Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Deriving a GENERIC system from a Hamiltonian system

Alexander Mielke[1], Mark A. Peletier[2], Johannes Zimmer[3]

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[1] Weierstrass Institute
    Mohrenstr. 39
    10117 Berlin
    Germany
    and
    Institut für Mathematik
    Humboldt-Universität zu Berlin
    Rudower Chaussee 25
    12489 Berlin
    Germany
    E-Mail: alexander.mielke@wias-berlin.de

[2] Department of Mathematics and Computer Science
    Eindhoven University of Technology
    The Netherlands
    E-Mail: m.a.peletier@tue.nl

[3] School of Computation, Information, and Technology
    Technische Universität München
    Germany
    E-Mail: jz@tum.de

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Deriving a GENERIC system from a Hamiltonian system

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Abstract

We reconsider the fundamental problem of coarse-graining infinite-dimensional Hamiltonian dynamics to obtain a macroscopic system which includes dissipative mechanisms. In particular, we study the thermodynamical implications concerning Hamiltonians, energy, and entropy and the induced geometric structures such as Poisson and Onsager brackets (symplectic and dissipative brackets).

We start from a general finite-dimensional Hamiltonian system that is coupled linearly to an infinite-dimensional heat bath with linear dynamics. The latter is assumed to admit a compression to a finite-dimensional dissipative semigroup (i.e., the heat bath is a dilation of the semigroup) describing the dissipative evolution of new macroscopic variables.

Already in the finite-energy case (zero-temperature heat bath) we obtain the so-called GENERIC structure (General Equations for Non-Equilibrium Reversible Irreversibe Coupling), with conserved energy, nondecreasing entropy, a new Poisson structure, and an Onsager operator describing the dissipation. However, their origin is not obvious at this stage. After extending the system in a natural way to the case of positive temperature, giving a heat bath with infinite energy, the compression property leads to an exact multivariate Ornstein-Uhlenbeck process that drives the rest of the system. Thus, we are able to identify a conserved energy, an entropy, and an Onsager operator (involving the Green-Kubo formalism) which indeed provide a GENERIC structure for the macroscopic system.

Contents

1   Introduction

1.1   Coarse-graining, GENERIC, and compressions

We revisit the classical topic of coarse-graining of Hamiltonian systems, and derive a thermodynamically consistent reduction for Hamiltonian systems which linearly couple a finite-dimensional Hamiltonian system to an infinite-dimensional Hamiltonian system acting as heat bath. A crucial element in

the reduction procedure is the theory of compressions. We now describe the main concepts in more detail.

Coarse-graining is the process by which less detailed ('coarse-grained') models of physical systems are derived from more detailed ones ('fine-grained'; see, e.g., [E11, Kue15]). One methodology for coarse-graining is the Mori-Zwanzig formalism, which allows to give macroscopic descriptions of microscopic systems such as those arising in molecular dynamics. In particular, this allows one to study the emergence of macroscopic dissipation from microscopically reversible Hamiltonian systems. In this paper we study a classical example of this type [JaP98a, Zwa01a].

GENERIC [Mor86, GrÖ97, ÖtG97] describes a class of thermodynamic evolution equations. If an evolution equation can be put in GENERIC form, then it is automatically thermodynamically consistent. In particular, it satisfies conservation of an energy and monotonicity of an entropy. In GENERIC, this thermodynamic consistency is implemented by combining a symplectic operator acting on the energy and a semidefinite operator acting on the entropy. In addition, the book [Ö05] describes a Mori-Zwanzig-type derivation of equations of GENERIC type from microscopic Hamiltonian systems with a clear separation of time scales. In this paper we derive a GENERIC form for the coarse-grained evolution, and this allows us to give an interpretation for the various components of the GENERIC structure.

A key ingredient in this mathematically rigorous derivation is the third component, *compressions*, which can be thought of the reverse of dilations. A *dilation* of a semigroup $\mathbb{S}_t$ on a space $\mathbf{Y}$ is a unitary group $\mathbb{U}_t$ on a larger Hilbert space $\mathbf{H}$ whose projection onto $\mathbf{Y}$ coincides with $\mathbb{S}_t$ [NF*10]. Conversely, compressions yield a projection of a unitary group on a large space onto a dissipative semigroup on a subspace. It is the existence of a suitable compression subspace that allows us to write the Mori-Zwanzig reduction in Markovian form and relate the dissipative part to the fluctuations.

1.2 Sketch of the microscopic Hamiltonian system

We first describe the starting point of this paper, which we call the 'microscopic' system. Later, from Section 1.4 onwards, we will describe how we apply a coarse-graining map to the state space of this system, which will lead to a system that we call 'macroscopic'. The terms 'microscopic' and 'macroscopic' do not refer to actual space or time scales, but are relative to the operation of coarse-graining. The coarse-graining map is highly non-injective, and therefore the macroscopic system has fewer degrees of freedom than the microscopic one.

The starting point of this paper, the 'microscopic system', resembles well-known models in the literature (see, e.g., [JaP98a, KS*02a, Rey06]). It couples two separate Hamiltonian systems: System A is finite-dimensional, and System B is infinite-dimensional and is interpreted as a heat bath. System A may be nonlinear, while System B and the coupling are linear. This is illustrated in Figure 1.1. The whole system is Hamiltonian, and in the interesting cases, the system also is reversible in time. The evolution is deterministic, while the initial data for the heat bath may be random, as we discuss below.
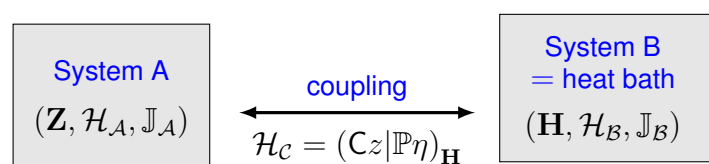

Figure 1.1: The microscopic system is a coupling of a fixed Hamiltonian system ('System A') and a heat bath ('System B'). See Section 1.2 for a discussion.

System A is described by a triple $(\mathbf{Z}, \mathcal{H}_{\mathcal{A}}, \mathbb{J}_{\mathcal{A}})$, where $\mathbf{Z}$ is a state space, $\mathcal{H}_{\mathcal{A}}$ is a Hamiltonian, and $\mathbb{J}_{\mathcal{A}}(z)\colon \mathbf{Z} \to \mathbf{Z}$ denotes the Poisson (also called co-symplectic) operators. We make the assumption that $\operatorname{div}_z \mathbb{J}_{\mathcal{A}} = 0$, corresponding to the Lebesgue measure being invariant (see Remark 4.7). The evolution of System A alone is given by the Hamiltonian evolution equation $\dot{z} = \mathbb{J}_{\mathcal{A}}(z)\mathrm{D}\mathcal{H}_{\mathcal{A}}(z)$.

System B, the heat bath, is described by a similar triple, $(\mathbf{H}, \mathcal{H}_{\mathcal{B}}, \mathbb{J}_{\mathcal{B}})$, where $\mathbf{H}$ is a Hilbert space, $\mathcal{H}_{\mathcal{B}}$ the Hamiltonian of the heat bath and $\mathbb{J}_{\mathcal{B}}$ a symplectic evolution operator. The evolution of the heat bath is linear. Specifically, we take

$$\mathcal{H}_{\mathcal{B}}(\eta) = \frac{1}{2}\|\eta\|_{\mathbf{H}}^2 \quad \text{for all } \eta \in \mathbf{H}.$$

The coupling between system A and system B is described by a Hamiltonian $\mathcal{H}_{\mathcal{C}}$, which couples the two systems linearly by

$$\mathcal{H}_{\mathcal{C}} = (\mathbb{A}z | \mathbb{P}\eta)_{\mathbf{H}}, \tag{1.1}$$

where $(\cdot|\cdot)_{\mathbf{H}}$ is the inner product in $\mathbf{H}$. Here $\mathbb{A}\colon \mathbf{Z} \to \mathbf{H}$ is a (linear) embedding operator; $\mathbb{P}$ is an orthogonal projection operator that is specified later. Since $\mathbb{P}$ is self-adjoint, we can alternatively define $\mathsf{C} := \mathbb{P}\mathbb{A}\colon \mathbf{Z} \to \mathbf{H}$ and write (1.1) as

$$\mathcal{H}_{\mathcal{C}} = (\mathsf{C}z | \eta)_{\mathbf{H}}. \tag{1.2}$$

The operator C satisfies $\mathsf{C} = \mathbb{P}\mathsf{C}$ and $\mathsf{C}^* = \mathsf{C}^*\mathbb{P}$.

The full (coupled) microscopic evolution for $(z, \eta) \in \mathbf{Z}\times\mathbf{H}$ is governed by the Hamiltonian

$$\mathcal{H}_{\text{total}}(z, \eta) = \mathcal{H}_{\mathcal{A}}(z) + \mathcal{H}_{\mathcal{B}}(\eta) + \mathcal{H}_{\mathcal{C}}(z, \eta), \tag{1.3}$$

together with the joint symplectic operator $\mathbb{J}_{\mathcal{A}} \oplus \mathbb{J}_{\mathcal{B}}$. The corresponding evolution equations are

$$\dot{z}_t = \mathbb{J}_{\mathcal{A}}(z)\big(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z_t) + \mathsf{C}^*\eta_t\big), \tag{1.4a}$$

$$\dot{\eta}_t = \mathbb{J}_{\mathcal{B}}\big(\eta_t + \mathsf{C}z_t\big), \tag{1.4b}$$

and the full Hamiltonian system is denoted by the triple $\big(\mathbf{Z}\times\mathbf{H}, \mathcal{H}_{\text{total}}, \mathbb{J}_{\mathcal{A}}\oplus\mathbb{J}_{\mathcal{B}}\big)$.

Example 1.1 (Running example, part 1)**.** To facilitate the understanding we provide a more explicit example for the whole theory that explains all the constructions in a concrete case.

For System A we consider a canonical Hamiltonian system with

$$z = (q, p) \in \mathbb{R}^n\times\mathbb{R}^n = \mathbf{Z}, \quad \mathcal{H}_{\mathcal{A}}(q, p) = \frac{1}{2}|p|^2 + V(q), \quad \text{and} \quad \mathbb{J}_{\mathcal{A}} = \begin{pmatrix} 0 & \mathbb{I}_{n\times n} \\ -\mathbb{I}_{n\times n} & 0 \end{pmatrix}.$$

For System B we choose

$$\mathbf{H} = \mathrm{L}^2(\mathbb{R}; \mathbb{R}^3), \quad \mathcal{H}_{\mathcal{B}}(\eta) = \frac{1}{2}\|\eta\|_{\mathrm{L}^2}^2, \quad \text{and} \quad \mathbb{J}_{\mathcal{B}} = \begin{pmatrix} -\partial_x & 0 & 0 \\ 0 & -\partial_x & 0 \\ 0 & 0 & -\partial_x \end{pmatrix}.$$

In particular, the unitary group $(\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}})_{t\in\mathbb{R}}$ is the group of shifts $\mathbb{S}_t f := f(\,\cdot\, -t)$. For the coupling we assume that only the state variable q (but not the momentum p) couples with the heat bath, i.e. $\mathcal{H}_{\mathcal{C}}(q, p, \eta) = (\mathsf{C}q | \eta)$ for a linear bounded operator $\mathsf{C}\colon \mathbb{R}^n \to \mathbf{H}$.

In summary, the example system has state $(q, p, \eta) \in \mathbb{R}^n\times\mathbb{R}^n\times\mathrm{L}^2(\mathbb{R}; \mathbb{R}^3)$ and is a coupled system of a nonlinear ODE and a linear transport equation for the three components of η:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q \\ p \\ \eta \end{pmatrix} = \begin{pmatrix} 0 & \mathbb{I}_{n\times n} & 0 \\ -\mathbb{I}_{n\times n} & 0 & 0 \\ 0 & 0 & -\partial_x \end{pmatrix}\begin{pmatrix} \mathrm{D}V(q) + \mathrm{D}_q\mathcal{H}_{\mathcal{C}}(q, \eta) \\ p \\ \eta + \mathrm{D}_\eta\mathcal{H}_{\mathcal{C}}(q, \eta) \end{pmatrix} = \begin{pmatrix} p \\ -\mathrm{D}V(q) - \mathsf{C}^*\eta \\ -\partial_x(\eta + \mathsf{C}q) \end{pmatrix}.$$

The first two equations are ODEs in $\mathbb{R}^d$, whereas the third equation is a transport equation in $\mathrm{L}^2(\mathbb{R}; \mathbb{R}^3)$ that has to be interpreted in a suitable weak or mild form, if we want to treat general initial conditions (see the abstract construction in Theorem 2.5). □

1.3 The compression property

We next choose the projection operator $\mathbb{P}$ and its range $\mathbf{W}$. The space $\mathbf{W}$ needs to be large enough to contain the range of C, but may also be larger. The central requirement that determines the choice of $\mathbf{W}$ and the projection $\mathbb{P}$ onto $\mathbf{W}$ is the following 'compression' property.

Assumption 1.2 (Compression property of the heat bath). *There exists a linear operator $\mathbb{D}$ on $\mathbf{W}$ such that*

$$\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\big|_{\mathbf{W}} = \begin{cases} \mathrm{e}^{-t\mathbb{D}} & t \geq 0 \\ \mathrm{e}^{t\mathbb{D}^*} & t \leq 0 \end{cases} \qquad on\ \mathbf{W}. \tag{1.5}$$

The eigenvalues of $\mathbb{D} + \mathbb{D}^*$ are strictly positive.

The left-hand side in the identity (1.5) should be interpreted as follows. If we evolve the heat bath starting from $w \in \mathbf{W}$, the result $\mathrm{e}^{t\mathbb{J}_\mathcal{B}}w$ typically is not an element of $\mathbf{W}$. Then $\mathbb{P}$ on the left-hand side projects $\mathrm{e}^{t\mathbb{J}_\mathcal{B}}w$ back onto $\mathbf{W}$, as one does in the Mori-Zwanzig framework. In particular, with the compression property the flow map $w \mapsto \mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}w$ is equivalent to the memory-less evolution $\dot{w} = -\mathbb{D}w$ for $t \geq 0$.

Assumption 1.2 in fact implies that $\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}$ is a strictly dissipative semigroup, since

$$\left\|\mathrm{e}^{-t\mathbb{D}}w\right\|_{\mathbf{H}} \leq \mathrm{e}^{-\alpha t}\|w\|_{\mathbf{H}} \qquad \text{for all } t \geq 0 \text{ and } w \in \mathbf{W},$$

where $\alpha > 0$ is the smallest eigenvalue of $(\mathbb{D} + \mathbb{D}^*)/2$.

Remark 1.3. In Assumption 1.2, it is equivalent to assume only the behavior for $t \geq 0$: the unitary nature of $\mathrm{e}^{t\mathbb{J}_\mathcal{B}}$ then implies that $\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\mathbb{P} = \mathbb{P}\big(\mathrm{e}^{-t\mathbb{J}_\mathcal{B}}\big)^*\mathbb{P} = \big(\mathbb{P}\mathrm{e}^{-t\mathbb{J}_\mathcal{B}}\mathbb{P}\big)^* = \mathrm{e}^{t\mathbb{D}^*}\mathbb{P}$ for $t \leq 0$. □

The context of the compression property is the theory of (dilations and) compressions. The relevant background is summarised in Appendix C. In essence, the theory of dilations states that for any contraction semigroup $(C_t)_{t \geq 0}$ one can find a unitary group $(S_t)_{t \in \mathbb{R}}$ on a sufficiently larger Hilbert space such that C_t is a 'coarse-grained version' of S_t. Conversely, one can in this setting regard the dissipative semigroup as a compression of a given unitary group. In our context, the unitary group is $\mathrm{e}^{t\mathbb{J}_\mathcal{B}}$ and represents the linear Hamiltonian system and $\mathrm{e}^{-t\mathbb{D}}$ is the contraction semigroup. We interpret a compression as a coarse-graining of a unitary group.

The crucial implication of the Compression Property 1.2 is that the evolution $\mathrm{e}^{-t\mathbb{D}}$ on $\mathbf{W}$ is a semigroup. It is thus in particular Markovian in the sense that the evolution equation does not involve the past. In (2.5b), we give a representation of the heat bath variable η which involves a memory term. The compression property allows us to rewrite that memory term as a local term.

For the coupled system, the projection onto $\mathbf{W}$, i.e., the part of the heat bath which interacts with System A, yields a compression semigroup. The existence of a compression, and with it the associated compression subspace $\mathbf{W}$ is related to the theory of Markovian subspaces in linear systems theory, see [LiP15, Ch. 10]. Necessary and sufficient conditions for the existence of compression subspaces are given in [Pic86, Th. 5.4]. We discuss the Compression Property 1.2 in more detail in Section 3.

