An optimization principle for deriving nonequilibrium statistical models of Hamiltonian dynamics

Bruce Turkington
Department of Mathematics and Statistics
University of Massachusetts Amherst

Abstract

A general method for deriving closed reduced models of Hamiltonian dynamical systems is developed using techniques from optimization and statistical estimation. As in the standard projection operator methodology of statistical mechanics, a set of resolved variables is selected to capture the slow, macroscopic behavior of the system, and the family of quasi-equilibrium probability densities on phase space corresponding to these resolved variables is employed as a statistical model. The macroscopic dynamics of the mean resolved variables is determined by optimizing over paths of these probability densities. Specifically, a cost function is introduced that quantifies the lack-of-fit of a feasible path to the underlying microscopic dynamics; it is an ensemble-averaged, squared-norm of the residual that results from submitting a path of trial densities to the Liouville equation. The evolution of the macrostate is estimated by minimizing the time integral of the cost function over such paths. Thus, the defining principle for the reduced model takes the form of Hamilton’s principle in mechanics, in which the Lagrangian is the cost function and the configuration variables are the parameters of the statistical model. The value function for this optimization, which plays the role of the action integral, satisfies the associated Hamilton-Jacobi equation, and it determines the optimal relation between the statistical parameters and the irreversible fluxes of the resolved variables, thereby closing the reduced dynamics. The resulting equations for the macroscopic variables have the generic form of governing equations for nonequilibrium thermodynamics, and they furnish a rational extension of the classical equations of linear irreversible thermodynamics beyond the near-equilibrium regime. In particular, the value function is a thermodynamic potential that extends the classical dissipation function and supplies the nonlinear relation between thermodynamics forces and fluxes.

Key Words and Phrases: model reduction, statistical closure, dynamical optimization, nonequilibrium thermodynamics.
1 Introduction

A main goal of nonequilibrium statistical mechanics is the derivation of effective equations for macroscopic behavior from the equations of motion that govern an underlying microscopic dynamics [2, 16, 25, 26, 39, 40, 45]. Unlike equilibrium statistical mechanics, which rests on the firm foundation of conserved variables and Gibbsian ensembles, this endeavor is necessarily imperfect and approximate. First, it relies on the choice of relevant macroscopic variables, which is not universal. Even though in traditional settings such as hydrodynamics, the local equilibrium hypothesis can be invoked to justify the use of locally conserved quantities, in many situations it may be advantageous to consider reduced or extended sets of relevant variables [24]. Second, the selection of a macroscopic description depends on the existence of a separation of time scales between the relevant variables that evolve on a slow time scale and the remaining microscopic variables that are expected to equilibrate on fast time scales. But, in some problems for which a statistical mechanical description is sought, such as fluid turbulence, a wide separation between fast and slow variables may not be present [32]. Third, when equations of motion for the relevant variables are derived by standard projection operator methods, they contain finite-memory effects and non-Markovian stochastic forcing terms, which are clumsy to handle until further approximations or limits are adopted to bring them to more tractable forms [11, 12]. As a consequence, most statistical treatments of nonequilibrium phenomena are restricted to idealized physical models having special microscopic dynamics. Often a key simplification is to replace a deterministic microscopic dynamics by a stochastic process at the outset of the analysis, constructing the process to be compatible with equilibrium fluctuations [19].

In the present paper we take a different approach, in that we seek to characterize the governing equations for a given set of relevant, or resolved, variables by applying a statistical model reduction procedure to the underlying deterministic dynamics itself, which we take to be a general Hamiltonian system having finitely-many degrees of freedom. The central idea in our approach is a dynamical optimization principle over paths of macrostates, which may be outlined as follows. (i) Relative to a given set of resolved variables, a parametric statistical model of the system is imposed using quasi-equilibrium probability densities with parameters conjugate to the expectations of the resolved variables. (ii) A macroscopic evolution is identified with a path in the parameter space of these trial probability densities, and the lack-of-fit of such a path to the underlying Hamiltonian dynamics is quantified by a certain cost functional, which is a time-integrated, weighted, squared norm of the residual of those densities with respect to the Liouville equation. (iii) The estimated, or predicted, evolution of the macrostate is determined by that path which minimizes the lack-of-fit cost functional. In this way we derive an irreversible, dissipative dynamics that is closed in the macrovariables and is optimally compatible with the underlying conservative, reversible microdynamics in a quantified, statistical sense.

A particularly desirable feature of the closed reduced equations derived via our approach is that they have the structure of the general equations for nonequilibrium thermodynamics proposed by contemporary researchers [35, 21, 38, 37, 4, 3]. In particular, our model reduction strategy may be viewed as a dynamical variational principle that
justifies the so-called GENERIC (General Equations of NonEquilibrium Reversible Irreversible Coupling) format for out-of-equilibrium dynamics [37]. In the notation used in the body of our paper, these equations have the form

$$\frac{da_i}{dt} = \sum_j \Omega_{ij} \frac{\partial h}{\partial a_j} - \frac{\partial v}{\partial \lambda^i},$$  \hspace{1cm} (1)

in which \( a = (a_1, \ldots, a_m) \) denotes the macrostate vector, which is the expectation of the given vector of resolved variables \( A = (A_1, \ldots, A_m) \) defined on the phase space of the Hamiltonian dynamics. The vector \( \lambda = (\lambda^1, \ldots, \lambda^m) \) consists of parameters conjugate to \( a \), given by \( \lambda^i = -\partial s/\partial a_i \), where \( s = s(a) \) is the entropy of the macrostate \( a \). The first term in (1) is a generalized Hamiltonian vector field having an energy function \( h = h(s, a) \) and a Poisson matrix \( \Omega = \Omega(a) \), which is anti-symmetric; the partial derivatives \( \partial h/\partial a \), are at constant entropy \( s = s(a) \). This term governs the reversible part of the reduced dynamics. The second term in (1) is a gradient vector field with respect to the parameter vector \( \lambda \) having the potential function \( v = v(\lambda) \). This term governs the irreversible part of the reduced dynamics. In our variational formulation the thermodynamic potential \( v(\lambda) \) is the value function for the optimization principle; that is, \( v(\lambda) \) equals the optimal value of the lack-of-fit cost functional in the minimization over paths emanating from the macrostate with parameter vector \( \lambda \) and tending to equilibrium in infinite time. The value function therefore solves the time-independent Hamilton-Jacobi equation associated with optimization principle. The functions \( h(s, a) \) and \( \Omega(a) \) in the reversible term are entirely dictated by the form of the trial probability densities defining the statistical model. By contrast, the value function \( v(\lambda) \) depends on the weights introduced into the lack-of-fit cost function, and these weights determine the adjustable parameters of the ensuing closure theory.

Under the near-equilibrium approximation, the closed reduced equations (1) take the classical form of linear irreversible thermodynamics [15]. Namely, a linear system of differential equations relates the fluxes \( da_i/dt \) to the affinities (or thermodynamic forces) \(-\lambda^i\); namely,

$$\frac{da_i}{dt} = \sum_j \left[ \beta^{-1} \Omega_{ij} - M_{ij} \right] \lambda^j, \hspace{1cm} a_i = \sum_j C_{ij} \lambda^j. \hspace{1cm} (2)$$

The coefficients in these equations are evaluated at equilibrium, \( a = 0; \beta \) is the inverse temperature, and the matrix \( (C_{ij}) \) is the inverse of the matrix \(-((\partial^2 s/\partial a_i \partial a_j))\). In this formula \( M \) is the symmetric and positive-definite matrix that defines the near-equilibrium value function, which is the quadratic form

$$v(\lambda) = \frac{1}{2} \sum_{i,j} M_{ij} \lambda^i \lambda^j.$$  

The physical meaning of the value function becomes transparent from these identities, which imply that \( ds/dt = 2v(\lambda) \). That is, the optimal value of the cost functional coincides with half the entropy production along the best-fit path.
Beyond the regime in which these near equilibrium approximations hold, the closed reduced equations (1) remain valid as the nonlinear equations that determine the best fit of the statistical model to the underlying dynamics. The utility of these equations depends on the choice of the resolved variables and the separation of time scales between the resolved and unresolved variables in the statistical model, not on the closeness of the modeled macrostates to equilibrium. In the far-from-equilibrium regime the value function \( v(\lambda) \) furnishes a natural extension of the classical dissipation function that is justified by a statistical mechanical derivation. Accordingly, our optimization-based derivation of the GENERIC theory offers both a new interpretation of the potential for the irreversible part of the governing equations (1), and a systematic way to calculate nonlinear corrections to the classical linear equations (2).

The paper is organized as follows. Section 2 presents the background on the general closure problem and introduces the family of trial probability densities that constitute the statistical model. In Section 3 the stationary version of the defining optimization principle is formulated and the general nonequilibrium equations for the best-fit reduced model are derived. Properties of these equations are discussed in Section 4, as well as the near-equilibrium linearization of the reduced model. In Section 5 the theory is extended to include an initial period of development during which the entropy production increases from zero. This plateau effect is encountered when the specified initial statistical state is itself a quasi-equilibrium ensemble. The value function then becomes time-dependent, \( v = v(\lambda, t) \), and solves a time-dependent Hamilton-Jacobi equation. Section 6 discusses the conceptual framework of the best-fit approach to closure and points to some specific test cases and applications.

