ contains a sum over all the eigenvalues of $\hat{\mathcal{L}}_{\lambda(t)}$.

It becomes necessary now to distinguish between covariant and contravariant quantities; therefore from this point onward in the discussion we will write control variables with raised indices, as λ^i .

We can explicitly check that $\zeta(\lambda)$ transforms correctly under a change of coordinates. Using the representation

Eq. (73), it is simple to see that under a continuous, invertible transformation (diffeomorphism) $\lambda \rightarrow \phi(\lambda)$, the elements of the new metric $\tilde{\zeta}(\phi)$ in ϕ -space are given by

$$\tilde{\zeta}_{kl} = \sum_{i,j} \zeta_{ij} \frac{\partial \lambda^i}{\partial \phi^k} \frac{\partial \lambda^j}{\partial \phi^l}. \quad (75)$$

This transformation law for the metric holds due to the two partial derivatives with respect to λ^i and λ^j in Eq. (73), which in turn derive from the two partial derivatives with respect to time in $\delta\rho^{(2)}(x; t)$. Therefore, even though Eq. (55) has no geometric structure in general that we can discover, the specific form of $\delta\rho^{(2)}(x; t)$ introduces geometric structure in the average dissipation. We will see shortly that this emergent structure persists in Eq. (55) to all orders in ν .

We emphasize that Eq. (72) is distinct from the formula for a thermodynamic metric given in Eq. 12 in [54], which was the first work to derive a thermodynamic metric for mesoscopic systems with time-varying relaxation times. As mentioned previously, this formula was derived in the linear response regime with a slow driving assumption. Evaluating it involves computing an integral with respect to time over the linear response function, which is the average two-point time correlation function of deviations of the conjugate forces from their equilibrium values.

Gathering the contributions from Eqs. (59), (64), (69) and (71), we have the following formula for the average

heat up to terms of order ν^2 in Eq. (45):

$$\beta \langle \Delta Q \rangle [\mathbf{\Lambda}] = 0 - \Delta S^{eq} + \int_0^\Omega dt \dot{\lambda}(t) \zeta(\lambda) \dot{\lambda}(t)^\top + \beta \Delta A. \quad (76)$$

To minimize Eq. (76) over protocols, we can define the action

$$S[\lambda(t)] = \beta \Delta A + 2 \int_0^\Omega dt \frac{1}{2} \dot{\lambda}(t) \zeta(\lambda) \dot{\lambda}(t)^\top. \quad (77)$$

The equations of motion follow by setting the variation $\frac{\delta S}{\delta \lambda^i}$ of S with respect to λ^i to zero, subject to the constraints $\delta \lambda^i(0) = \delta \lambda^i(\Omega) = 0 \forall i$. These constraints imply $\delta A(0) = \delta A(\Omega) = 0$, and therefore only the second term in Eq. (77) contributes to the equations of motion. These are the Euler-Lagrange equations of the Lagrangian $L = \frac{1}{2} \dot{\lambda}^\top \zeta \dot{\lambda}$:

$$\frac{d}{dt} \left(2 \sum_j \zeta_{pj} \dot{\lambda}^j \right) = \sum_{i,j} \dot{\lambda}^i \frac{\partial \zeta_{ij}}{\partial \lambda^p} \dot{\lambda}^j, \quad p \in (1, \dots, k). \quad (78)$$

Opening out the time derivative on the left-hand side of Eq. (78), a straightforward calculation shows that it is equivalent to

$$\ddot{\lambda}^p + \sum_{i,j} \Gamma_{ij}^p \dot{\lambda}^i \dot{\lambda}^j = 0, \quad p \in (1, \dots, k), \quad (79)$$

where Γ_{ij}^p is the Christoffel symbol of the second kind:

$$\Gamma_{ij}^p = \frac{1}{2} \sum_m \zeta^{pm} \left(\frac{\partial \zeta_{mi}}{\partial x^j} + \frac{\partial \zeta_{mj}}{\partial x^i} - \frac{\partial \zeta_{ij}}{\partial x^m} \right). \quad (80)$$

Eq. (79) are also the equations of motion of the Lagrangian $\tilde{L} = \sqrt{\dot{\lambda} \zeta \dot{\lambda}^\top}$ in the arc-length parameterization [84]. In other words, these are geodesic equations of the control parameter space \mathcal{C} .

