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Best-fit quasi-equilibrium ensembles: a general approach to statistical closure of underresolved Hamiltonian dynamics

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Abstract

A new method of deriving reduced models of Hamiltonian dynamical systems is developed using techniques from optimization and statistical estimation. Given a set of resolved variables that define a model reduction, the quasi-equilibrium ensembles associated with the resolved variables are employed as a family of trial probability densities on phase space. The residual that results from submitting these trial densities to the Liouville equation is quantified by an ensemble-averaged cost function related to the information loss rate of the reduction. From an initial nonequilibrium state, the statistical state of the system at any later time is estimated by minimizing the time integral of the cost function over paths of trial densities. Statistical closure of the underresolved dynamics is obtained at the level of the value function, which equals the optimal cost of reduction with respect to the resolved variables, and the evolution of the estimated statistical state is deduced from the Hamilton-Jacobi equation satisfied by the value function. In the near-equilibrium regime, or under a local quadratic approximation in the far-from-equilibrium regime, this best-fit closure is governed by a differential equation for the estimated state vector coupled to a Riccati differential equation for the Hessian matrix of the value function. Since memory effects are not explicitly included in the trial densities, a single adjustable parameter is introduced into the cost function to capture a time-scale ratio between resolved and unresolved motions. Apart from this parameter, the closed equations for the resolved variables are completely determined by the underlying deterministic dynamics.

Key Words and Phrases: nonequilibrium statistical mechanics, turbulence closure, model reduction, statistical estimation, optimization, Hamilton-Jacobi equation

1 Introduction

Complex nonlinear dynamical systems with many interacting degrees of freedom, or many coupled modes of motion, are formulated throughout the sciences for the purpose of making reliable predictions about the evolution of system states. But the practical usefulness of these high-dimensional models is limited unless they are combined with some kind of model reduction. Indeed, what is usually desired from a model of a complex system is a quantitative description of some robust, collective behavior. Such a description is not necessarily furnished by individual solution trajectories, owing to the generic presence of deterministic chaos. Moreover, in realistic problems neither the specification of initial states nor the measurement of evolved states is exact. It is generally desirable, therefore, to select some subset of the system's dynamical variables and declare them to be resolved, or relevant, variables, and to seek a reduced dynamical description in terms of them. For instance, in a spatially-extended system the resolved variables could furnish a coarse-grained description of the fully resolved, fine-grained dynamics. Aside from the practical considerations that constrain resolution in numerical simulations, the selection of these resolved variables is normally determined by two considerations: (1) how initial states are prepared and evolved states are observed, and (2) whether it is possible to achieve an approximate closure of the dynamics in terms of the resolved variables. In most instances there is no perfect selection. Also, there is a competition between these two criteria, because the first is more easily satisfied by a few resolved variables, while the second is better achieved by many. In this light, the modeler is often confronted with the general problem of deriving a reduced system of governing equations for a selected, though not unique, set of resolved variables.

This model reduction procedure is necessarily statistical, since it relegates all unresolved variables to a probabilistic description. A systematic approach to model reduction therefore naturally makes recourse to the methods of statistical mechanics, which furnishes a collection of methodologies for deriving macroscopic behavior from microscopic dynamics [2, 3, 7, 23]. But this field has traditionally developed in the narrower context of deriving thermodynamical properties of matter from the attributes and interactions of a huge number of elementary constituents. Moreover, since reduced equations governing statistically-averaged resolved variables for a complex system are analogous to transport equations for thermodynamics variables, the most pertinent methods are those of nonequilibrium statistical mechanics [2, 24, 40]. Unlike equilibrium statistical mechanics, which is a general theory resting on the secure foundation of Gibbs ensembles, nonequilibrium statistical mechanics is still an emerging field whose various branches treat particular physical processes and whose methods require special mathematical simplifications. As a result, there remain many problems in model reduction on which little progress has been made because they pertain to phenomena lying outside the range of existing nonequilibrium theory. For instance, many aspects of turbulence modeling suffer from the lack of systematic approximations that are analytically justified and computationally tractable, and it is mainly for this reason that the design of reliable statistical closures for turbulent dynamics remains such a challenging open problem.

In this paper we propose a new approach to model reduction for complex determin-

istic dynamics. In order to maintain contact with the fundamental notions of statistical mechanics, we focus on classical Hamiltonian systems. The essence of our approach to statistical closure is an optimization procedure in which we seek computationally tractable approximations to solutions of the Liouville equation, which governs the exact evolution of probability density on phase space [2, 23, 40]. Instead of manipulating exact but computationally inaccessible solutions of the Liouville equation, we use trial probability densities on phase space that form a parametric statistical model for which the given resolved variables are minimal sufficient statistics [6]. With respect to this family of trial densities, we seek paths in the statistical parameter space that have minimal lack-of-fit to the Liouville equation. Specifically, we minimize the time integral of an ensemble-averaged, quadratic cost function of the Liouville residual over those paths of trial densities which connect an initial nonequilibrium state to an estimated state at any later time. In this way we obtain a closure that is optimal relative to the resolved variables selected for model reduction.

To complete the derivation of the statistical closure, we deduce the set of differential equations governing the evolution of the estimated parameters for the statistical model. To do this we introduce the value function for our best-fit minimization problem, which is a function on the statistical parameter space that gives the optimal cost of reduction. As is known in optimization theory [12, 18], this value function satisfies a Hamilton-Jacobi equation with a Hamiltonian that is conjugate to the Lagrangian cost function. The desired equations governing the best-fit statistical state are therefore determined by the solution propagated by that Hamilton-Jacobi equation. Finally, computationally tractable simplifications of them are systematically extracted under some further approximations.

We restrict our attention here to the relaxation problem for Hamiltonian dynamical systems. Apart from mild regularity and growth conditions, we put no restrictions on the Hamiltonian defining the underlying complex dynamics or on the set of resolved variables defining the model reduction. In this general context we derive reduced equations that approximate the evolution toward equilibrium of ensemble-averaged resolved variables from incompletely specified, nonequilibrium initial values. Our purpose is to demonstrate how an irreversible statistical closure can be inferred from an underlying dynamics that is deterministic, reversible and conservative. Our approach to nonequilibrium statistical behavior differs from much of the current literature in that we do not assume that the microscopic dynamics is a known stochastic processes, nor do we interpose a stochastic model between the closed reduced dynamics and the Hamiltonian dynamics. While our general method could be adapted to forced and dissipative systems, we do not consider these systems in the present paper, nor do we address the much studied question of stationary statistical states for those dynamical systems.

For the sake of definiteness, we limit our presentation to the particular case of the best-fit estimation strategy in which the trial probability densities are quasi-equilibrium, or quasi-canonical, ensembles [38, 28, 32]. Namely, we use densities

$$\tilde{\rho}(z; \lambda) = \exp[\lambda^* A(z) - \phi(\lambda)] \rho_{eq}(z), \quad (1)$$

in which

$$\phi(\lambda) = \log \int_{\Gamma_n} \exp(\lambda^* A(z)) \rho_{eq}(z) dz .$$

The m -vector $A = (A_1, \dots, A_m)$ consists of the resolved variables in the reduced model, and ρ_{eq} denotes an equilibrium probability density. The family of densities (1) is parameterized by the real m -vector $\lambda = (\lambda^1, \dots, \lambda^m) \in \mathbb{R}^m$. Here and throughout the paper, $*$ denotes the transpose of a real vector or matrix (so that in these formulas, $\lambda^* A = \lambda^1 A_1 + \dots + \lambda^m A_m$); z denotes the generic point in the phase space $\Gamma_n \subset \mathbb{R}^{2n}$, and dz is the element of phase volume on Γ_n . For the purposes of our general development, the resolved variables, A_k , may be any independent, real-valued, smooth functions on Γ_n that are not conserved by the Hamiltonian dynamics, and ρ_{eq} , may be any invariant density, such as the canonical Gibbs ensemble. From the perspective of statistical inference, $\tilde{\rho}(z; \lambda)$ is an exponential family on Γ_n with the natural (or canonical) parameter λ , and the random vector A is a minimal sufficient statistic for this family [6].

In the reduced model the ensemble mean of A with respect to $\tilde{\rho}$ constitutes the macrostate

$$a = (a_1, \dots, a_m) = \langle A | \tilde{\rho} \rangle = \int_{\Gamma_n} A(z) \tilde{\rho}(z; \lambda) dz.$$

The parameter vector λ is dual to the macrostate vector a , and the convex function ϕ determines a one-to-one correspondence between λ and a through $a = \partial\phi/\partial\lambda$. The choice of the statistical model (1) defines a configuration space, \mathbb{R}^m , for the reduced model, the generic point of which is λ . The desired reduced dynamics is therefore characterized either by the evolution of λ or equivalently by the evolution of a . This point of view is familiar from the information-theoretic approach to nonequilibrium statistical mechanics [21, 22, 23, 38, 14, 28].

Our goal is to estimate the macrostate vector $a(t_1)$ at any time t_1 after an initial time t_0 at which a nonequilibrium initial state is specified. For simplicity in this Introduction, we assume that the initial density, $\rho(z, t_0) = \tilde{\rho}(z; \lambda_0)$, is a quasi-equilibrium ensemble of the form (1) corresponding to a specified $\lambda(t_0) = \lambda_0$, with $a(t_0) = a_0$; in the body of the paper we give a formulation in which the initial statistical state is incompletely specified. The exact density $\rho(z, t)$ at later times $t > t_0$ solves the Liouville equation, which can be written in exponential representation as

$$\frac{\partial \log \rho}{\partial t} + L \log \rho = 0,$$

where $L = \{\cdot, H\}$ denotes the Liouville operator associated to the Poisson bracket $\{\cdot, \cdot\}$. As ρ evolves it loses its quasi-equilibrium form and develops a more intricate structure than the trial probabilities $\tilde{\rho}$. The key to an effective statistical closure with respect to the given m -vector A of resolved variables is therefore to devise a good approximation to ρ within the quasi-equilibrium family $\tilde{\rho}$. To this end, we calculate the residual with respect to the Liouville equation of a trial density $\tilde{\rho}(z; \lambda(t))$ along any smooth path $\lambda(t)$ in the statistical parameter space \mathbb{R}^m :

$$R = \frac{\partial \log \tilde{\rho}}{\partial t} + L \log \tilde{\rho} = \dot{\lambda}^*(A - a) + \lambda^* L A.$$

This Liouville residual $R = R(z; \lambda, \dot{\lambda})$, or lack-of-fit of the trial density $\tilde{\rho}(z; \lambda)$ to the Liouville equation, has an interpretation as the instantaneous rate of information loss

within the statistical model. We therefore base our estimation strategy for $a(t_1)$ on minimizing R in an appropriate norm over the time horizon of estimation, $t_0 \leq t \leq t_1$. Namely, we evaluate the following time-integrated, ensemble-averaged cost functional:

$$\int_{t_0}^{t_1} \mathcal{L}(\lambda, \dot{\lambda}) dt = \frac{1}{2} \int_{t_0}^{t_1} \langle (P_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle + \epsilon^2 \langle (Q_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle dt \quad (2)$$

where P_λ is the orthogonal projection of $L^2(\Gamma_n, \tilde{\rho}(\lambda))$ onto the span of the resolved vector A , and $Q_\lambda = I - P_\lambda$ is the complementary projection. The constant $\epsilon \in (0, 1]$ is an adjustable parameter in our closure scheme, which assigns relative weights to the resolved and unresolved components of the Liouville residual.

