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EXISTENCE PROOF FOR ORTHOGONAL DYNAMICS AND THE MORI–ZWANZIG FORMALISM

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ABSTRACT

We study the existence of solutions to the orthogonal dynamics equation, which arises in the Mori–Zwanzig formalism in irreversible statistical mechanics. This equation generates the random noise associated with a reduction in the number of variables. If L is the Liouvillian, or Lie derivative associated with a Hamiltonian system, and P an orthogonal projection onto a closed subspace of L^2, then the orthogonal dynamics is generated by the operator $(I-P)L$. We prove the existence of classical solutions for the case where P has finite-dimensional range. In the general case, we prove the existence of weak solutions.

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1. Introduction

The Mori–Zwanzig formalism is a central paradigm in irreversible statistical mechanics [11, 20, 4]. It is a formal procedure whereby a dynamical system is reformulated as a lower-dimensional system for a selected set of variables (the "resolved" variables); the resulting system, which is often called a **generalized Langevin equation**, has memory (contains an integral over past values of the resolved variables) and contains a time-dependent function, often interpreted as "noise", which depends on the full initial data, and solves an auxiliary equation known as the **orthogonal dynamics equation**. Within an appropriate probabilistic setting, the noise function can be viewed as a random process. This formalism has an adjoint version which describes the evolution of marginal probability measures [12]. The Mori–Zwanzig formalism has recently received renewed attention within the context of variable reduction and stochastic modeling [1, 2, 10, 9].

The key element in the Mori–Zwanzig procedure is a projection operator. Functions that depend on all the coordinates of the system are projected onto a subspace of functions that depend only on the resolved variables; the projection is an orthogonal projection in the L^2 sense. There is freedom in the choice of projection, or equivalently, in the choice of the subspace onto which functions are projected. Most common is the projection onto the space of functions that are linear in the resolved variables. Another possibility is to project functions onto the subspace of all functions of the resolved variables; within the probabilistic setting this corresponds to a conditional expectation [20, 1]; this projection can be viewed as optimal, but may be difficult to compute. There exists a range of intermediate choices that can be viewed as increasingly high-dimensional approximations of the conditional expectation.

The validity of the Mori–Zwanzig formalism relies on the well-posedness of the orthogonal dynamics equation, which has always been taken for granted. The existence of solutions, i.e., the existence of a noise process, is however a subtle issue, which we address in the present paper. Our main results may be summarized as follows: if the range of the projection is a finite-dimensional subspace of L^2, as is the case in most of the statistical mechanics literature (see, e.g., [4]), then the existence of classical solutions may be proved. Our proof is constructive, based on a reduction of the orthogonal dynamics to an integral equation of Volterra type. In the more general case, for example, when the projection is a conditional expectation, we only prove the existence of weak solutions. The proof closely follows the lines of Friedrichs' existence proof for symmetric hyperbolic systems [6].

The paper is organized as follows. In Section 2 we present the Mori–Zwanzig formalism: we introduce the Hamiltonian dynamics, the corresponding probability space, various projection operators, the orthogonal dynamics, and derive the generalized Langevin equation. In Section 3 we address in general the existence of the orthogonal dynamics. In particular, we provide a simple example, which demonstrates how solutions may fail to exist in certain cases. The existence of orthogonal dynamics for the case where the range of the projection operator is finite dimensional is proved in Section 4. The existence of weak solution for general projections is proved in Section 5.

2. The Mori–Zwanzig formalism

Consider a Hamiltonian system,

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \tag{2.1}$$

where $q = (q_1, \dots, q_n)^T$ and $p = (p_1, \dots, p_n)^T$ are n-dimensional vectors and $H = H(q, p)$ is the Hamiltonian. Supplemented with $2n$ initial conditions, $q(0)$, $p(0)$, Hamilton's equations (2.1) govern the trajectory of a point in a $2n$-dimensional Euclidean space, $\Gamma = \mathbb{R}^{2n}$.

We rewrite equations(2.1) in a slightly more abstract form: let points in Γ be denoted by a $2n$-dimensional vector, $x = (x_1, \dots, x_{2n})^T$, where each of the components x_i is either a position or a momentum coordinate; let $x_{2i-1} = q_i$ and $x_{2i} = p_i$. Hamilton's equations induce a flow map, φ^t: $\Gamma \mapsto \Gamma$, which maps every initial value x to its evolute $\varphi^t(x)$ at time t. Equations(2.1) can be rewritten as a differential equation for $\varphi^t(x)$:

$$\begin{aligned} &\frac{d}{dt}\varphi_i^t(x) = b_i(\varphi^t(x)) \\ &\varphi_i^0(x) = x_i \end{aligned} \qquad i = 1, 2, \dots, 2n,$$

where $b(x) = (b_1(x), \dots, b_{2n}(x))^T$ is the Hamiltonian vector field, b: $\Gamma \mapsto \mathbb{R}^{2n}$. Hamiltonian vector fields are incompressible,

$$\sum_{i=1}^{2n} \partial_i b_i(x) = 0, \tag{2.2}$$

and as a result preserve the Lebesgue measure in Γ; we use ∂_i to denote the partial derivative with respect to the i-th variable. In particular, Hamiltonian dynamics preserve any absolutely continuous measure, $\mu(dx) = \varrho(x)dx$, if the density $\varrho(x)$ is a function of the Hamiltonian. An invariant (probability) measure of particular interest in statistical mechanics is the canonical measure, which corresponds to a probability density of $\varrho(x) = Z^{-1}e^{-\beta H(x)}$, where $\beta > 0$ is the inverse temperature and Z is a normalization constant.

Hamiltonian dynamics have an equivalent formulation in terms of an evolution equation for functions on Γ [14]. By adopting this alternative framework one obtains a linear evolution equation on an infinite-dimensional space. Let L be the differential operator

$$L = \sum_{i=1}^{2n} b_i(x)\partial_i, \tag{2.3}$$

known as the **Liouvillian**, or the Lie derivative associated with the vector field $b(x)$, and consider the linear differential equation

$$\begin{aligned} \frac{d}{dt}u^t(x) &= Lu^t(x) \\ u^0(x) &= g(x) \end{aligned} \tag{2.4}$$

for some function $g\colon \Gamma \mapsto \mathbb{R}$. Equation (2.4) is known as the **Liouville equation**. Its solution is $u^t(x) = g(\varphi^t(x))$ as we verify:

$$\begin{aligned} \frac{d}{dt}g(\varphi^t(x)) &= \sum_{i=1}^{2n} \partial_i g(\varphi^t(x)) b_i(\varphi^t(x)) \\ &= \sum_{i=1}^{2n} \partial_i g(\varphi^t(x)) \sum_{j=1}^{2n} \partial_j \varphi_i^t(x) \cdot b_j(x) \\ &= \sum_{j=1}^{2n} b_j(x)\partial_j[g(\varphi^t(x))] \\ &= Lg(\varphi^t(x)), \end{aligned}$$

where the identity $b_i(\varphi^t(x)) = \sum_{j=1}^{2n} \partial_j\varphi_i^t(x) \cdot b_j(x) = L\varphi_i^t(x)$ is an immediate consequence of the semigroup property $\varphi^t(\varphi^s(x)) = \varphi^s(\varphi^t(x))$; differentiate both sides with respect to s and set $s = 0$. The flow map $\varphi^t(x)$, x fixed, constitutes a family of characteristic curves for the hyperbolic system (2.4).