Example 1.4 (Running example, part 2)**.** Example 1.1 was chosen such that the unitary shift group $\mathbb{S}_t = \mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}$ admits an explicit and simple compression. We choose a linear operator $\mathbb{D}$ on $\mathbb{R}^3$ with eigenvalues $\vartheta_1 > 0$ and $\vartheta_2 \pm \mathrm{i}\varsigma$ with $\vartheta_2, \varsigma > 0$, and define the functions $f_j \colon \mathbb{R} \to \mathbb{R}^3$ by

$$f_1(y) = \frac{\chi_{\leq}(y)\mathrm{e}^{\vartheta_1 y}}{\sqrt{2\vartheta_1}}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \; f_2(y) = \frac{\chi_{\leq}(y)\mathrm{e}^{\vartheta_2 y}}{\sqrt{2\vartheta_2}}\begin{pmatrix} 0 \\ \cos(\varsigma y) \\ \sin(\varsigma y) \end{pmatrix}, \; f_3(y) = \frac{\chi_{\leq}(y)\mathrm{e}^{\vartheta_2 y}}{\sqrt{2\vartheta_2}}\begin{pmatrix} 0 \\ -\sin(\varsigma y) \\ \cos(\varsigma y) \end{pmatrix},$$

where $\chi_{\leq} = \mathbf{1}_{]-\infty,0]}$ is the indicator function for the negative part of the real line. We then define $\mathbf{W}$ to be the three-dimensional subspace $\mathbf{W} = \mathrm{span}\{f_1, f_2, f_3\}$, and the operator $\mathbb{P}$ to be the orthogonal projection onto $\mathbf{W}$. Note that $\{f_1, f_2, f_3\}$ forms an orthonormal basis of $\mathbf{W} \subset \mathbf{H}$.

The validity of the compression property can roughly be seen as follows: For $t > 0$ the functions $\mathbb{S}_t f_j = f_j(\cdot - t)$ immediately leave $\mathbf{W}$, but they return to $\mathbf{W}$, if we cut them off at $y = 0$ by multiplying with $\chi_{\leq}$, i.e. $\chi_{\leq}\mathbb{S}_t f_j \in \mathbf{W}$. Moreover, we can express this action by the contraction semigroup $\mathrm{e}^{-t\mathbb{D}}$, see the calculations in the proof of Proposition C.4.

Using the orthonormal basis $\{f_1, f_2, f_3\}$ we can identify $\mathbf{W}$ with $\mathbb{R}^3$ and using the orthogonal projections $\mathbb{P}$ from $\mathbf{H}$ to $\mathbf{W}$ we find

$$\mathbb{D} = \begin{pmatrix} \vartheta_1 & 0 & 0 \\ 0 & \vartheta_2 & -\varsigma \\ 0 & \varsigma & \vartheta_2 \end{pmatrix} \quad \text{and}$$

$$\mathbb{P}\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}\big|_{\mathbf{W}} = \mathrm{e}^{-t\mathbb{D}} = \begin{pmatrix} \mathrm{e}^{-\vartheta_1 t} & 0 & 0 \\ 0 & \mathrm{e}^{-\vartheta_2 t}\cos(\varsigma t) & \mathrm{e}^{-\vartheta_2 t}\sin(\varsigma t) \\ 0 & -\mathrm{e}^{-\vartheta_2 t}\sin(\varsigma t) & \mathrm{e}^{-\vartheta_2 t}\cos(\varsigma t) \end{pmatrix} \quad \text{for } t \geq 0.$$

Having the explicit representation of $\mathbf{W}$, the coupling $\mathsf{C} \colon \mathbb{R}^n \to \mathbf{W} \subset \mathbf{H}$ can be specified as $\mathsf{C}q = (\mathsf{c}^1 \cdot q)f_1 + (\mathsf{c}^2 \cdot q)f_2 + (\mathsf{c}^3 \cdot q)f_3$, where $\mathsf{c}^1, \mathsf{c}^2, \mathsf{c}^3 \in \mathbb{R}^n$ are given coupling vectors. Hence, the coupling energy reads

$$\mathcal{H}_{\mathcal{C}}(q, p, \eta) = (\mathsf{C}q | \mathbb{P}\eta)_{\mathbf{H}} = \sum_{j=1}^{3}(\mathsf{c}^j \cdot q)\int_{-\infty}^{0} f_j(x) \cdot \eta(x)\, \mathrm{d}x,$$

and the coupled ODE-PDE system takes the explicit form

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q \\ p \\ \eta \end{pmatrix} = \begin{pmatrix} p \\ -\mathrm{D}V(q) - \sum_1^3 \int_{-\infty}^0 f_j(y) \cdot \eta(y)\,\mathrm{d}y\, \mathsf{c}^j \\ -\partial_x\big(\eta + \sum_1^3(\mathsf{c}^j \cdot q)f_j(\cdot)\big) \end{pmatrix}.$$

We see that the coupling between the ODEs (first two equations) and the linear transport equation (third equation) occurs through the observable functions $f_j \in \mathbf{W}$, which are exponentially decaying.

As mentioned above, the transport equation has to be interpreted in a suitable weak or mild form if we want to treat general initial conditions. Note also that the functions f_j do not lie in the domain of the generator $\mathbb{J}_{\mathcal{B}}$ of the unitary group $\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}$, because $\mathrm{dom}(\mathbb{J}_{\mathcal{B}}) = \mathrm{H}^1(\mathbb{R};\mathbb{R}^3)$ and hence $\mathbf{W} \cap \mathrm{dom}(\mathbb{J}_{\mathcal{B}}) = \{0\}$. $\hfill\square$

1.4 Coarse-graining, part 1: Deterministic initial data

In Theorem 4.10, we rigorously derive an equation for a coarse-grained version of the microscopic system, and show how it can be recognized as a GENERIC equation. GENERIC equations are evolution

equations for an unknown $y(t) \in \mathbf{Y}$ that can be written in terms of two functionals $\mathcal{E}$ and $\mathcal{S}$ and two operators $\mathbb{J}$ and $\mathbb{K}$ as

$$\dot{y} = \mathbb{J}(y)\mathrm{D}\mathcal{E}(y) + \mathbb{K}(y)\mathrm{D}\mathcal{S}(y). \tag{1.6}$$

The quintuple $(\mathbf{Y}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ is used to denote the GENERIC system. Here $\mathcal{E}$ and $\mathcal{S}$ are referred to as the energy and entropy functionals, and D is an appropriate concept of derivative (see Remark 2.1). The operators $\mathbb{J}$ and $\mathbb{K}$ are called the *Poisson* and *Onsager* operators, and they define a Poisson bracket and a dissipative bracket. In the GENERIC framework, the components $\mathcal{E}$, $\mathcal{S}$, $\mathbb{J}$, and $\mathbb{K}$ are required to satisfy a number of additional conditions, which in particular imply that along any solution of (1.6) the functional $\mathcal{E}$ is constant and the functional $\mathcal{S}$ is non-decreasing. We describe the GENERIC framework in more detail in Section 4.

To describe this result precisely we first define the coarse-graining map,

$$\mathbf{Z} \times \mathbf{H} \ni (z, \eta) \overset{\pi_{z,w,e}}{\longmapsto} \left(z, \, w := \mathbb{P}\eta, \, e := \tfrac{1}{2}\|\eta\|_{\mathbf{H}}^2 - \tfrac{1}{2}\|w\|_{\mathbf{H}}^2 \right) \in \mathbf{Z} \times \mathbf{W} \times \mathbb{R}. \tag{1.7}$$

In the notation introduced for GENERIC, we have $\mathbf{Y} := \mathbf{Z} \times \mathbf{W} \times \mathbb{R}$. Note how this map $\pi_{z,w,e}$ preserves the System-A state variable z but projects the heat-bath variable η onto the finite-dimensional subspace $\mathbf{W}$. The third variable e allows us to recover an important piece of information from the missing part $\eta - w = \eta - \mathbb{P}\eta$, namely its total energy $\tfrac{1}{2}\|\eta - w\|_{\mathbf{H}}^2 = \tfrac{1}{2}\|\eta\|_{\mathbf{H}}^2 - \tfrac{1}{2}\|w\|_{\mathbf{H}}^2$. The variable e is only used to keep track of the energy exchanged with the heat bath. Already for $(z, w) = (z, \mathbb{P})$ we obtain the closed system of ODEs

$$\dot{z} = \mathbb{J}_{\mathcal{A}}(z)\big(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z) + \mathsf{C}^*w\big), \qquad \dot{w} = -\mathbb{D}w + \mathsf{C}z, \tag{1.8}$$

see Figure 1.2. However, this reduced model does not have a thermodynamical structure.
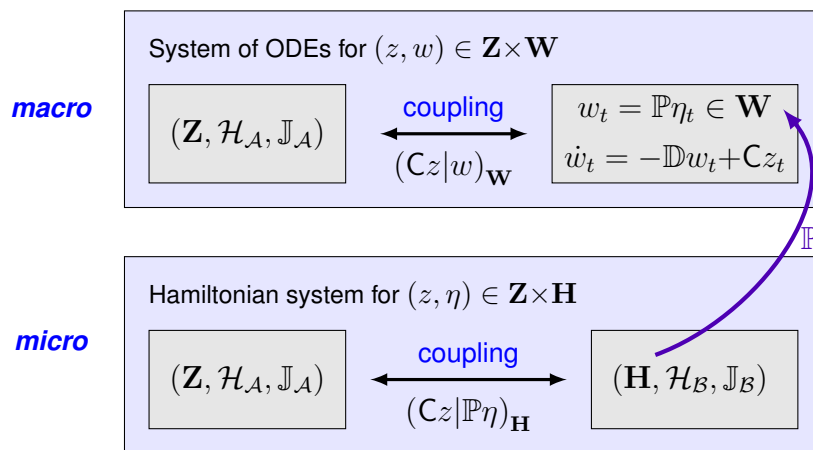
Figure 1.2: The special coupling and the compression property lead to the closed deterministic systems of ODEs (1.8) for $(z, w) \in \mathbf{Z} \times \mathbf{W}$, where w is the observable part $w = \mathbb{P}\eta$.

Using the additional scalar energy variable e, Part 1 of Theorem 4.10 states the following. If (z, η) evolves as described in Section 1.2, starting from a given point $z(t = 0) = z_0 \in \mathbf{Z}$ and $\eta(t = 0) = w_0 \in \mathbf{W}$, then $y(t) := \big(z(t), w(t), e(t)\big) := \pi_{z,w,e}\big(z(t), \eta(t)\big)$ is an exact solution of the ordinary

differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} z \\ w \\ e \end{pmatrix} = \underbrace{\begin{pmatrix} \mathbb{J}_{\mathcal{A}}(z) & 0 & 0 \\ 0 & -\mathbb{D}_{\mathrm{skw}} & 0 \\ 0 & 0 & 0 \end{pmatrix}}_{\mathbb{J}_{\mathrm{GEN}}(z,w,e)} \underbrace{\begin{pmatrix} \mathrm{D}\mathcal{H}_{\mathcal{A}}(z) + \mathsf{C}^* w \\ w + \mathsf{C}z \\ 1 \end{pmatrix}}_{\mathrm{D}\mathcal{E}_{\mathrm{GEN}}(z,w,e)}$$

$$+ \frac{1}{\beta} \underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbb{D}_{\mathrm{sym}} & -\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}z) \\ 0 & -(\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}z)|\square)_{\mathbf{H}} & (\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}z)|w+\mathsf{C}z)_{\mathbf{H}} \end{pmatrix}}_{\mathbb{K}_{\mathrm{GEN}}(z,w,e)} \underbrace{\begin{pmatrix} 0 \\ 0 \\ \beta \end{pmatrix}}_{\mathrm{D}\mathcal{S}_{\mathrm{GEN}}(z,w,e)} . \quad (1.9)$$

Here the operator $\mathbb{D}$ is decomposed into symmetric and skew-symmetric parts,

$$\mathbb{D} = \mathbb{D}_{\mathrm{sym}} + \mathbb{D}_{\mathrm{skw}} \quad \text{with } \mathbb{D}_{\mathrm{sym}} = \frac{1}{2}(\mathbb{D}+\mathbb{D}^*) \text{ and } \mathbb{D}_{\mathrm{skw}} := \frac{1}{2}(\mathbb{D}-\mathbb{D}^*), \qquad (1.10)$$

and we have defined

$$\mathcal{E}_{\mathrm{GEN}}(z, w, e) := \mathcal{H}_{\mathcal{A}}(z) + (\mathsf{C}z|w)_{\mathbf{H}} + \frac{1}{2}\|w\|_{\mathbf{H}}^2 + e,$$

$$\mathcal{S}_{\mathrm{GEN}}(z, w, e) := \beta e.$$

Here $\beta > 0$ is a parameter that will be discussed in Section 1.6.

The result (1.9) of Theorem 4.10 is interesting for a number of reasons. As we already noted in Section 1.3, it is remarkable that coarse-graining of this type leads to a closed system: typically, if in a dynamical system one disregards a part of the state space, then unique solvability tends to break down. In this case the Compression Property 1.2 guarantees that although knowledge of the initial values $z(0)$ and $w(0) = \mathbb{P}\eta(0)$ is not enough to uniquely solve for the microscopic system $(z(t), \eta(t))$, it *does* suffice for the prediction of the *projected* version of $(z(t), \eta(t))$. This points to a special role of the compression property in the study of this type of systems. The state space of the infinite-dimensional Hamiltonian system contains a finite-dimensional manifold that is exactly invariant under the full flow, and reduction of the flow to the manifold is described by a GENERIC equation.

Secondly, by following how the microscopic Hamiltonian-system components morph through coarse-graining into the GENERIC equation (1.9) we can gain some understanding about the GENERIC framework itself. In Sections 4.4, 4.5, and 4.6, we use the results of this paper to shed light on the modeling origin of the four components $\mathcal{E}$, $\mathcal{S}$, $\mathbb{J}$, and $\mathbb{K}$ and the relations between them.

1.5   Coarse-graining, part 2: Heat bath with positive temperature

In Section 1.4 the elements $\eta \in \mathbf{H}$ still have finite energy $\frac{1}{2}\|\eta\|^2$, and now we want to extend the theory to a heat bath with positive temperature $1/\beta$, which also implies infinite energy. We first only look to the interplay of the positive-temperature heat bath and the compression property. This will explain basic features of our theory without too much technicalities, because everything can be explained by Gaussian measures and processes. In Section 1.6 we will then do the same extension on the full Hamiltonian system $(\mathbf{Z}\times\mathbf{H}, \mathcal{H}_{\mathrm{total}}, \mathbb{J}_{\mathcal{A}}\otimes\mathbb{J}_{\mathcal{B}})$.