2 Statistical model and trial densities

The underlying microscopic dynamics is assumed to be a Hamiltonian system. In canonical form the equations of motion are

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

where \( z = (q, p) \) denotes a generic point in the phase space \( \Gamma_n = \mathbb{R}^{2n} \), \( n \) being the number of degrees of freedom of the system [1, 30]. Our theoretical development permits general systems of this kind, with time-independent, smooth Hamiltonians \( H \) on \( \Gamma_n \). In fact, our development only makes use of the general structure of the underlying microscopic dynamics — essentially, the conservation of energy and phase volume. Consequently it also applies without fundamental modifications to dynamical systems in a noncanonical Hamiltonian form. It is many such noncanonical systems, however, there are conserved quantities other than \( H \) which play an important role in conditioning the statistical behavior of the dynamics. A version of the theory appropriate to infinite-dimensional dynamics, such as occur in continuum models, could also be formulated. But it would be necessary to carry out a limiting analysis of discretized models in order to justify the statistical description. For the sake of definiteness, therefore, we restrict our discussion to finite-dimensional, canonical systems (3).
We are interested in making predictive estimates of some relevant macroscopic dynamical variables rather than following the details of the microscopic dynamics (3) itself. We therefore seek a statistical closure in terms of some resolved dynamical variables. In keeping with the general character of our approach, we allow any finite number of arbitrary resolved variables $A_k, k = 1, \ldots, m$, assuming that each is a smooth real-valued function on $\Gamma_n$ and the set $A_1, \ldots, A_m$ is linearly independent. We assemble them into the resolved vector $A = (A_1, \ldots, A_m)$. Typically, $m \ll n$.

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

$$\frac{dF}{dt} = \{F, H\}, \quad (4)$$

where $\{F, H\} = (\nabla F)^* J \nabla H$ is the Poisson bracket associated with the canonical Hamiltonian structure. Indeed, the statement that (4) holds for all smooth functions $F$ on $\Gamma_n$ is equivalent to the Hamiltonian dynamics (3). Fundamentally, the problem of closure in terms of the resolved variables $A_1, \ldots, A_m$ arises from the fact that, except under very special circumstances, the derived variables $\{A_1, H\}, \ldots, \{A_m, H\}$ are not expressible as functions of the resolved variables $A_1, \ldots, A_m$. This generic fact makes a statistical description of the unresolved variables necessary. The foundation for such a statistical description is provided by the Liouville equation, which governs the propagation of probability under the phase flow. Namely, for probability measures on $\Gamma_n$, $p(dz,t) = \rho(z,t)dz$, having smooth densities $\rho$ with respect to the invariant, $2n$-dimensional, phase volume element $dz = dq dp$,

$$\frac{\partial \rho}{\partial t} + L \rho = 0 \quad \text{in } \Gamma_n \times \mathbb{R}, \quad (5)$$

in which $L = \{\cdot, H\}$ denotes the Liouville operator. Given a density $\rho(z,t_0)$ at an initial time $t_0$, (5) completely determines the density $\rho(z,t)$ at any later time $t$, which is denoted formally by $\rho(\cdot, t) = e^{-(t-t_0)L} \rho(\cdot, t_0)$. We denote the expectation of any dynamical variable $F$ with respect to $\rho(t)$ by

$$\langle F|\rho(t) \rangle = \int_{\Gamma_n} F(z) \rho(z,t) \, dz.$$  

[This bracket notation is used for expectation throughout the paper.] The Liouville equation is equivalent to the statement that

$$\frac{d}{dt} \langle F|\rho(t) \rangle = \langle LF|\rho(t) \rangle$$  

for every dynamical variable $F$. In particular, the evolution of the mean of the resolved vector, $a(t) = \langle A|\rho(t) \rangle$, is determined by the exact solution of (5). But the exact density $\rho(z,t)$ evolving under the Liouville equation is highly intricate; it contains vastly more information than the resolved $m$-vector $a(t)$; and, it is excessively expensive to compute numerically, since it requires the integration of the microscopic trajectories starting from each sample point in an initial ensemble that approximates the given initial density.

For this reason we seek a statistical closure in terms of an analytically tractable family of trial probability densities having the same level of complexity as the resolved variables.
themselves. In the nomenclature of statistical inference, we impose a parametric statistical model for which the resolved vector $A$ is a minimal sufficient statistic $[9, 28]$. We denote this family of probability densities by $\hat{\rho}(z; \lambda)$, using a parameter vector $\lambda = (\lambda^1, \ldots, \lambda^m) \in \mathbb{R}^m$. The family is assumed to be regular, meaning that the densities depend smoothly on $\lambda$, the score variables are defined by

$$U(\lambda) = \frac{\partial \log \hat{\rho}(\lambda)}{\partial \lambda},$$

and the Fisher information matrix defined by

$$C(\lambda) = \langle (U(\lambda))^* \hat{\rho}(\lambda) \rangle$$

is nonsingular. [Here and throughout the paper we use the notation $M^*$ to denote the transpose of any matrix $M$; in particular, a column vector $V$ is taken to its dual row vector $V^*$. Also, we use the shorthand notation $\partial/\partial \lambda = (\partial/\partial \lambda^1, \ldots, \partial/\partial \lambda^m).$] The assumption that $A$ is a minimal sufficient statistic for the family $\hat{\rho}(\lambda)$ implies that there is a one-to-one correspondence between the expected resolved vector $a = \langle A \mid \hat{\rho}(\lambda) \rangle$ and the parameter vector $\lambda$. Accordingly, each macrostate can be identified with a unique parameter vector $\lambda$, which ranges over the configuration space $\mathbb{R}^m$, or perhaps a subset of it. We assume that the parameterization in terms of $\lambda$ is arranged so that the origin, $\lambda = 0$, is an equilibrium density, meaning that $L \hat{\rho}(0) = 0$.

Our interest centers on modeling the relaxation of the macrostate, $a(t) = \langle A \mid \hat{\rho}(\lambda(t)) \rangle$, from a specified nonequilibrium macrostate $a^0$ at time $t = 0$ towards equilibrium. Such a relaxation corresponds to a path $\lambda(t)$ in parameter space for which $\lambda(0) = \lambda_0 \neq 0$ and $\lambda(t) \to 0$ as $t \to +\infty$.

Even though we formulate the best-fit closure concept in such a general setting, we concentrate our attention in this paper on the model that uses the family of quasi-equilibrium, or quasi-canonical, densities $[22, 23, 31, 43]$,

$$\bar{\rho}(z; \beta, \lambda) = \exp[-\beta H + \lambda^* A - \psi(\beta, \lambda)],$$

in which

$$\psi(\beta, \lambda) = \log \int_{\Gamma_n} \exp(-\beta H + \lambda^* A) \, dz.$$  

[Here and throughout, $\lambda^* A = \sum_i \lambda^i A_i$.] These densities depend on the inverse temperature $\beta$ as well as the parameters $\lambda^1, \ldots, \lambda^m$ associated with the nonconserved resolved variables. Some growth conditions on $H$ and $A$ at infinity may be required to ensure that the normalization (10) exists and is finite; for simplicity in our exposition, we assume that these densities exist for all $\beta > 0$ and $\lambda \in \mathbb{R}^m$. The associated entropy function, $s(u, a)$, of the mean energy, $u$, and the mean resolved vector $a$, is determined by the maximum entropy principle,

$$s(u, a) = \max_{\rho} -\langle \log \rho \mid \rho \rangle \quad \text{subject to} \quad \langle H \mid \rho \rangle = u, \; \langle A \mid \rho \rangle = a, \; \langle 1 \mid \rho \rangle = 1. \quad (11)$$

The maximizer in (11) is the quasi-canonical density (9), and the parameter $\beta$ and parameter vector $-\lambda$ are Lagrange multipliers for the constraints on mean energy and mean
resolved vector, respectively. The entropy function \( s(u, a) \) is the negative of the convex conjugate function to \( \psi(\beta, \lambda) \) defined in (10); that is, \( -s(u, a) \) is the Legendre transform of \( \psi(\beta, \lambda) \), and hence all the following relations hold:

\[
-s(u, a) = -\beta u + \lambda^* a - \psi(\beta, \lambda), \quad -\frac{\partial \psi}{\partial \beta} = u, \quad \frac{\partial \psi}{\partial \lambda} = a, \quad \frac{\partial s}{\partial u} = \beta, \quad \frac{\partial s}{\partial a} = \lambda.
\]

There are two ways to handle the dependence of the family (9) on \( \beta \), or equivalently, on the mean energy \( u = \langle H | \bar{\rho} \rangle \), and this choice leads to two versions of the best-fit closure theory.