The integrand in the cost functional (2) may be viewed as a Lagrangian $\mathcal{L}(\lambda, \dot{\lambda})$ on the configuration space \mathbb{R}^m . In that light our best-fit strategy for closure is determined by an analogue to the classical principle of least action. We therefore use Hamilton-Jacobi theory [1, 18, 27, 16] to deduce the governing equations for our closed reduced dynamics. That is, we introduce the value function (or principal function)

$$v(\lambda_1, t_1) = \min_{\lambda(t_1)=\lambda_1} \int_{t_0}^{t_1} \mathcal{L}(\lambda, \dot{\lambda}) dt \quad \text{subject to} \quad \lambda(t_0) = \lambda_0, \quad (3)$$

which associates an optimal lack-of-fit to an arbitrary terminal state λ_1 at a terminal time t_1 . This minimization is over admissible paths $\lambda(t)$, $t_0 \leq t \leq t_1$, that connect the specified initial state λ_0 to λ_1 . The value function, $v = v(\lambda, t)$, satisfies the associated Hamilton-Jacobi equation

$$\frac{\partial v}{\partial t} + \mathcal{H}(\lambda, \frac{\partial v}{\partial \lambda}) = 0 \quad (4)$$

in which $\mathcal{H}(\lambda, \mu)$ is the Legendre transformation of $\mathcal{L}(\lambda, \dot{\lambda})$. The conjugate canonical variable, μ , has an interpretation as the irreversible part of the flux of the macrostate $a = \langle A | \tilde{\rho} \rangle$, in the sense that

$$\mu = \frac{\partial \mathcal{L}}{\partial \dot{\lambda}} = \langle RA | \tilde{\rho} \rangle = \frac{d}{dt} \langle A | \tilde{\rho} \rangle - \langle LA | \tilde{\rho} \rangle.$$

The Hamilton-Jacobi equation propagates the value function forward in time from the singular initial condition that all paths emanate from λ_0 . We designate the best-fit estimate of the statistical state at any time t to be the minimizer $\hat{\lambda}(t)$ of $v(\lambda, t)$; the corresponding best-fit macrostate is therefore $\hat{a}(t) = \langle A | \tilde{\rho}(\hat{\lambda}(t)) \rangle = \partial \phi / \partial \lambda(\hat{\lambda}(t))$.

The reduced dynamics governing the evolution of the best-fit macrostate can be deduced from the minimizing property of $\hat{\lambda}(t)$ and the Hamilton-Jacobi equation; the main result is

$$\frac{d\hat{a}}{dt} = \langle LA | \tilde{\rho}(\hat{\lambda}) \rangle - \epsilon^2 D^2 \phi(\hat{\lambda}) [D^2 v(\hat{\lambda}, t)]^{-1} \frac{\partial w}{\partial \lambda}(\hat{\lambda}), \quad (5)$$

where $w(\lambda) = \langle [Q_\lambda L(\lambda^* A)]^2 | \tilde{\rho}(\lambda) \rangle$, and $D^2 \phi$ and $D^2 v$ are Hessian matrices with respect to λ . The right hand side of this equation separates into an reversible term, which has a standard form, and an irreversible term scaled by ϵ^2 , which has a novel form. The irreversible part of the flux in (5) has a generalized gradient structure with a potential-type function $\epsilon^2 w(\lambda)$ that quantifies the influence of unresolved fluctuations. Besides

being scaled by ϵ^2 the irreversible term also depends on ϵ implicitly through the value function $v = v(\lambda, t; \epsilon)$.

The defining minimization over paths on the entire time interval of estimation partially compensates for the fact that the trial densities are memoryless, quasi-equilibrium ensembles. This feature of the best-fit closure is its primary advantage as a computational method, since no trajectories of the underlying Hamiltonian need be computed. However, this feature also requires that the scale factor ϵ be introduced into the cost function and be adjusted to give the correct dissipation rate in the reduced dynamics. It is not surprising that such adjustment is needed in light of known projection methods [40, 34, 8, 9], which furnish various expressions for the dissipative term in (5). These expressions involve time convolutions with respect to a memory kernel for autocorrelations with respect to a projected Liouville propagator, essentially e^{tQL} in our notation. The cost functional (2) incorporates a minimal representation of the memory of unresolved fluctuations by means of a single real parameter ϵ . This approach dispenses with the computation of any memory kernel at the expense of an adjustable parameter that must be tuned empirically.

A further approximation of the reduced dynamics (5) is desirable because evaluation of the value function requires solving the Hamilton-Jacobi equation, which is computational burdensome except when m is small. Accordingly, we derive a more explicit closure scheme for the pair $(\hat{\lambda}(t), \hat{M}(t))$, where $\hat{M}(t) = D^2 v(\hat{\lambda}(t), t)$ denotes the Hessian matrix of the value function at the best-fit state. To do so we make the local quadratic approximation $v(\lambda, t) \approx v(\hat{\lambda}(t), t) + (1/2)[\lambda - \hat{\lambda}(t)]^* \hat{M}(t)[\lambda - \hat{\lambda}(t)]$ in a neighborhood of $\hat{\lambda}$, and we find that the Hamilton-Jacobi equation reduces to a coupled system for $\hat{\lambda}$ and \hat{M} , in which \hat{M} satisfies a matrix Riccati differential equation with coefficient matrices that depend on $\hat{\lambda}$. The local quadratic approximation used to derive these closed reduced equations from the general best-fit theory has the character of a truncation of a closure hierarchy at the second order. In this sense it is a rational method of acquiring a computationally tractable statistical closure that could be applied far from equilibrium.

We also show that, in the near equilibrium regime under the standard linear response approximations [7, 40], this local quadratic representation of the value function is valid globally and the matrix Riccati equation has constant coefficients. Thus, for near equilibrium behavior we obtain a simpler system of closed reduced equations, which is comparable to the phenomenological equations of linear irreversible thermodynamics [13, 31], but with a time-dependent matrix of transport coefficients that is determined by the solution to the Riccati equation.

Our approach seems to have no antecedent in the literature. While we build on the ideas of Jaynes [21, 22] and Zubarev [38], as well as later workers [36, 28, 39], in that we utilize quasi-equilibrium densities, which maximize entropy subject to instantaneous macroscopic constraints, our strategy of minimizing a time-integrated cost function for the Liouville residual over paths of these densities appears to be new. Furthermore, our closed reduced equations have a different format from that of other theories. In particular, the differential equation for the estimated statistical state $\hat{\lambda}(t)$ is coupled to a differential equation for the Hessian matrix, $\hat{M}(t)$, which quantifies the information content in the estimate. In this sense our theory simultaneously estimates the evolving macrostate and quantifies the uncertainty inherent in that estimate. The format of our

closed reduced equations, therefore, resembles that of continuous-time optimal filtering theory [4, 11, 29, 30], and in the near equilibrium regime there is a close connection between our reduced equations and the Kalman-Bucy filter. Unlike the standard filtering problem, however, our statistical closure updates the reduced model by accessing the unresolved components of the deterministic equations of motion themselves, rather than assimilating some measurements.

The outline of the paper is as follows. We set the background for our approach in Section 2, and then we present the best-fit closure scheme in Sections 3 and 4. This theoretical development applies to nonequilibrium states that may be far from equilibrium. In Sections 5 and 6 we specialize our general formulation to the near-equilibrium version of our theory. In the case when all the resolved variables are symmetric under time reversal, we show that our near-equilibrium closure takes a form similar to that of linear irreversible thermodynamics. In Section 7 we give a heuristic analysis that supports the physical interpretation of the adjustable parameter ϵ as a time-scale ratio.

In a companion paper [33] we address the computational implementation of the general methodology developed in this paper, and we present comparisons of its predictions against fully-resolved numerical simulations for a particular Hamiltonian system.

2 Background

We consider a general Hamiltonian dynamics in canonical form

$$\frac{dz}{dt} = J \nabla_z H(z) \quad \text{with} \quad J = \begin{pmatrix} O & I \\ -I & O \end{pmatrix}, \quad (6)$$

where $z = (q, p)$ denotes a generic point in the phase space $\Gamma_n = \mathbb{R}^{2n}$, where n is the number of degrees of freedom of the system. We place no special restrictions on the Hamiltonian H other than it be a smooth function on Γ_n with a natural growth condition at infinity: $H(z) \geq b|z|^2 - c$, with $b > 0, c \geq 0$, for large $|z|$. Most of what follows holds for noncanonical Hamiltonian systems, but we will restrict our development in this paper to classical canonical systems for the sake of clarity.

We denote the phase flow for the Hamilton equations (6) by $\Phi(t) : \Gamma_n \rightarrow \Gamma_n$, so that

$$z(t_1) = \Phi(t_1 - t_0)(z(t_0)) \quad \text{for all } t_1 \geq t_0,$$

where $z(t)$ is any solution of (6). This deterministic phase flow $\Phi(t)$ is a volume-preserving diffeomorphism of Γ_n for all t , by Liouville's theorem. The invariant $2n$ -volume on Γ_n is denoted by dz .

We are interested in estimating or approximating the macroscopic behavior of a few dynamical variables rather than following the details of the microscopic dynamics (6) itself. We therefore suppose that some resolved, or relevant, dynamical variables are selected, and we seek a statistical closure in terms of these variables. We assume that each dynamical variable A_k is a smooth real-valued function on Γ_n , and that the set A_1, \dots, A_m is linearly independent. We assemble them into the resolved vector $A = (A_1, \dots, A_m)$. In

principle there is no restriction on m , but in practice the number m of relevant variables should be small compared to the dimension n of the phase space.