We introduce the semigroup notation [13],

$$g(\varphi^t(x)) = (e^{tL}g)(x),$$

where e^{tL} is the evolution operator associated with the Liouville equation (2.4). It is easily verified that $e^{tL}L = Le^{tL}$. In the particular case where g is the i-th coordinate, $g(x) = \pi_i(x) = x_i$, the solution is $(e^{tL}g)(x) = \pi_i(\varphi^t(x)) = \varphi_i^t(x)$, the i-th component of the trajectory.

Given a measure μ on Γ, functions g can be viewed as random variables, and $e^{tL}g$ can be viewed as a random function, or a stochastic process. Let $\mu(dx) = \varrho(x)dx$ be a probability measure, where the density $\varrho(x)$ is a function of $H(x)$; we assume that $\varrho(x)$ is continuous and strictly positive for all $x \in \Gamma$. The expected value of a function g with respect to the measure μ is given by

$$\mathbb{E}[g] = \int_\Gamma g(x)\varrho(x)dx.$$

We endow the space of functions on Γ with the inner product,

$$(f, g) = \mathbb{E}[fg],$$

which makes it a Hilbert space $L^2 = L^2(\mathbb{R}^{2n}, \mu)$. By the incompressibility condition (2.2) and the invariance of the measure, the operator L is skew-symmetric in this Hilbert space: $(Lf, g) = -(f, Lg)$, for all f, g in the domain of L.

Non-equilibrium statistical mechanics is based on the premise that one cannot solve the full system of equations(2.1), but can only follow the evolution of a smaller set of variables (the "resolved" coordinates). The remaining variables (the "unresolved" coordinates) are considered as random. For concreteness, we consider the case where the resolved variables are the first $2m$ coordinates $\hat{x} = (x_1, \ldots, x_{2m})$. Let $\tilde{x} = (x_{2m+1}, \ldots, x_{2n})$ denote the vector of unresolved coordinates; thus $x = (\hat{x}, \tilde{x})$. Similarly, let $\hat{\varphi}^t(x) = (\varphi_1^t(x), \ldots, \varphi_{2m}^t(x))$ denote the trajectories of the $2m$ coordinates of the solution that we focus on.

The Mori–Zwanzig formalism uses a projection operator, P, which projects functions in L^2 onto a subspace of functions that depend only on the resolved variables $\hat{x}$, i.e., functions on $\mathbb{R}^{2m}$. Let $f \in L^2$; most widely in use is the **linear projection**,

$$(Pf)(\hat{x}) = \sum_{i,j=1}^{2m} a_{ij}^{-1}(f, x_i)x_j, \tag{2.5}$$

where the a_{ij}^{-1} are the entries of the $2m \times 2m$ matrix whose inverse has entries $a_{ij} = (x_i, x_j)$. This is an orthogonal projection of functions in L^2 onto the subspace of linear functions of the resolved coordinates $\hat{x}$.

More generally, let $\hat{L}^2 \subset L^2$ denote the space of functions that depend only on $\hat{x}$. We may pick a set of functions in $\hat{L}^2$, say $h^\nu(\hat{x})$, $\nu = 1, 2, \ldots, M$; for convenience we make them orthonormal, $(h^\mu, h^\nu) = \delta_{\mu\nu}$. We define a projection

$$(Pf)(\hat{x}) = \sum_{\nu=1}^{M} (f, h^\nu) h^\nu(\hat{x}), \tag{2.6}$$

to which we refer as a **finite-rank projection**. Finally, we consider the projection of f onto the span of all functions in $\hat{L}^2$, given by

$$(Pf)(\hat{x}) = \frac{\int f(\hat{x}, \tilde{x}) \varrho(\hat{x}, \tilde{x}) d\tilde{x}}{\int \varrho(\hat{x}, \tilde{x}) d\tilde{x}}, \tag{2.7}$$

where $d\tilde{x} = dx_{2m+1} \cdots dx_{2n}$. In the context of probability theory, Pf is the **conditional expectation** of f given $\hat{x}$, usually denoted by $\mathbb{E}[f|\hat{x}]$ (see, e.g., Chung [3]). It is the best least-square approximation of f by a function of $\hat{x}$:

$$\mathbb{E}|f(x) - \mathbb{E}[f|\hat{x}]|^2 \leq \mathbb{E}|f(x) - g(\hat{x})|^2$$

for all functions $g \in \hat{L}^2$. Note that since $\hat{L}$ is separable, it follows that there exists an orthonormal set of functions, $\{h^\nu(\hat{x})\}_{\nu=1}^\infty$, such that

$$(Pf)(\hat{x}) = \sum_{\nu=1}^{\infty} (Pf, h^\nu) h^\nu(\hat{x}) = \sum_{\nu=1}^{\infty} (f, h^\nu) h^\nu(\hat{x}).$$

Thus, the conditional expectation is the limit of a finite-rank projection as $M \to \infty$ and the h^ν span $\hat{L}^2$.

Let P be any of the above three projections. The Mori–Zwanzig formalism starts by splitting the time derivative of the resolved components of the trajectory $\varphi_j^t(x) = e^{tL}\pi_j(x)$, $j = 1, 2, \dots, 2m$, into an expression that depends only on $\hat{\varphi}^t(x)$ plus a remainder:

$$\frac{d}{dt} e^{tL}\pi_j = e^{tL} L \pi_j = e^{tL} b_j = e^{tL} P b_j + e^{tL} Q b_j, \tag{2.8}$$

where $Q = I - P$. We define $R = Pb$, which is a vector field in $\mathbb{R}^{2m}$. The first term on the right-hand side, $e^{tL}R_j$, is consequently a function of the resolved components of the solution: $(e^{tL}Pb_j)(x) = R_j(\hat{\varphi}^t(x))$.