In one version we fix \( \beta > 0 \) and set \( \tilde{\rho}(\lambda) = \bar{\rho}(\beta, \lambda) \). The equilibrium density \( \tilde{\rho}(0) \) is the canonical Gibbs ensemble on \( \Gamma_n \),

\[
\rho_{eq}(z) = Z(\beta)^{-1} \exp(-\beta H(z)), \quad \text{with} \quad Z(\beta) = \int_{\Gamma_n} \exp(-\beta H(z)) \, dz. \tag{12}
\]

We let \( \langle F \rangle_{eq} \) denote expectation of any dynamical variable \( F \) with respect to \( \rho_{eq} \). The canonical statistical model with fixed inverse temperature therefore consists of the densities

\[
\tilde{\rho}(z; \lambda) = \exp(\lambda^* A - \phi(\lambda)) \rho_{eq}(z), \quad \text{with} \quad \phi(\lambda) = \log \langle \exp(\lambda^* A) \rangle_{eq}. \tag{13}
\]

Under this choice of trial densities the mean energy \( \langle H | \tilde{\rho}(\lambda) \rangle \) is allowed to vary along a path \( \lambda = \lambda(t) \). This version of the model is appropriate to a physical system in which an energy reservoir maintains a constant system temperature.

A standard motivation for using the family of densities (13) is that each member of the family minimizes relative entropy subject to the mean value of the resolved vector; that is, \( \tilde{\rho} \) solves

\[
-\tilde{s}(a) = \min_{\rho} \langle \log \frac{\rho}{\rho_{eq}} | \rho \rangle \quad \text{subject to} \quad \langle A | \rho \rangle = a, \quad \langle 1 | \rho \rangle = 1.
\]

From the perspective of information theory [13, 28], \( \tilde{\rho}(z; \lambda) \) is the least informative probability density relative to the equilibrium density \( \rho_{eq} \) that is compatible with the macrostate vector \( a = \langle A | \tilde{\rho} \rangle \). The relative entropy, \( -\tilde{s}(a) \), as a function of the mean resolved vector, \( a \), is the Legendre transform of \( \phi(\lambda) \), and the one-to-one correspondence between \( \lambda \) and \( a \) is a convex duality given by

\[
a = \frac{\partial \phi}{\partial \lambda}, \quad \lambda = -\frac{\partial \tilde{s}}{\partial a}. \tag{14}
\]

In statistical inference, (13) is called an exponential family relative to \( \rho_{eq} \) with natural parameter \( \lambda \) [9]. The score vector, \( U(\lambda) = A - a \), is the resolved vector centered around its mean, \( a = \langle A | \tilde{\rho}(\lambda) \rangle \). The Fisher information is \( C(\lambda) = \langle (A - a)(A - a)^* | \tilde{\rho}(\lambda) \rangle \), the covariance matrix for the resolved variables.

In the alternative version we impose the conservation of mean energy \( E = \langle H | \tilde{\rho}(\lambda(t)) \rangle \) exactly along paths \( \lambda(t) \). This constraint is achieved by allowing \( \beta = \beta(\lambda) \) to vary with \( \lambda \), and setting \( \tilde{\rho}(\lambda) = \tilde{\rho}(\beta(\lambda), \lambda) \). From a physical perspective this version is appropriate whenever the model system is isolated. Moreover, it leads to a closed reduced dynamics.
having precisely the form of GENERIC thermodynamics [37]. For these reasons, we also develop this version of the best-fit closure theory in the present paper, even though the version with fixed temperature is technically simpler.

The function $\beta(\lambda)$ is determined by the requirement that, for all admissible parameter vectors $\lambda$,

$$\langle H | \tilde{\rho}(\beta, \lambda) \rangle = -\frac{\partial \psi}{\partial \beta}(\beta, \lambda) = E,$$

where $E$ is the equilibrium energy corresponding to $\lambda = 0$. The unique solvability of this equation for $\beta = \beta(\lambda)$ is ensured by the strict convexity of $\psi$. Differentiating (15) with respect to $\lambda$ yields

$$0 = \frac{\partial}{\partial \lambda} \langle H | \tilde{\rho}(\lambda) \rangle = \langle (H - E)U(\lambda) | \tilde{\rho}(\lambda) \rangle,$$

where the score vector in this energy-conserving model is

$$U(\lambda) = (A - a) - \frac{\langle (H - E)(A - a) | \tilde{\rho} \rangle}{\langle (H - E)^2 | \tilde{\rho} \rangle} (H - E).$$

Thus, the score variables $U_i(\lambda)$ are the centered resolved variables $A_i$ projected onto the subspace of $L^2(\Gamma_n, \tilde{\rho})$ orthogonal to the centered Hamiltonian $H - E$. The Fisher information matrix (8) is the covariance matrix for these projected resolved variables:

$$C(\lambda) = \langle (A - a)(A - a)^* \rangle - \frac{\langle (H - E)(A - a) | \tilde{\rho} \rangle \langle (H - E)(A - a)^* \rangle}{\langle (H - E)^2 | \tilde{\rho} \rangle}. \quad (17)$$

Before proceeding to formulate our optimization principle over paths of macrostates, let us first review a naive closure procedure for the quasi-equilibrium probability densities $\tilde{\rho}(\lambda)$ that produces the reversible part of the closed reduced dynamics, but entirely suppresses the irreversible part [20]. Motivated by the moment equations (6), which hold for any dynamical variable $F$ and for the exact Liouville solution $\rho(\cdot, t)$, one may impose the $A$-moments of the Liouville equation on the trial densities $\tilde{\rho}(\lambda(t))$. Then the parameter path $\lambda(t) \in \mathbb{R}^m$ is required to satisfy the $m$ differential equations

$$0 = \langle A | \frac{\partial \tilde{\rho}}{\partial t} + L\tilde{\rho} \rangle = \frac{d}{dt} \langle A | \tilde{\rho} \rangle - \langle LA | \tilde{\rho} \rangle.$$

This simple moment closure with quasi-equilibrium densities is memoryless, and consequently it is entropy conserving. The entropy production calculation is:

$$\frac{ds}{dt} = -\lambda^* \frac{da}{dt} = -\langle L(\lambda^* A) | \tilde{\rho}(\lambda) \rangle$$

$$= -\int_{\Gamma_n} \{\lambda^* A, H\} \exp[-\beta H + \lambda^* A - \psi(\beta, \lambda)] dz$$

$$= -\int_{\Gamma_n} \{\exp[-\beta H + \lambda^* A - \psi(\beta, \lambda)], H\} dz = 0.$$

The last equality makes use of the general integration-by-parts identity,

$$\int_{\Gamma_n} \{F_1, F_2\} F_3 dz = -\int_{\Gamma_n} \{F_3, F_2\} F_1 dz,$$
which is also used in several calculations to follow.

The closed reduced equations governing this adiabatic closure can be written as

\[ \frac{da}{dt} = f(\lambda), \quad \text{with} \quad \lambda = -\frac{\partial s}{\partial a}, \tag{18} \]

introducing the vector field

\[
f(\lambda) = \langle \{LA|\tilde{\rho}(\lambda)\rangle \\
= \int_{\Gamma_n} \{A, H\} \exp[-\beta H + \lambda^* A - \psi(\beta, \lambda)] \, dz \\
= -\beta^{-1} \int_{\Gamma_n} \{A, \exp[-\beta H]\} \exp[\lambda^* A - \psi(\beta, \lambda)] \, dz \\
= \beta^{-1} \int_{\Gamma_n} \{A, \exp[\lambda^* A - \psi(\beta, \lambda)]\} \exp[-\beta H] \, dz \\
= \beta^{-1} \langle \{A, A^*\} | \tilde{\rho}(\lambda) \rangle \lambda.
\]

In either version of the model, with fixed \( \beta \) or fixed \( E \), it is possible to express \( f(\lambda) \) as a generalized Hamiltonian vector field. In both cases the energy representation, \( u = h(s,a) \), which inverts the entropy representation, \( s = s(u,a) \), plays a central role.

For the model with fixed \( \beta \), we introduce the associated free energy function

\[ \tilde{h}(\beta,a) = u - \beta^{-1} s. \tag{20} \]

Technically, \( \tilde{h} \) is the negative of the convex function conjugate to \( h(s,a) \) with respect to \( s \), considered as a function of the temperature \( \theta = \beta^{-1} = \partial h/\partial s \). A straightforward calculation using the properties of the Legendre transform yields

\[
\frac{\partial \tilde{h}}{\partial a} = -\beta^{-1} \frac{\partial s}{\partial a} = \beta^{-1} \lambda,
\]

in which the \( a \)-gradient of the free energy, \( \tilde{h} \), is a constant temperature. Substituting this expression into (19), we obtain the adiabatic closed reduced equation (18) in the form,

\[ \frac{da}{dt} = \Omega(a) \frac{\partial \tilde{h}}{\partial a}. \tag{21} \]

Here we introduce the Poisson matrix,

\[ \Omega = \langle \{A, A^*\} | \tilde{\rho}(\lambda) \rangle, \tag{22} \]

which we consider as a function of \( a \), recalling that there is a smooth, invertible mapping between \( \lambda \) and \( a \). The \( m \times m \) matrix \( \Omega \) is antisymmetric, state-dependent, and not necessarily invertible. Consequently, the reduced dynamics (21) is a generalized Hamiltonian system, or Poisson system, with a possibly degenerate symplectic structure. Nonetheless, it determines a well-defined reversible dynamics for any regular set of resolved variables \([4, 37]\).
For the energy-conserving model, entropy at fixed mean energy $E$ depends on $a$ alone: $s = s(E,a)$. Differentiating the identity $E = h(s(E,a),a)$ with respect to $a$ yields

$$0 = \frac{\partial h}{\partial s} \frac{\partial s}{\partial a} + \frac{\partial h}{\partial a} = \beta^{-1}(-\lambda) + \frac{\partial h}{\partial a}.$$

As in (21), we thereby obtain the adiabatic closed reduced dynamics in the form

$$\frac{da}{dt} = \Omega(a) \frac{\partial h}{\partial a},$$

in which the $a$-gradient of the mean energy, $h$, is at constant entropy.