For creating a Gaussian equilibrium measure corresponding to an energy distribution "$\mathrm{e}^{-\beta\|\eta\|_{\mathbf{H}}^2/2}\,\mathrm{d}\eta$" one embeds $\mathbf{H}$ into a bigger Hilbert space $\mathbf{X}$ by a symmetric and positive definite trace-class operator

$\mathbb{C} : \mathbf{X} \to \mathbf{X}$ such that $\mathbf{H} = \mathbb{C}^{1/2}\mathbf{X}$ and $\|\mathbb{C}^{1/2}\eta\|_{\mathbf{H}} = \|\eta\|_{\mathbf{X}}$. With this a Gaussian measure γ_β is defined such that the characteristic function $\chi = \mathcal{F}\gamma_\beta$ takes the form $\chi(\xi) = \exp\left(-\frac{1}{2\beta}\|\mathbb{C}^{1/2}\xi\|_{\mathbf{X}}^2\right)$. By the general theory of Gaussian measures, it follows that the orthogonal projector $\mathbb{P} : \mathbf{H} \to \mathbf{W} \subset \mathbf{H}$ extends to a random variable $\widehat{\mathbb{P}}$ on the space $\mathrm{L}^2(\mathbf{X}, \gamma_\beta)$, see Section 2.2. We show that it is also possible to choose $\mathbf{X}$ and $\mathbb{C}$ in such a way that the unitary group $(\mathrm{e}^{t\mathbb{J}_\mathcal{A}})_{t\in\mathbb{R}}$ on $\mathbf{H}$ extends by density to a strongly continuous group $(\widehat{S}_t)_{t\in\mathbb{R}}$ on $\mathbf{X}$ (see Section C.2). Thus, for each (infinite-energy) state $\eta \in \mathbf{X}$ of the heat bath, we can define the process

$$t \mapsto Y_t(\eta) := \widehat{\mathbb{P}}\widehat{S}_t\eta \ \in \mathbf{W}.$$

It turns out that the process Y is completely independent of the choice of $\mathbf{X}$ and $\mathbb{C}$ and is uniquely determined by the compression property alone. Indeed, it is a stationary multivariate Ornstein-Uhlenbeck process with mean $0 \in \mathbf{W}$ and covariance matrix

$$\mathbb{E}\big(Y_t \otimes Y_s\big) = \begin{cases} \frac{1}{\beta}\,\mathrm{e}^{-(t-s)\mathbb{D}} & \text{for } t \geq s, \\ \frac{1}{\beta}\,\mathrm{e}^{-(s-t)\mathbb{D}^*} & \text{for } t \leq s. \end{cases}$$

see Lemma 3.2. Hence, the paths $Y_t(\eta)$ are the solutions of the linear SDE

$$\mathrm{d}Y_t = -\mathbb{D}Y_t\,\mathrm{d}t + \Sigma\,\mathrm{d}B_t \quad \text{with } \Sigma = \left(\tfrac{1}{\beta}\big(\mathbb{D}+\mathbb{D}^*\big)\right)^{1/2}.$$

See Figure 1.3 for an explanation how the drift term and the noise term arise via the projection $\widehat{\mathbb{P}} : \mathbf{X} \to \mathbf{W}$ and the extended semigroup $\widehat{S}_t : \mathbf{X} \to \mathbf{X}$.
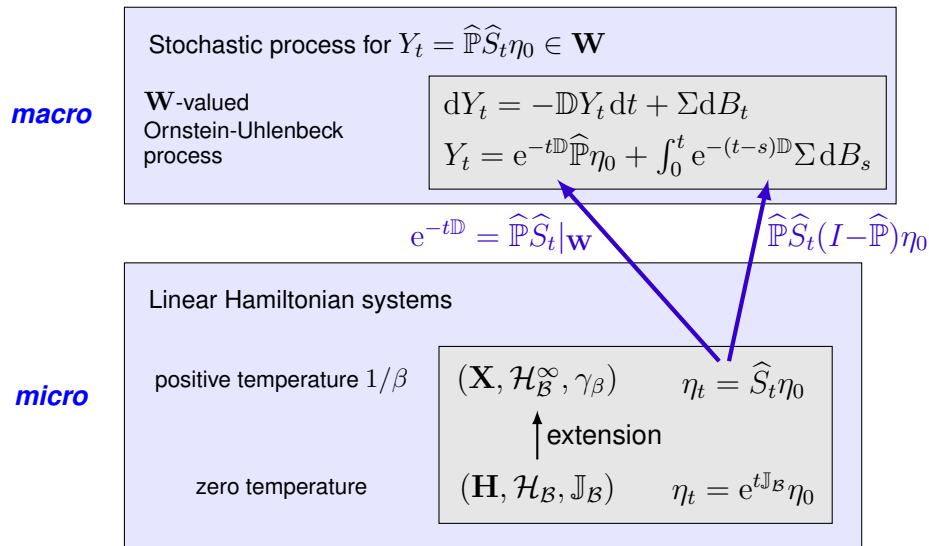
Figure 1.3: The Gaussian measure γ_β encodes the temperature $1/\beta > 0$. After extending $\mathbb{P} : \mathbf{H} \to \mathbf{W}$ and $\mathrm{e}^{t\mathbb{J}_\mathcal{B}}$ to $\widehat{\mathbb{P}}$ and $\widehat{S}_t$, respectively, the compression property implies that $t \mapsto Y_t = \widehat{\mathbb{P}}\widehat{S}_t\eta_0$ defines a Gaussian process, namely the $\mathbf{W}$-valued Ornstein-Uhlenbeck process with drift $\mathbb{D}Y_t$ and noise intensity Σ with $\Sigma\Sigma^* = \frac{1}{\beta}(\mathbb{D}+\mathbb{D}^*)$.

In the following we discuss how this construction can be coupled to the Hamiltonian System A.

1.6   Coarse-graining, part 3: Random initial data

In Section 1.4 we already derived a GENERIC structure for the case of a heat bath with zero temperature. But the result was ad hoc and didn't explain why this is the "correct form" of $\mathcal{E}_{\mathrm{GEN}}$, $\mathcal{S}_{\mathrm{GEN}}$, $\mathbb{J}_{\mathrm{GEN}}$, and $\mathbb{K}_{\mathrm{GEN}}$. This question can only be answered by looking at the coupled system at positive temperature $1/\beta > 0$. This means that we consider now initial conditions $(z_0, \eta_0) \in \mathbf{Z} \times \mathbf{X}$ that are random according to a suitable equilibrium measure.

This approach will reveal the deeper connections to the coarse-graining of systems with thermal fluctuations. For instance, it allows us to give a meaning to the parameter $\beta > 0$ in (1.9) as an inverse temperature and to 'entropy' $\mathcal{S}_{\mathrm{GEN}}(z, w, e) = \beta e$ as a micro-canonical surface area. In addition, it addresses the slightly unnatural initial datum of the previous section. There we started the heat bath at $\eta(t = 0) = w_0 \in \mathbf{W}$, which fixes the visible part of the bath to some non-zero w_0, while requiring the (infinite-dimensional) 'invisible' component to be zero. This is an unnatural choice in a Hamiltonian system with a Hamiltonian $\mathcal{H}_{\mathcal{B}}(\eta) = \frac{1}{2}\|\eta\|_{\mathbf{H}}^2$ that gives no special status to $\mathbf{W}$, and our choice of random initial data will also improve this aspect.

We choose a distribution for the random initial data that builds on the 'canonical' invariant measure $\mu_\beta := \text{"}\mathrm{e}^{-\beta \mathcal{H}_{\mathrm{total}}(z, \eta)}\text{"}$ of the microscopic Hamiltonian system, where $\mathcal{H}_{\mathrm{total}}$ is the total Hamiltonian given in (1.3). Like the Gaussian measure γ_β is defined on $\mathbf{X} \supset \mathbf{H}$, also μ_β can be rigorously defined on $\mathbf{Z} \times \mathbf{X}$ but is no longer Gaussian unless $\mathcal{H}_{\mathcal{A}}$ is also quadratic. For any $(z_0, w_0) \in \mathbf{Z} \times \mathbf{W}$ we then choose a random initial datum (z_0, η_0) from the conditional measure $\mu_\beta(\,\cdot\,|z_0, w_0)$ obtained by conditioning μ_β to $z = z_0$ and $\widehat{\mathbb{P}}\eta = w_0$. This leads to an initial datum with deterministic 'visible' part and random 'invisible' part in the heat bath. Once the initial datum is selected, the microscopic Hamiltonian system generates a deterministic evolution for $(z(t), \eta(t))$. This leads to a SDE for the variables (z, w) on the space $\mathbf{Z} \times \mathbf{W}$, see Figure 1.4. As in Section 1.5 it is the Gaussianity of γ_β and the Compression Property 1.2 that guarantee that the (Mori-Zwanzig type) coarse graining map

$$\mathbf{Z} \times \mathbf{X} \ni (z, \eta) \;\overset{\pi_{z,w}}{\longmapsto}\; (z, w := \widehat{\mathbb{P}}\eta) \in \mathbf{Z} \times \mathbf{W} \qquad \text{(see Section 2.2 for } \widehat{\mathbb{P}}\text{),} \qquad (1.11)$$

leads to a memory-less Markov process that can be described by a SDE.

Similarly to the deterministic case in Section 1.4 we also need the 'internal-energy' variable e. For random initial data the formula $e = \frac{1}{2}\|\eta\|_{\mathbf{H}}^2 - \frac{1}{2}\|w\|_{\mathbf{H}}^2$ is not available, however, since the Hamiltonian $\mathcal{H}_{\mathcal{B}}(\eta) = \frac{1}{2}\|\eta\|_{\mathbf{H}}^2$ is almost surely infinite (see Remark 2.2). We circumvent this problem by following an alternative but equivalent route: we first coarse-grain $(z, w) = \pi_{z,w}(z, \eta) = (z, \widehat{\mathbb{P}}\eta)$ and then reconstruct e *a posteriori* from $(z(t), w(t))$ as the energy exchanged with the heat bath.

The main result for this setup is the second part of Theorem 4.10, which shows that the curve $(z(t), w(t), e(t))$ constructed this way satisfies the following "GENERIC SDE":

$$\mathrm{d}\begin{pmatrix} z \\ w \\ e \end{pmatrix} = \Big[\mathbb{J}_{\mathrm{GEN}}\mathrm{D}\mathcal{E}_{\mathrm{GEN}}(z, w, e) + \mathbb{K}_{\mathrm{GEN}}(z, w)\mathrm{D}\mathcal{S}_{\mathrm{GEN}}(z, w, e) + \mathrm{div}\,\mathbb{K}_{\mathrm{GEN}}(z, w)\Big]\mathrm{d}t$$

$$+ \Sigma_{\mathrm{GEN}}(z, w)\,\mathrm{d}B(t), \quad (1.12)$$

where $\mathbb{J}_{\mathrm{GEN}}(z)$, $\mathbb{K}_{\mathrm{GEN}}$, $\mathcal{E}_{\mathrm{GEN}}$, and $\mathcal{S}_{\mathrm{GEN}}$ are as in Section 1.4, and the mobility Σ_{GEN} is given by

$$\Sigma_{\mathrm{GEN}}(z, w) := \begin{pmatrix} 0 \\ \Sigma \\ -(w + \mathsf{C}z|\Sigma\,\square)_{\mathbf{H}} \end{pmatrix} \quad \text{with } \Sigma\Sigma^* = \frac{1}{\beta}(\mathbb{D} + \mathbb{D}^*).$$
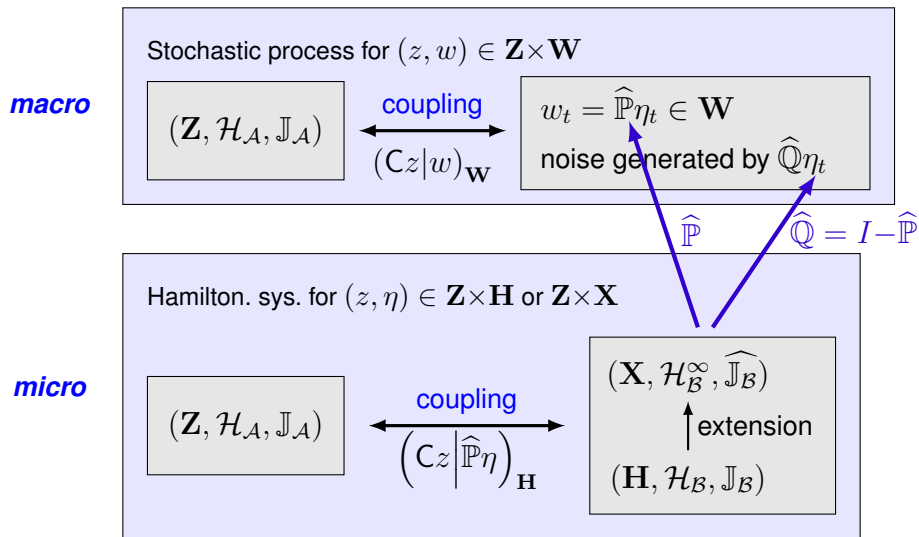
Figure 1.4: The coarse-graining step, illustrated as the transition from the bottom row to the top row. We separate the heat-bath variable η into the observable part $w = \widehat{\mathbb{P}}\eta$ and the remainder $\widehat{\mathbb{Q}}\eta = \eta - \widehat{\mathbb{P}}\eta$. The pair (z, w) can be considered a stochastic process driven by $\widehat{\mathbb{Q}}\eta$.

This equation is a natural stochastic counterpart of the deterministic GENERIC equation (1.6). We discuss equations of this form in more detail in Section 4.2.

Again, the derivation of (1.12) is interesting for a number of reasons. As in the deterministic case, the fact that this is an *exact* reduction is remarkable: not only is the drift term in (1.12) Markovian, as we already remarked in Section 1.3, but in addition the noise term is exact Brownian noise, and therefore memoryless. Considering that the evolution of the microscopic variable (z, η) is deterministic, and therefore 'maximally memory-full', this indeed is remarkable.

In addition, the mobility Σ_{GEN} that colors the noise is coupled to the Onsager operator $\mathbb{K}_{\mathrm{GEN}}$ by the fluctuation-dissipation relation

$$\Sigma_{\mathrm{GEN}}\Sigma_{\mathrm{GEN}}^* = 2\mathbb{K}_{\mathrm{GEN}}.$$

This underscores the shared origin of Σ_{GEN}, $\mathbb{K}_{\mathrm{GEN}}$, and $\mathcal{S}_{\mathrm{GEN}}$ in the randomness of the initial data. We indeed show in Section 4.6 how $\mathcal{S}_{\mathrm{GEN}}$ can be interpreted as the mass of a microcanonical measure, and how this leads to the corresponding drift $\mathbb{K}_{\mathrm{GEN}}\mathrm{D}\mathcal{S}_{\mathrm{GEN}}$ in (1.6) and (1.12).

1.7 Outline of this paper

The layout of this paper is as follows. The microscopic system is described in more detail in Section 2.

In Section 3 we employ a compression to derive the coarse-grained system. Specifically, in Section 3.1 we introduce compressions and derive an Ornstein-Uhlenbeck process on the projected space. In Section 3.2 we perform the coarse-graining described in Sections 1.4 and 1.6 above, which leads to deterministic and stochastic evolutions. At this stage they still are without GENERIC structure.

In Section 4 we describe the GENERIC structure in detail and establish some properties of so-called GENERIC SDEs. By taking into account the energy flowing in and out of the heat bath, as described in in Sections 1.4 and 1.6, we can formulate the equations obtained in Section 3.2 as a GENERIC system, either deterministic or stochastic, and identify the components. This also gives insight in how the GENERIC restrictions arise in the coarse-graining process.

In Section 5 we summarize the results of the paper, and discuss connections with various other developments. In Appendix A we collect a number of properties of Gaussian measures that we use, and in Appendix B we give the proofs of a number of lemmas.

List of notation, setting, and assumptions

We denote Hilbert spaces with boldface symbols and their elements with lower case letters. Below we will use Hilbert spaces $\mathbf{H}$, $\mathbf{W}$, and $\mathbf{X}$ satisfying $\mathbf{W} \subset \mathbf{H} \subset \mathbf{X}$; $\mathbf{W}$ and $\mathbf{H}$ share the same inner product $(\cdot|\cdot)_{\mathbf{H}}$, while $\mathbf{X}$ has a weaker inner product $(\cdot|\cdot)_{\mathbf{X}}$. We use the notation $\mathbb{A}^*$ for the Hilbert adjoint of an operator $\mathbb{A}$ between two Hilbert spaces.

We use the Lebesgue measure on general finite-dimensional Hilbert spaces; this is defined by identifying the Hilbert space with $\mathbb{R}^N$ through any orthonormal basis. The resulting measure is independent of the choice of basis. By the same type of identification any finite-dimensional Hilbert space admits a 'standard normal distribution' and a 'standard Brownian motion'. The 'narrow' convergence of measures on a Hilbert space $\mathbf{Y}$ is defined by duality with $\mathrm{C}_b(\mathbf{Y})$.