The formalism proceeds by splitting the remaining term, $e^{tL}Qb_j$, as follows. An auxiliary evolution operator, e^{tQL}, acting on functions in the null space of P is introduced: $w^t(x) = e^{tQL} g(x)$ is defined as the solution of the **orthogonal dynamics equation**:

$$\begin{aligned} &\frac{d}{dt} w^t(x) = QLw^t(x) \\ &w^0(x) = g(x) \end{aligned} \tag{2.9}$$

with $Pg = 0$. Assuming that e^{tQL} is well-defined, the evolution operators e^{tL} and e^{tQL} satisfy the Dyson formula

$$e^{tL} = \int_0^t e^{(t-s)L} PLe^{sQL} ds + e^{tQL},$$

which can be viewed as an application of Duhammel's principle. Thus the second term on the right-hand side of (2.8) takes the form

$$e^{tL} Qb_j = \int_0^t e^{(t-s)L} PLe^{sQL} Qb_j ds + e^{tQL} Qb_j.$$

Defining $F^t\colon \mathbb{R}^{2n} \mapsto \mathbb{R}^{2m}$ and $K^t\colon \mathbb{R}^{2m} \mapsto \mathbb{R}^{2m}$ with components,

$$F_j^t = e^{tQL} Qb_j, \quad K_j^t = PLF_j^t,$$

equation (2.8) reduces to the **generalized Langevin equation**

$$\frac{d}{dt} e^{tL} \pi_j = e^{tL} R_j + \int_0^t e^{(t-s)L} K_j^s ds + F_j^t,$$

or, in a more transparent form,

$$\frac{d}{dt} \varphi_j^t(x) = R_j(\hat{\varphi}^t(x)) + \int_0^t K_j^s(\hat{\varphi}^{t-s}(x)) ds + F_j^t(x). \tag{2.10}$$

Equation (2.10) is an identity between functions. Its right-hand side has a conventional interpretation. The first term depends only on the instantaneous value of the resolved variables, and is therefore called the **Markovian** vector field. The second term depends on x only through the value of $\hat{\varphi}^s(x)$ at times s between 0 and t; it therefore embodies **memory** effects. The third term depends on the full knowledge of the initial conditions x; it is viewed as a **noise** term with statistics determined by the initial conditions. The orthogonal dynamics (2.9) can therefore be viewed as the noise generator for the generalized Langevin equation (2.10).

While the Mori–Zwanzig formalism is usually presented based on a canonical measure, it is also of interest to consider it within a micro-canonical framework, i.e., assuming that the total energy of the system is given, so that the dynamics take place on an energy manifold. The geometrical background needed for such a formulation is presented in the Appendix.

3. Existence of orthogonal dynamics: general considerations

The Mori–Zwanzig formalism relies on the well-posedness of the auxiliary evolution operator e^{tQL}, defined by (2.9). Note that e^{tQL} acts on Qb_j, which belongs to the orthogonal complement of the range of the projection P. We introduce the following subspaces of L^2:

$$\mathscr{M} = \left\{u \in L^2 : Pu = u\right\}, \quad \mathscr{M}_\perp = \left\{u \in L^2 : Pu = 0\right\}.$$

The Mori–Zwanzig formalism relies on the assumption that QL is the generator of a semigroup in $\mathscr{M}_\perp$ (for general references on semigroup theory see [13, 15, 5]). Since L itself is a generator of a unitary semigroup, then by Stone's theorem [18] it is not only skew-symmetric, but also skew-adjoint in L^2. The projection operators P and Q are self-adjoint operators in L^2, from which it immediately follows that PLP and QLQ are skew-symmetric operators in L^2, hence PL and QL are skew-symmetric in $\mathscr{M}$ and $\mathscr{M}_\perp$ respectively. Resorting again to Stone's theorem, the existence of orthogonal dynamics boils down to the question whether QL is a skew-adjoint operator in $\mathscr{M}_\perp$.

Naively, it may seem that the composition of a (self-adjoint) projection and a skew-adjoint operator is always skew-adjoint. This is the case when A is a bounded, skew-symmetric operator and Q is an orthogonal projection. Then, QAQ has an extension $\overline{QAQ}$ which is skew-adjoint and the semigroup $\exp(t\overline{QAQ})$ is unitary in L^2. This may fail for unbounded operators as the following example shows.

Example: Consider the Hilbert space $L^2(\mathbb{R})$ and let $(Au)(x) = (d/dx)u(x)$ with domain $\mathscr{D}(A) = W_0^{1,2}(\mathbb{R}_-) \oplus W_0^{1,2}(\mathbb{R}_+) \subset L^2(\mathbb{R})$ (this domain coincides with the set of absolutely continuous functions in $L^2(\mathbb{R})$ that vanish at the origin, and whose derivative is in $L^2(\mathbb{R})$). A direct calculation shows that A is a closed, skew-symmetric operator which has a skew-adjoint extension with domain $W^{1,2}(\mathbb{R})$. Let Q be the orthogonal projection:

$$(Qu)(x) = \begin{cases} 0, & x < 0, \\ u(x), & x \geq 0. \end{cases}$$

Then QAQ is also skew-symmetric on $W_0^{1,2}(\mathbb{R}_-) \oplus W_0^{1,2}(\mathbb{R}_+)$, but has no skew-adjoint extension as its deficiency indexes are not equal [19]. In particular, QA does not generate a semigroup on the range of Q.

While the skew-adjointness of QL in $\mathscr{M}_\perp$ turns out to be a subtle issue when P is the conditional expectation (2.7), it is possible to show, under quite general conditions, that PL is skew-adjoint in $\mathscr{M}$, or equivalently, generates a unitary semigroup in $\mathscr{M}$. This is interesting because $QL = L - PL$ is then the sum of two skew-adjoint operators. This does not imply anything for QL, however, since L and QL are defined on different subspaces.

Specifically, let L be as in (2.3) and let $f \in \mathscr{D}(L) \cap \mathscr{M}$, i.e., $f = f(\hat{x})$. Then,

$$(Lf)(x) = \sum_{j=1}^{2n} b_j(x)\partial_j f(\hat{x}) = \sum_{j=1}^{2m} b_j(x)\partial_j f(\hat{x}),$$

and

$$(PLf)(\hat{x}) = \sum_{j=1}^{2m} (Pb_j)(\hat{x})\partial_j f(\hat{x}) = \sum_{j=1}^{2m} R_j(\hat{x})\partial_j f(\hat{x}),$$

where, as before, $R_j = Pb_j$ is the Markovian vector field.