Due to the spectral properties of $\hat{\mathcal{H}}_S$, Eq. (74) also indicates that the quadratic form $\dot{\lambda}^\top \zeta \dot{\lambda}$ is always finite. Therefore, if $V_{\lambda(t)}$ is such that $U_{\lambda(t)}$ is confining, and the perturbative expansion Eq. (45) holds over the time period Ω , we are guaranteed that $\zeta(\lambda)$ exists and is well-defined over the course of driving. Then, up to terms of order ν^2 in Eq. (45), optimal protocols $\mathbf{\Lambda}^{\text{opt}}$ are geodesics in \mathcal{C} with respect to the length measure defined by $\zeta(\lambda)$.

We note that in a specific optimal problem, the invariance of the geodesic equations to reparameterizations of \mathcal{C} is broken by the boundary conditions, in which the *identities* of the control parameters, along with their initial and final values, are specified. For example, in the next section, we consider the harmonic potential $V_{\lambda(t)}(x) = \kappa x^2/2 + Ex$ with time-dependent electric field E and spring constant κ . The choice of these two control parameters breaks the diffeomorphism invariance of Eq. (79) for this problem instance.

The diffeomorphism invariance of the geodesic equations suggests that it is appropriate to write $V_{\lambda(t)}$ in such a way that all components of λ have matching units. One way to do this is to introduce a fixed length scale ℓ and rescale x as $x \rightarrow x/\ell$. For example, in the harmonic potential defined previously, the control parameters κ and E have different units. Rescaling x by ℓ , we can instead write $V_{\lambda(t)}(x/\ell) = (\ell^2 \kappa)(x/\ell)^2/2 + (\ell E)x/\ell$. The new control vector is $\lambda = (\ell^2 \kappa, \ell E)$, both components of which have units of energy. Applying diffeomorphisms that may scramble the two control parameters now makes sense. We can choose ℓ to be such that $\beta \ell E = 1$, or, equivalently, such that $\beta \ell^2 \kappa = 1$.

We end this section with a note on higher-order terms in the average heat production. By calculations analogous to those for $\langle \Delta Q \rangle_2$, it is straightforward to establish that for any $w \geq 2$, the contribution to Eq. 55 from $\delta \rho^{(w)}(x; t)$ takes the form

$$\beta \langle \Delta Q \rangle_w = \beta \Delta A_w + \int_0^\Omega dt \sum_{i_1, \dots, i_w} \dot{\lambda}^{i_1} \dots \dot{\lambda}^{i_w} \Xi_{i_1 \dots i_w}^{(w)}, \quad (81)$$

where A_w is a term that depends only on the values of λ and $\dot{\lambda}$ at times 0 and Ω , and $\Xi^{(w)}$ is an object with w indices. (In the notation of Eq. (81), the quantity A defined in Eq. (70) is A_2 , and the thermodynamic metric ζ is $\Xi^{(2)}$.) Due to the fact that $\delta \rho^{(w)}(x; t)$ contains exactly w derivatives with respect to time, under a reparameterization $\lambda \rightarrow \phi(\lambda)$, $\Xi^{(w)}$ obeys the transformation law $\tilde{\Xi}_{j_1 \dots j_w}^{(w)} = \sum_{i_1, \dots, i_w} \Xi_{i_1 \dots i_w}^{(w)} \partial_{\phi^{j_1}} \lambda^{i_1} \dots \partial_{\phi^{j_w}} \lambda^{i_w}$, and is therefore a rank- w tensor. Thus, if the conditions for the existence of Eq. (45) are met, geometric structure is emergent in Eq. (55) at all orders in ν .