The quality of any choice of resolved variables is determined by the ability of the resulting reduced model to approximate the collective behavior of the system. The assessment of any particular selection of resolved variables therefore first requires the formulation of a closure scheme. Nonetheless, in most practical problems there will be some natural choices of A in terms of which it is reasonable to expect a good approximation. We mention just two such physical systems: molecular dynamics and dispersive wave turbulence. For a coupled system of particles in which a few tagged particles interact with many particles constituting a “heat bath,” the canonical variables of the tagged particles furnish natural resolved variables for reduction [17, 19]. For a nonlinear wave system with many interacting modes, a kinetic description of the power spectrum (perhaps in some selected bands) is a customary reduction for “weak turbulence” theory [37, 5]. Even in these cases, though, improved approximations may result from expanding or otherwise modifying the set of resolved variables. In light of considerations of this kind, we proceed without putting any special restrictions on the resolved vector A .

The evolution of any dynamical variable, F , resolved or not, is determined by the equation

$$\frac{dF}{dt} = \{F, H\}, \quad (7)$$

where $\{F, H\} = (\nabla F)^* J \nabla H$ is the Poisson bracket associated with the canonical Hamiltonian structure. Indeed, the statement that (7) holds for all smooth functions F on Γ_n is equivalent to the Hamiltonian dynamics (6). Fundamentally, the problem of closure in terms of the resolved variables A_1, \dots, A_m arises from the fact that, except under very special circumstances, the derived variables $\dot{A}_1 = \{A_1, H\}, \dots, \dot{A}_m = \{A_m, H\}$ are not expressible as functions of A_1, \dots, A_m . For instance, in the exceptional case when $\dot{A} = \Omega A$ identically on Γ_n for some $m \times m$ constant matrix Ω , a deterministic closure is immediate from (7). We are however interested in the generic case, and hence we adopt a statistical description defined by that evolving probability measure $p(dz, t)$ on the phase space Γ_n which is induced by the phase flow; namely,

$$\int_{\Phi(t_1 - t_0)(B)} p(dz, t_1) = \int_B p(dz, t_0) \quad \text{for all Borel subsets } B \subset \Gamma_n, \quad \text{and any } t_1 \geq t_0.$$

We consider only probability measures, $p(dz, t) = \rho(z, t)dz$, having densities ρ that are smooth in z and t , because all trial densities in our reduced model have this regularity. Then the propagation of probability by the phase flow is governed by the Liouville equation

$$\frac{\partial \rho}{\partial t} + L\rho = 0 \quad \text{in } \Gamma_n \times \mathbb{R}, \quad (8)$$

in which we introduce the Liouville operator $L = \{\cdot, H\}$. Given a density $\rho(z, t_0)$ at an initial time t_0 , (8) completely determines the density $\rho(z, t)$ at any later time t , denoted formally by $\rho(\cdot, t) = e^{-(t-t_0)L} \rho(\cdot, t_0)$. The statistical mean of any dynamical variable F at time t is given by

$$\langle F | \rho(t) \rangle = \int_{\Gamma_n} F(z) \rho(z, t) dz = \int_{\Gamma_n} F \circ \Phi(t - t_0)(z) \rho(z, t_0) dz,$$

where the first equality defines our notation for expectation. In particular, the evolution of the statistical average of the relevant vector $\langle A | \rho(t) \rangle$ is determined by the exact solution of (8). From the point of view of a numerical computation, however, solving the Liouville equation is impractical because it requires the simulation of an ensemble of exact trajectories for the complex dynamics (6). For this reason we resort to the following natural approximation procedure.

We seek to approximate the exact density $\rho(t)$ by a family of trial densities, $\tilde{\rho}(t)$, that have a simple and tractable analytical form. For reduction relative to a given resolved vector A , a natural choice is supplied by the so-called quasi-equilibrium, or quasi-canonical, densities [21, 22, 38, 32] already displayed in (1). A standard motivation for using the family of densities (1) to construct a statistical closure is that each member of the family maximizes information entropy subject to the mean value of the resolved vector; that is, $\tilde{\rho}$ solves

$$\text{maximize } S(\rho) = - \int_{\Gamma_n} \rho \log \frac{\rho}{\rho_{eq}} dz \quad \text{subject to } \int_{\Gamma_n} A \rho dz = a, \quad \int_{\Gamma_n} \rho dz = 1.$$

From the perspective of information theory [10, 25], $\tilde{\rho}(z, \lambda)$ is the least informative probability density relative to the equilibrium density ρ_{eq} that is compatible with the macrostate vector

$$a = \langle A | \tilde{\rho} \rangle = \int_{\Gamma_n} A(z) \tilde{\rho}(z; \lambda) dz. \quad (9)$$

The parameter vector $\lambda \in \mathbb{R}^m$ then consists of the Lagrange multipliers for the vector constraint (9), and there is a one-to-one correspondence between λ and a given by

$$a = \frac{\partial \phi}{\partial \lambda}, \quad \lambda = - \frac{\partial s}{\partial a}, \quad (10)$$

where $s(a) = S(\tilde{\rho})$ denotes the entropy of the macrostate a . This correspondence is a convex duality, and $-s(a)$ is the convex conjugate function to $\phi(\lambda)$.

In this formulation we fix an equilibrium density ρ_{eq} on Γ_n and construct the family of quasi-equilibrium trial densities $\tilde{\rho}$ relative to it. An alternative formulation is to include the Hamiltonian H among the resolved variables, by forming an augmented resolved vector $A = (A_0, A_1, \dots, A_m)$ with $A_0 = H$. Then the trial densities $\tilde{\rho} = \exp[\lambda_0 A_0 + \dots + \lambda_m A_m - \phi(\lambda)]$ have the augmented parameter vector $\lambda \in \mathbb{R}^{m+1}$ and are respect to phase volume dz . This alternative leads to a parallel theory. Our formulation in terms of a non-conserved resolved vector A focuses the discussion of nonequilibrium concepts and facilitates the derivation of the near-equilibrium theory via the linear response approximation.

In physical terms the quasi-equilibrium description establishes a nonequilibrium statistical mechanics without memory, in the sense that $\tilde{\rho}(z, \lambda(t))$ depends only on the instantaneous macrostate $a(t)$, not on its history, $a(t')$ for $t' < t$. Such a memoryless description might be justified when there is a wide separation between the time scale of evolution of the resolved vector, A , and the time scale of conditional equilibration of the unresolved variables. In the limit of an infinite time-scale separation, an instantaneous statistical closure with respect to these quasi-equilibrium densities is obtained by imposing the A -moment of the Liouville equation, namely,

$$\frac{d}{dt} \langle A(z) | \tilde{\rho}(z; \lambda(t)) \rangle = \langle LA(z) | \tilde{\rho}(z; \lambda(t)) \rangle.$$

But the resulting statistical closure is exactly entropy conserving, as the following straightforward calculation shows:

$$\frac{d}{dt}S(\tilde{\rho}) = -\lambda^* \frac{da}{dt} = \int_{\Gamma_n} L \lambda^* A \exp[\lambda^* A - \phi(\lambda)] \rho_{eq} dz = 0.$$

Thus, the combination of a quasi-equilibrium ansatz and an instantaneous moment closure results in a reversible reduced dynamics [14, 20]. The inability of this adiabatic closure to capture the dissipation, or entropy production, of the actual nonequilibrium statistical behavior is a serious defect, making it useful only for certain short-time phenomena.

In much previous work [38, 39, 28, 35, 20], the remedy for this defect has been to include memory effects into the relevant probability densities by replacing $\lambda(t)^* A$ with time-weighted averages of the dynamical variables, $\int_0^\infty \lambda(t-\tau)^* A \circ \Phi(-\tau) w(\tau) d\tau$. Closure is then obtained by taking instantaneous A -moments with respect to these memory-dependent densities. The resulting reduced equations, however, depend upon the weighting function w , for which there is no universal choice. Moreover, they involve convolutions over time, and therefore require the evaluation of various correlations of A and $LA = \{A, H\}$ over a range of time shifts τ . The statistical closures derived in this manner are consequently difficult to justify theoretically and expensive to implement computationally.

The new approach that we propose in the next section is fundamentally different. Rather than use memory-dependent densities and moment closure, we retain the quasi-equilibrium densities as natural trial densities in a parametric statistical model. With respect to this model we obtain closure by best-fitting trajectories of trial densities to the Liouville equation over the entire time interval from when the initial statistical state is specified to when the evolved state is estimated.

3 Formulation of best-fit closure

As outlined in the Introduction, we quantify the lack-of-fit of the quasi-equilibrium trial probability densities (1) to the Liouville equation (8) over an interval of time $t_0 \leq t \leq t_1$ by a cost functional

$$\Sigma[\lambda; t_0, t_1] = \int_{t_0}^{t_1} \mathcal{L}(\lambda, \dot{\lambda}) dt. \quad (11)$$

In this formulation the cost functional is analogous to an action integral for a Lagrangian \mathcal{L} , which is a function of λ and $\dot{\lambda} = d\lambda/dt$, and the configuration space is the parameter space \mathbb{R}^m for the statistical model (1). To construct an appropriate (running) cost function $\mathcal{L}(\lambda, \dot{\lambda})$, we introduce the residual of the log-likelihood, $\log \tilde{\rho}$, of the trial densities with respect to the Liouville operator:

$$R(\cdot; \lambda, \dot{\lambda}) = \left(\frac{\partial}{\partial t} + L \right) \log \tilde{\rho}(\cdot; \lambda(t)) = \dot{\lambda}(t)^* (A - a(\lambda(t))) + \lambda(t)^* LA. \quad (12)$$

There are two related expressions for this Liouville residual R that reveal its significance in the statistical closure problem.

First, for any $z \in \Gamma_n$ and any smooth parameter path $\lambda(t)$, we examine the log-likelihood ratio between the exact density and the trial density after a short interval of time Δt :

$$\log \frac{e^{-(\Delta t)L} \tilde{\rho}(z; \lambda(t))}{\tilde{\rho}(z; \lambda(t + \Delta t))} = -(\Delta t)R(z; \lambda(t), \dot{\lambda}(t)) + O((\Delta t)^2) \quad \text{as } \Delta t \rightarrow 0.$$

This expansion shows that, to leading order locally in time, $-R(z; \lambda(t), \dot{\lambda}(t))$ represents the information in the sample point z for discriminating the exact density against the trial density [25]. By considering arbitrary smooth paths passing through a point λ with a tangent vector $\dot{\lambda}$, we may consider $R(z; \lambda, \dot{\lambda})$ evaluated at z as a function of $(\lambda, \dot{\lambda})$ in the tangent space to the configuration space, and we may interpret it to be the local rate of information loss in the sample point z for the pair $(\lambda, \dot{\lambda})$.