PL generates a semigroup in $\mathscr{M}$ for the same reason that L generates a semigroup in L^2—because the equation

$$\frac{d}{dt}u^t(\hat{x}) = PLu^t(\hat{x}) = \sum_{j=1}^{2m} R_j(\hat{x})\partial_j u^t(\hat{x}) \tag{3.1}$$

is hyperbolic and can be solved by the method of characteristics. Indeed, let $\psi^t(\hat{x})$ be the flow map associated with the vector field R:

$$\begin{aligned} &\frac{d}{dt}\psi_j^t(\hat{x}) = R_j(\psi^t(\hat{x})), \\ &\psi_j^0(\hat{x}) = x_j, \end{aligned} \qquad j = 1, 2, \ldots, 2m. \tag{3.2}$$

Then

$$u^t(\hat{x}) = u^0(\psi^t(\hat{x}))$$

solves (3.1). To complete the argument it is necessary to determine under what conditions the ODEs (3.2) have a solution. In most cases of interest, the functions $b_j(x)$ are differentiable and the projection P preserves differentiability, hence the functions $R_j(\hat{x})$ are differentiable and (3.2) has a unique (local) solution. Note, moreover, that if $\varrho = \varrho(H)$, then

$$\mathcal{H}(\hat{x}) = \int \eta(H(x))d\tilde{x},$$

with $\eta(H) = \int_H^\infty \varrho(s)ds$, is a constant of motion for solutions of (3.2).

4. Existence of orthogonal dynamics: finite rank projection

In this section we show the existence of orthogonal dynamics for the case where the projection P is given by the finite-rank projection (2.6), i.e., has finite-dimensional range. Our proof is constructive and is based on a reduction of (2.9) to a Volterra equation.

THEOREM 4.1: *Let $h^\nu \in \hat{L}^2$, $\nu = 1, 2, \ldots, M$, be an orthonormal set, $h^\nu \in \mathscr{D}(L)$. For any function $g \in \mathscr{M}_\perp$ the orthogonal dynamics equation (2.9) has a unique solution on any bounded time interval.*

Proof: We start by rewriting the orthogonal dynamics equations (2.9) in the following equivalent form:

$$\begin{aligned}&\frac{d}{dt}w^t(x) - Lw^t(x) = -PLw^t(x),\\ &w^0(x) = g(x),\end{aligned}$$

where g belongs to the null space of P. Using Duhammel's principle with the left-hand side as an inhomogeneous term, we obtain the integral equation

$$w^t(x) = e^{tL}w^0(x) - \int_0^t e^{(t-s)L}PLw^s(x)ds.$$

Substituting the explicit expression (2.6) for the projection, we have

$$w^t(x) = e^{tL}w^0(x) - \sum_{\nu=1}^{M}\int_0^t c^\nu(s)e^{(t-s)L}h^\nu(\hat{x})ds, \tag{4.1}$$

where

$$c^\nu(s) = (Lw^s, h^\nu).$$

Given the functions $c^\nu(t)$, (4.1) is an explicit representation of $w^t(x)$ in terms of the solution operator e^{tL} of the Hamiltonian dynamics.

To find the coefficient functions $c^\nu(s)$ we apply L on both sides of (4.1), and take an inner product with each of the basis functions h^μ, $\mu = 1, 2, \ldots, M$. This yields the Volterra equation

$$c^\mu(t) = f^\mu(t) - \sum_{\nu=1}^{M}\int_0^t H^{\mu\nu}(t-s)c^\nu(s)ds, \tag{4.2}$$

with a kernel matrix

$$H^{\mu\nu}(t) = (Le^{tL}h^\nu, h^\mu) = -(e^{tL}h^\nu, Lh^\mu) = -(h^\nu, Le^{-tL}h^\mu) = -H^{\nu\mu}(-t),$$

and a forcing vector

$$f^\mu(t) = (Le^{tL}w^0, h^\mu) = -(w^0, Le^{-tL}h^\mu).$$

The problem of solving the orthogonal dynamics (2.9) has been thus reduced to that of solving the Volterra equation (4.2). Note that both the forcing $f^\mu(t)$ and the kernel $H^{\mu\nu}(t)$ are autocorrelation functions with respect to the Liouvillian time evolution e^{tL}. These quantities can be calculated by averaging over a collection of experiments or numerical simulations, with initial conditions drawn from the equilibrium distribution.

By the unitarity of the evolution operator e^{tL} it follows that

$$|H^{\mu\nu}(t)| \le \|h^\nu\|\|Lh^\mu\|, \quad |f^\mu(t)| \le \|w^0\|\|Lh^\mu\|.$$

Since, as a result of the continuity of the semigroup e^{tL}, $H^{\mu\nu}(t)$ and $f^\mu(t)$ are continuous functions of time, then there exist solutions to (4.2) on any bounded time interval (see, e.g., [7] for a general reference on the Volterra equation). ∎

5. Existence of weak solutions

Henceforth we consider P to be the conditional expectation (2.7). We prove the existence of a *weak* solution to the orthogonal dynamics (2.9). The main results are stated in Theorem 5.11 and Corollary 5.12. Our approach follows Friedrichs' construction of weak solutions for a symmetric hyperbolic system [6] (see also John [8]). For Friedrichs' method to be applicable, we first need to show that L^2 functions in the null space of P can be approximated, within this subspace, by smooth functions with compact support. This is done in Lemmas 5.1 and 5.2. Throughout this section it is assumed that the vector field $b(x)$ is differentiable, and that the density $\varrho(x)$ is continuous and strictly positive.

We prove the existence of solutions on a finite time interval $[0, T_0]$; T_0 may be taken arbitrarily large. Functions $w^t(x)$ are defined on the domain $\mathcal{R} = [0, T_0] \times \mathbb{R}^{2n}$, which is bounded by the two surfaces

$$\mathcal{S} = \{0\} \times \mathbb{R}^{2n}, \quad \mathcal{T} = \{T_0\} \times \mathbb{R}^{2n}.$$

Following standard notations, we denote by $C(\mathcal{R})$ the set of continuous functions on $\mathcal{R}$, and by $C^k(\mathcal{R})$, $k = 1, 2, \ldots, \infty$, the set of k times differentiable functions. We denote by $C_c(\mathcal{R})$ and $C_c^k(\mathcal{R})$ the sub-classes of functions that have compact support in the x variables; specifically, $u \in C_c^k(\mathcal{R})$ if it is in $C^k(\mathcal{R})$, and in addition $\operatorname{supp}(u) \subset [0,T_0] \times K$ for some $K \subset \mathbb{R}^{2n}$ compact. Given a function $u \in C^k(\mathcal{R})$, we denote by Su and Tu its restriction to the surfaces $\mathcal{S}$ and $\mathcal{T}$, respectively. Clearly, $Su \in C^k(\mathcal{S})$ and $Tu \in C^k(\mathcal{T})$. The same holds for C^k replaced by C_c^k.