### 3 Stationary formulation

The adiabatic closure discussed in the previous section imposes the $A$-moment of the Liouville equation on the quasi-equilibrium probability densities $\tilde{\rho}(\lambda)$, for $\lambda = \lambda(t) \in \mathbb{R}^m$, and thereby determines $m$ ordinary differential equations of first order for the evolution of the macrostate $a(t) = \langle A | \tilde{\rho}(\lambda(t)) \rangle$. This dissipationless closure is clearly deficient as a model of the statistical behavior of the resolved vector $A \in \mathbb{R}^m$, because it suppresses the influence of the unresolved variables on the resolved variables. The traditional remedy for this deficiency is to obtain closure by taking the $A$-moment with respect to a family of probability densities on phase space having memory [31, 43, 44]. The customary choice is given by the so-called theory of nonequilibrium statistical operators, in which the densities have the form

$$\rho_\epsilon(\cdot,t) = \int_0^\infty e^{-\tau L} \tilde{\rho}(\cdot;\lambda(t-\tau)) \epsilon e^{-\epsilon \tau} d\tau.$$  

(24)

Such a density $\rho_\epsilon(\cdot,t)$ is a functional of the path $\lambda(t)$ corresponding to a macroscopic evolution. It depends on the values of the resolved vector $A$ at times prior to $t$ via the propagator $e^{-\tau L}$ for the Liouville equation in elapsed time $\tau > 0$, and includes an artificial decay rate $\epsilon > 0$ for the memory. The nonequilibrium statistical operator (24) at time $t$ is thus a time-weighted superposition of exactly propagated solutions from quasi-equilibrium densities at earlier times $t - \tau$. The density (24) satisfies the inhomogeneous Liouville equation

$$\frac{\partial \rho_\epsilon}{\partial t} + L \rho_\epsilon = -\epsilon [ \rho_\epsilon - \tilde{\rho} ].$$

This equation shows that the nonequilibrium statistical operator $\rho_\epsilon$ becomes a formal solution of the Liouville equation in the limit as $\epsilon \to 0+$. The usual procedure to obtain a closure in terms of the mean resolved vector $a(t)$ is to impose the following two equations:

$$\frac{da}{dt} = \langle LA | \rho_\epsilon \rangle, \quad \text{and} \quad a(t) = \langle A | \rho_\epsilon(\cdot,t) \rangle = \langle A | \tilde{\rho}(\cdot;\lambda(t)) \rangle,$$

(25)

for sufficiently small $\epsilon > 0$ (or in an appropriate limit as $\epsilon \to 0+$). The first equation, which is precisely the $A$-moment of the Liouville equation itself, defines the closed reduced equations for the macrostate $a$; the second equation is a consistency condition between
that determines $\lambda$ in terms of a common mean resolved vector $a$. Since $\rho_e$ relies on the memory of $A$ under the phase flow, the resulting closure is governed by integrodifferential equations in $a$, in which the propagator for the Liouville equation appears explicitly.

The main justification for the closure theory based on nonequilibrium statistical operators is that an irreversible thermodynamic formalism is achieved. In this theory the irreversibility of the closed reduced dynamics for $a$ is produced by the slowly fading memory of the density $\rho_e$ used to form the instantaneous $A$-moment equations. That is, the use of $\rho_e$ rather than $\tilde{\rho}$ breaks the time-reversal symmetry of the adiabatic closure. The reduction obtained in this way, however, is nearly an identity, as opposed to a systematic method of approximating the influence of the unresolved variables on the resolved variables. Implementation of the reduced equations requires that ensembles of trajectories of the underlying Hamiltonian system be computed over a time interval over which the memory fades. In situations in which there is a wide separation of time scales between the resolved and unresolved variables, a further analysis is required to deduce the autonomous ordinary differential equations that govern the macrostate.

In these respects, the theory of nonequilibrium statistical operators shares the main features of the well-known projection methods of nonequilibrium statistical mechanics [2, 45, 41, 36]. In that methodology, a stochastic integro-differential equation is produced by projecting the Liouville propagators onto the resolved variables. The result is an exact identity that includes a time-convolution with a memory kernel, and random forcing terms that are related to the kernel via the fluctuation-dissipation theorem. At least in the near-equilibrium regime, the outcome of either theory is essentially the same, as are the challenges faced when implementing the reduced equations in a specific problem.

For these reasons we pursue a fundamentally different approach in the present work. In our approach the quasi-equilibrium densities, $\tilde{\rho}(\lambda)$, are retained to establish the thermodynamic structure of the reduced dynamics, but moment closure is replaced by an optimization procedure over paths of trial densities, $\tilde{\rho}(\lambda(t))$. The cost functional in this optimization is designed so that the optimal path is that path which is most compatible with the underlying Hamiltonian phase flow in a statistical, or information-theoretic, sense. No other densities need be introduced to yield an irreversible closure, nor is there a need for a stochastic representation intermediate between the deterministic microscopic dynamics and the macroscopic reduced equations.

The lack-of-fit cost function that is the basis of this procedure is constructed as follows. We introduce the residual of log $\tilde{\rho}$ with respect to the Liouville operator, namely,

$$ R(\cdot; \lambda, \dot{\lambda}) = \left( \frac{\partial}{\partial t} + L \right) \log \tilde{\rho}(\cdot; \lambda(t)). $$

[Here and throughout, $\dot{\lambda} = d\lambda/dt$.] There are two related expressions for this statistic $R$, which we call the Liouville residual, that reveal its significance to the closure problem.

First, for any $z \in \Gamma$, and any smooth parameter path $\lambda(t)$, the log-likelihood ratio between the density propagated for a short interval of time $\Delta t$ under the Liouville equation
and the evolving trial density is
\[
\log \frac{e^{-(\Delta t)L}\tilde{\rho}(z; \lambda(t))}{\tilde{\rho}(z; \lambda(t+\Delta t))} = -(\Delta t)R(z; \lambda(t), \dot{\lambda}(t)) + O((\Delta t)^2) \quad \text{as} \quad \Delta t \to 0.
\]

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 \([13, 28]\). By considering arbitrary smooth paths passing through a point \(\lambda\) 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 \(F : \Gamma_n \to \mathbb{R}\), the \(F\)-moment of the Liouville equation with respect to the trial densities along a path \(\lambda(t)\) is
\[
\frac{d}{dt} \langle F | \tilde{\rho}(\lambda(t)) \rangle - \langle LF | \tilde{\rho}(\lambda(t)) \rangle = \langle FR | \tilde{\rho}(\lambda(t)) \rangle.
\]

Thus, while an exact solution \(\rho(t)\) of the Liouville equation satisfies (6) for all \(F\), a trial solution \(\tilde{\rho}(\lambda(t))\) 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 quantify the dynamical lack-of-fit of the statistical model in terms 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 \(P_\lambda\) denote the orthogonal projection of the Hilbert space \(L^2(\Gamma_n, \tilde{\rho}(\lambda))\) onto the span of the score functions \(U_1(\lambda), \ldots, U_m(\lambda)\), and let \(Q_\lambda = I - P_\lambda\) denote the complementary projection; specifically, for any \(F \in L^2(\Gamma_n, \tilde{\rho}(\lambda))\),
\[
P_\lambda F = \langle FU(\lambda)^* | \tilde{\rho}(\lambda) \rangle C(\lambda)^{-1}U(\lambda),
\]

where \(C(\lambda)\) is given in (8). We declare the lack-of-fit cost function to be
\[
\mathcal{L}(\lambda, \dot{\lambda}) = \frac{1}{2} \langle (P_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle + \frac{1}{2} \langle (W_\lambda Q_\lambda R)^2 | \tilde{\rho}(\lambda) \rangle. \quad (27)
\]
\(\mathcal{L}\) is a weighted, mean-squared norm, with respect to a linear operator \(W_\lambda\) on \(L^2(\Gamma_n, \tilde{\rho})\) that assigns relative weights to the resolved and unresolved components of the Liouville residual. \(W_\lambda\) is assumed to be self-adjoint, and to satisfy \(W_\lambda P_\lambda = P_\lambda W = P_\lambda\). It follows that the resolved and unresolved subspaces are invariant under \(W_\lambda\), and that unit weights are assigned to the resolved subspace. The weights assigned by \(W_\lambda\) to the unresolved subspace constitute the adjustable parameters in the closure theory.