Other notation

$\beta > 0$	inverse temperature	
γ_β	canonical Gaussian measure on the heat bath	(2.7)
C, $\mathbb{A}$	coupling operator	(1.2), (2.2)
D	derivative operator	Rem. 2.1
$\mathbb{D}$	generator of the compressed semigroup	Ass. 1.2
$\mathbb{D}_{\mathrm{sym}}$, $\mathbb{D}_{\mathrm{skw}}$	symmetric and skew-symmetric parts of $\mathbb{D}$	(1.10)
$\mathcal{H}_{\mathcal{A},\mathcal{B},\mathcal{C},\mathrm{total}}$	components of the microscopic Hamiltonian	Sec. 1.2
$\mathcal{H}_{\mathcal{B}}^{\infty}$	Extension of $\mathcal{H}_{\mathcal{B}}$ from $\mathbf{H}$ to $\mathbf{X}$	Sec. 1.6
$\mathbb{I}$ or $\mathbb{I}_{n \times n}$	identity operator or matrix	
$\mathbb{J}_{\mathcal{A}}$, $\mathbb{J}_{\mathcal{B}}$	Poisson operators of microscopic system	Secs 1.2, 2.1
$\mathrm{Lin}(\mathbf{X}, \mathbf{Y})$	bounded linear maps from $\mathbf{X}$ to $\mathbf{Y}$	
μ_β	invariant measure for the microscopic system	Secs 1.6, 2.4
$\mu_{\beta,\mathbf{Z}}$	invariant measure for System A	(1.13), (2.12)
$\mathcal{N}(m, \mathbb{C})$	normal distribution	App. A
$\mathbb{P}$, $\widehat{\mathbb{P}}$	projection onto $\mathbf{W}$ from $\mathbf{H}$ or $\mathbf{X}$	Secs 2.1, 2.2
$\pi_{z,w}$	projection onto coarse-grained variables (z, w)	(1.11)
$\pi_{z,w,e}$	projection onto coarse-grained variables (z, w, e)	(1.7)
$\mathbb{Q}$, $\widehat{\mathbb{Q}}$	complementary projections: $\mathbb{Q} = I - \mathbb{P}$, $\widehat{\mathbb{Q}} = I - \widehat{\mathbb{P}}$	Secs 2.1, 2.2
$\widehat{S}_t$	extension of the group $\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}$ from $\mathbf{H}$ to $\mathbf{X}$	Ass. 2.3
$\mathbb{U}_t$	evolution operator of the microscopic system	Th. 2.5

Key assumptions (see Section 2 for details)

- $\mathbf{H}$, $\mathbf{X}$, and $\mathbf{Z}$ are real separable Hilbert spaces, with $\dim \mathbf{Z} < \infty$ and with compact embedding $\mathbf{H} \hookrightarrow \mathbf{X}$ such that $\mathbf{H} = \mathbb{C}^{1/2}\mathbf{X}$, where $\mathbb{C} = \mathbb{C}^* : \mathbf{X} \to \mathbf{X}$ is positive definite and trace class;

- $\mathbb{J}_{\mathcal{B}}$ is the generator of both a strongly continuous unitary group $\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}$ on $\mathbf{H}$, and $\widehat{S}_t$ is an extension forming a strongly continuous group on $\mathbf{X}$;

- $\mathbb{P}$ is the orthogonal projection in $\mathbf{H}$ onto the finite-dimensional linear subspace $\mathbf{W} \subset \mathbf{H}$;

- ■ C is a bounded linear map from $\mathbf{Z}$ to $\mathbf{H}$ satisfying $\mathbb{P}\mathsf{C} = \mathsf{C}$;
- ■ $\beta > 0$ and $\mathcal{H}_\mathcal{A} \in \mathrm{C}^2(\mathbf{Z}; \mathbb{R})$ is such

$$\exp\big(-\beta\big(\mathcal{H}_\mathcal{A}(z) - \tfrac{1}{2}\|\mathsf{C}z\|_\mathbf{H}^2\big)\big) \in L^1(\mathbf{Z}),$$

  and $\mathrm{D}\mathcal{H}_\mathcal{A}$ is globally Lipschitz continuous;
- ■ $\mathbb{J}_\mathcal{A}(z)$ is a skew-adjoint linear operator on $\mathbf{Z}$;
- ■ $\gamma_\beta = \mathcal{N}_\mathbf{X}(0, \beta^{-1}\mathbb{C})$, $\mu_\beta = \mu_{\beta,\mathbf{Z}}(\mathrm{d}z)\mathcal{N}_\mathbf{X}(-\mathsf{C}z, \beta^{-1}\mathbb{C})(\mathrm{d}\eta)$, and

$$\mu_{\beta,\mathbf{Z}}(\mathrm{d}z) = \frac{1}{Z_\beta}\exp\big(-\beta\mathcal{H}_\mathcal{A}(z) + \frac{\beta}{2}\|\mathsf{C}z\|_\mathbf{H}^2\big)\,\mathrm{d}z; \tag{1.13}$$

- ■ Compression Property 1.2: $\mathbb{P}\,\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\big|_\mathbf{W} = \mathrm{e}^{-t\mathbb{D}}$ for $t \geq 0$; and $\mathbb{D} + \mathbb{D}^*$ has strictly positive eigenvalues.

Data availability statement

No datasets were generated in the preparation of this paper.

2 The microscopic system

The microscopic setup of this paper is a well-known model (see, e.g., [JaP98a, KS*02a, Rey06]). As mentioned above, two separate Hamiltonian systems are coupled, where one is finite-dimensional ('System A'), and the other is infinite-dimensional and is interpreted as a heat bath ('System B'). System A may be nonlinear, while System B and the coupling will be linear. This is illustrated in Figure 1.1.

We construct the microscopic system and its properties in the following steps:

1. We define the two subsystems in spaces $\mathbf{Z}$ and $\mathbf{H}$ and their coupling in state space $\mathbf{Z} \times \mathbf{H}$ (Section 2.1);
2. We consider the heat-bath subsystem at positive temperature, which requires extending the state space $\mathbf{H}$ to a larger space $\mathbf{X}$ (Section 2.2);
3. We study the evolution of the heat bath on this larger state space, and characterize the observable part (Lemma 2.4);
4. We use the properties of the heat bath to establish existence of solutions of the coupled system (Theorem 2.5).

2.1 Finite energy, deterministic evolution

We first recall from the Introduction the microscopic system at finite energy and without randomness. System A is a fixed Hamiltonian system $(\mathbf{Z}, \mathcal{H}_\mathcal{A}, \mathbb{J}_\mathcal{A})$, where $\mathbf{Z}$ is a finite-dimensional real Hilbert space, $\mathcal{H}_\mathcal{A}$ is a nonlinear Hamiltonian on $\mathbf{Z}$ satisfying some conditions (see below), and $\mathbb{J}_\mathcal{A}$ defines a possibly state-dependent Poisson structure, i.e. $\mathbb{J}_\mathcal{A}(z)\colon \mathbf{Z} \to \mathbf{Z}$ is a skew-symmetric linear operator satisfying $\mathrm{div}_z\,\mathbb{J}_\mathcal{A} = 0$ and Jacobi's identity (4.2). We write $z \in \mathbf{Z}$ for the variables in System A, and the uncoupled motion of System A is governed by the equation $\dot{z} = \mathbb{J}_\mathcal{A}(z)\mathrm{D}\mathcal{H}_\mathcal{A}(z)$.

System B is imagined to be a 'heat bath'. Concretely, System B is a Hamiltonian system $(\mathbf{H}, \mathcal{H}_\mathcal{B}, \mathbb{J}_\mathcal{B})$, where $\mathbf{H}$ is an infinite-dimensional separable real Hilbert space, $\mathcal{H}_\mathcal{B} := \frac{1}{2}\|\cdot\|_\mathbf{H}^2$, and $\mathbb{J}_\mathcal{B}$ is a densely

defined, unbounded skew-adjoint operator on $\mathbf{H}$ that generates a strongly continuous, unitary group $(\mathrm{e}^{t\mathbb{J}_\mathcal{B}})_{t\in\mathbb{R}}$. We write $\eta \in \mathbf{H}$ for the states of the heat bath, and the uncoupled evolution of the heat bath is formally given by $\dot{\eta} = \mathbb{J}_\mathcal{B}\eta = \mathbb{J}_\mathcal{B}\mathrm{D}\mathcal{H}_\mathcal{B}(\eta)$. In particular, $\eta(t) = \mathrm{e}^{t\mathbb{J}_\mathcal{B}}\eta(0)$ describes the evolution of the heat bath.

We assume that the heat bath is 'large'[1], but that only part of the heat bath is observable by System A. This limited observability is implemented by an orthogonal projection operator $\mathbb{P}\colon \mathbf{H} \to \mathbf{W} = \mathbb{P}\mathbf{H} \subset \mathbf{H}$ and its complement $\mathbb{Q} := \mathbb{I} - \mathbb{P}$. System A only perceives the heat bath through the operator $\mathbb{P}$. The range $\mathbf{W}$ of $\mathbb{P}$ is assumed to be a finite-dimensional subspace of $\mathbf{H}$, and we use the important Compression Property 1.2 about $\mathbb{P}$ and $\mathbf{W}$ that we already mentioned in the introduction. Note that $\mathbb{P}$ is self-adjoint in $\mathbf{H}$.

The coupling between the macroscopic system and the heat bath is given via a linear coupling operator $\mathsf{C}\colon \mathbf{Z} \to \mathbf{H}$ defining the bilinear coupling Hamiltonian

$$\mathcal{H}_\mathcal{C}(z,\eta) := (\mathbb{A}z|\mathbb{P}\eta)_\mathbf{H} = \big(\underbrace{\mathbb{P}\mathbb{A}}_{\mathsf{C}}z|\eta\big)_\mathbf{H}.$$

This expression shows how the impact of the heat bath on System A is mediated by the operator $\mathbb{P}$. The total microscopic Hamiltonian system then is the sum of the three parts,

$$\mathcal{H}_{\mathrm{total}}(z,\eta) = \mathcal{H}_\mathcal{A}(z) + \mathcal{H}_\mathcal{B}(\eta) + \mathcal{H}_\mathcal{C}(z,\eta) \tag{2.1}$$

$$= \mathcal{H}_\mathcal{A}(z) + \frac{1}{2}\|\eta\|_\mathbf{H}^2 + (\mathsf{C}z|\eta)_\mathbf{H} \tag{2.2}$$

$$= \mathcal{H}_\mathcal{A}(z) - \frac{1}{2}\|\mathsf{C}z\|_\mathbf{H}^2 + \frac{1}{2}\|\eta + \mathsf{C}z\|_\mathbf{H}^2. \tag{2.3}$$

We can now make the conditions on $\mathcal{H}_\mathcal{A}$ concrete: we assume that $\mathcal{H}_\mathcal{A} \in C^2(\mathbf{Z})$ such that $\mathrm{D}\mathcal{H}_\mathcal{A}$ is globally Lipschitz continuous, and that for our chosen $\beta > 0$ we have

$$\exp\big(-\beta\big(\mathcal{H}_\mathcal{A}(z) - \tfrac{1}{2}\|\mathsf{C}z\|_\mathbf{H}^2\big)\big) \in L^1(\mathbf{Z}). \tag{2.4}$$

The coupled (finite-energy) microscopic system is defined in terms of the total Hamiltonian system $(\mathbf{Z}\times\mathbf{H}, \mathcal{H}_{\mathrm{total}}, \mathbb{J}_\mathcal{A}\oplus\mathbb{J}_\mathcal{B})$, where the Poisson operator $\mathbb{J}_{\mathrm{total}}(z) := \mathbb{J}_\mathcal{A}(z)\oplus\mathbb{J}_\mathcal{B} : \mathbf{Z}\times\mathrm{dom}(\mathbb{J}_\mathcal{B}) \to \mathbf{Z}\times\mathbf{H}$ still is skew-adjoint and satisfies Jacobi's identity (4.2), since $\mathbb{J}_\mathcal{B}$ is constant. The associated Hamiltonian equations are (1.4), repeated here for convenience

$$\dot{z}_t = \mathbb{J}_\mathcal{A}(z)\big(\mathrm{D}\mathcal{H}_\mathcal{A}(z_t) + \mathsf{C}^*\eta_t\big), \tag{2.5a}$$

$$\dot{\eta}_t = \mathbb{J}_\mathcal{B}\big(\eta_t + \mathsf{C}z_t\big). \tag{2.5b}$$

Here we follow the convention from probability to denote the time-dependence of a variable with a subscript t. When necessary for better readability we write the time dependence in parentheses, as in $z(s)$. Existence and uniqueness of solutions of these equations is proved in Theorem 2.5 below. This will need a suitable weak formulation of (2.5b) because $\mathrm{range}(\mathsf{C}) \subset \mathbf{W}$ is not contained in the domain of the unbounded operator $\mathbb{J}_\mathcal{B}$ (see Remark C.2).

Remark 2.1 (Convention for the derivative D). In the context of Hilbert spaces, there is a choice to consider either the Fréchet derivative, which is an element of the dual space, or the 'gradient', which

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[1]In the context of this paper, the heat bath being 'large' translates into assumptions that the heat bath has many dimensions and a large total energy; in the limit this becomes an assumption of infinite-dimensionality and a Gaussian measure. We explore this limit in detail in Section 4.6.

is the Riesz representative of the Fréchet derivative and therefore an element of the primal space. In this paper we always choose the second interpretation, as the Riesz representatitive of the Fréchet derivative. With this choice, we have for instance for all $\eta \in \mathbf{H}$ and $z \in \mathbf{Z}$,

$$\mathrm{D}_\eta \frac{1}{2}\|\eta\|_{\mathbf{H}}^2 = \eta, \qquad \mathrm{D}_\eta \left(\mathsf{C}z|\eta\right)_{\mathbf{H}} = \mathsf{C}z, \qquad \text{and} \qquad \mathrm{D}_z \left(\mathsf{C}z|\eta\right)_{\mathbf{H}} = \mathrm{D}_z \left(z|\mathsf{C}^*\eta\right)_{\mathbf{Z}} = \mathsf{C}^*\eta.$$

This choice also implies that an operator such as $\mathbb{J}_{\mathcal{B}}$ is an unbounded operator from $\mathbf{H}$ to $\mathbf{H}$ (and not from $\mathbf{H}^*$ to $\mathbf{H}$). $\qquad\qquad\square$

2.2 Positive temperature: The heat bath

We now extend this setup to positive temperature, first focusing on just the heat bath and its evolution. We recall in Appendix A the properties of Gaussian measures that we use.

Let $\beta > 0$ be interpreted as inverse temperature. Since the heat-bath Hamiltonian is $\mathcal{H}_{\mathcal{B}}(\eta) = \frac{1}{2}\|\eta\|_{\mathbf{H}}^2$, a thermodynamic or statistical-mechanical point of view (see Section 4.6) suggests to consider a Gaussian measure with the formal expression

$$\gamma_\beta(\mathrm{d}\eta) = \exp\left(-\frac{\beta}{2}\|\eta\|_{\mathbf{H}}^2\right)\mathrm{d}\eta \tag{2.6}$$

on a suitable space containing $\mathbf{H}$. This measure should be the natural invariant measure for the Hamiltonian evolution $\dot{\eta}_t = \mathbb{J}_{\mathcal{B}}\eta_t$ of the isolated heat bath. To define such a Gaussian measure on an infinite-dimensional Hilbert space $\mathbf{H}$, an embedding into a bigger space is required, and is provided by the Cameron-Martin setting sketched below. A reason is that, unlike in finite dimensions, a special structure, namely trace-class nature, of the covariance is required. For example, in infinite dimensions there is no Gaussian measure with the identity as covariance, unlike in finite dimensions.

We briefly recall the Cameron-Martin setting which establishes a meaning for this expression; see Appendix A for more detail. Let the Hilbert space $\mathbf{H}$ be embedded into a larger separable Hilbert space $\mathbf{X}$, in such a way that the identity map $\mathrm{id} : \mathbf{H} \to \mathbf{X}$ is a Hilbert-Schmidt operator. Then $\mathbb{C} := \mathrm{id}\,\mathrm{id}^* : \mathbf{X} \to \mathbf{X}$ is of trace class, and we rigorously define γ_β as the centered Gaussian measure

$$\gamma_\beta := \mathcal{N}_{\mathbf{X}}\big(0, \beta^{-1}\mathbb{C}\big). \tag{2.7}$$

The space $\mathbf{H}$ can be considered to be the 'Cameron-Martin space' of γ_β.

From now on we will consider the larger space $\mathbf{X}$ as the state space for the heat bath, and the larger space $\mathbf{Z} \times \mathbf{X}$ as the state space for the whole system. We therefore need to extend the operator $\mathbb{P}$ from $\mathbf{H}$ to $\mathbf{X}$. By Lemma A.7, the operator $\mathbb{P}: \mathbf{H} \to \mathbf{W} \subset \mathbf{H}$ has a *measurable linear extension* $\widehat{\mathbb{P}}: \mathbf{X} \to \mathbf{W} \subset \mathbf{H}$, which is γ_β-a.e. uniquely characterized by the property that it is linear and coincides with $\mathbb{P}$ on $\mathbf{H}$ (see Definition A.6). The complementary operator $\widehat{\mathbb{Q}} := \mathrm{id} - \widehat{\mathbb{P}} : \mathbf{X} \to \mathbf{X}$ similarly is a measurable linear extension of $\mathbb{Q}$. We also define $\widehat{\mathsf{C}^*} := \mathsf{C}^*\widehat{\mathbb{P}}: \mathbf{X} \to \mathbf{Z}$, which is a measurable extension of $\mathsf{C}^*: \mathbf{H} \to \mathbf{Z}$.