Up to terms of order ν^k in $\rho(x; t)$, the Lagrangian of the optimal control problem is given by $L^{(w)} = \sum_{w=2}^k \sum_{i_1, \dots, i_w} \dot{\lambda}^{i_1} \dots \dot{\lambda}^{i_w} \Xi_{i_1 \dots i_w}^{(w)}$; like Eq. (70), the ΔA_w for $w \geq 3$ do not participate in the Euler-Lagrange equations for $\mathbf{\Lambda}^{\text{opt}}$. Predictions of optimal protocols can be refined beyond the solutions of Eq. (79) by including terms of order $w = 3$ and higher in $L^{(w)}$. The $\Xi^{(w)}$ —and therefore $L^{(w)}$ —can easily be expressed in terms of $\rho_{\lambda(t)}^{eq}$ and $G_{\lambda(t)}$. For example, the elements of $\Xi^{(3)}$ are given by

$$\Xi_{ijk}^{(3)} = - \int dx dx' \frac{\partial \log \rho_{\lambda(t)}^{eq}(x)}{\partial \lambda^i} G_{\lambda(t)}(x; x') \frac{\partial}{\partial \lambda^j} \left(\int dx'' G_{\lambda(t)}(x'; x'') \rho_{\lambda(t)}^{eq}(x'') \frac{\partial \log \rho_{\lambda(t)}^{eq}(x'')}{\partial \lambda^k} \right). \quad (82)$$

We leave the study of possible interpretations of $\Xi^{(w)}$ for $w \geq 3$ and the development of solutions of the Euler-Lagrange equations of $L^{(w)}$ for $w \geq 3$ to future work.

B. Relationship of ζ to previously proposed formula for a thermodynamic metric

In [63], the authors propose an approximate formula for a thermodynamic metric involving only $\rho_{\lambda(t)}^{eq}$. Call this metric χ . Using the notation $\Pi_{\lambda(t)}^{eq}$ to refer to the cumulative distribution function

$$\Pi_{\lambda(t)}^{eq}(x) = \int_{-\infty}^x dx' \rho_{\lambda(t)}^{eq}(x'), \quad (83)$$

the elements of χ are given by

$$\chi_{ij} = \int dx \frac{\gamma\beta}{\rho_{\lambda(t)}^{eq}(x)} \left(\frac{\partial}{\partial\lambda_i} \Pi_{\lambda(t)}^{eq}(x) \right) \left(\frac{\partial}{\partial\lambda_j} \Pi_{\lambda(t)}^{eq}(x) \right). \quad (84)$$

The advantage of this formula is that it is entirely local in x , depending only on $\rho_{\lambda(t)}^{eq}$ and not on $G_{\lambda(t)}$, which is nonlocal in x and contains all the natural timescales of the system. In the case of a harmonic potential, it can be checked by explicit calculation that ζ and χ are identical. For more general potentials, we show that in a certain limit, Eq. (72) can be written as Eq. (84) plus correction terms.

For this part of the discussion only, we restrict ourselves to potentials of the form

$$V_{\lambda(t)}(x) = g(x) + \sum_{i=1}^m a_i x^i, \quad (85)$$

where $m \geq 4$ is even, and $a_m > 0$. The a_i are functions of $\lambda(t)$. $g(x)$ is any function of x and λ that is finite in the limit $|x| \rightarrow \infty$. At large x , this potential is dominated by the x^m term. In fact, it contains a natural length scale, x_0 , defined as the value of x at which the ratio $V_{\lambda(t)}(x_0)/a_m x_0^m$ is of order 1. For such a potential, it is the case that

$$\lim_{|x| \rightarrow \infty} e^{\beta V_{\lambda(t)}(x)/2} \frac{\partial}{\partial\lambda_i} \Pi_{\lambda(t)}^{eq}(x) = 0, \quad (86)$$

and integrals over x of the quantity in the limit converge. This can be established using the asymptotic expansion of $1 - \Pi_{\lambda(t)}^{eq}(x_0) \sim \int_{x_0}^{\infty} dy e^{-\beta a_m y^m}$:

$$\int_{x_0}^{\infty} dy e^{-\beta a_m y^m} \approx \frac{e^{-\beta a_m x_0^m}}{x_0^{m-1}} \left(1 + \mathcal{O}\left(\frac{1}{x_0}\right) \right). \quad (87)$$

The first term in the expansion can be verified by differentiating both sides of Eq.(87) with respect to x_0 .

In the following, we drop the subscript $\lambda(t)$ for brevity. We use the notation $\zeta_{ij}^{x_0}$ and $\chi_{ij}^{x_0}$ to denote Eqs. (72) and (84) with all integrals evaluated between $-x_0$ and x_0 .