A more explicit formula for \(\mathcal{L}\) is derived as follows. The Liouville residual has zero mean, \(\langle R | \tilde{\rho}(\lambda) \rangle = 0\), and its orthogonal components are given by
\[
P_\lambda R = [\dot{\lambda} - C(\lambda)^{-1} \langle LU(\lambda) | \tilde{\rho}(\lambda) \rangle]^*U(\lambda), \quad Q_\lambda R = Q_\lambda L \log \tilde{\rho}(\lambda).
\]
The calculation of $P_R$ employs the string of equations,

$$\langle [L \log \tilde{\rho}(\lambda)] U(\lambda) | \tilde{\rho} \rangle = \int_{\Gamma_n} \{\tilde{\rho}(\lambda), H\} U(\lambda) \, dz$$

$$= - \int_{\Gamma_n} \{U(\lambda), H\} \tilde{\rho}(\lambda) \, dz$$

$$= - \langle L U(\lambda) | \tilde{\rho} \rangle.$$  

In light of these formulas the lack-of-fit cost function can be written in the form,

$$L(\lambda, \dot{\lambda}) = \frac{1}{2} [\dot{\lambda} - C(\lambda)^{-1} f(\lambda)]^* C(\lambda) [\dot{\lambda} - C(\lambda)^{-1} f(\lambda)] + w(\lambda),$$  

where, compatibly with (19), we employ the vector field

$$f(\lambda) = \langle LU(\lambda) | \tilde{\rho}(\lambda) \rangle,$$  

and we define the non-negative function

$$w(\lambda) = \frac{1}{2} \langle [W_\lambda Q_\lambda L \log \tilde{\rho}(\lambda)]^2 | \tilde{\rho}(\lambda) \rangle.$$  

We now formulate the stationary version of the optimization principle that defines our statistical closure. For an initial time, $t_0$, we consider the dynamical minimization problem

$$v(\lambda_0) = \min_{\lambda(t_0) = \lambda_0} \int_{t_0}^{+\infty} L(\lambda, \dot{\lambda}) \, dt,$$  

in which the lack-of-fit cost function (28) defines the cost functional over admissible paths $\lambda(t)$, $t_0 \leq t < +\infty$, in the configuration space of the statistical model, with the constraint that each path starts at $\lambda_0$ at time $t_0$. In conformity with optimization and control theory, we refer to $v(\lambda_0)$ as the value function for the minimization problem (31) [8, 14, 18]. Since the cost function $L(\lambda, \dot{\lambda})$ is independent of $t$, and the optimization extends to infinity in time, $v(\lambda_0)$ is independent of $t_0$; indeed, the time variable in (31) can be shifted so that $t_0$ is replaced by 0. It is in this sense that we refer to (31) as the stationary formulation of the best-fit principle.

By analogy to analytical mechanics, one may regard (31) as a principle of least action for the “Lagrangian” $L(\lambda, \dot{\lambda})$ and interpret the first member in (28) as its “kinetic” term and the second member as its “potential” term [1, 30]. The kinetic term is a quadratic form in the generalized velocities $\dot{\lambda}$ with positive-definite Fisher information matrix $C(\lambda)$, and it is entirely determined by the expressions that also arise in the adiabatic closure presented in the previous section. The potential term $w(\lambda)$ embodies the influence of the unresolved variables on the resolved variables, and it depends on the weight operator $W_\lambda$ that quantifies that influence. Accordingly, we call $w(\lambda)$ the closure potential. Of course, these mechanical analogies are not literal: $L$ has the units of a rate of entropy production, not of an energy, and it is a sum of its “kinetic” and “potential” terms, not a difference.

An extremal path $\hat{\lambda}(t)$, with $\hat{\lambda}(t_0) = \lambda_0$, for (31) determines the best-fit evolution of the statistical macrostate $\tilde{\rho}(\cdot; \hat{\lambda}(t))$, in the sense that the time-integral of the lack-of-fit cost function $L$ is minimized along the path $\hat{\lambda}(t)$. Thus, the extremal paths for
(31) define the estimated, or predicted, evolution in our reduced model, and the closed equations governing this evolution are derived from the optimization principle (31).

The derivation of the closed reduced equations that follow from the optimality conditions for (31) makes use of Hamilton-Jacobi theory [1, 30, 18, 17]. The value function, $v(\lambda)$, on $\lambda \in \mathbb{R}^m$, defined by (31), is analogous to an action integral, or Hamilton principal function, and it therefore satisfies the associated time-independent Hamilton-Jacobi equation,

$$
\mathcal{H} \left( \lambda, -\frac{\partial v}{\partial \lambda} \right) = 0,
$$

(32)

where $\mathcal{H}(\lambda, \mu)$ is the Legendre transform of $\mathcal{L}(\lambda, \dot{\lambda})$. That is, $\mathcal{L}$ and $\mathcal{H}$ are convex conjugate functions with respect to their second arguments, and

$$
\mu = \frac{\partial \mathcal{L}}{\partial \lambda} = C(\lambda) \dot{\lambda} - f(\lambda)
$$

(33)

$$
\mathcal{H}(\lambda, \mu) = \dot{\lambda}^* \mu - \mathcal{L}(\lambda, \dot{\lambda}) = \frac{1}{2} \mu^* C(\lambda)^{-1} \mu + f(\lambda)^* C(\lambda)^{-1} \mu - w(\lambda).
$$

These calculations are straightforward and explicit because $\mathcal{L}(\lambda, \dot{\lambda})$ is a quadratic function of $\dot{\lambda}$. According to Hamilton-Jacobi theory, the conjugate variable $\mu = \dot{\mu}(t)$ along an extremal path $\lambda = \dot{\lambda}(t)$ is given by the relation

$$
\dot{\mu} = -\frac{\partial v}{\partial \lambda}(\dot{\lambda}).
$$

(34)

This basic relation together with (33) closes the reduced dynamics along the extremal path, in that it yields the (vector) differential equation

$$
C(\dot{\lambda}) \frac{d\dot{\lambda}}{dt} = f(\dot{\lambda}) - \frac{\partial v}{\partial \lambda}(\dot{\lambda}).
$$

(35)

In summary, the choice of a statistical model of trial probability densities $\tilde{\rho}(\lambda)$ and the specification of a weight operator $W_\lambda$ determine the lack-of-fit Lagrangian $\mathcal{L}$ and its associated Hamiltonian $\mathcal{H}$, and thereby the value function $v(\lambda)$ for the best-fit optimization principle. All the terms in (35) are then uniquely defined, and this equation governs the evolution of best-fit statistical states in the reduced model. The modeled relaxation is described by an extremal path $\dot{\lambda}(t)$ satisfying $\lim_{t \to +\infty} \dot{\lambda}(t) = 0$, since the trial densities $\tilde{\rho}(\lambda)$ are parameterized so that $\tilde{\rho}(0)$ is an equilibrium density.

The value function satisfies the equilibrium conditions

$$
v(0) = 0, \quad \frac{\partial v}{\partial \lambda}(0) = 0;
$$

(36)

the first is immediate from (31), and the second is a direct consequence of (32). Moreover, the Hessian matrix of second partial derivatives of the value function is non-negative, semi-definite at equilibrium,

$$
\xi^* \frac{\partial^2 v}{\partial \lambda \partial \lambda^*}(0) \xi \geq 0, \quad \text{for all } \xi \in \mathbb{R}^m.
$$
In the non-degenerate case when the resolved variables do not contain any conserved quantities, this matrix is actually positive-definite. These properties reflect that fact that the equilibrium state $\lambda = 0$ is a local minimum of $v(\lambda)$, and in the non-degenerate case a strict local minimum. The value function defined by (31) is the so-called viscosity solution of (32) validating these equilibrium conditions. The reader is referred to [17] for the modern theory of existence and uniqueness of solutions to Hamilton-Jacobi equations, including the time-dependent equations encountered in Section 5.

The foregoing discussion applies to the most general form of the reduction using any regular family of densities $\tilde{\rho}(\lambda)$ as the statistical model. We now specialize the results contained in (35) to the models that use quasi-equilibrium densities (9), for either fixed inverse temperature $\beta$ or fixed mean energy $E$.

For the family (13) with fixed $\beta > 0$, the lack-of-fit Lagrangian takes the form (28) with $C(\lambda) = \langle (A - a)(A - a)^* \mid \tilde{\rho}(\lambda) \rangle$ and $f(\lambda) = \langle LA \mid \tilde{\rho}(\lambda) \rangle$. The closure potential can be expressed in the explicit form

$$w(\lambda) = \frac{1}{2} \lambda^* \langle [W_\lambda Q_\lambda LA] [W_\lambda Q_\lambda LA^*] \mid \tilde{\rho}(\lambda) \rangle \lambda = \frac{1}{2} \lambda^* D(\lambda) \lambda,$$

where the second equality defines the $m \times m$ Gram matrix $D(\lambda)$. Thus, $w(\lambda)$ is expressed as a non-negative quadratic form in $\lambda$, with a symmetric, semi-definite matrix $D(\lambda)$ which, in general, is $\lambda$-dependent. It is important to note that the weight operator $W_\lambda$ enters into the best-fit closure scheme only through the matrix $D(\lambda)$, and so all the adjustable parameters introduced into the scheme as weight factors in the lack-of-fit cost function are assembled in $D(\lambda)$ alone. The practical utility of this approach to closure rests on the requirement that in problems of interest there be a natural choice of weights via $W_\lambda$ that leads to a tractable number of adjustable parameters in $D(\lambda)$ and hence in $w(\lambda)$.