Second, for any dynamical variable $F : \Gamma_n \rightarrow \mathbb{R}$, we evaluate the F -moment of the Liouville equation with respect to the trial densities along a path $\lambda(t)$ and we obtain the identities

$$\frac{d}{dt} \langle F | \tilde{\rho}(\lambda(t)) \rangle - \langle LF | \tilde{\rho}(\lambda(t)) \rangle = \langle F | (\partial/\partial t + L) \tilde{\rho}(\lambda(t)) \rangle = \langle FR | \tilde{\rho}(\lambda(t)) \rangle$$

where the second equality follows directly from the definition (12). Thus we find that, while an exact solution $\rho(t)$ of the Liouville equation satisfies the identities, $d/dt \langle F | \rho(t) \rangle - \langle LF | \rho(t) \rangle = 0$, for all test functions F , a trial solution $\tilde{\rho}$ produces a departure that coincides with the covariance between F and R . This representation of R furnishes a natural linear structure for analyzing the fit of the trial densities to the Liouville equation.

In light of these two interpretations of the Liouville residual R , we proceed to measure the dynamical lack-of-fit of the statistical model in terms of it. To do so, we consider the components of R in the resolved and unresolved subspaces. At any configuration point $\lambda \in \mathbb{R}^m$, let P_λ denote the orthogonal projection of the Hilbert space $L^2(\Gamma_n, \tilde{\rho}(\lambda))$ onto the span of the functions $A_1 - a_1(\lambda), \dots, A_m - a_m(\lambda)$, and let $Q_\lambda = I - P_\lambda$ denote the complementary projection; specifically, for any $F \in L^2(\Gamma_n, \tilde{\rho}(\lambda))$,

$$P_\lambda F = \langle F(A - a(\lambda))^* | \tilde{\rho}(\lambda) \rangle C(\lambda)^{-1} (A - a(\lambda)).$$

where

$$C(\lambda) = \langle (A - a(\lambda))(A - a(\lambda))^* | \tilde{\rho}(\lambda) \rangle. \quad (13)$$

We take the cost function in (11) to be

$$\mathcal{L}(\lambda, \dot{\lambda}) = \frac{1}{2} \langle (P_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle + \frac{\epsilon^2}{2} \langle (Q_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle \quad (14)$$

for a constant $\epsilon \in (0, 1]$. This lack-of-fit norm is of mean-squared type, but with an adjustable parameter ϵ that controls the weight given to the unresolved component of the residual versus the resolved component.

By duality, $\mathcal{L}(\lambda, \dot{\lambda})$ can be characterized in terms of test functions F as follows:

$$2\mathcal{L}(\lambda, \dot{\lambda}) = \max \{ \langle FR | \tilde{\rho} \rangle^2 : \langle (P_\lambda F)^2 | \tilde{\rho} \rangle + \epsilon^{-2} \langle (Q_\lambda F)^2 | \tilde{\rho} \rangle \leq 1, \quad F \in L^2(\Gamma_n, \tilde{\rho}) \}.$$

This dual form of the norm highlights the fact that \mathcal{L} weights departures in the unresolved dynamical variables less than departures in the resolved variables, depending on ϵ . In particular, when ϵ is small the constraint in this maximization gives preference to those F which have a relatively small component in the unresolved subspace. Thus, as the adjustable parameter ϵ is decreased, the contribution of the unresolved variables to the cost function \mathcal{L} is correspondingly decreased; and, in the limit as $\epsilon \rightarrow 0$, it vanishes entirely. In Section 7 we explain how ϵ is related to time scales and memory effects.

Before presenting the optimization problem that defines our best-fit closure, we first exhibit the Lagrangian \mathcal{L} in a more explicit form. The Liouville residual has zero mean, $\langle R|\tilde{\rho}(\lambda)\rangle = 0$, and its orthogonal components are given by

$$P_\lambda R = [\dot{\lambda} - C(\lambda)^{-1}\langle LA|\tilde{\rho}(\lambda)\rangle]^*(A - a), \quad Q_\lambda R = \lambda^*(Q_\lambda LA).$$

The calculation of $P_\lambda R$ employs the string of equations,

$$\langle LA|\tilde{\rho}\rangle = \langle (LA)e^{\lambda^*A-\phi(\lambda)}|\rho_{eq}\rangle = -\langle (A-a)Le^{\lambda^*A-\phi(\lambda)}|\rho_{eq}\rangle = -\langle (A-a)L(\lambda^*A)|\tilde{\rho}\rangle$$

in which the anti-symmetry of the operator L with respect to ρ_{eq} is used. Hence the Lagrangian cost function can be written in the explicit form,

$$\mathcal{L}(\lambda, \dot{\lambda}) = \frac{1}{2}[\dot{\lambda} - C(\lambda)^{-1}\langle LA|\tilde{\rho}(\lambda)\rangle]^*C(\lambda)[\dot{\lambda} - C(\lambda)^{-1}\langle LA|\tilde{\rho}(\lambda)\rangle] + \frac{\epsilon^2}{2}\lambda^*D(\lambda)\lambda, \quad (15)$$

where

$$D(\lambda) = \langle (Q_\lambda LA)(Q_\lambda LA^*)|\tilde{\rho}(\lambda)\rangle. \quad (16)$$

By analogy to analytical mechanics, one may regard the first member in (15) as the “kinetic” term and the second member as the “potential” term. The kinetic term is a quadratic form in the generalized velocities $\dot{\lambda}$ with positive-definite matrix $C(\lambda)$. In fact, this matrix is the Fisher information matrix [25, 6] for the exponential family (1), having components

$$C_{ij}(\lambda) = \langle \frac{\partial \log \tilde{\rho}}{\partial \lambda_i} \frac{\partial \log \tilde{\rho}}{\partial \lambda_j} |\tilde{\rho}(\lambda)\rangle.$$

It defines a natural Riemannian metric, $ds^2 = \sum_{i,j} C_{ij}(\lambda)d\lambda^i d\lambda^j$, on the configuration space \mathbb{R}^m . The potential term equals ϵ^2 times the function

$$w(\lambda) = \frac{1}{2}\lambda^*D(\lambda)\lambda = \frac{1}{2}\langle [Q_\lambda L \log \tilde{\rho}]^2 |\tilde{\rho}(\lambda)\rangle, \quad (17)$$

which we call the closure potential because it embodies the influence of the unresolved variables on the resolved variables. Of course, these mechanical analogies are not literal. Indeed, even though we refer to \mathcal{L} as a “Lagrangian,” it has the units of a rate of entropy production, not of an energy, and it is a sum of two positive-definite terms, not a difference.

For a given initial time t_0 , we define the value function [4, 12]

$$v(\lambda_1, t_1) = \min_{\lambda(t)=\lambda_1} v_0(\lambda(t_0)) + \Sigma[\lambda; t_0, t_1], \quad (18)$$

in which the minimization is over all regular paths $\lambda(t)$ on the interval $t_0 \leq t \leq t_1$ that terminate at an arbitrary (admissible) state $\lambda_1 \in \mathbb{R}^m$ at time t_1 . The optimization problem in (18) is the foundation of our best-fit closure scheme. The value function (18) quantifies a total lack-of-fit of the statistical state λ_1 at time t_1 with respect to evolution from an incompletely specified statistical state at time t_0 . As explained above, the second member of the objective functional in (18) is a dynamically intrinsic norm on the Liouville residual for a path of densities $\tilde{\rho}(\lambda(t))$ over the time interval, $t_0 \leq t \leq t_1$. The first member of the objective functional determines the initial value function, $v_0(\lambda)$, which is given data in the optimization problem. In the special case when initial density, ρ_0 , is specified to be a quasi-equilibrium density, $\tilde{\rho}(\cdot; \lambda_0)$, for a known m -vector λ_0 , the initial value function v_0 is singular; namely,

$$v_0(\lambda) = \begin{cases} +\infty & \lambda \neq \lambda_0 \\ 0 & \lambda = \lambda_0 \end{cases}$$

In this case the first member in the objective functional in (18) can be dropped and the constraint $\lambda(t_0) = \lambda_0$ imposed instead. This singular initial condition can also be obtained as the limit of penalty functions $v_0(\lambda) = b(\lambda - \lambda_0)^2/2$ as $b \rightarrow +\infty$. In the general case when there is some uncertainty in the initial statistical state, $\lambda(t_0)$ is free and is penalized by the nonsingular initial value function v_0 , which represents the degree of specification of the initial statistical state.

It is a fundamental fact from the calculus of variations that such a value function satisfies a corresponding Hamilton-Jacobi equation [27, 18, 16]. Since \mathcal{L} is quadratic and convex in $\dot{\lambda}$, the required Legendre transformation can be calculated explicitly. The conjugate canonical variable is

$$\mu = \frac{\partial \mathcal{L}}{\partial \dot{\lambda}} = C(\lambda) \dot{\lambda} - \langle LA | \tilde{\rho}(\lambda) \rangle, \quad (19)$$

and the Hamiltonian associated with \mathcal{L} is

$$\mathcal{H}(\lambda, \mu) = \dot{\lambda}^* \frac{\partial \mathcal{L}}{\partial \dot{\lambda}} - \mathcal{L} = \frac{1}{2} \mu^* C^{-1} \mu + \langle LA | \tilde{\rho}(\lambda) \rangle^* C^{-1} \mu - \epsilon^2 w(\lambda), \quad (20)$$

where we recall the closure potential $w(\lambda)$ defined in (17). The value function in (18) therefore satisfies the Hamilton-Jacobi equation

$$\frac{\partial v}{\partial t} + \mathcal{H}(\lambda, \frac{\partial v}{\partial \lambda}) = 0, \quad \text{for } t > t_0, \quad \text{with } v(\lambda, t_0) = v_0(\lambda). \quad (21)$$

At this juncture of our development we have a complete formulation of the desired model reduction scheme. Given a resolved vector, A , and an equilibrium density, ρ_{eq} , the lack-of-fit Hamiltonian (20) is entirely determined up to a choice of the parameter $\epsilon \in (0, 1]$, and the Hamilton-Jacobi equation (21) propagates the value function $v = v(\lambda, t)$ forward in time from any suitable initial value function $v_0(\lambda)$. We may view this Hamilton-Jacobi equation as the appropriate contraction of the Liouville equation relative to our statistical model reduction in the following sense. For each instant of time $t > t_0$, $v = v(\lambda, t)$ is a function on the statistical parameter space that may be conceptualized as

a dynamical analogue of a minus-log-likelihood function [6, 25]. The minimizer, $\hat{\lambda} = \hat{\lambda}(t)$, of $v(\lambda, t)$ defines the best-fit estimate of the parameter λ at time t , and thus $\hat{\lambda}$ is analogous to a maximum likelihood estimate. Moreover, the second-order behavior of $v(\lambda, t)$ in a neighborhood of $\hat{\lambda}$ represents the confidence in, or information content of, the best-fit estimate. Thus, we may say that, just as the Liouville equation propagates the ensemble probability on phase space, the Hamilton-Jacobi equation (21) propagates the uncertainty in the reduced model, which is quantified by v . In this light, we discover that the desired reduced model closes at the level of the value function v on configuration space, not at the level of the estimated configurations themselves. This property of our best-fit closure reflects the fact that the value function governs both the best-fit estimate, at first order, and its uncertainty, at second order.