Using $\partial_x \Pi^{eq}(x) = \rho^{eq}(x)$, Eq. (72) can be rewritten as

$$\zeta_{ij}^{x_0} = - \int_{-x_0}^{x_0} dx' dx'' \frac{\partial^2 \Pi^{eq}(x'')}{\partial\lambda_i \partial x''} \frac{G(x'; x'')}{\rho_{\lambda(t)}^{eq}(x')} \frac{\partial^2 \Pi^{eq}(x')}{\partial\lambda_j \partial x'}. \quad (88)$$

Integrating by parts twice, this is

$$\zeta_{ij}^{x_0} = - \int_{-x_0}^{x_0} dx' dx'' \frac{\partial \Pi^{eq}(x'')}{\partial\lambda_i} \Theta(x', x'') \frac{\partial \Pi^{eq}(x')}{\partial\lambda_j}, \quad (89)$$

where

$$\Theta(x', x'') = \frac{\partial^2}{\partial x' \partial x''} \frac{G(x'; x'')}{\rho^{eq}(x')}. \quad (90)$$

For potentials of the form Eq. (85), the boundary terms in Eq. (89) are exponentially suppressed in x_0 , that is, they are of order $e^{-\beta a_m x_0^m}$. Opening out the derivatives in Θ , we find that it satisfies the differential equation

$$\frac{1}{\gamma\beta} \frac{\partial}{\partial x'} \rho^{eq}(x') \Theta(x', x'') = \hat{\mathcal{L}}(x') \frac{\partial G(x'; x'')}{\partial x''}. \quad (91)$$

Applying Eq. (41), this is

$$\frac{\partial}{\partial x'} (\rho^{eq}(x') \Theta(x', x'')) + \gamma\beta \delta(x' - x'') = 0. \quad (92)$$

The solution to this differential equation is a family of functions $h_{x'}(x'')$ parameterized by x' . We choose to work with h evaluated at $x' = x_0$, henceforth notated simply as $h(x'')$:

$$h(x'') = \rho^{eq}(x_0) \Theta(x_0, x'') + \gamma\beta \delta(x_0 - x''). \quad (93)$$

In terms of h , Eq. (90) can be written as

$$\Theta(x', x'') = \frac{1}{\rho^{eq}(x')} (-\beta\gamma \delta(x' - x'') + h(x'')). \quad (94)$$

Substituting this in Eq. (89), we find

$$\zeta_{ij}^{x_0} = \chi_{ij}^{x_0} + \Delta_{ij}^{x_0}, \quad (95)$$

where

$$\Delta_{ij}^{x_0} = - \int_{-x_0}^{x_0} dx' dx'' \frac{\beta\gamma}{\rho^{eq}(x')} \frac{\partial \Pi^{eq}(x')}{\partial\lambda_j} h(x'') \frac{\partial \Pi^{eq}(x'')}{\partial\lambda_i}. \quad (96)$$

Once again using the asymptotic expansion Eq. (87), it can be shown that $\Delta_{ij}^{x_0}$ is of order $e^{-\beta a_m x_0^m}$. We note that it is necessary to evaluate the function $h_{x'}$ at $x' \geq x_0$ to arrive at this conclusion, otherwise it is not clear how to estimate the size of $\Delta_{ij}^{x_0}$. Therefore we finally arrive at

$$\zeta_{ij}^{x_0} = \chi_{ij}^{x_0} + \mathcal{O}(e^{-\beta a_m x_0^m}). \quad (97)$$

From Eq. (97), we see that in the limit $|x_0| \rightarrow \infty$, all correction terms go to zero, and we have $\zeta_{ij} - \chi_{ij} \rightarrow 0$. However, this limit is not physically valid—it is simple to check that as $x_0 \rightarrow \infty$, Eq.(1) is trivialized to $0 = 0$. Thus, for general potentials, we cannot expect the two formulae ζ and χ to be equivalent. As previously mentioned, the quadratic potential is an interesting exception

for which it can be explicitly checked that both ζ and χ evaluate to the same quantity.