We endow the spaces $C_c^\infty(\mathcal{R})$, $C_c^\infty(\mathcal{S})$, and $C_c^\infty(\mathcal{T})$ with the inner products

$$\begin{aligned}(u_1,u_2)_{\mathcal{R}} &= \int_{\mathcal{R}} u_1^t(x) u_2^t(x) \varrho(x)\, dx dt,\\ (v_1,v_2)_{\mathcal{S}} &= \int_{\mathcal{S}} v_1(x) v_2(x) \varrho(x)\, dx,\\ (w_1,w_2)_{\mathcal{T}} &= \int_{\mathcal{T}} w_1(x) w_2(x) \varrho(x)\, dx.\end{aligned}$$

The corresponding norms are denoted by $\|\cdot\|_{\mathcal{R}}$, $\|\cdot\|_{\mathcal{S}}$, and $\|\cdot\|_{\mathcal{T}}$, respectively. These spaces can be completed into Hilbert spaces, $L^2(\mathcal{R})$, $L^2(\mathcal{S})$, and $L^2(\mathcal{T})$.

Lemma 5.1: *The space of functions*

$$C_{c,0}^\infty(\mathcal{R}) = \{u \in C_c^\infty(\mathcal{R}) : Su = Tu = 0\}$$

is dense in $L^2(\mathcal{R})$.

Proof: $C_c^\infty(\mathcal{R})$ is dense in $L^2(\mathcal{R})$ by definition. Functions in $C_c^\infty(\mathcal{R})$ can further be approximated by functions in $C_{c,0}^\infty(\mathcal{R})$ as is well known (see [16]). ∎

Consider now the conditional expectation, P, which is a projection operator on $L^2(\mathbb{R}^{2n})$. Since $L^2(\mathcal{S})$ and $L^2(\mathcal{T})$ are isomorphic to $L^2(\mathbb{R}^{2n})$, the projection is automatically defined on these spaces. On $L^2(\mathcal{R})$ we define, with a slight abuse of notation, P to act pointwise in time:

$$(Pu)^t(\hat{x}) = \frac{\int u^t(\hat{x},\tilde{x}) \varrho(\hat{x},\tilde{x})\, d\tilde{x}}{\int \varrho(\hat{x},\tilde{x})\, d\tilde{x}}.$$

It is easily verified that P is an orthogonal projection on a closed subspace of $L^2(\mathcal{R})$.

The orthogonal dynamics (2.9) takes place in the null space of P, hence we introduce the following spaces:

$$\begin{aligned}L_\perp^2(\mathcal{R}) &= L^2(\mathcal{R}) \cap \mathscr{N}(P),\\ L_\perp^2(\mathcal{S}) &= L^2(\mathcal{S}) \cap \mathscr{N}(P),\\ L_\perp^2(\mathcal{T}) &= L^2(\mathcal{T}) \cap \mathscr{N}(P).\end{aligned}$$

The following approximation lemma is analogous to Lemma 5.1. It states that functions in $L_\perp^2(\mathcal{R})$ can be approximated by smooth functions of compact support within this subspace.

LEMMA 5.2: *The space of functions $C^\infty_{c,0}(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ is dense in $L^2_\perp(\mathcal{R})$.*

Proof: Let $u \in L^2_\perp(\mathcal{R})$. Since $L^2_\perp(\mathcal{R}) \subset L^2(\mathcal{R})$, then by Lemma 5.1 there exists, for all $\epsilon > 0$, a function $v \in C^\infty_{c,0}(\mathcal{R})$ such that

$$\operatorname{supp} v \subset [0, T_0] \times [-b, b] \times \cdots \times [-b, b] \subset [0, T_0] \times \mathbb{R}^{2n},$$

for some $b > 0$, and $\|u - v\|_\mathcal{R} \leq \epsilon/3$. There is, however, no guarantee that $v \in L^2_\perp(\mathcal{R})$; we can only deduce that the projection of v on $L^2_\perp(\mathcal{R})$ is small,

$$\|Pv\|_\mathcal{R} = \|P(u - v)\|_\mathcal{R} \leq \|u - v\|_\mathcal{R} \leq \epsilon/3.$$

On the other hand, $(I - P)v \in C^\infty(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$, but will, in general, not have compact support.

We next define

$$g(\hat{x}) = \int \varrho(\hat{x}, \tilde{x}) d\tilde{x},$$

which is a positive, differentiable function of $\hat{x}$, and

$$f(\hat{x}, a) = \int_{|x_i| \leq a} \varrho(\hat{x}, \tilde{x}) d\tilde{x},$$

which is a differentiable, increasing function of a, with $f(\hat{x}, 0) = 0$. Since $\lim_{a\to\infty} f(\hat{x}, a) = g(\hat{x})$, then it follows that for every $\hat{x}$ there exists an $a = A(\hat{x})$ such that $f(\hat{x}, a) = \frac{1}{2} g(\hat{x})$. Then we set

$$R = \max_{|x_i| \leq b} A(\hat{x}) + b$$

(here we use the fact that $A(\hat{x})$ is a continuous function of $\hat{x}$, which follows from the implicit function theorem).

Let now $\eta(\tilde{x})$ be a non-negative $C^\infty(\mathbb{R}^{2(n-m)})$ function with compact support, $0 \leq \eta(\tilde{x}) \leq 1$, and $\eta(\tilde{x}) = 1$ if $|x_i| \leq R$, $i = 2m + 1, \ldots, 2n$. By our choice of R it follows that for all $\hat{x}$ such that $|x_i| \leq b$, $i = 1, \ldots, 2m$,

$$(P\eta)(\hat{x}) = \frac{\int \eta(\tilde{x}) \varrho(\hat{x}, \tilde{x}) d\tilde{x}}{\int \varrho(\hat{x}, \tilde{x}) d\tilde{x}} \geq \frac{\int_{|x_i| \leq R} \varrho(\hat{x}, \tilde{x}) d\tilde{x}}{\int \varrho(\hat{x}, \tilde{x}) d\tilde{x}} \geq \frac{1}{2},$$

hence

$$\left| \frac{\eta(\tilde{x})}{(P\eta)(\hat{x})} \right| \leq 2.$$

Finally, consider the function

$$w^t(\hat{x}, \tilde{x}) = v^t(\hat{x}, \tilde{x}) - (Pv)^t(\hat{x}) \frac{\eta(\tilde{x})}{(P\eta)(\hat{x})}.$$

Clearly, $Pw = 0$, hence $w \in L^2_\perp(\mathcal{R})$. It has compact support in $\mathcal{R}$ as Pv has compact support in the $(t, \hat{x})$ variables and η has compact support in the $\tilde{x}$ variables; since all the functions are also smooth we have $w \in C^\infty_{c,0}(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$.