Summarizing, we define the best-fit parameter and macrostate by

$$\hat{\lambda}(t) = \arg \min_{\lambda} v(\lambda, t), \quad \hat{a}(t) = \frac{\partial \phi}{\partial \lambda}(\hat{\lambda}(t)) \quad \text{for each } t \geq t_0. \quad (22)$$

Accordingly, our best-fit closure is entirely determined by the solution of the Hamilton-Jacobi equation (21). Moreover, this best-fit estimation of time-dependent, nonequilibrium statistical states is valid far from equilibrium. While this general result is a certainly satisfactory from a theoretical viewpoint, it suffers from the fact that the nonlinear partial differential equation (21) is difficult to solve except when the number m of resolved variables is very small. For this reason, we now proceed to derive ordinary differential equations for $\hat{\lambda}(t)$, or equivalently $\hat{a}(t)$, and investigate to what extent it is possible to circumvent solving the Hamilton-Jacobi equation.

4 Derivation of closed reduced dynamics

We are primarily interested in the evolution of the best-fit parameter $\hat{\lambda}(t)$, and correspondingly the best-fit macrostate $\hat{a}(t)$, since they determine our estimates of the expectations $\langle B | \tilde{\rho}(\hat{\lambda}(t)) \rangle$ of any dynamical variable B . We therefore seek the system of ordinary differential equations for $\hat{\lambda}(t)$.

By definition $\hat{\lambda}(t)$ is the minimizer for $v(\lambda, t)$ for each $t > t_0$, and consequently it satisfies

$$\hat{\mu}(t) = \frac{\partial v}{\partial \lambda}(\hat{\lambda}(t), t) = 0 \quad \text{for all } t > t_0. \quad (23)$$

Differentiating this relation with respect to t , and invoking the Hamilton-Jacobi equation, we get

$$\begin{aligned} 0 &= \frac{\partial^2 v}{\partial \lambda \partial \lambda^*} \cdot \frac{d\hat{\lambda}}{dt} + \frac{\partial^2 v}{\partial \lambda \partial t} \\ &= \frac{\partial^2 v}{\partial \lambda \partial \lambda^*} \cdot \frac{d\hat{\lambda}}{dt} - \frac{\partial}{\partial \lambda} \mathcal{H}(\lambda, \frac{\partial v}{\partial \lambda})|_{\lambda=\hat{\lambda}} \\ &= \frac{\partial^2 v}{\partial \lambda \partial \lambda^*} \cdot \frac{d\hat{\lambda}}{dt} - \frac{\partial \mathcal{H}}{\partial \lambda}(\hat{\lambda}, 0) - \frac{\partial^2 v}{\partial \lambda \partial \lambda^*} \cdot \frac{\partial \mathcal{H}}{\partial \mu}(\hat{\lambda}, 0), \end{aligned}$$

where

$$\frac{\partial^2 v}{\partial \lambda \partial \lambda^*} = \left(\frac{\partial^2 v}{\partial \lambda^i \partial \lambda^j} \right)_{i,j=1,\dots,m}$$

denotes the Hessian matrix of v with respect to λ . The second and third terms in this final expression are calculated from \mathcal{H} to be

$$\frac{\partial \mathcal{H}}{\partial \lambda}(\hat{\lambda}, 0) = -\epsilon^2 \frac{\partial w}{\partial \lambda}(\hat{\lambda}), \quad \frac{\partial \mathcal{H}}{\partial \mu}(\hat{\lambda}, 0) = C(\hat{\lambda})^{-1} \langle LA | \tilde{\rho}(\hat{\lambda}) \rangle.$$

Solving for $d\hat{\lambda}/dt$, we arrive at the equation governing the reduced dynamics:

$$\frac{d\hat{\lambda}}{dt} = C(\hat{\lambda})^{-1} \langle LA | \tilde{\rho}(\hat{\lambda}) \rangle - \epsilon^2 \left[\frac{\partial^2 v}{\partial \lambda \partial \lambda^*}(\hat{\lambda}, t) \right]^{-1} \frac{\partial w}{\partial \lambda}(\hat{\lambda}). \quad (24)$$

This is a first-order system of ordinary differential equations is closed in $\hat{\lambda}$, but it involves the value function $v(\lambda, t)$, which in turn is determined by the Hamilton-Jacobi equation. The first term on the right-hand side of (24) is exactly what is obtained from the adiabatic closure when the moment condition $\langle R(A-a) | \tilde{\rho} \rangle = 0$ is imposed instantaneously at each time t ; and thus the adiabatic closure is recovered from the best-fit closure in the limit as $\epsilon \rightarrow 0$. The dissipation, or irreversibility, in the reduced dynamics is produced by second term on the right hand side of (24). The magnitude of this dissipation depends on the adjustable parameter ϵ , but it does not necessarily scale like ϵ^2 , owing to the ϵ -dependence of v through the Hamilton-Jacobi equation.

We now attempt to find a governing equation for the Hessian matrix,

$$\hat{M}(t) = \frac{\partial^2 v}{\partial \lambda \partial \lambda^*}(\hat{\lambda}(t), t) \quad (25)$$

since the inverse of this matrix enters into (24). To do so, we calculate the matrix of all second partial derivatives with respect to λ of the Hamilton-Jacobi equation (21), and thereby obtain a partial differential equation for the matrix-valued function

$$M(\lambda, t) = \frac{\partial^2 v}{\partial \lambda \partial \lambda^*}(\lambda, t).$$

The result is

$$0 = \frac{\partial M}{\partial t} + \frac{\partial^2 \mathcal{H}}{\partial \lambda \partial \lambda^*} + \frac{\partial^2 \mathcal{H}}{\partial \lambda \partial \mu^*} M + M \frac{\partial^2 \mathcal{H}}{\partial \mu \partial \lambda^*} + M \frac{\partial^2 \mathcal{H}}{\partial \mu \partial \mu^*} M + \sum_{k=1}^m \frac{\partial \mathcal{H}}{\partial \mu_k} \frac{\partial M}{\partial \lambda_k}. \quad (26)$$

In order to set $\lambda = \hat{\lambda}$ and $\hat{\mu} = 0$ in this matrix equation, we need to evaluate the various coefficients in it, using the expression (20) for \mathcal{H} . We introduce the shorthand notation

$$f(\lambda) = C(\lambda)^{-1} \langle LA | \tilde{\rho}(\lambda) \rangle,$$

which coincides with $d\lambda/dt$ under the adiabatic closure. The required coefficients are

$$\frac{\partial \mathcal{H}}{\partial \mu}(\hat{\lambda}, 0) = f(\hat{\lambda}),$$

$$\begin{aligned}\frac{\partial^2 \mathcal{H}}{\partial \lambda \partial \lambda^*}(\hat{\lambda}, 0) &= -\epsilon^2 \frac{\partial^2 w}{\partial \lambda \partial \lambda^*}(\hat{\lambda}), & \frac{\partial^2 \mathcal{H}}{\partial \mu \partial \mu^*}(\hat{\lambda}, 0) &= C(\hat{\lambda})^{-1}, \\ \frac{\partial^2 \mathcal{H}}{\partial \lambda \partial \mu^*}(\hat{\lambda}, 0) &= \frac{\partial f}{\partial \lambda}(\hat{\lambda}), & \frac{\partial^2 \mathcal{H}}{\partial \mu \partial \lambda^*} &= \left[\frac{\partial f}{\partial \lambda}(\hat{\lambda}) \right]^*.\end{aligned}$$

Substituting these identities into (26) we obtain:

$$0 = \frac{\partial M}{\partial t}(\hat{\lambda}, t) - \epsilon^2 \frac{\partial^2 w}{\partial \lambda \partial \lambda^*} + \frac{\partial f}{\partial \lambda} \hat{M} + \hat{M} \left[\frac{\partial f}{\partial \lambda} \right]^* + \hat{M} C^{-1} \hat{M} + f \cdot \frac{\partial M}{\partial \lambda}(\hat{\lambda}, t),$$

in which all the coefficient functions are evaluated at $\lambda = \hat{\lambda}(t)$. Now using the governing equation (24) for $\hat{\lambda}$, which can be written as,

$$\frac{d\hat{\lambda}}{dt} = f(\hat{\lambda}) - \epsilon^2 \hat{M}^{-1} \frac{\partial w}{\partial \lambda}(\hat{\lambda}),$$

we find that the matrix-valued function $\hat{M}(t) = M(\hat{\lambda}(t), t)$ satisfies

$$\frac{d\hat{M}}{dt} = -\frac{\partial f}{\partial \lambda} \hat{M} - \hat{M} \left[\frac{\partial f}{\partial \lambda} \right]^* - \hat{M} C^{-1} \hat{M} + \epsilon^2 \frac{\partial^2 w}{\partial \lambda \partial \lambda^*} - \epsilon^2 \left[\hat{M}^{-1} \frac{\partial w}{\partial \lambda} \right] \cdot \frac{\partial M}{\partial \lambda}(\hat{\lambda}, t), \quad (27)$$

in which again $\lambda = \hat{\lambda}(t)$ throughout this equation.

Our goal is to close the differential equation (24) for the best-fit parameter $\hat{\lambda}$ by coupling it to a differential equation for \hat{M} . But the last term in (27) involves the partial derivatives $\partial M / \partial \lambda$, and consequently it is not closed in \hat{M} . In fact, the pair of first-order differential equations (24) and (27) constitute the first and second members of a closure hierarchy. In principle, we could generate a third member of the hierarchy by deriving a differential equation for $\partial M / \partial \lambda(\hat{\lambda}, t)$, and so forth. We will not pursue the hierarchy of ordinary differential equations any further, since the best-fit estimation scheme closes elegantly at the level of the Hamilton-Jacobi equation for the value function.