The closed reduced equations governing the evolution of the best-fit macrostate are

$$\frac{d\hat{a}}{dt} = f(\hat{\lambda}) - \partial v \partial \lambda (\hat{\lambda}), \quad \text{with} \quad \hat{a}(t) = \langle A \mid \tilde{\rho}(\hat{\lambda}) \rangle.$$  

(38)

Referring to (18) we see that (38) differs from the adiabatic reduced equation derived in the previous section by the presence of the gradient of $v(\lambda)$. In the subsequent section, this gradient term is shown to be the source of entropy production in the closed reduced dynamics, and consequently the best-fit evolution governed by (38) is irreversible. It is illuminating to display the Hamilton-Jacobi equation satisfied by $v(\lambda)$, namely,

$$\frac{1}{2} \left( \partial v \partial \lambda \right)^* C(\lambda)^{-1} \left( \partial v \partial \lambda \right) - f(\lambda)^* C(\lambda)^{-1} \left( \partial v \partial \lambda \right) = \frac{1}{2} \lambda^* D(\lambda) \lambda.$$

(39)

The source term in this partial differential equation for $v(\lambda)$ is the closure potential with matrix $D(\lambda)$. This matrix quantifies the magnitude of the unresolved Liouville residual and, in turn, generates the irreversible part of the closed reduced equation for $\hat{a}(t)$ via (39). In this way the irreversible reduced macrodynamics ensues from the reversible, conservative microdynamics.

The same governing equations hold for the version of the reduction in which the mean energy $\langle H \mid \tilde{\rho} \rangle = E$ is fixed. Specifically, the closed reduced equation governing this version
is identical to (38), the only change being that \( C(\lambda) \) is replaced by the appropriate matrix \( (17) \); the terms \( f(\lambda) \) and \( w(\lambda) \) take the same forms as in the version with fixed \( \beta \).

The reversible term in either of these reduced equations is expressible as a Hamiltonian vector field in the same way as in Section 2. That is, the effective Hamiltonian for the version with fixed \( \beta \) is the free-energy function, \( \tilde{h} \), while for fixed \( E \) it is the mean energy function, \( h \).

4 Properties of the reduced model

The best-fit statistical closures developed in the preceding section result in reduced equations for the macrostate \( a \) which possess the so-called GENERIC (General Equations of NonEquilibrium Reversible-Irreversible Coupling) format, a general framework for the equations of thermodynamics and hydrodynamics [21, 38, 37]. Let us consider the formulation with a fixed mean energy \( \langle H | \tilde{\rho}(\lambda) \rangle = E \), for which the reversible dynamics is given by (23). The governing equation (35) for the best-fit closure has both reversible and irreversible terms, which are expressible in the form

\[
\frac{d\hat{a}}{dt} = \Omega(\hat{a}) \frac{\partial h}{\partial a}(\hat{a}) - \frac{\partial v}{\partial \lambda}(\hat{\lambda}) , \quad \hat{\lambda} = -\frac{\partial s}{\partial a}(\hat{a}) .
\] (40)

As in Section 2, \( s = s(E, a) \) denotes the entropy relation \( s = s(u, a) \) in (11) evaluated at fixed energy, \( E \), and the mean energy function, \( u = h(s, a) \), is defined by inverting this relation. The reversible term in (40) is a Hamiltonian vector field with Hamiltonian \( h \) and cosympletic matrix, \( \Omega \); the gradient \( \partial h / \partial a \) is at fixed entropy. The irreversible term in (40) is a gradient vector field of the value function \( v \) with respect to \( \lambda = -\partial s / \partial a \). This form of the irreversible term conforms precisely with the general, nonlinear GENERIC form proposed by Grmela and Öttinger [21, 38]. Other closely related formats have also been developed [35, 4, 3].

By virtue of (34), the irreversible term in (40) is exactly the conjugate vector \( \hat{\mu} \). This correspondence furnishes the thermodynamic interpretation of the vectors \( \lambda \) and \( \mu \) in our optimization-based theory. Namely, the variables \( \lambda_1, \ldots, \lambda_m \), which are the “coordinates” of the Hamilton-Jacobi theory, may be interpreted as (minus) thermodynamic forces, or affinities; and, the variables \( \mu_1, \ldots, \mu_m \), which are the conjugate “momenta”, may be interpreted as corresponding thermodynamic fluxes. [Our notation introduces a minus sign in \( \lambda \) compared to much of the physical literature.] Thus, the duality naturally attached to our variational principle (31) coincides with the duality between “forces” and “fluxes” in nonequilibrium thermodynamics [15, 26].

The value function, \( v(\lambda) \), which mediates this duality, is closely related to the entropy production. Namely, an immediate implication of (40) is the fundamental identity,

\[
\frac{d\dot{s}}{dt} = -\dot{\lambda}^* \dot{\mu} = \dot{\lambda}^* \frac{\partial v}{\partial \lambda}(\dot{\lambda}) .
\] (41)

An entropy production inequality follows from this identity, provided that \( v(\lambda) \) is convex. This convexity is guaranteed whenever the cost function \( \mathcal{L}(\lambda, \dot{\lambda}) \) is jointly convex in the
pair \((\lambda, \dot{\lambda})\); but, for large \(|\lambda|\) the dependence of the coefficient functions \(C(\lambda)\) and \(D(\lambda)\), as well as the nonlinearity of \(f(\lambda)\), may result in a loss of convexity. Nonetheless, the convexity of \(v(\lambda)\) always holds in some neighborhood of equilibrium, \(\lambda = 0\). Thus, apart from a far-from-equilibrium regime in which convexity may be lost, we are assured that entropy increases at a rate bounded below by \(\dot{\lambda}\):

\[
\frac{d\dot{s}}{dt} \geq v(\dot{\lambda}) \geq 0.
\]

(42)

This inequality follows from the fact that \(0 = v(0) \geq v(\lambda) - \lambda^* \partial v / \partial \lambda(\lambda)\) for \(\lambda\) in the domain of convexity of \(v\). The value function is thus found to be the key thermodynamic potential in the nonequilibrium reduced model, and its close relation to entropy production further reinforces the information-theoretic basis of the optimization principle (31).

Since nonequilibrium behavior is most readily understood in the near-equilibrium regime, we now present the best-fit closure theory in its approximate form for small \(|\lambda|\); that is, for paths \(\lambda(t)\) in a neighborhood of \(\lambda = 0\) having trial densities \(\tilde{\rho}(\lambda(t))\) close to \(\rho_{eq}\). We assume that the resolved vector \(A\) is normalized so that \(\langle A \rangle_{eq} = 0\). We also assume that \(\langle AH \rangle_{eq} = 0\); this is easily obtained by replacing each \(A_i\) by \(A_i - \alpha_i(H - E)\) for appropriate \(\alpha_i\). Under these normalizations the linearization of the closure is identical for the versions that fix either \(\beta\) or \(E\) along paths.

The near-equilibrium form of the cost function (28) is simply

\[
\mathcal{L}(\lambda, \dot{\lambda}) = \frac{1}{2} [\dot{\lambda} - C^{-1}J\lambda]^* C [\dot{\lambda} - C^{-1}J\lambda] + \frac{1}{2} \lambda^* D\lambda,
\]

in which the coefficient matrices are constant, being evaluated at equilibrium; specifically,

\[ C = C(0) = \langle AA^* \rangle_{eq}, \quad D = D(0) = \langle(WQLA)(WQLA^*) \rangle_{eq}, \quad J = \frac{\partial f}{\partial \lambda}(0) = \langle(LA)A^* \rangle_{eq}. \]

\(C\) is a positive-definite symmetric matrix, \(D\) is a semi-definite symmetric matrix, and \(J\) is an anti-symmetric matrix. The cost function (43), which is a quadratic form in \((\lambda, \dot{\lambda})\), governs the linear relaxation from near-equilibrium initial states \(\lambda_0\), a phenomenon treated by familiar linear-response theory [10, 45]. The value function associated with \(\mathcal{L}\) is therefore also a quadratic form, and in light of (36) it is simply

\[
v(\lambda) = \frac{1}{2} \lambda^* M\lambda,
\]

for some constant, symmetric \(m \times m\) matrix \(M\). The Legendre transform yields the following expressions for the conjugate vector of fluxes and the Hamiltonian:

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

Along an extremal path, \(\dot{\lambda}(t)\), the relation between flux and force is linear, \(\dot{\mu} = -M\dot{\lambda}\). Consequently, the closed reduced equation for near-equilibrium relaxation is the constant-coefficient linear system of ODEs,

\[
\frac{d\dot{\lambda}}{dt} = (J - M)\dot{\lambda}, \quad \dot{\lambda} = C\dot{\lambda}.
\]

(45)
The matrix, \( M \), is determined by an algebraic Riccati equation, to which the stationary Hamilton-Jacobi equation (32) reduces \([29]\); namely,

\[
MC^{-1}M + JC^{-1}M - MC^{-1}J = D.
\]

(46)

The coefficient matrices, \( C \) and \( J \), are determined entirely by the parametric statistical model, whereas the source matrix, \( D \), depends on the choice of the adjustable constants in the closure. \( M \) is the unique, semi-definite matrix solution of (46). The matrix of transport coefficients in (45) thus includes an antisymmetric (reversible) part and a symmetric (irreversible) part, and while the irreversible part, \(-M\), responds directly to the choice of closure matrix \( D \), it is also modified by the reversible part, \( J \), via the coupling terms in the Riccati equation.