It remains to show that w approximates u. Indeed,

$$\begin{aligned}\|u - w\|_\mathcal{R} &\le \|u - v\|_\mathcal{R} + \|v - w\|_\mathcal{R} \\ &\le \frac{\epsilon}{3} + \left\| Pv \cdot \frac{\eta}{P\eta} \right\|_\mathcal{R} \\ &\le \frac{\epsilon}{3} + 2 \cdot \frac{\epsilon}{3}.\end{aligned}$$

This completes the proof. ∎

We are going to prove the existence of a (weak) solution $u \in L^2_\perp(\mathcal{R})$ to the orthogonal dynamics equation

$$Eu^t(x) = \left(\frac{d}{dt} - QL \right) u^t(x) = 0,$$

with $u^0 \in L^2_\perp(\mathcal{S})$. Since the flow field $b(x)$ is continuous, then L, which is a first-order differential operator, maps $C^1_c(\mathcal{R})$ into $C_c(\mathcal{R})$. Note, however, that Qu does not necessarily have compact support even if u does. Hence, the operator E maps $C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ into $C(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$. Weak solutions are defined with respect to a weak extension of the operator E. We construct operators $\tilde{E}, \tilde{S}$, which we show to be extensions of E, S (called weak extensions), and prove that for every $g \in L^2_\perp(\mathcal{S})$ there corresponds a $u \in L^2_\perp(\mathcal{R})$ such that $\tilde{E}u = 0$ and $\tilde{S}u = g$. The definition of $\tilde{E}, \tilde{S}$ is based on the following adjointness formula:

Lemma 5.3: *The identity*

$$(v, Ew)_\mathcal{R} + (Ev, w)_\mathcal{R} + (Sv, Sw)_\mathcal{S} - (Tv, Tw)_\mathcal{T} = 0 \tag{5.1}$$

holds for all $v, w \in C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$.

Proof: This is an immediate consequence of the skew-symmetry of QL in $C^1_c(\mathbb{R}^{2n}) \cap L^2_\perp(\mathbb{R}^{2n})$:

$$\begin{aligned}(v, Ew)_\mathcal{R} &= \int_\mathcal{R} v^t(x) \left[\frac{d}{dt} w^t(x) - QLw^t(x) \right] \varrho(x) dx dt \\ &= \int_\mathcal{R} \left\{ \frac{d}{dt}[v^t(x) w^t(x)] - w^t(x) \frac{d}{dt} v^t(x) - v^t(x)[QLw^t(x)] \right\} \varrho(x) dx dt \\ &= (Tv, Tw)_\mathcal{T} - (Sv, Sw)_\mathcal{S} - \int_\mathcal{R} w^t(x) \left[\frac{d}{dt} v^t(x) - QLv^t(x) \right] \varrho(x) dx dt \\ &= (Tv, Tw)_\mathcal{T} - (Sv, Sw)_\mathcal{S} - (Ev, w)_\mathcal{R}. \quad ∎\end{aligned}$$

The weak extensions $\tilde{E}, \tilde{S}$ of the operators E, S are defined on a space $L^2_{\perp,w}(\mathcal{R})$, which we define next:

Definition 5.4: The space $L^2_{\perp,w}(\mathcal{R})$ consists of all functions $v \in L^2_\perp(\mathcal{R})$ for which there exist functions $f \in L^2_\perp(\mathcal{R})$ and $g \in L^2_\perp(\mathcal{S})$, such that the relation

$$(v, Ew)_\mathcal{R} + (f, w)_\mathcal{R} + (g, Sw)_\mathcal{S} = 0 \tag{5.2}$$

holds for all $w \in C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ for which $Tw = 0$.

By definition $L^2_{\perp,w}(\mathcal{R}) \subseteq L^2_\perp(\mathcal{R})$; by the adjointness formula (5.1), $v \in C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ satisfies (5.2) with $f = Ev$ and $g = Sv$, thus we have the following hierarchy:

$$C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R}) \subseteq L^2_{\perp,w}(\mathcal{R}) \subseteq L^2_\perp(\mathcal{R}).$$

The following two lemmas are needed to establish that the mappings $v \mapsto f$ and $v \mapsto g$ are uniquely defined, and extend the operators E, S.

Lemma 5.5: *Equation (5.2) is satisfied for $v = 0$ only if $f = 0$ and $g = 0$.*

Proof: Let $v = 0$ and suppose that (5.2) is satisfied for some $f \in L^2_\perp(\mathcal{R})$ and $g \in L^2_\perp(\mathcal{S})$. Since (5.2) holds for all $w \in C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ for which $Tw = 0$, it certainly holds if we further restrict w to satisfy $Sw = 0$. In this case, we remain with

$$(f, w)_\mathcal{R} = 0$$

for all $w \in C^1_{c,0}(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$. By Lemma 5.2 this set is dense in $L^2_\perp(\mathcal{R})$, therefore $f = 0$. Lifting now the restriction on Sw, (5.2) reduces to

$$(g, Sw)_\mathcal{S} = 0$$

for all $w \in C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ which satisfy $Tw = 0$. It is easy to see that the restriction of $C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ functions to the surface $t = 0$ is dense in $L^2_\perp(\mathcal{S})$, hence $g = 0$. ∎

Lemma 5.6: *Let $v \in L^2_{\perp,w}(\mathcal{R})$; then the functions f, g in (5.2) are uniquely and linearly determined by v.*

Proof: Suppose that (5.2) is satisfied by two sets of functions f_1, g_1 and f_2, g_2:

$$(v, Ew)_\mathcal{R} + (f_1, w)_\mathcal{R} + (g_1, Sw)_\mathcal{S} = 0,$$
$$(v, Ew)_\mathcal{R} + (f_2, w)_\mathcal{R} + (g_2, Sw)_\mathcal{S} = 0.$$

Subtracting one from another we get

$$(0, Ew)_{\mathcal{R}} + (f_1 - f_2, w)_{\mathcal{R}} + (g_1 - g_2, Sw)_{\mathcal{S}} = 0,$$

for all $w \in C_c^1(\mathcal{R}) \cap L_\perp^2(\mathcal{R})$ which satisfy $Tw = 0$. By the previous lemma this implies $f_1 = f_2$ and $g_1 = g_2$. The linearity of $v \mapsto f$ and $v \mapsto g$ is an immediate consequence of the bilinearity of the inner product. ∎

Corollary 5.7: *Let $v \in L^2_{\perp,w}(\mathcal{R})$: the linear mappings $v \mapsto f$, $v \mapsto g$, which we denote by $f = \tilde{E}v$ and $g = \tilde{S}v$, are* **weak extensions** *(the so-called Friedrichs extension) of the operators E and S in the sense that*

$$(v, Ew)_{\mathcal{R}} + (\tilde{E}v, w)_{\mathcal{R}} + (\tilde{S}v, Sw)_{\mathcal{S}} = 0 \tag{5.3}$$

for all $w \in C_c^1(\mathcal{R}) \cap L_\perp^2(\mathcal{R})$ for which $Tw = 0$.