Nonetheless, it is important to achieve an approximate closure scheme that is more computationally tractable than solving the Hamilton-Jacobi equation itself. Perhaps the most natural approximation of this kind is to set $\partial M / \partial \lambda(\hat{\lambda}, t) = 0$ identically. We call this the local quadratic approximation, because it amounts to replacing the solution $v(\lambda, t)$ of the Hamilton-Jacobi equation by its second-order Taylor expansion around $\hat{\lambda}$; that is,

$$v(\lambda, t) \approx v(\hat{\lambda}, t) + \frac{1}{2}(\lambda - \hat{\lambda}(t))^* \hat{M}(t)(\lambda - \hat{\lambda}(t)) \quad \text{for } \lambda \text{ near } \hat{\lambda}(t).$$

Moreover, recalling that the value function v may be viewed as a dynamical analogue of a minus-log-likelihood function, we may regard this local quadratic approximation as comparable to a quasi-Gaussian approximation. Under this approximation, the last term in (27) disappears and consequently we obtain a closed first-order differential equation for \hat{M} ; namely,

$$\frac{d\hat{M}}{dt} = -\frac{\partial f}{\partial \lambda}(\hat{\lambda}) \hat{M} - \hat{M} \left[\frac{\partial f}{\partial \lambda}(\hat{\lambda}) \right]^* - \hat{M} C(\hat{\lambda})^{-1} \hat{M} + \epsilon^2 \frac{\partial^2 w}{\partial \lambda \partial \lambda^*}(\hat{\lambda}). \quad (28)$$

We thus arrive at the desired closed reduced equations in the pair $(\hat{\lambda}, \hat{M})$. The coupled pair of governing equations for the statistical closure consists of a state equation (24) for $\hat{\lambda}$ and a matrix Riccati equation (28) for \hat{M} . The parameter vector $\hat{\lambda}$ determines the best-fit macrostate, while the matrix \hat{M} characterizes the uncertainty in the best-fit estimate, up to the local quadratic approximation. The initial condition for (28) is

$$\hat{M}(t_0) = \frac{\partial^2 v_0}{\partial \lambda \partial \lambda^*}(\lambda_0), \quad \text{where } \lambda_0 = \arg \min_{\lambda} v_0(\lambda).$$

We assume that the initial value function v_0 is strictly convex, and hence that $\hat{M}(t_0)$ is positive-definite.

We note that the matrix solution $\hat{M}(t)$ of (28) for $t \geq t_0$ is necessarily symmetric and positive-definite whenever the closure potential w is convex along the solution $\hat{\lambda}$. This conclusion follows from known properties of solutions of matrix Riccati equations, which hold for (28) provided that the symmetric matrices C and $\partial^2 w / \partial \lambda \partial \lambda^*$ are both positive-semidefinite, and the initial condition is positive-definite [26]. While the Fisher information matrix $C(\lambda)$ is positive-definite for arbitrary λ , the convexity of the closure potential is ensured only near to equilibrium; indeed,

$$\frac{\partial^2 w}{\partial \lambda \partial \lambda^*}(\lambda) = D(0) + O(|\lambda|) \quad \text{as } \lambda \rightarrow 0,$$

and matrix $D(\lambda)$ defined in (16) is positive-semidefinite by construction. Far from equilibrium the closure potential could lose its convexity, however, and the solution matrix \hat{M} could become singular. In that situation the closed reduced equations would no longer be well-defined. This behavior would signify a bifurcation in the best-fit parameter trajectory, which we would interpret as a dynamic phase transition in the reduced model.

5 Near-equilibrium approximation

In this section we present the simpler and more explicit form of best-fit quasi-equilibrium closure that results from applying a linear response approximation [7, 40] in a neighborhood of the statistical equilibrium state ρ_{eq} . As in the preceding developments, the equilibrium density can be any invariant probability density for the underlying Hamiltonian dynamics. For instance, it can be a canonical Gibbs ensemble:

$$\rho_{eq}(z) = \exp(-\beta[H(z) - \psi(\beta)]), \quad \text{with } \psi(\beta) = \beta^{-1} \log \int_{\Gamma_n} \exp(-\beta H(z)) dz,$$

for some inverse temperature $\beta > 0$. We denote the equilibrium mean of any dynamical variable or vector F on Γ_n by $\langle F \rangle_{eq}$.

Since the quasi-equilibrium densities (1) reduce to the equilibrium density ρ_{eq} when $\lambda = 0$, the near-equilibrium theory is the linearization of the general theory around $\lambda = 0$. Throughout this analysis we assume that the resolved vector A is normalized relative to equilibrium by $\langle A \rangle_{eq} = 0$. We make the usual linear response approximation

$$\tilde{\rho}(z; \lambda) \approx [1 + \lambda^* A(z)] \rho_{eq}(z). \quad (29)$$

Under this approximation the Lagrangian $\mathcal{L}(\lambda, \dot{\lambda})$ defined in (14) becomes a quadratic form in the pair $(\lambda, \dot{\lambda})$:

$$\mathcal{L}(\lambda, \dot{\lambda}) \approx \frac{1}{2}[\dot{\lambda} - C^{-1}J\lambda]^* C [\dot{\lambda} - C^{-1}J\lambda] + \frac{\epsilon^2}{2}\lambda^* D \lambda, \quad (30)$$

where

$$C = \langle A A^* \rangle_{eq}, \quad J = \langle (LA) A^* \rangle_{eq}, \quad D = \langle (QLA) (QLA^*) \rangle_{eq} \quad (31)$$

The major simplification that occurs in the near equilibrium regime is that the coefficient matrices C, J, D defining (30) are constants determined by the equilibrium state ρ_{eq} . These matrices have the symmetry properties: $C^* = C$, $J^* = -J$, $D^* = D$. The projections P and $Q = I - P$ are also independent of λ , being orthogonal operators on $L^2(\Gamma_n, \rho_{eq})$. The Legendre transformation (19) and (20) now yields

$$\mu = C\dot{\lambda} - J\lambda, \quad \mathcal{H}(\lambda, \mu) = \frac{1}{2}\mu^* C^{-1} \mu - \lambda^* J C^{-1} \mu - \frac{\epsilon^2}{2}\lambda^* D \lambda,$$

in which the conjugate canonical variable, μ , is linear in the pair $(\lambda, \dot{\lambda})$, and the Hamiltonian, $H(\lambda, \mu)$, is a quadratic form. The closure potential w is the quadratic form,

$$w(\lambda) = \frac{1}{2}\lambda^* D \lambda, \quad \text{where} \quad D = \langle (LA)(LA^*) \rangle_{eq} + J C^{-1} J \quad (32)$$

Since the Hamiltonian is exactly quadratic, the Hamilton-Jacobi equation (21) admits a solution that is a quadratic form in λ :

$$v(\lambda, t) = \hat{v}(t) + \frac{1}{2}(\lambda - \hat{\lambda}(t))^* \hat{M}(t)(\lambda - \hat{\lambda}(t))$$

for some $m \times m$ symmetric matrix $\hat{M}(t)$, m -vector $\hat{\lambda}(t)$ and scalar $\hat{v}(t)$. Substitution of this ansatz into the Hamilton-Jacobi equation produces equations corresponding to the quadratic, linear and constant terms in λ . Namely,

$$0 = \frac{d\hat{M}}{dt} + \hat{M}C^{-1}\hat{M} - JC^{-1}\hat{M} + \hat{M}C^{-1}J - \epsilon^2 D,$$

$$0 = -\hat{M}\frac{d\hat{\lambda}}{dt} + \hat{M}C^{-1}J\hat{\lambda} - \epsilon^2 D\hat{\lambda},$$

$$0 = \frac{d\hat{v}}{dt} - \frac{\epsilon^2}{2}\hat{\lambda}^* D \hat{\lambda}.$$

The first of these equations is a matrix Riccati equation for \hat{M} . It is supplemented by the initial condition $\hat{M}(t_0) = M_0$ for a given positive-definite, symmetric matrix M_0 . The second of these equations determines the best-fit vector $\hat{\lambda}(t)$, and its initial condition is $\hat{\lambda}(t_0) = \lambda_0$. The third equation merely generates the additive constant $\hat{v}(t)$, and its initial condition may be set to zero, $\hat{v}(t_0) = 0$.

It is transparent that the near-equilibrium approximation produces a best-fit closure theory for which the local quadratic approximation discussed in the preceding section

holds globally. The structure of the governing equations for the parameter vector $\hat{\lambda}$ and the matrix \hat{M} is the same as in the general case, given in the preceding section, except that the coefficient matrices are constant and the Riccati equation decouples from the state equation. It is worthwhile to summarize the closed reduced equations governing near-equilibrium:

$$\begin{aligned}\frac{d\hat{\lambda}}{dt} &= [C^{-1}J - \epsilon^2\hat{M}^{-1}D]\hat{\lambda} \\ \frac{d\hat{M}}{dt} &= JC^{-1}\hat{M} - \hat{M}C^{-1}J - \hat{M}C^{-1}\hat{M} + \epsilon^2D\end{aligned}\tag{33}$$

The positive-definite, symmetric matrix $\hat{M}(t)$ has the interpretation as the confidence, or information, in the best-fit estimate $\hat{\lambda}(t)$ at each time t . In particular, if all the eigenvalues of $\hat{M}(t)$ are large, then the value function $v(\lambda, t)$ increases rapidly away from its minimum point at $\hat{\lambda}$, meaning that the best-fit estimate is sharp with respect to the lack-of-fit norm for the Liouville equation. In general, the eigenvalues and associated eigenvectors of $\hat{M}(t)$ characterize the multivariate sensitivity of the best-fit estimate, and their evolution in time quantifies the propagation of uncertainty in the reduced model. The inverse matrix, $\hat{G}(t) = \hat{M}(t)^{-1}$, furnishes an alternative characterization of uncertainty in the sense that it is comparable to a covariance matrix for the parameter vector λ . Moreover, as a straightforward calculation shows, the near-equilibrium closed reduced equations (33) have the following equivalent form in terms of $\hat{\lambda}$ and \hat{G} :

$$\begin{aligned}\frac{d\hat{\lambda}}{dt} &= [C^{-1}J - \epsilon^2\hat{G}D]\hat{\lambda} \\ \frac{d\hat{G}}{dt} &= C^{-1}J\hat{G} - \hat{G}JC^{-1} - \epsilon^2\hat{G}D\hat{G} + C^{-1}.\end{aligned}\tag{34}$$

This form has the attractive feature that matrix inversion is eliminated from the closed reduced dynamics. Moreover, the fully specified initial condition, $\lambda(0) = \lambda_0$ with improper v_0 or M_0 , is readily handled by the homogeneous initial condition $\hat{G}(0) = 0$ on the Riccati equation in (34).