Under the near-equilibrium approximation the entropy production identity (41) becomes

\[
\frac{ds}{dt} = 2v(\dot{\lambda}) = \int_0^\infty 2\mathcal{L}(\dot{\lambda}(t'), d\dot{\lambda}/dt') dt' \geq 0,
\]

since \( v \) is homogeneous of degree 2, and hence \( \lambda^* \partial v/\partial \lambda = 2v \). Thus the time-integrated, squared-norm of the lack-of-fit along the extremal \( \dot{\lambda} \) equals the entropy production of the predicted evolution. In this light it is evident that the dynamical optimization principle defining our best-fit closure theory establishes the tight relationship between the rate of information loss in the reduced dynamics and the quantified lack-of-fit of the trial densities to the Liouville equation. The one-to-one correspondence between \( M \) and \( D \) in (46) expresses this relationship for relaxation in a neighborhood of equilibrium.

5 Nonstationary formulation

The stationary formulation of the best-fit closure developed in the preceding sections has an irreversible term that is time-independent, being the minus gradient of the solution \( v(\lambda) \) of the time-independent Hamilton-Jacobi equation (32). But when the modeled evolution is initiated by a quasi-equilibrium density \( \bar{\rho}(\lambda_0) \) for a given initial state \( \lambda_0 \in \mathbb{R}^m \), there is an early phase of the relaxation in which the entropy production increases from zero. After a sufficiently long time, the entropy production and the irreversible flux approach their stationary values. This “plateau” effect can be demonstrated by expanding an exact solution of the Liouville equation in a power series in time about \( t = 0 \). For small \( t \), the mean resolved vector corresponding to the exact solution is given by

\[
a(t) = \langle e^{t\mathcal{L}}A | \bar{\rho}(\lambda_0) \rangle = \langle A | \bar{\rho}(\lambda_0) \rangle + tf(\lambda_0) + O(t^2),
\]

recalling the definition of \( f(\lambda) \) in (19). If we attach to \( a(t) \) a path of trial densities, \( \bar{\rho}(\lambda(t)) \), with \( \lambda(t) \) determined so that \( a(t) = \langle A | \bar{\rho}(\lambda(t)) \rangle \), then

\[
\lambda(t) = \lambda_0 + tC(\lambda_0)^{-1}f(\lambda_0) + O(t^2).
\]

The entropy production along this path is then

\[
\frac{ds}{dt}(a(t)) = -\lambda(t)^*\frac{da}{dt}(t) = \lambda_0^*f(\lambda_0) + O(t);
\]
and the constant term in this equation vanishes,

\[
\lambda^*_0 f(\lambda_0) = \langle L(\lambda^*_0 A) | \tilde{\rho}(\lambda_0) \rangle = \int_{\Gamma_n} L\tilde{\rho}(\lambda_0) \, dz = 0.
\]

Thus, we see that the entropy production of a perfectly fitted path of trial densities grows from zero linearly in time, given an initial density that is itself a trial density.

Physically, such an initial condition is naturally created by applying constant external perturbations with strengths proportional to \(\lambda_1^0, \ldots, \lambda_m^0\) via the resolved variables and allowing the system to equilibrate with respect to the perturbed Hamiltonian \(H - \beta^{-1} \lambda_0^* A\). When these external perturbations are switched off at time \(t = 0\), a relaxation occurs that is the object of the modeling exercise. Moreover, in numerical experiments that test a closure theory it is often convenient to use initial ensembles defined by quasi-equilibrium trial densities. For these reasons, we now modify the defining optimization principle (31) to include such a plateau effect. We refer to this as the nonstationary formulation, in that the value function \(v = v(\lambda, t)\) becomes time dependent.

The nonstationary optimization principle has the value function

\[
v(\lambda_1, t_1) = \min_{\lambda(t_1) = \lambda_1} \int_0^{t_1} \mathcal{L}(\lambda, -\dot{\lambda}) \, dt ,
\]

in which the admissible paths \(\lambda(t), \ 0 \leq t \leq t_1\), in the configuration space of the statistical model are constrained to terminate at \(\lambda_1 \in \mathcal{C}^n\) at time \(t_1 \geq 0\), while \(\lambda(0)\) is unconstrained. The integrand in (47) is modified to account for time-reversal, and the admissible paths may be viewed as evolving in reversed time, \(\tau = t_1 - t\), starting from \(\lambda_1\) at \(\tau = 0\). The value function \(v(\lambda_1, t_1)\) quantifies the optimal lack-of-fit of a time-reversed path connecting the current state \(\lambda_1\) to an unspecified initial state \(\lambda(0)\). By contrast, the stationary formulation ties the value function to the time at which the initial condition is specified, while the stationary formulation ties the value function to equilibration at infinite time.

The value function (47) is the unique solution of the initial value problem (with \((\lambda, t)\) replacing \((\lambda_1, t_1)\))

\[
\frac{\partial v}{\partial t} + \mathcal{H} \left(\lambda, -\frac{\partial v}{\partial \lambda}\right) = 0 , \quad \text{for } t > 0 , \quad \text{with } v(\lambda, 0) = 0 ,
\]

which is a time-reversed Hamilton-Jacobi equation. That is, keeping \(\mathcal{H}(\lambda, \mu)\) the Legendre transform of \(\mathcal{L}(\lambda, \dot{\lambda})\) as in (33), the Hamiltonian corresponding to \(\mathcal{L}(\lambda, -\dot{\lambda})\) is \(\mathcal{H}(\lambda, -\mu)\); thus (48) follows from (47).

In terms of the time-dependent value function, \(v(\lambda, t)\), closure is achieved by setting

\[
\hat{\mu}(t) = -\frac{\partial v}{\partial \lambda}(\hat{\lambda}, t) .
\]

This relation is the nonstationary analogue to (34). The nonstationary reduced equations are determined by this relation in the same way that (35) follows from (34); namely,

\[
C(\hat{\lambda}) \frac{d \hat{\lambda}}{dt} = f(\hat{\lambda}) - \frac{\partial v}{\partial \lambda}(\hat{\lambda}, t) .
\]
But, in contrast to the stationary case, the solution \( \hat{\lambda}(t) \) of (50) is not itself an extremal of the defining optimization principle; the extremal paths that define \( v(\lambda, t) \) for each \((\lambda, t)\) vary with \( t \) as well as with \( \lambda \), and they instantaneously determine the flux of the predicted evolution \( \hat{\lambda}(t) \).

Since \( \mathcal{H}(\lambda, \mu) \) is positive-definite in \( \mu \), the viscosity solution \( v(\lambda, t) \) of (48) exists for all time \( t > 0 \), is unique, and coincides with the value function defined by (47) [17]. Moreover, \( v(\lambda, t) \to v(\lambda) \), the stationary value function, as \( t \to +\infty \). Thus, the nonstationary best-fit closure is a natural generalization of the stationary closure that straightforwardly includes an intrinsic plateau effect.

We remark that it is possible to consider solutions of (48) having nonzero initial conditions \( v(\lambda, 0) \). One natural alternative is to optimize over time-reversed admissible paths \( \lambda(t) \) that attach to the given initial state, so that \( \lambda(0) = \lambda_0 \). This requirement produces a value function, \( V(\lambda, t; \lambda_0) \), that is singular at \( t = 0 \) in the sense that \( V(\lambda, t; \lambda_0) \sim (\lambda - \lambda_0)^* C(\lambda_0)(\lambda - \lambda_0)/2t \) as \( t \to 0^+ \). A theory based on this value function, and using (50) with \( V \) replacing \( v \), constitutes another natural formulation of the plateau effect. The resulting reduced equations, however, are less attractive as a tractable closure because they are inhomogeneous in the mean resolved vector \( \hat{a} \), they require a more intricate solution of (48), and their properties are more difficult to deduce. Consequently, even though this approach incorporates the plateau effect in a strong form, we prefer the nonstationary theory that follows from the homogeneous initial condition \( v(\lambda, 0) = 0 \) in (48), and that shares the general properties the stationary theory.

In particular, the entropy production identity (41) and the inequality (42) remain valid in the homogeneous, nonstationary closure theory, since the time-dependent value function \( v(\lambda, t) \) continues to satisfy the equilibrium conditions (36). Moreover, the Hessian matrix of second partial derivatives of the value function evaluated at equilibrium,

\[
M(t) = \frac{\partial^2 v}{\partial \lambda \partial \lambda^*}(0, t),
\]

satisfies the Riccati differential equation

\[
\frac{dM}{dt} + MC^{-1}M + JC^{-1}M - MC^{-1}J = D, \quad M(0) = 0. \tag{51}
\]

The derivation of (51) merely requires taking the matrix of second partial derivatives of (48) and evaluating the result at \( \lambda = 0 \). This equation implies that \( M(t) \) is semi-definite, because the source term \( D \) is semi-definite; in the non-degenerate case when \( D \) is positive-definite, which is the case whenever none of the resolved variables is a dynamical invariant, \( M(t) \) is positive-definite for \( t > 0 \) [29]. The equilibrium point \( \lambda = 0 \) is then a strict local minimum for \( v(\lambda, t) \) for all \( t > 0 \).