Next, we define a **strong extension** of the operators E and S:

Definition 5.8: The space $L^2_{\perp,s}(\mathcal{R})$ consists of all functions $v \in L^2_\perp(\mathcal{R})$, for which there exist functions $f \in L^2_\perp(\mathcal{R})$, $g \in L^2_\perp(\mathcal{S})$, and a sequence of functions $v_n \in C_c^1(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$, $Tv_n = 0$, such that

$$\lim_{n\to\infty} \|v_n - v\|_{\mathcal{R}} = 0, \qquad \lim_{n\to\infty} \|Ev_n - f\|_{\mathcal{R}} = 0, \qquad \lim_{n\to\infty} \|Sv_n - g\|_{\mathcal{S}} = 0. \tag{5.4}$$

Lemma 5.9: *If $v \in L^2_{\perp,s}(\mathcal{R})$ then $v \in L^2_{\perp,w}(\mathcal{R})$, i.e.,*

$$C_c^1(\mathcal{R}) \cap L^2_\perp(\mathcal{R}) \subseteq L^2_{\perp,s}(\mathcal{R}) \subseteq L^2_{\perp,w}(\mathcal{R}) \subseteq L^2_\perp(\mathcal{R}).$$

Proof: Let $v \in L^2_{\perp,s}(\mathcal{R})$ and v_n be a sequence in $C_c^1(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$, $Tv_n = 0$, satisfying (5.4). For all $w \in C_c^1(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ for which $Tw = 0$, the adjointness formula (5.1) reads

$$(v_n, Ew)_{\mathcal{R}} + (Ev_n, w)_{\mathcal{R}} + (Sv_n, Sw)_{\mathcal{S}} = 0.$$

Taking the limit $n \to \infty$ we have

$$(v, Ew)_{\mathcal{R}} + (f, w)_{\mathcal{R}} + (g, Sw)_{\mathcal{S}} = 0,$$

which by Definition 5.4 implies that $v \in L^2_{\perp,w}(\mathcal{R})$ with $\tilde{E}v = f$ and $\tilde{S}v = g$. ∎

Thus, the mappings $v \mapsto f$, $v \mapsto g$ in Definition 5.8 are extensions of the operators E, S; they are called **strong extensions** and are denoted by $f = \bar{E}v$, $g = \bar{S}v$.

We next derive a so-called energy inequality, which holds for all functions in $L^2_{\perp,s}(\mathcal{R})$:

LEMMA 5.10: *There exists a number $\gamma > 0$ such that for all $v \in L^2_{\perp,s}(\mathcal{R})$,*

$$\|v\|^2_{\mathcal{R}} + \|\bar{S}v\|^2_{\mathcal{S}} \le \gamma^2 \|\bar{E}v\|^2_{\mathcal{R}}. \tag{5.5}$$

Proof: Consider first $v \in C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$, $Tv = 0$. For all $0 \le t \le T_0$ we have

$$\begin{aligned}
\frac{d}{dt}\|v^{T_0-t}\|^2_{L^2(\mathbb{R}^{2n})} &= -2\Big(v^{T_0-t}, \frac{d}{dt}v^{T_0-t}\Big)_{L^2(\mathbb{R}^{2n})} \\
&= -2\left(v^{T_0-t}, Ev^{T_0-t} + QLv^{T_0-t}\right)_{L^2(\mathbb{R}^{2n})} \\
&= -2\left(v^t, Ev^t\right)_{L^2(\mathbb{R}^{2n})} \\
&\le 2\|v^{T_0-t}\|_{L^2(\mathbb{R}^{2n})}\|Ev^{T_0-t}\|_{L^2(\mathbb{R}^{2n})} \\
&\le \|v^{T_0-t}\|^2_{L^2(\mathbb{R}^{2n})} + \|Ev^{T_0-t}\|^2_{L^2(\mathbb{R}^{2n})},
\end{aligned}$$

where we have used the skew-symmetry of QL in $C^1_c(\mathbb{R}^{2n}) \cap L^2_\perp(\mathbb{R}^{2n})$ in the passage from the second to the third line.

Rewriting this differential inequality as

$$\frac{d}{dt}\left(e^{T_0-t}\|v^{T_0-t}\|^2_{L^2(\mathbb{R}^{2n})}\right) \le e^{T_0-t}\|Ev^{T_0-t}\|^2_{L^2(\mathbb{R}^{2n})} \tag{5.6}$$

and integration over $[0, T_0]$ gives

$$\|Sv\|^2_{\mathcal{S}} \le e^{T_0}\|Ev\|^2_{\mathcal{R}}. \tag{5.7}$$

Integrating (5.6) over $[0, t]$, followed by a second integration over $[0, T_0]$, yields on the other hand

$$\|v\|^2_{\mathcal{R}} \le (e^{T_0} - 1)\|Ev\|^2_{\mathcal{R}}. \tag{5.8}$$

Combining (5.7) and (5.8) we obtain (5.5) with $\gamma^2 = 2e^{T_0} - 1$. This inequality holds for all $v \in L^2_{\perp,s}(\mathcal{R})$ by the very definition of this space and the corresponding operators $\bar{E}$ and $\bar{S}$. ∎

We are now in measure to prove the main theorem from which follows the existence of weak solutions to the orthogonal dynamics equation.

THEOREM 5.11: *For all $f \in L^2_\perp(\mathcal{R})$ and $g \in L^2_\perp(\mathcal{S})$ there exists a function $u \in L^2_{\perp,w}(\mathcal{R})$ for which*

$$\tilde{E}u = f, \quad \tilde{S}u = g.$$

Proof: Consider the set of functions $v \in C^1_c(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$ for which $Tv = 0$, endowed with the inner product

$$(v, w)_{\mathscr{H}} = (Ev, Ew)_{\mathcal{R}}.$$

The corresponding norm is denoted by $\|\cdot\|_{\mathscr{H}}$ (note that $Ev = 0$ implies by the energy inequality (5.5) that $v = 0$). The Hilbert space obtained by the completion of this space is denoted by $\mathscr{H}$.