Finally, the pair of equations (34) has a strong resemblance to the equations for a Kalman-Bucy filter [4, 11, 12]. That is, we may view the pair of equations (34) as a state estimate equation for $\hat{\lambda}$ coupled to a variance equation for \hat{G} . This similarity might be expected from the fact that our best-fit closure scheme is derived from a dynamic optimization principle, as are filtering algorithms. However, our problem is not a standard filtering problem, because we are concerned with fitting a statistical model to underresolved, deterministic dynamics rather than blending a stochastic dynamics with noisy measurements. Nonetheless, we can put our closure problem into a filtering format by regarding the linear mapping, $\lambda \mapsto QL(\lambda^*A)$, which takes a state λ into the unresolved component of the Liouville residual, as the measurement process. In this formal analogy the measured data is the zero function identically in time, so that the measurement error corresponds to the L^2 -norm of $QL(\lambda^*A)$. The defining minimization principle for our best-fit closure is thereby identified with a filtering principle for a squared-norm that blends

the resolved and unresolved components of the Liouville residual using a weight factor ϵ^2 . This interpretation may have some utility beyond providing a conceptual connection. Namely, it suggests that our best-fit closure scheme could be combined naturally with actual continuous measurements, and in this way the estimation of the resolved variables could be continually improved by a hybrid of closure and filtering. But we will not pursue this line of development in the present paper.

6 Simplification under time reversal symmetry

Before discussing the role of the adjustable parameter ϵ , which scales the dissipative effects in the best-fit closure, it is convenient first to display the simplified closed reduced equations that result from symmetry with respect to time reversal. Accordingly, we consider the special case in which each of the resolved variables, A_k ($k = 1, \dots, m$), composing A is even under time reversal. In this case, and in the case when $m = 1$ and $A = A_1$ is an arbitrary scalar variable, the near equilibrium equations can be solved explicitly and the thermodynamic properties of its solutions can be derived easily. Moreover, this case pertains to reduced models that are purely dissipative, a physically important situation [13].

Let $\Theta : \Gamma_n \rightarrow \Gamma_n$ denote the time reversal operator defined by $\Theta(q, p) = (q, -p)$ for $z = (q, p) \in \Gamma_n$. A dynamical variable F is even under time reversal if $F \circ \Theta = F$ on Γ_n . We assume that the Hamiltonian and ρ_{eq} are even. Then the phase flow $\Phi(t)$ on Γ_n satisfies $\Phi(t) = \Theta \circ \Phi(-t) \circ \Theta$. For any even dynamical variable, F , it follows that $F \circ \Phi(t) = F \circ \Phi(-t) \circ \Theta$.

For a resolved vector, $A = (A_1, \dots, A_m)$, composed of even component variables A_k , the matrix $J = \langle (LA)A^* \rangle_{eq}$ vanishes. This result follows directly from the fact that LA is odd under time reversal, which is easily seen from the identities:

$$\begin{aligned} (LA) \circ \Theta &= \lim_{\Delta t \rightarrow 0} \frac{A \circ \Phi(\Delta t) \circ \Theta - A \circ \Theta}{\Delta t} \\ &= \lim_{\Delta t \rightarrow 0} \frac{A \circ \Phi(-\Delta t) - A}{\Delta t} = -(LA). \end{aligned}$$

That $J = 0$ for any scalar resolved variable, $A \in \mathbb{R}^1$, is immediate from the skew-symmetry of J .

In the case of even resolved variables, the closed reduced equations (34) have a scaling structure with respect to the adjustable parameter ϵ . In terms of the rescaled time $\tau = \epsilon(t - t_0)$, we introduce the fundamental solution matrix, $\hat{\Psi}(\tau)$, for the state equation in (34) expressed as an equation for the macrostate $\hat{a}(t) = C\hat{\lambda}(t)$:

$$\frac{d\hat{a}}{dt} = -\epsilon^2 C \hat{G}(t; \epsilon) D C^{-1} \hat{a}$$

Representing the solution, $\hat{a}(t) = \hat{\Psi}(\epsilon t) a_0$, in terms of its initial state a_0 , and rewriting the solution of the Riccati equations in (34) in terms of the rescaled matrix $\hat{K}(\tau) =$

$\epsilon C \hat{G}(\tau/\epsilon; \epsilon) D$, we find that (34) is equivalent to the following pair of matrix equations:

$$\frac{d\hat{\Psi}}{d\tau} = -\hat{K} C^{-1} \hat{\Psi}, \quad \frac{d\hat{K}}{d\tau} = D - \hat{K} C^{-1} \hat{K}. \quad (35)$$

These equations are supplemented by the initial conditions, $\hat{\Psi}(0) = I$, $\hat{K}(0) = 0$, which are appropriate to the situation when the arbitrary initial macrostate $a_0 \in \mathbb{R}^m$ is completely specified; incomplete specification of the initial statistical state changes $\hat{K}(0)$.

The pair of matrix equations (35) can be simultaneously diagonalized and hence solved explicitly. Let W be a matrix of normalized eigenvectors of D relative to C , and let Δ be the corresponding diagonal matrix of eigenvalues, all of which are real and nonnegative. The nonsingular matrix W diagonalizes D relative to C , meaning that

$$W^* D W = \Delta \quad \text{and} \quad W^* C W = I.$$

Making the substitutions, $\bar{\Psi}(\tau) = W^* \hat{\Psi}(\tau) (W^*)^{-1}$ and $\bar{K}(\tau) = W^* \hat{K}(\tau) W$, in (35), we get the diagonalized matrix equations,

$$\frac{d\bar{\Psi}}{d\tau} = -\bar{K} \bar{\Psi}, \quad \frac{d\bar{K}}{d\tau} = \Delta - \bar{K}^2.$$

Their solutions are elementary: $\bar{\Psi}(\tau) = \text{sech}(\sqrt{\Delta} \tau)$ and $\bar{K}(\tau) = \sqrt{\Delta} \tanh(\sqrt{\Delta} \tau)$, where $\sqrt{\Delta}$ denotes the nonnegative square root of the nonnegative diagonal matrix Δ , and the hyperbolic functions act in the obvious way. Inverting the transformation, we obtain the desired solutions of (35); namely,

$$\hat{\Psi}(\tau) = (W^*)^{-1} \text{sech}(\sqrt{\Delta} \tau) W^*, \quad \hat{K}(\tau) = (W^*)^{-1} \sqrt{\Delta} \tanh(\sqrt{\Delta} \tau) W^{-1} \quad (36)$$

Returning to the closed reduced equations (34) expressed in unscaled time t , we now have a relaxation equation for the best-fit macrostate with an explicit, scaled, time-dependent coefficient matrix:

$$\frac{d\hat{a}}{dt} = -\epsilon \hat{K}(\epsilon(t - t_0)) \hat{\lambda}(t). \quad (37)$$

The format of (37) is reminiscent of the linear transport equations of phenomenological nonequilibrium thermodynamics [13, 24, 31]. In that setting, a separation of time scales between the evolution of the macrostate and the fluctuations of the microstate is assumed, and linear relaxation equations are posited to relate fluxes to forces. In our notation the thermodynamic forces are $-\hat{\lambda}$, while the thermodynamic fluxes are $d\hat{a}/dt$. In the well-known Onsager theory of near-equilibrium relaxation, the matrix of transport coefficients is usually denoted by L , and is constant in time, so that the phenomenological equations are

$$\frac{d\hat{a}}{dt} = -L \hat{\lambda}, \quad \text{with} \quad \hat{a}(t) = C \hat{\lambda}(t).$$

For a resolved vector A that is even under time reversal, the celebrated reciprocity relations imply that L must be symmetric. The entropy production is then $d\hat{s}/dt = \hat{\lambda}^* L \hat{\lambda}$,

and this expression is invoked to imply that L must be positive-definite. These classical results rely on a number of assumptions concerning the format of the macroscopic transport equations and the statistical properties of the microscopic fluctuations, namely the Onsager regression hypothesis.

By contrast, our relaxation equation (37) has a time-dependent transport matrix, $\epsilon \hat{K}(\epsilon(t - t_0))$, that is derived from the underlying dynamics via the best-fit model reduction, up to the adjustable parameter ϵ . Moreover, the best-fit transport matrix is necessarily positive-definite and symmetric by virtue of the Riccati equation [26]. Thus, our best-fit reduced dynamics shares the key qualitative properties of phenomenological irreversible thermodynamics: for the near-equilibrium, even-variable regime, it possesses positive entropy production and reciprocity relations. Furthermore, the derivation of the relaxation equation (37) from the Liouville equation does not require an extreme separation of time scales. Indeed, the time dependence of \hat{K} implies that there is a plateau effect during which $\hat{K}(\tau)$ increases from 0 to its asymptotic limit, \hat{K}_∞ , which is determined by $\hat{K}_\infty C^{-1} \hat{K}_\infty = D$. This plateau effect is regulated by the matrices C and D . More precisely, there are m plateau time scales, τ_1, \dots, τ_m , defined by $\text{diag} \{1/\tau_1, \dots, 1/\tau_m\} = \sqrt{\Delta}$, which give the rates at which the eigenvectors of $\hat{K}(\tau)$ equilibrate. Thus, we see that the scaled time variable $\tau = \epsilon(t - t_0)$ applies to the plateau effect, while the original time variable t pertains to the relaxation.

7 Irreversibility and the parameter ϵ

In this section we turn our attention to the role that the adjustable parameter ϵ plays in the best-fit approach to model reduction.

Broadly speaking, a reduced model for a complex dynamics with finitely-many degrees of freedom may be expected to exhibit three distinct time scales: (1) the relaxation time scale, T_r , over which the macroscopic resolved variables decay (and possibly oscillate); (2) a plateau time, T_p , over which fluctuations in the unresolved variables influence the resolved variables; and (3) a memory time, T_m , over which the unresolved fluctuations decorrelate. Moreover, these time scales generically have the ordering: $T_r > T_p > T_m$. In fact, a strong separation of time scales, $T_r \gg T_p \gg T_m$ is necessary to justify a Markovian stochastic model of the resolved variables. In the absence of such an extreme separation of time scales, the reduced dynamics is described by well-known generalized transport equations that are derived by the Mori-Zwanzig projection method [40]. This formal identity has recently been employed as the starting point for statistical closure for underresolved Hamiltonian dynamics [8, 9, 19]. This work follows a line of development in nonequilibrium statistical mechanics that have been pursued by various investigators in the past [2, 34, 36, 35, 39, 28]. While our approach is fundamentally different than these works, the generalized transport equations furnish a means of interpretation of our adjustable parameter ϵ and an explanation of how ϵ is related to the relevant times scales in the statistical closure.