The calculation leading to Eq. (95) is a proof of the formula Eq. (84) for polynomial potentials. In [63], the class of potentials for which Eq. (84) converges was not established. We further note that we expect a relation similar to Eq. (97) to hold for potentials that grow faster than Eq. (85); for example, $V(x) = e^{b|x|}$ with $b > 0$. The specifics of the asymptotic analysis proving this point will differ from what is presented here.

III. THE HARMONIC OSCILLATOR IN AN ELECTRIC FIELD

We calculate ζ for a one-dimensional system of charge q in a harmonic potential with time-dependent spring constant $\kappa(t)$ and subject to an external electric field $E(t)$. The control vector is $\lambda(t) = (\kappa(t), E(t))$, where $\kappa > 0$ and $E \in \mathbb{R}$. The potential is

$$V_{\lambda(t)}(x) = \frac{1}{2}\kappa x^2 - qEx = \frac{1}{2}\kappa(x - \theta)^2 - \frac{\kappa}{2}\theta^2. \quad (98)$$

In the second equality we have defined the new variable $\theta = E/\kappa$. The electric field can be interpreted as an offset in the center of the harmonic trap.

$$\begin{aligned} \zeta_{\kappa\kappa} = & - \int dx \int dy \sqrt{\frac{\beta\kappa}{2\pi}} e^{-\frac{1}{2}\beta\kappa(y-\theta)^2} \left(\frac{1}{2\kappa} - \frac{\beta(x-\theta)^2}{2} \right) \left(\frac{1}{2\kappa} - \frac{\beta(y-\theta)^2}{2} \right) \\ & \sum_{n \neq 0} -\frac{\gamma}{\kappa n} \frac{1}{2^n n!} \sqrt{\frac{\beta\kappa}{2\pi}} e^{-\frac{1}{2}\beta\kappa(x-\theta)^2} H_n \left(\sqrt{\frac{\beta\kappa}{2}}(x-\theta) \right) H_n \left(\sqrt{\frac{\beta\kappa}{2}}(y-\theta) \right). \end{aligned} \quad (102)$$

Transforming to the variables $x' = \sqrt{\beta\kappa/2}(x - \theta)$, $y' = \sqrt{\beta\kappa/2}(y - \theta)$, and using $\frac{1}{2} - x'^2 = -\frac{1}{4}H_2(x')$, this is

$$\zeta_{\kappa\kappa} = \frac{1}{\pi} \frac{\gamma}{\kappa^3} \frac{1}{16} \sum_{n \neq 0} \frac{1}{n 2^n n!} \left(\int dx' e^{-x'^2} H_2(x') H_n(x') \right)^2. \quad (103)$$

Applying the orthogonality property

$$\int dx' e^{-x'^2} H_m(x') H_n(x') = \delta_{mn} 2^n n! \sqrt{\pi}, \quad (104)$$

we have

$$\zeta_{\kappa\kappa} = \frac{\gamma}{4\kappa^3}. \quad (105)$$

Similarly, the elements $\zeta_{\theta\kappa}$ and $\zeta_{\kappa\theta}$ are proportional to the product

$$\int dx' e^{-x'^2} \frac{1}{4} H_2(x') H_n(x') \int dy' e^{-y'^2} \frac{1}{2} H_1(y') H_n(y'), \quad (106)$$

The Fokker-Planck operator for this system is

$$\hat{\mathcal{L}}_{\lambda(t)}(x) = \frac{1}{\gamma} \left[\kappa(t) + \kappa(t)(x - \theta(t)) \frac{\partial}{\partial x} + \frac{1}{\beta} \frac{\partial^2}{\partial x^2} \right]. \quad (99)$$

The eigenfunctions ψ_n of the corresponding Schrödinger operator are given by the Hermite functions [74]. Using H_n to denote the n^{th} Hermite polynomial, the right and left eigenfunctions are

$$\rho_{r,n}(x) = \frac{1}{\sqrt{2^n n!}} \sqrt{\frac{\beta\kappa}{2\pi}} e^{-\frac{1}{2}\beta\kappa(x-\theta)^2} H_n \left(\sqrt{\frac{\beta\kappa}{2}}(x-\theta) \right), \quad (100a)$$

$$\rho_{l,n}(x) = \frac{1}{\sqrt{2^n n!}} H_n \left(\sqrt{\frac{\beta\kappa}{2}}(x-\theta) \right). \quad (100b)$$