Let $v_n \in C_c^1(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$, $Tv_n = 0$, be a Cauchy sequence in $\mathscr{H}$. By definition,

$$\|Ev_n - Ev_m\|^2_{\mathcal{R}} = \|v_n - v_m\|^2_{\mathscr{H}} \to 0,$$

whereas by the energy inequality (5.5)

$$\|v_n - v_m\|^2_{\mathcal{R}} + \|Sv_n - Sv_m\|^2_{\mathcal{S}} \leq \gamma^2 \|Ev_n - Ev_m\|^2_{\mathcal{R}} \to 0.$$

Since $L^2_\perp(\mathcal{R})$ and $L^2_\perp(\mathcal{S})$ are complete spaces, there exist $v, f \in L^2_\perp(\mathcal{R})$ and $g \in L^2_\perp(\mathcal{S})$ such that $v_n \to v$, $Ev_n \to f$, $Sv_n \to g$, and $Tv_n = 0$, i.e., $v \in L^2_{\perp,s}(\mathcal{R})$ with $f = \bar{E}v$ and $g = \bar{S}v$. Moreover, v can be identified with the limit in $\mathscr{H}$ of the Cauchy sequence v_n, which implies that $\mathscr{H} \subseteq L^2_{\perp,s}(\mathcal{R})$ and

$$(v, w)_{\mathscr{H}} = (\bar{E}v, \bar{E}w)_{\mathcal{R}}.$$

Let $f \in L^2_\perp(\mathcal{R})$ and $g \in L^2_\perp(\mathcal{S})$ be given and consider the linear functional on $\mathscr{H}$ given by

$$\Phi(w) = -(f, w)_{\mathcal{R}} - (g, \bar{S}w)_{\mathcal{S}}.$$

We show that this functional is bounded, i.e., $\Phi \in \mathscr{H}^*$ (the dual space of $\mathscr{H}$): For all $w \in C_c^1(\mathcal{R}) \cap L^2_\perp(\mathcal{R})$, $Tw = 0$,

$$\begin{aligned}
|\Phi(w)| &\leq |(f, w)_{\mathcal{R}}| + |(g, \bar{S}w)_{\mathcal{S}}| \\
&\leq \|f\|_{\mathcal{R}} \|w\|_{\mathcal{R}} + \|g\|_{\mathcal{S}} \|\bar{S}w\|_{\mathcal{S}} \\
&\leq \sqrt{\|f\|^2_{\mathcal{R}} + \|g\|^2_{\mathcal{S}}} \sqrt{\|w\|^2_{\mathcal{R}} + \|\bar{S}w\|^2_{\mathcal{S}}} \\
&\leq \gamma \sqrt{\|f\|^2_{\mathcal{R}} + \|g\|^2_{\mathcal{S}}} \|\bar{E}w\|_{\mathcal{R}} \\
&\leq \text{const}\, \|w\|_{\mathscr{H}},
\end{aligned}$$

where Cauchy–Schwarz has been used in the passage from the first to the second line, and the energy inequality has been used in the passage to the fourth line. Thus, $\Phi(w)$ is a bounded functional that can be extended to the whole $\mathscr{H}$.

By the Riesz representation theorem there exists a $v \in \mathscr{H}$ such that

$$\Phi(w) = (v, w)_{\mathscr{H}}$$

for all $w \in \mathscr{H}$, that is,

$$(\bar{E}v, \bar{E}w)_{\mathcal{R}} + (f, w)_{\mathcal{R}} + (g, \bar{S}w)_{\mathcal{S}} = 0.$$

Since this holds, in particular, for all $w \in C_c^1(\mathcal{R}) \cap L_\perp^2(\mathcal{R})$ for which $Tw = 0$, it follows by Definition 5.4 that $u = \bar{E}v \in L_{\perp,w}^2(\mathcal{R})$, with $\tilde{E}u = f$ and $\tilde{S}u = g$. This completes the proof. ∎

COROLLARY 5.12 (Existence of weak solutions): *Let $g \in L_\perp^2(\mathcal{S})$; then there exists a weak solution $u \in L_{\perp,w}^2(\mathcal{R})$ to the orthogonal dynamics, such that $\tilde{E}u = 0$ and $\tilde{S}u = g$. Explicitly,*

$$(u, Ew)_{\mathcal{R}} + (g, Sw)_{\mathcal{S}} = 0$$

for all $w \in C_c^1(\mathcal{R}) \cap L_\perp^2(\mathcal{R})$ for which $Tw = 0$.

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Appendix A. Flow on manifolds: the micro-canonical ensemble

In this appendix we describe how to adapt the Mori–Zwanzig formalism for a micro-canonical ensemble, where the invariant measure is concentrated on a level set of the Hamiltonian (an "energy shell").

Assume that the Hamiltonian H is $C^\infty(\mathbb{R}^{2n})$. According to Sard's theorem [17] H has only a null set of singular values. Let c be a regular value of H, and define $M = \{x \in \mathbb{R}^{2n} : H(x) = c\}$. M is an orientable manifold with measure dP, induced by the Lebesgue measure on $\mathbb{R}^{2n}$. Recall that the Lebesgue measure can be constructed using a volume, which is a $2n$-form in $\mathbb{R}^{2n}$. The induced measure on M is constructed using a $(2n-1)$-form defined on the tangent bundle of M; it is the Lebesgue $2n$-form, with one of its arguments fixed to be the unit vector normal to M, divided by $|\nabla H|$. The induced measure dP is the micro-canonical measure. It is invariant under the Hamiltonian flow.

Let b: $M \mapsto TM$ be the Hamiltonian vector field, where TM is the tangent bundle of M; the equations of motion are:

$$\frac{d}{dt}\varphi^t(m) = b(\varphi^t(m)),$$
$$\varphi^0(m) = m.$$

Since H is a constant of motion, $m \in M$ implies $\varphi^t(m) \in M$ for all t.

We next introduce the equivalent Liouville dynamics. For every $f \in C^\infty(M)$ let df denote its differential form. The differential operator L: $C^\infty(M) \mapsto C^\infty(M)$, defined by

$$Lf(m) = df(m) \cdot b(m),$$

is the Liouvillian, of the Lie derivative associated with the vector space B. One can show that the Liouville equation

$$\begin{aligned} &\frac{d}{dt} u^t(m) = (Lu^t)(m) \\ &u^0(m) = g(m) \end{aligned}$$

has for solution $u^t(m) = g(\varphi^t(m))$, i.e., that the Hamiltonian trajectories $\varphi^t(m)$ are the characteristic curves for the Liouville equation.

The space $C^\infty(M)$ is endowed with an inner product,

$$(f, g) = \int fg dP,$$

and can be completed into a Hilbert space $L^2(M)$. It is straightforward to show that the Lie derivative L is skew-symmetric with respect to this inner product.

To carry out the Mori–Zwanzig decomposition it is necessary to choose the resolved variables, and define a projection operator which maps functions in $L^2(M)$ into a closed subspace of functions of the resolved variables. We show here how to define a projection which is the conditional expectation given the resolved variables. We demonstrate it for a single resolved variable $g \in C^\infty(M)$. The generalization to several variables is straightforward.

Let $g \in C^\infty(M)$ by given. By Sard's theorem, if c is a regular value of g, then $M_c = \{m \in M : g(m) = c\}$ is an orientable sub-manifold of M, with induced measure dP_c. The conditional expectation of a function $f \in L^2(M)$ given g is

$$E[f|g](m) = \frac{\int_{g^{-1}(g(m))} f dP_{g(m)}}{\int_{g^{-1}(g(m))} dP_{g(m)}}.$$

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