Remark 2.2 (Positive temperature means infinite energy)**.** The properties of Gaussian measures imply that if $\eta \sim \gamma_\beta$, then $\mathcal{H}_{\mathcal{B}}(\eta) = \frac{1}{2}\|\eta\|_{\mathbf{H}}^2 = +\infty$ almost surely—despite the fact that $\mathcal{H}_{\mathcal{B}}(\eta)$ appears in the exponent in (2.6). This can be recognized by choosing an orthonormal basis $\{e_k\}_{k\in\mathbb{N}}$ of $\mathbf{H}$, and observing that the vector $\big((\eta|e_1)_{\mathbf{H}}, \ldots, (\eta|e_n)_{\mathbf{H}}\big)$ of the first n coordinates of η in this basis has variance n/β (see (A.16)); therefore the expectation of $\|\eta\|_{\mathbf{H}}^2$ can not be finite. See, e.g., [Rey06, Sec. 2.1] or [Bog98, Rem. 2.2.3] for a discussion of this property.

As a result, 'finite energy' requires 'zero temperature'; positive temperature implies infinite energy. □

We formally denote the extended system with finite temperature (and infinite energy) by $\mathfrak{S}_\beta :=$ $(\mathbf{Z} \times \mathbf{X}, \mathcal{H}^\infty_{\text{total}}, \mathbb{J}_\mathcal{A} \oplus \mathbb{J}_\mathcal{B}, \gamma_\beta)$, such that the new ingredients $\mathbf{X} \supset \mathbf{H}$ and $\gamma_\beta = \mathcal{N}_\mathbf{X}(0, \beta^{-1}\mathbb{C})$ are visible. Here $\mathcal{H}^\infty_{\text{total}}$ coincides with $\mathcal{H}_{\text{total}}$ on $\mathbf{Z} \times \mathbf{H}$ and equals $+\infty$ for $\eta \in \mathbf{X} \setminus \mathbf{H}$. In Section 2.3 we discuss how the solution operator for the finite-energy microscopic system $(\mathbf{Z} \times \mathbf{H}, \mathcal{H}_{\text{total}}, \mathbb{J}_\mathcal{A} \oplus \mathbb{J}_\mathcal{B})$ can be extended to the infinite-energy system $\mathfrak{S}_\beta$.

The evolution operator $\mathrm{e}^{t\mathbb{J}_\mathcal{B}}$, that describes the heat-bath unitary evolution in the smaller space $\mathbf{H}$, can similarly be extended γ_β-a.e. to a operators $\widehat{S}_t$ on $\mathbf{X}$. Without loss of generality we make the following simplifying assumption (see Section C.2 for a discussion):

Assumption 2.3 (Continuous evolution of the heat bath)**.** *The operator* $\mathrm{e}^{t\mathbb{J}_\mathcal{B}} : \mathbf{H} \to \mathbf{H}$ *can be extended to a strongly continuous group* $(\widehat{S}_t)_{t \in \mathbb{R}}$ *of bounded linear operators* $\widehat{S}_t$ *from* $\mathbf{X}$ *to* $\mathbf{X}$.

The extended operators $\widehat{S}_t$ leave γ_β invariant as is shown in Lemma A.9.

For random initial datum $\eta_0 \sim \gamma_\beta$, the process

$$t \mapsto \widehat{S}_t\eta_0 \in \mathbf{X}$$

is a stochastic process in $\mathbf{X}$; its evolution is deterministic in time, but the randomness of the initial datum implies that the process as a whole is stochastic. Under Assumption 2.3, this process has continuous sample paths in $\mathbf{X}$. The next lemma states some properties of the *projected* version of this process, which has values in $\mathbf{W}$, which is equipped with the stronger norm of $\mathbf{H}$.

Lemma 2.4. *Adopt the setup above, including Assumption 2.3, and set*

$$Y_t(\eta_0) := \widehat{\mathbb{P}}\widehat{S}_t\eta_0 \quad \text{for all} \quad t \in \mathbb{R},\ \eta_0 \in \mathbf{X}.$$

Then, the following holds:

1. *For every* $\eta_0 \in \mathbf{H}$ *we have* $t \mapsto Y_t(\eta_0) \in C(\mathbb{R}; \mathbf{W})$.
2. *Choose the probability space* $(\mathbf{X}, \mathcal{B}(\mathbf{X})_{\gamma_\beta}, \gamma_\beta)$, *where* $\mathcal{B}(\mathbf{X})_{\gamma_\beta}$ *is the* γ_β-*completion of the Borel* σ-*algebra* $\mathcal{B}(\mathbf{X})$. *If* η_0 *is drawn from* $\mathbf{X}$ *with law* γ_β, *then both* $Y = Y(\eta_0)$ *and* $Y = Y(\widehat{\mathbb{Q}}\eta_0)$ *are measurable* $\mathbf{W}$-*valued stochastic processes with sample paths in* $L^2_{\text{loc}}(\mathbb{R}; \mathbf{W})$; *in addition* $Y(\eta_0)$ *is stationary.*

The proof is given in Appendix B. Part 1, the continuity in $\mathbf{H}$, follows directly from the definitions; but more interesting is part 2, where we re-interpret the evolution as a stochastic process. The randomness of this process is naturally parametrized by the starting point η_0 drawn from γ_β, leading to the choice of probability space $(\mathbf{X}, \mathcal{B}(\mathbf{X})_{\gamma_\beta}, \gamma_\beta)$. The fact that the sample paths are in L^2_{loc} follows from the fact that for fixed t, $Y_t(\eta_0)$ is a Gaussian random variable in $\mathbf{W}$ with finite and t-independent variance, so that

$$\mathbb{E}_{\eta_0 \sim \gamma_\beta} \int_a^b \|Y_t(\eta_0)\|^2_\mathbf{H} \, \mathrm{d}t = \int_a^b \mathbb{E}_{\eta_0} \|Y_t(\eta_0)\|^2_\mathbf{H} = C\,(b-a) \qquad \text{for } -\infty < a < b < \infty.$$

The additional characterization of $Y(\widehat{\mathbb{Q}}\eta_0)$ will be useful below, when we solve the initial-value problem with a given value of $w_0 := \widehat{\mathbb{P}}\eta_0$.

2.3 Well-posedness of the stochastic process on the product space

With the characterization of the process Y by Lemma 2.4 we can now construct the solution of the coupled microscopic system on the product space $\mathbf{Z} \times \mathbf{H}$ (deterministic and with finite energy) or $\mathbf{Z} \times \mathbf{X}$ (random and with infinite energy).

Theorem 2.5. *Assume that* $\mathrm{D}\mathcal{H}_{\mathcal{A}}$ *is globally Lipschitz continuous on* $\mathbf{Z}$*. Then there exists a collection of nonlinear operators* $\{\mathbb{U}_t\}_{t \in \mathbb{R}}$ *on* $\mathbf{Z} \times \mathbf{X}$ *with the following properties:*

1 *For* $(z_0, \eta_0) \in \mathbf{Z} \times \mathbf{H}$*, the mapping* $t \mapsto (z_t, \eta_t) := \mathbb{U}_t(z_0, \eta_0)$ *has the regularity* $z \in C^1(\mathbb{R}; \mathbf{Z})$ *and* $\eta \in C(\mathbb{R}; \mathbf{H})$*, and it satisfies*

$$\dot{z}_t = \mathbb{J}_{\mathcal{A}}(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z_t) + \mathsf{C}^*\eta_t) \qquad\qquad \text{for } t \in \mathbb{R} \qquad (2.8a)$$

$$\eta_t = \mathrm{e}^{\mathbb{J}_{\mathcal{B}}t}(\eta_0 + \mathsf{C}z_0) - \mathsf{C}z_t + \int_0^t \mathrm{e}^{\mathbb{J}_{\mathcal{B}}(t-s)}\mathsf{C}\dot{z}_s\,\mathrm{d}s \qquad \text{for } t \in \mathbb{R}. \qquad (2.8b)$$

2 *For all* $z_0 \in \mathbf{Z}$ *and* γ_β*-a.e.* $\eta_0 \in \mathbf{X}$*, the function* $t \mapsto (z_t, \eta_t) := \mathbb{U}_t(z_0, \eta_0)$ *has the regularity* $z \in W_{\mathrm{loc}}^{1,2}(\mathbb{R}; \mathbf{Z})$, $\eta \in C(\mathbb{R}; \mathbf{X})$ *and it satisfies*

$$\dot{z}_t = \mathbb{J}_{\mathcal{A}}(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z_t) + \widehat{\mathsf{C}}^*\eta_t), \qquad\qquad \text{a.e. } t \in \mathbb{R} \qquad (2.9a)$$

$$\eta_t = \widehat{S}_t(\eta_0 + \mathsf{C}z_0) - \mathsf{C}z_t + \int_0^t \mathrm{e}^{\mathbb{J}_{\mathcal{B}}(t-s)}\mathsf{C}\dot{z}_s\,\mathrm{d}s \qquad t \in \mathbb{R} \qquad (2.9b)$$

(note the extended operators $\widehat{\mathsf{C}}^*$ *in* (2.9a) *and* $\widehat{S}_t$ *in* (2.9b)*). For fixed* z_0 *and random* $\eta_0 \sim \gamma_\beta$*, the resulting stochastic process* $(z_t, \eta_t)_{t \in \mathbb{R}}$ *is a measurable* $\mathbf{Z} \times \mathbf{X}$*-valued process on the probability space* $(\mathbf{X}, \mathcal{B}(\mathbf{X})_{\gamma_\beta}, \gamma_\beta)$*.*

3 *Fix* $z_0 \in \mathbf{Z}$ *and* $w_0 \in \mathbf{W}$*, and let* $\eta_0 = w_0 + \xi_0$ *with* $\xi_0 \in \widehat{\mathbb{Q}}\mathbf{X}$ *and* $\xi_0 \sim \widehat{\mathbb{Q}}_{\#}\gamma_\beta$*. For almost every such* ξ_0 *the curve* $(z_t, \eta_t) := \mathbb{U}_t(z_0, \eta_0)$ *has the same properties as under part 2 above.*

Proof. By integrating (2.5b) and substituting into (2.5a) we find the equation for z alone,

$$\dot{z}_t = \mathbb{J}_{\mathcal{A}}\mathsf{C}^*Y_t + \mathbb{J}_{\mathcal{A}}\big(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z) + \mathsf{C}^*(\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}\mathsf{C}z_0 - \mathsf{C}z_t)\big) + \mathbb{J}_{\mathcal{A}}\int_0^t \mathsf{C}^*\mathrm{e}^{(t-s)\mathbb{J}_{\mathcal{B}}}\mathsf{C}\dot{z}_s\,\mathrm{d}s, \qquad (2.10)$$

where $Y = Y(\eta_0)$. For $(z_0, \eta_0) \in \mathbf{Z} \times \mathbf{H}$, the process $t \mapsto Y_t(\eta_0)$ is continuous with values in $\mathbf{W}$ by Lemma 2.4, and a standard ODE proof based on contraction for small times gives short-time existence and uniqueness of a solution of (2.10) with the specified regularity. The global Lipschitz bound on $\mathrm{D}\mathcal{H}_{\mathcal{A}}$ implies that the time of existence does not depend on the initial datum, and we obtain existence globally in time. Equation (2.8a) can then be recovered from (2.10) by differentiating in time, and equation (2.8b) can be used to reconstruct η. This proves the part 1 of the theorem.

For $z_0 \in \mathbf{Z}$ and $\eta_0 \sim \gamma_\beta$, the stochastic process $Y(\eta_0)$ has sample paths almost surely in $L_{\mathrm{loc}}^2(\mathbb{R}; \mathbf{W})$ by Lemma 2.4. Again an ODE contraction proof gives the unique existence of a solution of (2.10) with regularity $z \in W_{\mathrm{loc}}^{1,2}(\mathbb{R}; \mathbf{Z})$. To recover η, remark that $X = X_t(\eta_0) := \widehat{S}_t\eta_0 \in \mathbf{X}$ has sample paths in $C(\mathbb{R}; \mathbf{X})$; again equation (2.8b) can be used to define η in terms of z. This proves the existence in part 2. The measurability of (z, η) jointly in t and η_0 follows from observing that $(t, \eta_0) \mapsto Y_t(\eta_0)$ is measurable by Lemma 2.4, and by Fubini the measurability transfers to the integral in time.

For part 3, we use that $Y_t(\eta)$ is linear in η and split Y_t in the first term on the right-hand side in (2.10) as

$$Y_t(\eta_0) = Y_t(\widehat{\mathbb{Q}}\eta_0) + Y_t(\widehat{\mathbb{P}}\eta_0) = Y_t(\widehat{\mathbb{Q}}\eta_0) + \mathbb{P}\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}\widehat{\mathbb{P}}\eta_0.$$

The second term on the right-hand side above equals $\mathbb{P}e^{t\mathbb{J}_\mathcal{B}}w_0$ and is continuous in time; the first term again has sample paths almost surely in $L^2_{\mathrm{loc}}(\mathbb{R}; \mathbf{W})$ by Lemma 2.4. The sum therefore almost surely is in $L^2_{\mathrm{loc}}(\mathbb{R}; \mathbf{W})$ and can be treated the same way as in the proof of part 2. □

Example 2.6 (Running example, part 3). For our model discussed in Examples 1.1 and 1.4 we can explicitly construct the larger Hilbert space $\mathbf{X} \supset \mathbf{H} = L^2(\mathbb{R}; \mathbb{R}^3) = L^2(\mathbb{R})^3$. In fact, this can be done independently for each of the three components. We follow the classical construction in [Rey06] and choose

$$\mathbf{X} = X \times X \times X \quad \text{with } X := \mathrm{H}^{-2}(\mathbb{R}) + \mathrm{L}^2_{-2}(\mathbb{R}).$$

Here X contains distributions T that can be decomposed into $T = T_1 + T_2$ with $T_2 \in \mathrm{H}^{-2}(R)$ and $T_2 \in \mathrm{L}^2_{-2}(\mathbb{R})$, i.e. $x \mapsto (1+x^2)^{-1}T_2(x) \in \mathrm{L}^2(\mathbb{R})$. Clearly, the shift operator $\widehat{S}_t : T \mapsto T(\,\cdot-t)$ generates a continuous semigroup that is the extension of the unitary shift group $(e^{t\partial_x})_{t\in\mathbb{R}}$ on $\mathrm{L}^2(\mathbb{R})$.

The regularity theory for Brownian motion shows that for all $\alpha \in [0, 1/2)$ the paths $t \mapsto B_t$ lie in $\mathrm{H}^\alpha_{\mathrm{loc}}(\mathbb{R})$ almost surely, but not in $\mathrm{H}^{1/2}_{\mathrm{loc}}(\mathbb{R})$ (see e.g. [HyV08]). Thus, the white-noise distributions $\eta = \mathrm{d}B_t$ lie in $H^{\alpha-1}_{\mathrm{loc}}(\mathbb{R})$ only. Moreover, our dilation functions f_j, $j = 1, 2, 3$, in Example 1.4 have a jump at $y = 0$ and are otherwise smooth. Hence, they lie in $\mathrm{H}^\beta(\mathbb{R})$ with $\beta < 1/2$, but not in $H^{1/2}(\mathbb{R})$. Thus, the extension of the projection $\mathbb{P} : h \to \sum_{j=1}^3 (f_j|h) f_j$ to $\widehat{\mathbb{P}}$ remains nontrivial in the sense that the subspace L of $\mathbf{X}$ of full measure needs to be constructed by the abstract methods of Lemma A.7. □

2.4 Invariant measure on the product space $\mathbf{Z} \times \mathbf{X}$

Since the stochastic process on $\mathbf{Z} \times \mathbf{X}$ is a Hamiltonian system with the Hamiltonian $\mathcal{H}_{\mathrm{total}}$ given in (2.1), a natural stationary measure should be of the (formal) form

$$\exp\big(-\beta \mathcal{H}_{\mathrm{total}}(z, \eta)\big) \,\mathrm{d}z\,\mathrm{d}\eta.$$

We make this expression rigorous by splitting off the infinite-dimensional Gaussian component, as in (2.3):

$$\exp(-\beta \mathcal{H}_{\mathrm{total}}(z,\eta)) = \exp\left(-\beta\big(\mathcal{H}_\mathcal{A}(z) + \frac{1}{2}\|\mathsf{C}z\|^2_{\mathbf{H}}\big)\right) \exp\left(-\frac{\beta}{2}\|\eta+\mathsf{C}z\|^2_{\mathbf{H}}\right).$$

This leads to the rigorous definition

$$\mu_\beta(\mathrm{d}z\,\mathrm{d}\eta) := \mu_{\beta,\mathbf{Z}}(\mathrm{d}z)\mathcal{N}_{\mathbf{X}}(-\mathsf{C}z, \beta^{-1}\mathbb{C})(\mathrm{d}\eta), \tag{2.11}$$

where

$$\mu_{\beta,\mathbf{Z}}(\mathrm{d}z) = \frac{1}{\mathsf{Z}_\beta}\exp\left(-\beta\big(\mathcal{H}_\mathcal{A}(z) - \frac{1}{2}\|\mathsf{C}z\|^2_{\mathbf{H}}\big)\right)\mathrm{d}z. \tag{2.12}$$

The following result shows that the measure μ_β as defined above is indeed invariant under the flow. The proof needs some nontrivial steps because of the coupling of the finite-dimensional and the infinite-dimensional system. On the one hand, $\mathbf{W}$ is not contained in the domain of $\mathbb{J}_\mathcal{A}$ and hence not in the domain of the generator of the extended group $(\widehat{S}_t)_{t\in\mathbb{R}}$. On the other hand, the measure γ_β is invariant under $(\widehat{S}_t)_{t\in\mathbb{R}}$, but the covariance matrix $\mathbb{C}: \mathbf{X} \to \mathbf{X}$ is not, see the proof of Lemma A.9.