The corresponding eigenvalues are $-\kappa n/\gamma$. The equilibrium distribution at any given time t is a normalized Gaussian distribution with mean θ and variance $1/\beta\kappa$:

$$\rho_{\lambda(t)}^{eq}(x) = \sqrt{\frac{\beta\kappa}{2\pi}} e^{-\frac{1}{2}\beta\kappa(x-\theta)^2}. \quad (101)$$

We proceed to calculate the four elements, beginning with $\zeta_{11} = \zeta_{\kappa\kappa}$:

which evaluates to zero for all n . Finally

$$\zeta_{\theta\theta} = \frac{2\beta\gamma}{\pi} \sum_{n \neq 0} \frac{1}{n 2^n n!} \left(\int dx' \frac{1}{2} H_1(x') H_n(x') \right)^2 = \beta\gamma. \quad (107)$$

Gathering elements, we have

$$\zeta = \gamma \begin{bmatrix} (4\kappa^3)^{-1} & 0 \\ 0 & \beta \end{bmatrix}. \quad (108)$$

As mentioned in the previous section, the same result is obtained by evaluating Eq. (84) for this system. Eq. (108) is also identical to the result obtained by evaluating the formula for a thermodynamic metric given in [54] for a harmonic potential with time-varying spring constant and trap center.

We can now calculate optimal protocols for the harmonic oscillator. For the metric Eq. (108), Eq. (71) takes the form

$$\int_0^\Omega dt \gamma \left(\frac{\dot{\kappa}^2}{4\kappa^3} + \beta \dot{\theta}^2 \right) = \int_0^\Omega dt \gamma \left(\dot{\mu}^2 + \beta \dot{\theta}^2 \right). \quad (109)$$

In the second equality above we have made the change of variables $\mu = \sqrt{\kappa}$. This is a diffeomorphism for $\kappa > 0$. From Eq. (109) it is clear that the potential Eq. (98) gives rise to a flat geometry in (μ, θ) -space. However, the protocols have a nontrivial structure in the physical control parameter space (κ, θ) due to the existence of the forbidden region $\kappa \leq 0$. The Euler-Lagrange equations corresponding to Eq. (109) are $\ddot{\mu} = \ddot{\theta} = 0$. The solutions are straight lines in the (μ, θ) plane. Given initial and final values of the physical parameters— κ_Ω and κ_0 , and similarly for θ —the protocol that minimizes Eq. (71) is

$$\theta^{\text{opt}}(t) = \frac{\theta_\Omega - \theta_0}{\Omega} t + \theta_0 \quad (110a)$$

$$\kappa^{\text{opt}}(t) = \left(\frac{\sqrt{\kappa_\Omega} - \sqrt{\kappa_0}}{\Omega} t + \sqrt{\kappa_0} \right)^2. \quad (110b)$$

The optimal protocol demands a constant rate of change for θ and $\sqrt{\kappa}$.

In this example, we can explicitly check the consistency conditions of Section I D. To do so, it is convenient to rescale the optimal control problem so that all control parameters are dimensionless. This is easily done by first rescaling $x \rightarrow x/\ell$ where the length measure ℓ is defined by $\beta \ell^2 \kappa = 1 = E \ell \beta$, as discussed at the end of Section II A, and then multiplying the potential (Eq. (98)) by β . These rescalings do not disturb the optimal control problem. We have the following optimal protocols for the dimensionless control parameters $(\tilde{\mu}, \tilde{\theta}) = (\sqrt{\beta \kappa \ell^2}, E/\kappa \ell)$:

$$\tilde{\theta}^{\text{opt}}(t) = \frac{\tilde{\theta}_\Omega - \tilde{\theta}_0}{\Omega} t + \tilde{\theta}_0 \quad (111a)$$

$$\tilde{\mu}^{\text{opt}}(t) = \frac{\tilde{\mu}_\Omega - \tilde{\mu}_0}{\Omega} t + \tilde{\mu}_0. \quad (111b)$$

These are of precisely the same form as Eq. (110). In terms of the dimensionless control parameters, the eigenvalues of the Fokker-Planck operator for the harmonic oscillator are given by $-\tilde{\mu}^2 n / \beta \ell^2 \gamma$. Therefore, under the optimal protocol, the relaxation time of the Brownian system is $\tau_{\alpha_1} = \beta \ell^2 \gamma / (\tilde{\mu}^{\text{opt}})^2$.