We focus on the near-equilibrium of our theory and of the projection operator identity. To within the linear response approximation we are given an initial ensemble

$\rho_0 = \exp[\lambda_0^* A - \phi(\lambda_0)] \rho_{eq} \approx [1 + \lambda_0^* A] \rho_{eq}$, and we are interested in the evolution of the ensemble-averaged macrostate $a_{ex}(t) = \langle e^{(t-t_0)L} A | \rho_0 \rangle \approx \langle (e^{(t-t_0)L} A) A^* \rangle_{eq} \lambda_0$. The following Mori-Zwanzig formula, which is an exact consequence of the Liouville equation up to the near-equilibrium approximations, states that

$$\frac{da_{ex}}{dt} = JC^{-1}a_{ex} - \int_{t_0}^t Z(t-t') C^{-1}a_{ex}(t') dt', \quad (38)$$

where $Z(\theta) = \langle [e^{\theta QL}(QLA)](QLA^*) \rangle_{eq}$. The central difficulty faced when implementing this formula in practice is to find tractable approximations to the exact memory kernel $Z(\theta)$, which involves the complementary orthogonal propagator, $e^{\theta QL}$, in memory time θ .

To relate this formula to our best-fit closure, let us attach a quasi-equilibrium density to the exact macrostate, $a_{ex}(t)$, at each instant of time. That is, we define the corresponding parameter vector $\lambda_{ex}(t) = C^{-1}a_{ex}(t)$ and density $\rho_{ex}(t) = \tilde{\rho}(\lambda_{ex}(t))$. Of course, the goal of our closure scheme is to approximate the exact state $\lambda_{ex}(t)$ by the estimated state $\hat{\lambda}(t)$, which is computed without evaluation of the memory kernel $Z(\theta)$ or equivalent quantities. For the purposes of interpreting ϵ , we examine the entropy, $s_{ex} = \phi(\lambda_{ex}) - \lambda_{ex}^* a_{ex}$, of the quasi-equilibrium states attached to the exact states and calculate the associated entropy production. From (38) we find that

$$\frac{ds_{ex}}{dt} = \int_{t_0}^t \lambda_{ex}(t)^* Z(t-t') \lambda_{ex}(t') dt' \quad (39)$$

Correspondingly, the entropy production for our best-fit closure in the near-equilibrium regime is given by

$$\frac{d\hat{s}}{dt} = \epsilon^2 \hat{\lambda}(t)^* C \hat{G}(t; \epsilon) D \hat{\lambda}(t), \quad (40)$$

where \hat{G} is determined by the Riccati equation in (34). Roughly speaking, the free parameter ϵ should be adjusted so that the entropy production in (40) approximately matches that in (39). Since the memory kernel is not accessible in the best-fit reduced model, this adjustment is an empirical tuning [33].

To proceed further with the heuristic analysis, let us suppose that the resolved variable A is a scalar. Then, $J = 0$, and $C, D > 0$. Recalling the discussion in the preceding section, the plateau time is $T_p = \sqrt{D/C}$. We write the memory kernel in the form, $Z(\theta) = D\zeta(\theta/T_m)$, for a dimensionless function $\zeta(u)$ with $\zeta(0) = 1$ and $\lim_{u \rightarrow \infty} \zeta(u) = 0$; in other words, Z decays with a characteristic memory time scale T_m . Then assuming that the relaxation time scale, T_r , is large compared to T_m , we have

$$\frac{ds_{ex}}{dt} = \frac{C}{T_p^2} \int_{t_0}^t \lambda_{ex}(t) \zeta\left(\frac{t-t'}{T_m}\right) \lambda_{ex}(t') dt' \approx \frac{C T_m}{T_p^2} \lambda_{ex}(t)^2 \int_0^\infty \zeta(u) du.$$

On the other hand, in this scalar case the best-fit closure gives the approximation

$$\frac{d\hat{s}}{dt} \approx \frac{C\epsilon}{T_p} \hat{\lambda}(t)^2,$$

supposing that the T_r is large compared to T_p , and hence replacing $\hat{G}(t; \epsilon)$ by its asymptotic value $\hat{G}_\infty = T_p/C\epsilon$. These approximate expressions for the entropy production agree (up to some absolute constants) provided that $\epsilon \sim T_m/T_p$. Thus, we conclude that ϵ effectively sets the memory time scale, which is not evaluated in the best-fit closure scheme, relative to the plateau time, which is known. Moreover, a similar analysis applied to the relaxation equation for \hat{a} in (34) shows that its decay rate is approximately $\epsilon^2 \hat{G}_\infty D = \epsilon/T_p$. Consequently, we obtain the complementary result that $\epsilon \sim T_p/T_r$. The fact that $T_p/T_r \sim T_m/T_p$ is already implied by (38) when there is a separation of time scales.

In essence, the single adjustable parameter ϵ represents the minimal amount of extra information about memory effects that must be included into the best-fit closure scheme. Since ϵ enters into the lack-of-fit Lagrangian as a scale factor for the closure potential w that determines the irreversible terms in the closed reduced equations, it is manifest that ϵ regulates the magnitude of dissipation in the reduced model. As the discussion in this section shows, the appropriate value of ϵ is related to a common ratio of the characteristic time scales in the model reduction problem. But, from the point of view of implemented computations, these rough estimates do not suffice to determine ϵ quantitatively. Rather, ϵ must be estimated from some observations or simulations that are not part of the best-fit closure itself.

Our presentation throughout this paper has been restricted to a single adjustable parameter ϵ , and the heuristic analysis given above applies only to a single scalar resolved variable A . In a companion paper [33], we implement the model reduction in this form and investigate quantitatively how well the statistical closure scheme approximates fully resolved statistical solutions. In such investigations, and in other potential applications, the single parameter theory can be expected to perform well when it is possible to identify a memory time and a plateau time, at least approximately, that pertain to all the resolved variables. In general, when multiple time scales operate, a better approximation might be obtained by a more intricate construction of the lack-of-fit functional. Specifically, we could replace the Lagrangian (14) by

$$\mathcal{L}(\lambda, \dot{\lambda}) = \frac{1}{2} \langle (P_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle + \frac{1}{2} \langle (E_\lambda Q_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle,$$

in which E_λ is a self-adjoint, positive operator on $L^2(\Gamma_n, \tilde{\rho}(\lambda))$, possibly depending on λ , with operator norm, $\|E_\lambda\| \leq 1$. Throughout the present paper $E_\lambda = \epsilon I$. By designing other operators E_λ the resulting closure potential w might more faithfully represent the influence of the unresolved fluctuations on the resolved variables. The best-fit strategy would carry over to this generalization, but its practical implementation would require multiple tuned parameters.

8 Discussion and conclusions

The methodology presented in this paper offers a new approach to the general problem of constructing a reduced statistical-dynamical description of a complex Hamiltonian system.

Most approaches to problems of this kind in nonequilibrium statistical mechanics interpose a stochastic model between the given microscopic dynamics and the derived macroscopic dynamics, while our approach deduces an irreversible macrodynamics for the selected set of resolved variables directly from the deterministic and reversible microdynamics. Our method is based on an optimization principle for parameterized paths of trial probability densities on phase space: paths that achieve the least residual with respect to the Liouville equation determine the evolution of the estimated macrostates. This approach provides an information-theoretic meaning to the statistical closure, since the best-fit paths minimize a cost functional that measures the rate of information loss incurred by the model reduction. Moreover, it leads to a closure theory having a form analogous to optimal filtering theory. That is, the best-fit closure blends unresolved microdynamics into the reduced equations for the resolved macrostate via a matrix of transport coefficients in much the same way that the Kalman-Bucy filter assimilates continuous measurements into a stochastic state equation via a gain matrix. By formulating the prediction of underresolved dynamics as optimal estimation, the best-fit approach furnishes a new perspective on statistical closure of complex, chaotic, or turbulent dynamics.

The value function for the defining optimization principle is a key ingredient in the best-fit closure theory. It has the units of entropy production, it represents the optimal cost of reduction with respect to the selected resolved variables, and it solves the Hamilton-Jacobi equation associated with the cost function. The best-fit macrostate corresponds to the evolving minimizer of the value function, while the uncertainty of the best-fit estimate is measured by the Hessian matrix of the value function at the minimizer. We may say that our Hamilton-Jacobi equation plays a role analogous to that of the Fokker-Planck equation for a stochastic model whose resolved variables are described by a Langevin dynamics. One conclusion of our work is that irreversible behavior can be derived from an optimization principle and its related Hamilton-Jacobi theory, without explicitly introducing diffusive processes.

Criteria for the choice of the resolved variables are not considered in this paper, but this is an important aspect of any model reduction strategy. In some physical problems it may be evident that certain variables offer a thermodynamic, or kinetic, description, and thus are natural resolved variables. The separation of time scales between resolved and unresolved motions often informs this choice. More generally, though, there may be latitude in the selection of the resolved variables, and the design of a good model reduction may require examining a variety of sets of resolved variables. In the best-fit closure, a preferred choice would be one for which the uncertainty of the estimated macrostate, as measured by the second-order behavior of the value function, is relatively small. In principle, therefore, the theory itself offers a method of distinguishing the predictive power of different sets of resolved variables. We leave the issue of designing reduced descriptions, however, to future investigations of particular problems with the best-fit methodology.

The framework for statistical model reduction that we propose in this work is intended to be implemented on complex, multi-scale dynamical problems. To this end, the local quadratic approximation of the value function in the far-from-equilibrium regime and the related simplification in the near-to-equilibrium regime are developed so that the numerical solution of the Hamilton-Jacobi equation itself is avoided. Under these approxi-

mations the best-fit closure theory admits a computationally effective implementation, since sophisticated and powerful numerical methods exist for the integration of Riccati matrix differential equations. The best-fit approach does not require the computation of memory kernels, which arise in approaches through Mori-Zwanzig projection methods and necessitate either simulations of cumbersome propagators or analytical approximations available only in limiting situations. Instead, the tunable parameter ϵ introduces a single time-scale separation into the best-fit reduction strategy. We recognize, though, that extensions of our basic methodology would likely involve more elaborate trial densities and more detailed lack-of-fit norms, which would include multiple time-scale parameters.

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