Theorem 2.7 (Invariance of μ_β). *Assume the above setting, including Assumption 1.2, as well as*

$$\mathbb{J}_\mathcal{A} \in \mathrm{C}^1_{\mathrm{b}}(\mathbf{Z}; \mathrm{Lin}(\mathbf{Z})) \quad \text{and} \quad \mathrm{div}\,\mathbb{J}_\mathcal{A}(z) = 0 \text{ on } \mathbf{Z}, \tag{2.13}$$

$$z \mapsto \big(1 + \|\mathrm{D}\mathcal{H}_\mathcal{A}(z) - \mathsf{C}^*\mathsf{C}z\|\big)e^{-\beta(\mathcal{H}_\mathcal{A}(z)-\|\mathsf{C}z\|^2/2)} \quad \text{lies in } \mathrm{L}^1(\mathbf{Z}). \tag{2.14}$$

Then, the measure μ_β defined in (2.11) *is invariant under the flow generated by* (2.9).

Proof. We do a coordinate transformation to simplify the structure of μ_β as well as of the evolution equation.

By introducing the new variables $(z, \zeta) = \widetilde{M}_t(z, \eta) = \big(z, \widehat{S}_{-t}(\eta + \mathsf{C}z)\big)$ the measure μ_β is transformed into

$$\widetilde{\mu}_\beta = (\widetilde{M}_t)_\# \mu_\beta = \mu_{\beta,\mathbf{Z}}(\mathrm{d}z)\, \gamma_\beta(\mathrm{d}\zeta).$$

The result is simple for $t = 0$ because we only shift by the mean value. This leads to $\widetilde{\mu}_\beta$. The subsequent transformation by $\widehat{S}_t$ does not change the resulting product measure because γ_β is invariant (see Lemma A.9).

Thus, it remains to show that the measure $\widetilde{\mu}_\beta$ is invariant under the transformed evolution equation for (z, ζ). Using the linear structure of $\widetilde{M}_t$ we see that (z_t, η_t) is a solution of (2.9) if and only if $(z_z, \zeta_t) = \widetilde{M}_t(z_t, \eta_t)$ solves

$$\dot{z}_t = \mathbb{J}_\mathcal{A}(z_t)\big(\mathrm{D}\mathcal{H}_\mathsf{C}(z_t) + \mathsf{C}^*\widehat{\mathbb{P}}\widehat{S}_t\zeta_t\big), \quad \zeta_t = \zeta_0 + \int_0^t \mathrm{e}^{-s\mathbb{J}_\mathcal{B}}\mathsf{C}\dot{z}_s\,\mathrm{d}s,$$

where $\mathcal{H}_\mathsf{C}(z) := \mathcal{H}_\mathcal{A}(z) - \frac{1}{2}\|\mathsf{C}z\|^2$. In particular, we conclude that $t \mapsto \zeta_t \in \mathbf{X}$ is differentiable with a derivative in the smaller space $\mathbf{H}$. Hence, we can use that ζ_t satisfies the differential equation

$$\dot{\zeta}_t = \mathrm{e}^{-t\mathbb{J}_\mathcal{B}}\mathsf{C}\dot{z}_t \in \mathbf{H} \quad \text{with initial condition } \zeta_0 = \eta_0 + \mathsf{C}z_0 \in \mathbf{X}.$$

The advantage of using ζ is that the unbounded generator $\widehat{\mathbb{J}_\mathcal{B}}$ of the group $(\widehat{S}_t)_{t\in\mathbb{R}}$ does not appear.

We will show in Lemma 3.2 that $\zeta_0 \sim \gamma_\beta$ implies that $Y_t = \widehat{\mathbb{P}}\widehat{S}_t\zeta_0$ is an Ornstein-Uhlenbeck process, such that the function $t \mapsto Y_t$ is almost surely continuous. As a consequence one can show as in Theorem 2.5 that $t \mapsto (z_t, \zeta_t - \zeta_0)$ lies in $\mathrm{C}^1_{\mathrm{loc}}(\mathbb{R}; \mathbf{Z} \times \mathbf{H})$.

Let us denote by $\Phi_t \colon \mathbf{Z} \times \mathbf{X} \to \mathbf{Z} \times \mathbf{X}$ with $(z_t, \zeta_t) = \Phi_t(z_0, \zeta_0)$ the corresponding flow map. Then, invariance of $\widetilde{\mu}_\beta$ means $\widehat{\mu}_\beta^{(t)} := (\Phi_t)_\# \widetilde{\mu}_\beta = \widetilde{\mu}_\beta$ for all $t \in \mathbb{R}$. The invariance follows from the transport equation for $t \mapsto \widetilde{\mu}_\beta^{(t)}$, namely

$$\partial_t \widehat{\mu}_\beta^{(t)} + \mathrm{div}_{\mathbf{Z}\times\mathbf{x}}\big(V_t(z, \zeta)\widehat{\mu}_\beta^{(t)}\big) = 0,$$

$$\text{with } V_t(z, \zeta) = \begin{pmatrix} \mathbb{J}_\mathcal{A}(z)\,(\mathrm{D}\mathcal{H}_\mathsf{C}(z) + \mathsf{C}^*\widehat{\mathbb{P}}\widehat{S}_t\zeta) \\ \widehat{S}_{-t}\,\mathsf{C}\,\mathbb{J}_\mathcal{A}(z)\,(\mathrm{D}\mathcal{H}_\mathsf{C}(z) + \mathsf{C}^*\widehat{\mathbb{P}}\widehat{S}_t\zeta) \end{pmatrix},$$

which is to be understood in the sense of distributions by applying suitable test functions in $\mathrm{C}^1_\mathrm{b}(\mathbf{Z} \times \mathbf{X})$. (For clarity, we have written $\mathsf{C}^*\widehat{\mathbb{P}}$ instead of $\widehat{\mathsf{C}^*}$, which emphasizes that the only unbounded term is $\widehat{\mathbb{P}}$.)

Thus, it remains to show the identity

$$\int_{\mathbf{Z}\times\mathbf{X}} \left\langle \begin{pmatrix} \mathrm{D}_z\check{\Phi}(z, \zeta) \\ \mathrm{D}_\zeta\check{\Phi}(z, \zeta) \end{pmatrix}, V_t(z, \zeta) \right\rangle \widetilde{\mu}_\beta(\mathrm{d}z, \mathrm{d}\zeta) = 0 \text{ for all } \check{\Phi} \in \mathrm{C}^1_\mathrm{b}(\mathbf{Z}\times\mathbf{X}). \tag{2.15}$$

Indeed, testing with functions $\check{\Phi}(z, \zeta) = \widetilde{\Phi}(z, \widehat{S}_t\zeta)$ and using the invariance of $\widetilde{\mu}_\beta = \mu_{\beta,\mathbf{Z}}\,\gamma_\beta$ under $\mathrm{id}_\mathbf{Z} \oplus \widehat{S}_t$ we see that it suffices to prove (2.15) for $t = 0$ only.

For the final step we work with cylindrical test functions, see [AGS05, Def. 5.1.11]. For this, we choose the orthogonal basis generated by $\mathbb{C} = \mathbb{C}^* > 0$ in $\mathbf{X}$, and denote by $\mathsf{Q}_n \colon \mathbf{X} \to \mathbf{X}$ the orthogonal projection on to the span of the eigenfunctions associated with the n largest eigenvalues. Because $\mathbf{H} = \mathbb{C}^{1/2}\mathbf{X}$ we have $\mathbf{H}_n :- \mathsf{Q}_n\mathbf{X} \subset \mathbf{H}$ and we may use the decomposition $\mathbf{X} = \mathbf{H}_n \otimes \mathbf{Y}_n$ with

$\mathbf{Y}_n = (\mathbb{I}-\mathbb{Q}_n)\mathbf{X}$. Moreover, since the kernel of $\mathbb{C}$ is trivial, the restriction $\mathbb{C}_n = \mathbb{C}|_{\mathbf{H}_n} : \mathbf{H}_n \to \mathbf{H}_n$ is invertible and we may choose the scalar product of $\mathbf{H}$ on the finite-dimensional space $\mathbf{H}_n$.

Writing $\eta = h + y$ with $h \in \mathbf{H}_n$ and $y \in \mathbf{Y}_n$, we now consider the cylindrical test functions $\check{\Phi}(z,\eta) = \Psi(z,h)$ with $\Psi \in \mathrm{C}^1_{\mathrm{b}}(\mathbf{Z}{\times}\mathbf{H}_n)$, i.e. we restrict to a finite-dimensional space, where computations are classical.

To integrate over the infinite-dimensional space $\mathbf{Y}_n$ we observe that assumption (2.14) implies that the integrand in (2.15) lies in $\mathrm{L}^1(\mathbf{Z}{\times}\mathbf{H}_n{\times}\mathbf{Y}_n, \widetilde{\mu}_\beta)$. For this we also use that $\mathbf{X} \ni \eta \mapsto \widehat{\mathbb{P}}\eta \in \mathbf{W}$ lies in $\mathrm{L}^2(\mathbf{X}, \gamma_\beta)$, see part 2 of Lemma A.7, i.e. equation (A.16).

Hence, we can apply Fubini's theorem and integrate first over $y \in \mathbf{Y}_n$. Here we can exploit that the integrand has the affine form $a_\Psi(z,h) + \big(b_\Psi(z,h)\big|\widehat{\mathbb{P}}y\big)_{\mathbf{H}}$ and that the measure on $\mathbf{Y}_n$ is a centered Gaussian. Thus, the linear term vanishes, and we are left with an integral over $\mathbf{Z}{\times}\mathbf{H}_n$, namely

$$\mathsf{LHS}(2.15) = \int_{\mathbf{Z}\times\mathbf{H}_n} \left\langle \begin{pmatrix} \mathrm{D}_z\Psi(z,h) \\ \mathrm{D}_y\Psi(z,h) \end{pmatrix}, \begin{pmatrix} \mathbb{J}_{\mathcal{A}}(z)(\mathrm{D}\mathcal{H}_{\mathsf{C}}(z){+}\mathsf{C}^*h) \\ \mathsf{C}\mathbb{J}_{\mathcal{A}}(z)(\mathrm{D}\mathcal{H}_{\mathsf{C}}(z){+}\mathsf{C}^*h) \end{pmatrix} \right\rangle \frac{\mathrm{e}^{-\beta(\mathcal{H}_{\mathsf{C}}(z)+\frac{1}{2}\|h\|^2_{\mathbf{H}})}}{\widetilde{Z}_\beta} \, \mathrm{d}z \, \mathrm{d}h,$$

where we used that $h \in \mathbf{H}_n \subset \mathbf{H}$ which implies that $\widehat{\mathbb{P}}y = \mathbb{P}y$ and hence $\mathsf{C}^*\widehat{\mathbb{P}}y = \mathsf{C}^*\mathbb{P}y = \mathsf{C}^*y$. Moreover, the induced measure from γ_β on the subspace $\mathbf{H}_n$ is $\widehat{Z}_\beta^{-1}\mathrm{e}^{-\beta\|h\|^2_{\mathbf{H}}/2}\,\mathrm{d}h$.

Neglecting the irrelevant normalization constant $\widetilde{Z}_\beta$ and integrating by parts we obtain

$$\int_{\mathbf{Z}\times\mathbf{H}_n} \Psi(z,h)\big(-M_1(z,h) - M_2(z,h) + \beta M_3(z,h)\big)\mathrm{e}^{-\beta(\mathcal{H}_{\mathsf{C}}(z)+\frac{1}{2}\|h\|^2_{\mathbf{H}})}\,\mathrm{d}z\,\mathrm{d}h$$

$$\text{with } M_1(z,h) = \mathrm{div}_{\mathbf{Z}}(\mathbb{J}_{\mathcal{A}}(z)(\mathrm{D}\mathcal{H}_{\mathsf{C}}(z){+}\mathsf{C}^*h)),$$
$$M_2(z,h) = \mathrm{div}_{\mathbf{H}_n}(\mathsf{C}\mathbb{J}_{\mathcal{A}}(z)(\mathrm{D}\mathcal{H}_{\mathsf{C}}(z){+}\mathsf{C}^*h)),$$
$$\text{and } M_3(z,h) = \big\langle \begin{pmatrix} \mathrm{D}\mathcal{H}_{\mathsf{C}}(z) \\ h \end{pmatrix}, V_0(z,h) \big\rangle.$$

Explicit calculations show that all three terms are zero. Indeed, using $\mathrm{div}\,\mathbb{J}_{\mathcal{A}} \equiv 0$ (see (2.13)) and $\mathbb{J}_{\mathcal{A}}(z)^* = -\mathbb{J}_{\mathcal{A}}(z)$ we have

$$M_1(z,h) = \big(\mathrm{div}\,\mathbb{J}_{\mathcal{A}}\big)(\mathrm{D}\mathcal{H}_{\mathsf{C}}(z){+}\mathsf{C}^*h) + \mathbb{J}_{\mathcal{A}}(z){:}(\mathrm{D}^2\mathcal{H}_{\mathsf{C}}(z) + 0) = 0,$$

where ":" means matrix scalar product, $A{:}B = \sum_{i,j} A_{ij}B_{ij}$. Similarly, we have

$$M_2(z,h) = \mathsf{C}\mathbb{J}_{\mathcal{A}}(z) : \mathsf{C}^*\nabla_y h = (\mathsf{C}\mathbb{J}_{\mathcal{A}}(z)\mathsf{C}^*) : \mathbb{I} = 0.$$

Finally, the third term can be rearranged as

$$M_3(z,h) = (\mathrm{D}\mathcal{H}_{\mathsf{C}}(z){+}\mathsf{C}^*h|\mathbb{J}_{\mathcal{A}}(z)(\mathrm{D}\mathcal{H}_{\mathsf{C}}(z){+}\mathsf{C}^*h))_{\mathbf{Z}} = 0,$$

because of the skew-symmetry of $\mathbb{J}_{\mathcal{A}}(z)$.

Using the transport theory from [AGS05, Ch. 8] we see that the projected measures $(\mathsf{Q}_n)_\#\widehat{\mu}_\beta^{(t)}$ are constant, namely

$$(\mathsf{Q}_n)_\#\widehat{\mu}_\beta^{(t)} = (\mathsf{Q}_n)_\#\widehat{\mu}_\beta^{(0)} = (\mathsf{Q}_n)_\#\widetilde{\mu}_\beta.$$

We can now take the limit $n \to \infty$ and use $(\mathsf{Q}_n)_\#\widetilde{\mu}_\beta = (\mathsf{Q}_n)_\#\mu_\beta^{(t)} \to \mu_\beta^{(t)}$, see [AGS05, Prop. 8.3.3]. Thus, we obtain $\widetilde{\mu}_\beta^{(t)} = \widetilde{\mu}_\beta$, which is the desired invariance.   □

3   Compression and the coarse-grained system

3.1   Compressions and dilations

The theory of dilations, developed in the 1950s by Béla Sz.-Nagy and Foias [Sz.53, SzF70], provides an embedding of a strongly continuous semigroup in a unitary group. This can be interpreted as the embedding of irreversible dynamics in reversible dynamics on a larger space, such that the irreversible dynamics can be obtained by projection to a subspace. For us, the 'reverse' procedure is of interest, namely the compression of a unitary group to a contraction semigroup.

While for coarse-graining compressions are the natural concept, the theory of dilations provides crucial motivation for the choice of the model discussed in this paper. For a given strongly continuous contraction semigroup (thought of as a large-scale, thermodynamic description), the theory of dilations provides the existence of a unitary semigroup which is unique up to isomorphism, and has a representation as time shift in a suitable space (the theory of dilations is closely related to one-dimensional scattering theory, cf. [LaS89, Cha. III.2]). We give an explicit construction of this dilation in Appendix C.