Without loss of generality, we can assume $\dot{\tilde{\mu}}^{\text{opt}} \geq \dot{\tilde{\theta}}^{\text{opt}}$. For ease of notation in what follows, we write the difference $\tilde{\mu}_\Omega - \tilde{\mu}_0$ as $\Delta \tilde{\mu}$. The longest driving timescale set by the optimal protocol is then given by $\tau_\lambda = 1/\dot{\tilde{\mu}}^{\text{opt}} = \Omega/\Delta \tilde{\mu}$.

Therefore we have

$$\nu = \frac{\tau_{\alpha_1}}{\tau_\lambda} = \frac{\beta \ell^2 \gamma}{(\tilde{\mu}^{\text{opt}})^2} \frac{\Delta \tilde{\mu}}{\Omega} = \mathcal{O}\left(\frac{1}{\Omega}\right). \quad (112)$$

ν can be made small by choosing Ω , the duration of the protocol, to be sufficiently long.

From Eq. (111), we see that $\dot{\tilde{\mu}}^{\text{opt}}$ is of order $1/\Omega$. The rate of change of the spectrum of the Fokker-Planck operator, too, goes as $1/\Omega$. To see this, note that $|\dot{\alpha}_1| = 1/\tau_{\alpha_1}$. Differentiating this with respect to time,

we find $|\dot{\alpha}_1| = 2\dot{\tilde{\mu}}^{\text{opt}} \tilde{\mu}^{\text{opt}} / \beta \ell^2 \gamma = \mathcal{O}(1/\Omega)$ since $\dot{\tilde{\mu}}^{\text{opt}}$ is $\mathcal{O}(1/\Omega)$. Thus, both the control parameters and the spectrum of the Fokker-Planck operator vary appreciably only on the timescale of the control parameters, and are roughly constant on the timescale of the system if Ω is chosen to be large.

Lastly, differentiating Eq. (112) with respect to time, we find that $\dot{\nu}$ is of order $1/\Omega^2$, i.e., $\mathcal{O}(\nu^2)$, and is therefore suppressed on the control timescale.

IV. SUMMARY AND FUTURE WORK

We have developed a precise perturbative solution to Eq. (1) and used it to calculate the heat generated in the environment when the external parameters of a small stochastic system are varied in time. In so doing, we derived a new formula for the thermodynamic metric and all correction terms at the same order in the perturbation theory.

Both [54] and [63] propose formulae for thermodynamic metrics but do not establish the class of potentials for which those formulae are valid. The formula we have derived, Eq. (72), holds for potentials $V_{\lambda(t)}$ such that both $V_{\lambda(t)}$ and the associated Schrödinger potential $U_{\lambda(t)}$ are confining. We have shown that for a subset of such potentials, namely, those in Eq. (85), the formula Eq. (84) of [63] is approximately valid.

We found that the expansion in ν has an emergent local diffeomorphism symmetry not present in the original formula, Eq. (55), for average heat production. Every term of this expansion transforms as a tensor of this diffeomorphism symmetry. Restricting to the symmetric 2-tensor (metric) in the expansion, we explicitly worked out the equations for an optimal protocol. These equations of motion describe geodesics in the space of control parameters.

In future work, it would be interesting to study the physical interpretation of the tensors $\Xi^{(w)}$ for $w \geq 3$, and to develop methods of calculating Λ^{opt} when these tensors are retained in the Lagrangian. Additional directions for future research include extending the perturbation theory to underdamped systems, and to higher spatial dimensions. For the latter, much of the formalism developed here will be applicable but it will be necessary to study the spectral properties of the Schrödinger operator in higher dimensions.

In this paper we derived a formula for the thermodynamic metric corresponding to the confining potential $U_{\lambda(t)}$. This invites the following question: given a metric, what is the class of potentials that give rise to it? This may be especially interesting and tractable in the case of two-dimensional Riemannian geometries.

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