The near-equilibrium linearization of the nonstationary best-fit closure theory has a time-varying linear relation between flux and force along an extremal path, \( \dot{\mu} = -M(t)\dot{\lambda} \). Consequently, the nonstationary version of the closed reduced equation is a nonautonomous linear system of ODEs entirely analogous to (45); namely,

\[
\frac{d\hat{a}}{dt} = [J - M(t)] \hat{\lambda}, \quad \hat{a} = C\hat{\lambda}. \tag{52}
\]
The value function $v(\lambda, t)$ is the time-dependent quadratic form (44).

As a simple illustration let us consider the near-equilibrium, nonstationary closure for a single resolved variable $A \in \mathbb{R}^1$, that is, for $m = 1$. Then $C > 0$, $J = 0$, and there is a single closure parameter $D \geq 0$. The solution to the scalar Riccati differential equation (51) and the closed reduced equation (52) are, respectively,

$$M(t) = \sqrt{CD} \tanh \sqrt{\frac{D}{C} t}, \quad a(t) = a_0 \sech \sqrt{\frac{D}{C} t}.$$  

This solution clearly shows the plateau effect for small $t$ and the exponential relaxation for large $t$.

The analogous multivariate form of this result holds for $m > 1$ provided that all the resolved variables $A_1, \ldots, A_m$, as well as $H$, are even under time-reversal; that is, $A_k(q, -p) = A_k(q, p)$, for $k = 1, \ldots, m$. Then, each $L A_k$ is odd, and consequently $J = \langle (L A) A^* \rangle_{eq} = 0$. And the same holds if all the $A_k$ are odd. In these situations the closed reduced dynamics governed by (52) and (51) is diagonalizable. Namely, let $V$ be the $m \times m$ matrix of eigenvectors for $D$ relative to $C$; that is, $V$ is the matrix for which $V^* C V = I$ and $V^* D V = \Delta$, where $\Delta$ is the diagonal matrix whose diagonal consists of the associated eigenvalues $\gamma_1, \ldots, \gamma_m \geq 0$. In the transformed variables, $b(t) = V^* a(t)$ and $N(t) = V^* M(t) V$, the closed reduced dynamics (52) and (51) become

$$\frac{d \hat{b}}{dt} = -N(t) \hat{b}, \quad \frac{dN}{dt} + N^2 = \Delta.$$

The solution $N(t)$ of this transformed Riccati equation is the diagonal matrix having diagonal elements, $\sqrt{\gamma_1} \tanh \sqrt{\gamma_1} t, \ldots, \sqrt{\gamma_m} \tanh \sqrt{\gamma_m} t$. In turn, the solution of the relaxation equation is $\hat{b}(t) = \left( b_1(0) \sech \sqrt{\gamma_1} t, \ldots, b_m(0) \sech \sqrt{\gamma_m} t \right)$. In the original variables the relaxation is given by $\hat{a}(t) = (V^*)^{-1} \hat{b}(t)$ and $\hat{\lambda}(t) = V^{-1} \hat{b}(t)$. Thus, the best-fit closure theory for these resolved variables predicts a linear relaxation that combines a plateau effect with an exponential decay for $m$ normal modes with $m$ characteristic time scales $1/\sqrt{\gamma_k}$.

In the general near-equilibrium relaxation for which special symmetries are not present in the selected resolved variables, the antisymmetric matrix $J$ is nonzero, and it participates in the Riccati matrix equation (51) that determines $M(t)$. Consequently, $J$, which defines the reversible part of closed reduced dynamics, also influences the irreversible part controlled by $M(t)$. A central prediction of the best-fit closure theory, therefore, is the coupling between the reversible and irreversible parts of the closed reduced equations, which implies a quantitative coupling between the time scales of reversible oscillations and the time scales of irreversible relaxation.
6 Discussion

We have developed a methodology for constructing nonequilibrium statistical models of Hamiltonian dynamical systems based on the recognition that such models are essentially estimation strategies. When seeking closure in terms of a reduced description, it is desirable to have the flexibility to expand or contract the set of resolved, or macroscopic, variables, while maintaining a consistent approximation strategy. Expansion increases accuracy at the expense of model complexity, while contraction improves tractability at the expense of model fidelity. Whatever the compromise between accuracy and tractability, the goal of the modeling exercise is to obtain a dynamical closure that is as effective as possible for the selected macrovariables. Motivated by these considerations, we have developed a best-fit criterion for canonical statistical models associated with any independent set of resolved variables.

Our optimization principle produces an irreversible, dissipative macrodynamics that minimizes a certain lack-of-fit of the selected statistical model to the reversible, conservative microdynamics. The structure of the cost function in this principle conforms to the separation of the reduced dynamics into reversible and irreversible parts, in that it assigns relative weights to the resolved and unresolved components of the Liouville residual. In particular, the contribution of the unresolved component to the cost function is the source of irreversibility in the best-fit closure, and the rates of relaxation of the macrovariables scale with the weights assigned to the unresolved component.

The closed reduced equations that follow from the optimality conditions have the form of governing equations for nonequilibrium thermodynamics. The value function, which is the central quantity in the optimization theory, becomes the pivotal quantity in the thermodynamic formalism. Specifically, the gradient of the value function with respect to the vector of affinities is the vector of corresponding fluxes. The value function is therefore the natural extension of the Rayleigh-Onsager dissipation function beyond the range of linear irreversible thermodynamics. The main novelty of our variational formulation is that this key thermodynamic potential is realized as the minimal lack-of-fit of macroscopic paths to the underlying microscopic dynamics.

The utility of reduced models and statistical closures for any particular system depends upon two factors: (i) a convenient set of the resolved variables with some separation of time scales between the the resolved (slow) and unresolved (fast) variables; (ii) an expression for, or approximation of, the dissipation function in terms of a manageable number of adjustable parameters. Traditionally, thermodynamic modeling has tended to concentrate on special physical situations where these two requirements are met very strongly. But a closure theory can also be worth pursuing even in situations that are not extremely favorable. For instance, coarse-grained models of turbulent behavior or sub-grid scale parameterizations for complex systems in which coherent structures interact with fluctuations over a range of scales may necessitate somewhat crude closures, or perhaps a hierarchy of closures. In problems of this kind, our optimization approach furnishes a systematic method for deriving closures approximations that share the formal structure of thermodynamics.

As one concrete example we mention an implementation of our general methodol-
ogy to the truncated Burgers-Hopf equation [27]. This system has been proposed as a good testbed for model reduction techniques because it is a relatively simple prototype of turbulent fluid systems [33, 34]. The continuum dynamics of the Burgers-Hopf PDE is truncated to $n$ Fourier modes, and then a reduction to the lowest $m \ll n$ modes is considered. The truncated system, though it has a noncanonical Hamiltonian structure, possesses a Gaussian invariant measure, and for $n > 20$ its computed dynamics are observed to be ergodic and mixing and to have nearly Gaussian statistics. A best-fit closure theory based on Gaussian trial densities produces explicit, closed reduced equations for the relaxation of the $m$ resolved modes from nonequilibrium initial conditions. These equations have the form of the $m$-mode truncation itself but with strong mode-dependent dissipation and modified nonlinear modal interactions. Even though this closure has only one adjustable parameter and the time-scale separation is meager, the predictions of the best-fit closure with 5 resolved modes agree quite well with direct numerical simulations of large ensembles of solutions of a 50-mode dynamics. Moreover, this agreement holds for far-from-equilibrium initial conditions as well as near-to-equilibrium conditions. In light of the structure of the Burgers-Hopf dynamics — essentially a quadratic nonlinearity of hydrodynamic type — these results suggest that more realistic systems of this kind may be amenable to a best-fit closure.

The present paper has focussed exclusively on the relaxation from nonequilibrium statistical initial conditions of conservative, deterministic dynamical systems. It remains to develop the analogous theory for forced systems with nonconservative or stochastic dynamics. In the latter context, a promising connection exists between our approach and the studies of nonequilibrium steady states of driven diffusive systems by Bertini et al. [5, 6, 7]. In that work a natural variational principle over paths also arises as well as an associated Hamilton-Jacobi equation. In contrast to our approach, though, these authors are primarily concerned with characterizing theoretically the thermodynamic limits of stochastic microscopic models, not with deriving computationally tractable, predictive reduced models of complex dynamical systems. Nonetheless, the common features of all these reduction strategies and nonequilibrium thermodynamic structures would benefit from further investigations.

7 Acknowlegments

In the course of this work the author benefited from conversations with R.S. Ellis, M. Katsoulakis, R. Kleeman, A.J. Majda, and P. Plechac. This research was initiated during a sabbatical stay at the University of Warwick partly supported by an international short visit fellowship from the Royal Society, and was completed during a two-month visit to the Courant Institute of Mathematical Sciences. This work received funding from the National Science Foundation under grant DMS-0604071.
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Contact Information:

Bruce E. Turkington
Department of Mathematics and Statistics
University of Massachusetts
Amherst, MA 01003

turk@math.umass.edu