An important aspect of this specific construction is that it can simulaneously be used to define the larger space $\mathbf{X}$ and the extension of the unitary group $(\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}})_{t\in\mathbb{R}}$ on $\mathbf{H}$ to a strongly continuous group $(\widehat{S}_t)_{t\in\mathbb{R}}$ on the space $\mathbf{X}$, as required by Assumption 2.3.

Definition 3.1 (Contractions, dilations and compressions)**.** *A strongly continuous semigroup* $(C_t)_{t\geq 0}$ *of bounded linear operators on a Hilbert space* $\mathbf{G}$ *is called a* contraction semigroup *if* $\|C_t z\| \leq \|z\|$ *for all* $t \geq 0$ *and* $z \in \mathbf{G}$.

A dilation *of the contraction semigroup* $(C_t)_{t\geq 0}$ *on* $\mathbf{G}$ *is a pair* $\big(\mathbf{H}, (S_t)_{t\in\mathbb{R}}\big)$ *of a Hilbert space* $\mathbf{H}$ *that contains* $\mathbf{G}$ *as a closed subspace (with the same scalar product) and a strongly continuous unitary group* $(S_t)_{t\in\mathbb{R}}$ *such that*

$$\mathbb{P}S_t\big|_{\mathbf{G}} = C_t \in \mathrm{Lin}(\mathbf{G}; \mathbf{G}) \quad \text{for all } t \geq 0,$$

where $\mathbb{P}\colon \mathbf{H} \to \mathbf{G} \subset \mathbf{H}$ *is the orthogonal projection of* $\mathbf{H}$ *onto* $\mathbf{G}$. *In this case,* $(C_t)_{t\geq 0}$ *is called a* compression *of the group* $(S_t)_{t\in\mathbb{R}}$.

Every contraction semigroup has a dilation; however, one cannot expect a general unitary group to have a compression. We come back to this point in Appendix C.

In light of this definition, the important Compression Property 1.2 states that the evolution of the heat bath can be compressed to a contraction semigroup $C_t = \mathrm{e}^{-\mathbb{D}t}$. With the additional structure of Assumption 1.2 we can say much more about the process $Y_t(\eta_0) := \widehat{\mathbb{P}}\widehat{S}_t\eta_0$ than in Lemma 2.4:

Lemma 3.2. *Under the same assumptions as Lemma 2.4, and in addition Assumption 1.2,* $t \mapsto Y_t(\eta_0)$ *is a stationary* $\mathbf{W}$-*valued Ornstein-Uhlenbeck process with drift* $-\mathbb{D}Y$ *and mobility* Σ *satisfying* $\Sigma\Sigma^* = \frac{1}{\beta}(\mathbb{D} + \mathbb{D}^*)$.

That is, $Y_t = Y_t(\eta_0)$ *is a stationary solution of the stochastic differential equation*

$$\mathrm{d}Y_t + \mathbb{D}Y_t\mathrm{d}t = \Sigma\,\mathrm{d}B_t, \tag{3.1}$$

where B *is a standard* $\mathbf{W}$-*valued Brownian motion. The process* Y *has covariance matrix*

$$\mathbb{E}Y_t\otimes Y_s = \mathbf{R}(s,t) := \begin{cases} \frac{1}{\beta}\mathrm{e}^{-(t-s)\mathbb{D}} & \text{for } t \geq s, \\ \frac{1}{\beta}\mathrm{e}^{-(s-t)\mathbb{D}^*} & \text{for } t \leq s. \end{cases}$$

In particular, Y_t is a Gaussian process with continuous sample paths.

Similarly, if $\xi_0 \sim \widehat{\mathbb{Q}}_\# \gamma_\beta$, then $Y(\xi_0)$ is a (non-stationary) Ornstein-Uhlenbeck process satisfying (3.1) and $Y_0(\xi_0) = 0$ almost surely.

Proof. For any $t_1, \ldots, t_n \in \mathbb{R}$, the vector $(Y_{t_1}(\eta_0), \ldots, Y_{t_n}(\eta_0)) \in \mathbf{W}^n$ consists of n measurable linear maps applied the Gaussian random variable η_0, and therefore is a multivariate Gaussian random variable. This means that the process $t \mapsto Y_t(\eta_0)$ is a Gaussian process. Since η_0 is centered, Y_t also is centered, and since $t \mapsto \widehat{S}_t \eta_0$ is stationary, the same holds for Y_t.

We calculate the covariance function of $Y_t(\eta_0)$ for $\eta_0 \sim \gamma_\beta$. First remark that by the Compression Property 1.2

$$\mathbf{R}(s,t) = \frac{1}{\beta} \mathbb{P} \mathrm{e}^{(t-s)\mathbb{J}_\mathcal{B}} \mathbb{P}.$$

For fixed $h_1, h_2 \in \mathbf{H}$ and $s, t \in \mathbb{R}$ we then calculate the expectation with respect to η_0,

$$\mathbb{E}\,(Y_t | h_1)_H\,(Y_s | h_2)_H = \mathbb{E}\left(\widehat{\mathbb{P}}\widehat{S}_t \eta_0 \Big| h_1\right)_H \left(\widehat{\mathbb{P}}\widehat{S}_s \eta_0 \Big| h_2\right)_H = \mathbb{E}\left(\eta_0 \big| \mathrm{e}^{-t\mathbb{J}_\mathcal{B}} \mathbb{P} h_1\right)_H \left(\eta_0 \big| \mathrm{e}^{-s\mathbb{J}_\mathcal{B}} \mathbb{P} h_2\right)_H$$

$$\overset{\text{(A.14)}}{=} \frac{1}{\beta}\left(\mathrm{e}^{-t\mathbb{J}_\mathcal{B}} \mathbb{P} h_1 \big| \mathrm{e}^{-s\mathbb{J}_\mathcal{B}} \mathbb{P} h_2\right)_H = \frac{1}{\beta}\left(h_1 \big| \mathbb{P} \mathrm{e}^{(t-s)\mathbb{J}_\mathcal{B}} \mathbb{P} h_2\right)_H = (h_1 | \mathbf{R}(s,t) h_2)_H.$$

Therefore Y is a stationary centered Gaussian process with covariance matrix $\mathbf{R}(s,t)$; this property characterizes the Ornstein-Uhlenbeck process with drift $-\mathbb{D}Y$ and mobility Σ.[2]

If $\xi_0 \sim \widehat{\mathbb{Q}}_\# \gamma_\beta$, then by choosing $w_0 \in \mathbf{W}$ randomly according to $\widehat{\mathbb{P}}_\# \gamma_\beta$, the sum $\eta_0 := w_0 + \xi_0$ is distributed according to γ_β (see Lemma A.7), and the remarks above apply. Writing for $t \geq 0$

$$Y_t(\xi_0) = Y_t(\eta_0) - Y_t(w_0) = Y_t(\eta_0) - \mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}} w_0 = Y_t(\eta_0) - \mathrm{e}^{-t\mathbb{D}} w_0,$$

we calculate that

$$\mathrm{d}Y_t(\xi_0) = \mathrm{d}Y_t(\eta_0) - \mathrm{d}\mathrm{e}^{-t\mathbb{D}} w_0 = -\mathbb{D}Y_t(\eta_0)\,\mathrm{d}t + \Sigma\,\mathrm{d}B_t + \mathbb{D}\mathrm{e}^{-t\mathbb{D}} w_0\,\mathrm{d}t$$

$$= -\mathbb{D}Y_t(\xi_0)\,\mathrm{d}t + \Sigma\,\mathrm{d}B_t. \qquad \square$$

3.2   Derivation of the coarse-grained equations

With the characterisation of the projected stochastic process $Y = Y(\eta_0)$ of Lemma 3.2, we can now derive the coarse-grained system, i.e., the evolution in (z, w).

Theorem 3.3. *Consider the setup of Section 2, including the Compression Property 1.2.*

   1 *For $z_0 \in \mathbf{Z}$ and $w_0 \in \mathbf{W}$ consider $(z_t, \eta_t) = \mathbb{U}_t(z_0, w_0)$ as in part 1 of Theorem 2.5. Then the pair $(z_t, w_t := \mathbb{P}\eta_t)$ satisfies the ODE in $\mathbf{Z} \times \mathbf{W}$*

$$\dot{z}_t = \mathbb{J}_\mathcal{A}(z_t)(\mathrm{D}\mathcal{H}_\mathcal{A}(z_t) + \mathsf{C}^* w_t) \tag{3.2a}$$

$$\dot{w}_t = -\mathbb{D}(w_t + \mathsf{C} z_t). \tag{3.2b}$$

---

[2]This follows from recognizing that covariance functions uniquely determine stationary centered Gaussian processes, that for solutions of (3.1) and $t > s$, we have

$$\partial_t \mathbb{E} Y_t \otimes Y_s = -\mathbb{D}\,\mathbb{E} Y_t \otimes Y_s \qquad \text{and} \qquad \partial_t \mathbb{E} Y_s \otimes Y_t = -\mathbb{E} Y_s \otimes Y_t\,\mathbb{D}^*,$$

and that $\mathbb{E} Y_0 \otimes Y_0 = \beta^{-1} \mathbb{I}$ since $\mathrm{e}^{-\beta \|y\|_\mathbf{W}^2/2}\,\mathrm{d}y$ is stationary. See also [MüS85, Sec. 9.1].

2 For $z_0 \in \mathbf{Z}$, $w_0 \in \mathbf{W}$, and $\xi_0 \sim \widehat{\mathbb{Q}}_\# \gamma_\beta$, consider $(z_t, \eta_t) = \mathbb{U}_t(z_0, w_0 + \xi_0)$ as in part 3 of Theorem 2.5. Set $w_t := \widehat{\mathbb{P}}\eta_t$. Then the pair (z_t, w_t) satisfies the SDE

$$\mathrm{d}z_t = \mathbb{J}_{\mathcal{A}}(z_t)(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z_t) + \mathsf{C}^* w_t)\mathrm{d}t \tag{3.3a}$$

$$\mathrm{d}w_t = -\mathbb{D}(w_t + \mathsf{C}z_t)\,\mathrm{d}t + \Sigma\,\mathrm{d}B_t, \tag{3.3b}$$

where Σ is a square root of $(\mathbb{D} + \mathbb{D}^*)/\beta$, and $(z_t, w_t)|_{t=0} = (z_0, w_0)$. Here B_t is a standard $\mathbf{W}$-valued Brownian motion.

3 Similarly, if $(z_0, \eta_0) \sim \mu_\beta$ and $(z_t, \eta_t) = \mathbb{U}_t(z_0, \eta_0)$, then (z_t, w_t) is a stationary solution of the SDE (3.3). The single-time marginal is

$$\nu_\beta(\mathrm{d}z\,\mathrm{d}w) := (\pi_{z,w})_\# \mu_\beta(\mathrm{d}z\,\mathrm{d}w) \overset{(*)}{=} \mu_{\beta,\mathbf{z}}(\mathrm{d}z)\mathcal{N}_{\mathbf{W}}(-\mathsf{C}z, \beta^{-1})(\mathrm{d}w) \tag{3.4}$$

(and this measure is therefore invariant under the SDE (3.3)). It can alternatively be written as

$$\nu_\beta(\mathrm{d}z\,\mathrm{d}w) = \frac{1}{Z_\beta}\exp\left[-\beta\left(\mathcal{H}_{\mathcal{A}}(z) + \tfrac{1}{2}\|w\|_{\mathbf{H}}^2 + (\mathsf{C}z|w)_{\mathbf{H}}^2\right)\right]\mathrm{d}z\,\mathrm{d}w. \tag{3.5}$$

Remark 3.4. From here onward the implicit probability space will be always the same as in Lemma 2.4 and Theorem 2.5, namely $(\mathbf{X}, \mathcal{B}(\mathbf{X})_{\gamma_\beta}, \gamma_\beta)$. □

Remark 3.5. This coarse-graining approach is similar to many approaches in the Mori-Zwanzig style, but nonetheless different; we comment on this in Section 5.1. □

Proof. We first prove part 2. Since $\widehat{\mathsf{C}}^* = \mathsf{C}^*\widehat{\mathbb{P}}$, equation (3.3a) follows directly from (2.9a). To show that w satisfies (3.3b), we apply $\widehat{\mathbb{P}}$ to (2.9b) and use the compression property. We then integrate by parts to obtain

$$w_t = \widehat{\mathbb{P}}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}(w_0 + \xi_0 + \mathsf{C}z_0) - \mathsf{C}z_t + \int_0^t \mathbb{P}\mathrm{e}^{(t-s)\mathbb{J}_\mathcal{B}}\mathsf{C}\dot{z}_s\,\mathrm{d}s$$

$$= \mathrm{e}^{-t\mathbb{D}}w_0 + Y_t(\xi_0) + \mathrm{e}^{-t\mathbb{D}}\mathsf{C}z_0 - \mathsf{C}z_t + \int_0^t \mathrm{e}^{-(t-s)\mathbb{D}}\mathsf{C}\dot{z}_s\,\mathrm{d}s$$

$$= \mathrm{e}^{-t\mathbb{D}}w_0 + Y_t(\xi_0) + \mathbb{D}\int_0^t \mathrm{e}^{-(t-s)\mathbb{D}}\mathsf{C}z_s\,\mathrm{d}s,$$

which is a mild form of the SDE

$$\mathrm{d}w_t = -\mathbb{D}(w_t + \mathsf{C}z_t)\mathrm{d}t + \mathrm{d}Y_t(\xi_0) + \mathbb{D}Y_t(\xi_0)\mathrm{d}t.$$

Equation (3.3b) then follows from Lemma 3.2. For part 1 the calculation is identical, but with the choice $\xi_0 = 0$.

Finally, for part 3, Th. 2.7 implies that $t \mapsto (z_t, \eta_t)$ is a stationary stochastic process with single-time marginal μ_β, and therefore $t \mapsto (z_t, w_t) = \pi_{z,w}(z_t, \eta_t)$ also is a stationary stochastic process, with single-time marginal $(\pi_{z,w})_\# \mu_\beta$. By part 2, (z_t, w_t) is a solution of the SDE (3.3).

The characterization $(*)$ in (3.4) follows from part 2 of Lemma A.7. Taking $\mathbb{O} := \mathbb{P}$ in that lemma, we find that if $\eta \sim \mathcal{N}_{\mathbf{X}}(0, \beta^{-1}\mathbb{C})$, then $w := \widehat{\mathbb{P}}\eta$ has distribution $\mathcal{N}_{\mathbf{H}}(0, \beta^{-1}\mathbb{P}) = \mathcal{N}_{\mathbf{W}}(0, \beta^{-1}\mathbb{I}_{\mathbf{W}})$. By translating the distributions by $\mathsf{C}z$ we find the identity $(*)$. Finally, the version (3.5) is a rewriting of (3.4). □

Remark 3.6 (Invariance of ν_β)**.** The invariance of the measure in (3.5) can also be seen by explicit computation. The generator associated with the stochastic process (3.3) is

$$\mathcal{L} = \mathbb{J}_{\mathcal{A}}(z)\big(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z) + \mathsf{C}^*w\big) \cdot \nabla_z - \mathbb{D}(w + \mathsf{C}z) \cdot \nabla_w + \frac{1}{\beta}\mathbb{D}_{\mathrm{sym}} : \nabla_w^2,$$

with adjoint operator

$$\mathcal{L}^{\star}\rho = -\operatorname{div}_z\big[\rho\mathbb{J}_{\mathcal{A}}(z)(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z)+\mathsf{C}^*w)\big] + \operatorname{div}_w\big[\rho\mathbb{D}(w + \mathsf{C}z)\big] + \frac{1}{\beta}\operatorname{div}_w\big[\operatorname{div}_w(\rho\mathbb{D}_{\mathrm{sym}})\big].$$

To show that ν_β is invariant, we show that $\mathcal{L}^{\star}\nu_\beta = 0$. Identifying ν_β with its Lebesgue density, note that

$$\nabla_z\nu_\beta = -\beta\nu_\beta(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z) + \mathsf{C}^*w), \qquad \nabla_w\nu_\beta = -\beta\nu_\beta(w+\mathsf{C}z),$$

$$\text{and} \qquad \frac{1}{\beta}\operatorname{div}_w(\nu_\beta\mathbb{D}_{\mathrm{sym}}) = -\mathbb{D}_{\mathrm{sym}}\nabla_w\nu_\beta.$$

We then calculate

$$\operatorname{div}_z\big[\nu_\beta\mathbb{J}_{\mathcal{A}}(z)(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z)+\mathsf{C}^*w)\big] = -\frac{1}{\beta}\operatorname{div}_z\big[\mathbb{J}_{\mathcal{A}}(z)\nabla_z\nu_\beta\big]$$

$$= -\frac{1}{\beta}\underbrace{\operatorname{div}_z\big[\mathbb{J}_{\mathcal{A}}(z)\big]}_{=\,0\text{ by assumption}}\cdot\nabla_z\nu_\beta - \frac{1}{\beta}\underbrace{\mathbb{J}_{\mathcal{A}}(z):\nabla_z^2\nu_\beta}_{=\,0\text{ by }\mathbb{J}_{\mathcal{A}}^* = -\mathbb{J}_{\mathcal{A}}} = 0,$$

and

$$\operatorname{div}_w\left[\nu_\beta\mathbb{D}(w+\mathsf{C}z) + \frac{1}{\beta}\operatorname{div}_w(\nu_\beta\mathbb{D}_{\mathrm{sym}})\right] = \operatorname{div}_w\left[-\frac{1}{\beta}\mathbb{D}\nabla_w\nu_\beta + \frac{1}{\beta}\mathbb{D}_{\mathrm{sym}}\nabla_w\nu_\beta\right]$$

$$= -\frac{1}{\beta}\underbrace{\operatorname{div}_w[\mathbb{D}_{\mathrm{skw}}\nabla_w\nu_\beta]}_{=\,0\text{ by }\mathbb{D}_{\mathrm{skw}}^* = -\mathbb{D}_{\mathrm{skw}}} = 0.$$

Therefore ν_β is invariant.

For a harmonic potential V, existence of an invariant measure can be shown using controllability as in [JPS17]. $\qquad\square$

4 GENERIC

4.1 Deterministic GENERIC

The GENERIC framework combines dissipative and conservative evolutions in way that respects thermodynamic principles. An evolution equation for an unknown $y(t)$ in a reflexive Banach space $\mathbf{Y}$ is said to be in GENERIC form if it can be written in terms of two functionals $\mathcal{E}$ and $\mathcal{S}$ and two operators $\mathbb{J}$ and $\mathbb{K}$ as

$$\dot{y} = \mathbb{J}(y)\mathrm{D}\mathcal{E}(y) + \mathbb{K}(y)\mathrm{D}\mathcal{S}(y). \tag{4.1}$$

Here the functionals $\mathcal{E}$, $\mathcal{S}$ and operators $\mathbb{J}$, $\mathbb{K}$ should satisfy the following (formal) requirements:

1 The 'energy' $\mathcal{E}$ and 'entropy' $\mathcal{S}$ are sufficiently smooth functionals on $\mathbf{Y}$.

2 For each $y \in \mathbf{Y}$, $\mathbb{J}(y)$ and $\mathbb{K}(y)$ are (possibly unbounded) linear operators from $\mathbf{Y}^*$ to $\mathbf{Y}$.

3 For each $y \in \mathbf{Y}$, the Poisson operator $\mathbb{J}(y)$ is skew-adjoint and satisfies Jacobi's identity:

$$\forall\, y \in \mathbf{Y} \,\forall\, \mu_1, \mu_2, \mu_3 \in \mathbf{Y}^* : \quad \big\langle \mu_1, \mathrm{D}\mathbb{J}(y)[\mathbb{J}(y)\mu_2]\mu_3 \big\rangle_{\mathbf{Y}} + \text{cyclic perm.} = 0, \qquad (4.2)$$

where $\langle \cdot, \cdot \rangle_{\mathbf{Y}}$ denotes the duality paring on $\mathbf{Y}^* \times \mathbf{Y}$ and $\mathrm{D}\mathbb{J}(y)[v]$ is the directional derivative in the direction $v \in \mathbf{Y}$.

4 For each $y \in \mathbf{Y}$, the Onsager operator $\mathbb{K}(y)$ is symmetric and non-negative.

5 The following *non-interaction conditions* are satisfied:

$$\mathbb{J}(y)\mathrm{D}\mathcal{S}(y) \stackrel{\text{(a)}}{=} 0 \quad \text{and} \quad \mathbb{K}(y)\mathrm{D}\mathcal{E}(y) \stackrel{\text{(b)}}{=} 0 \quad \text{for all } y \in \mathbf{Y}. \qquad (4.3)$$

We call the quintuple $(\mathbf{Y}, \mathcal{E}, \mathcal{S}, \mathbb{J}, \mathbb{K})$ a GENERIC system if the conditions 1.-5. hold.

A pre-form of this structure was introduced by Morrison [Mor86] under the name *metriplectic systems*, and further developed by Öttinger and Grmela as *General Equation for the Non-Equilibrium Reversible-Irreversible Coupling*, abbreviated as GENERIC [GrÖ97, ÖtG97, Ö05]. In [Mor86] the structures $\mathbb{J}$ and $\mathbb{K}$ feature together with one function $\mathcal{F} = \mathcal{E} - \mathcal{S}$. The importance of keeping $\mathcal{E}$ and $\mathcal{S}$ separate and the role of the non-interaction conditions was emphasized for the first time in [GrÖ97, ÖtG97]. Grmela and Öttinger's treatment includes extensions to stochastic evolutions, which are central to this paper, and we therefore follow the GENERIC terminology.

Remark 4.1 (Hamiltonian and Poisson systems). The property 3 above implies that $\mathbb{J}$ generates a Poisson manifold (see e.g. [MaR99, Ch. 10] for the theory of Poisson manifolds). An evolution equation of the form $\dot{y} = \mathbb{J}(y)\mathrm{D}\mathcal{E}(y)$ is therefore formally a Poisson system. This also implies that the GENERIC structure contains the class of Hamiltonian systems as a special case, corresponding to $\mathbb{K}\mathrm{D}\mathcal{S} \equiv 0$.

The non-interaction condition $\mathbb{J}\mathrm{D}\mathcal{S} = 0$ implies that the corresponding Poisson structure is degenerate: the flow of any evolution equation $\dot{y} = \mathbb{J}(y)\mathrm{D}\mathcal{F}(y)$ preserves the value of $\mathcal{S}$; the full space is therefore foliated into sets of the form $\{\mathcal{S} = \text{constant}\}$, and the flow preserves each of these leaves [MaR99, Th. 10.4.4]. We will see examples of this in Section 4.6. □

Remark 4.2. The non-interaction conditions (4.3) imply that the 'energy' $\mathcal{E}$ and the 'entropy' $\mathcal{S}$ have the properties that one expects from thermodynamics: if $y = y(t)$ satisfies (4.1) then $\mathcal{E}$ is preserved and $\mathcal{S}$ is non-decreasing:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(y(t)) = \big\langle \mathrm{D}\mathcal{E}, \dot{y} \big\rangle = \underbrace{\big\langle \mathrm{D}\mathcal{E}, \mathbb{J}\mathrm{D}\mathcal{E} \big\rangle}_{=\,0 \text{ by skew-symmetry of } \mathbb{J}} + \underbrace{\big\langle \mathrm{D}\mathcal{E}, \mathbb{K}\mathrm{D}\mathcal{S} \big\rangle}_{=\,0 \text{ by (4.3)(b)}} = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}(y(t)) = \big\langle \mathrm{D}\mathcal{S}, \dot{y} \big\rangle = \underbrace{\big\langle \mathrm{D}\mathcal{S}, \mathbb{J}\mathrm{D}\mathcal{E} \big\rangle}_{=\,0 \text{ by (4.3)(a)}} + \underbrace{\big\langle \mathrm{D}\mathcal{E}, \mathbb{K}\mathrm{D}\mathcal{S} \big\rangle}_{\geq\,0 \text{ by non-negativity of } \mathbb{K}} \geq 0.$$

□

Remark 4.3 (Special cases: Hamiltonian systems and gradient flows). We already mentioned that any Hamiltonian system is also a GENERIC system, corresponding to $\mathbb{K}\mathrm{D}\mathcal{S} \equiv 0$. Similarly, all gradient flows are also GENERIC systems, corresponding to $\mathbb{J}\mathrm{D}\mathcal{E} \equiv 0$. Note that with this choice of sign the driving functional $\mathcal{S}$ increases along solutions, in contrast to the more common decreasing case. □

Remark 4.4 (Coordinate invariance). The GENERIC equation (4.1) is coordinate-invariant: under linear or nonlinear changes of variables the equations retain the same form (see e.g. [Ö05, Sec. 1.2.4] or [Mie11, Sec. 2]). □

4.2 GENERIC SDEs

In this paper we encounter versions of GENERIC that include noise. We define a 'GENERIC SDE' to be a stochastic differential equation for a process Y_t in a finite-dimensional Hilbert space $\mathbf{Y}$ of the form

$$\mathrm{d}Y_t = \Big(\mathbb{J}(Y_t)\mathrm{D}\mathcal{E}(Y_t) + \mathbb{K}(Y_t)\mathrm{D}\mathcal{S}(Y_t) + \operatorname{div}\mathbb{K}(Y_t)\Big)\mathrm{d}t + \Sigma(Y_t)\,\mathrm{d}B_t, \qquad (4.4)$$

where B_t is a standard finite-dimensional Brownian motion. Note that we restrict ourselves to finite-dimensional spaces $\mathbf{Y}$ for simplicity. We require that the noise intensity Σ and the dissipation operator $\mathbb{K}$ are related by a fluctuation-dissipation relation:

$$\Sigma\Sigma^*(y) = 2\mathbb{K}(y) \qquad \text{for all } y. \qquad (4.5)$$

Fluctuation-dissipation relations of the form (4.5) have a long history; see e.g. the discussion in [ÖPM21, MPÖ21]. The GENERIC SDE (4.4) and the fluctuation-dissipation relation (4.5) seem to appear for the first time in [GrÖ97]; Öttinger refers to equations of the form (4.4) as 'GENERIC with fluctuations' [Ö05, Sec. 1.2.5].

The GENERIC SDE inherits energy conservation from the deterministic structure, and the fluctuation-dissipation relation (4.5) and conservation condition (4.6) imply that the measure $\mathrm{e}^{\mathcal{S}(y)}\,\mathrm{d}y$ is stationary:

Lemma 4.5 (Properties of a GENERIC SDE). *Assume that $\mathcal{E}$, $\mathcal{S}$, $\mathbb{J}$, and $\mathbb{K}$ satisfy the GENERIC conditions 1–5 above and the additional condition*

$$\operatorname{div}\mathbb{J} = 0 \qquad \text{on } \mathbf{Y}. \qquad (4.6)$$

In addition, assume that the equation (4.4) *has unique weak solutions for any given starting point Y_0. Then*

 1 *The evolution deterministically preserves $\mathcal{E}$, i.e. for any $Y_0 \in \mathbf{Y}$,*

$$\mathcal{E}(Y_t) = \mathcal{E}(Y_0) \qquad \text{almost surely, for all } t \geq 0.$$

 2 *The measure*

$$\mathrm{e}^{\mathcal{S}(y)}\,\mathrm{d}y$$

 is preserved by the flow of (4.4).

Proof. To show the conservation of $\mathcal{E}$, we calculate by Itō's lemma that

$$\mathrm{d}\mathcal{E}(Y_t) = \mathrm{D}\mathcal{E}(Y_t)^*\Big(\mathbb{J}(Y_t)\mathrm{D}\mathcal{E}(Y_t) + \mathbb{K}(Y_t)\mathrm{D}\mathcal{S}(Y_t) + \tfrac{1}{2}\operatorname{div}\big[\Sigma\Sigma^*\big](Y_t)\Big)\mathrm{d}t$$

$$\qquad + \mathrm{D}\mathcal{E}(Y_t)^*\Sigma(Y_t)\,\mathrm{d}B_t + \frac{1}{2}\mathrm{D}^2\mathcal{E}(Y_t) : \Sigma\Sigma^*(Y_t)\,\mathrm{d}t$$

$$\overset{(*)}{=} \frac{1}{2}\Big(\mathrm{D}\mathcal{E}(Y_t)^*\operatorname{div}\big[\Sigma\Sigma^*\big](Y_t) + \mathrm{D}^2\mathcal{E}(Y_t) : \Sigma\Sigma^*(Y_t)\Big)\mathrm{d}t$$

$$\qquad + \mathrm{D}\mathcal{E}(Y_t)^*\Sigma(Y_t)\,\mathrm{d}B_t$$

$$= \frac{1}{2}\operatorname{div}[\mathrm{D}\mathcal{E}(Y_t)^*\Sigma\Sigma^*(Y_t)]\,\mathrm{d}t + \mathrm{D}\mathcal{E}(Y_t)^*\Sigma(Y_t)\,\mathrm{d}B_t$$

$$= 0.$$

The identity $(*)$ follows from the non-interaction conditions (4.3), and the final two terms vanish because the range of Σ is included in the range of $\mathbb{K}$ by (4.5), which is orthogonal to $\mathrm{D}\mathcal{E}$ for the same reason.

To show that $\mathrm{e}^{\mathcal{S}(y)}\mathrm{d}y$ is stationary, note that the dual generator of the process Y_t in (4.4) is given by

$$\mathcal{L}^*\rho = \mathrm{div}\Big[\rho\mathbb{J}\mathrm{D}\mathcal{E} + \mathbb{K}(\rho\mathrm{D}\mathcal{S} - \mathrm{D}\rho)\Big].$$

One checks that $\rho(y) = \mathrm{e}^{\mathcal{S}(y)}$ satisfies $\mathcal{L}^*\rho = 0$:

$$\mathrm{div}\big[\mathrm{e}^{\mathcal{S}}\mathbb{J}\mathrm{D}\mathcal{E}\big] = \underbrace{\mathrm{e}^{\mathcal{S}}\mathrm{D}\mathcal{S}\cdot\mathbb{J}\mathrm{D}\mathcal{E}}_{=0\text{ by }(4.3)} + \underbrace{\mathrm{e}^{\mathcal{S}}\mathrm{D}\mathcal{E}\cdot\mathrm{div}\,\mathbb{J}}_{=0\text{ by }(4.6)} + \underbrace{\mathrm{e}^{\mathcal{S}}\mathbb{J}:\mathrm{D}^2\mathcal{E}}_{=0\text{ by }\mathbb{J}^*=-\mathbb{J}} = 0, \tag{4.7}$$

$$\mathrm{div}\big[\mathbb{K}(\mathrm{e}^{\mathcal{S}}\mathrm{D}\mathcal{S} - \mathrm{D}\mathrm{e}^{\mathcal{S}})\big] = 0.$$

This implies that $\mathrm{e}^{\mathcal{S}(y)}\mathrm{d}y$ is an invariant measure of the process (4.4). $\qquad\square$

Remark 4.6 (Additional invariant measures). In fact, the conservation of $\mathcal{E}$ by the SDE (4.4) implies that there is a very large class of invariant meaures. For instance, any measure of the form $f(\mathcal{E}(y))\mathrm{e}^{\mathcal{E}(y)}\,\mathrm{d}y$ also is conserved, for any measurable function $f\colon\mathbb{R}\to\mathbb{R}$. As another example, in Section 4.5 we construct invariant measures $\nu_\beta^{\mathcal{E}_0}$ that can be interpreted as "$\mathrm{e}^{\mathcal{S}}(y)\,\mathrm{d}y$ restricted to a level set $\mathcal{E} = \mathcal{E}_0$", which can be seen as an extreme version of $f(\mathcal{E}(y))\mathrm{e}^{\mathcal{E}(y)}\,\mathrm{d}y$. $\qquad\square$

Remark 4.7 (Interpretation of $\mathrm{div}\,\mathbb{J} = 0$). The proof of Lemma 4.5 illustrates the role of the condition $\mathrm{div}\,\mathbb{J} = 0$ in (4.6). In (4.7) this condition is combined with the skew-symmetry and non-interaction conditions to show that the measure $\mathrm{e}^{\mathcal{S}(y)}\mathrm{d}y$ is stationary for the Hamiltonian flow $\mathbb{J}\mathrm{D}\mathcal{E}$.

However, the condition $\mathrm{div}\,\mathbb{J} = 0$ is not coordinate-invariant; the corresponding coordinate-invariant setup is as follows. Let $m = m(y)$ be a smooth and positive density on $\mathbf{Y}$, and assume that

$$\mathrm{div}(m\mathbb{J}) = 0. \tag{4.8}$$

(The case (4.6) corresponds to $m \equiv 1$.) Weinstein [Wei97] discusses equations of this type in the context of Poisson geometry. If such a density m exists, then $\mu(\mathrm{d}y) = m(y)\mathrm{d}y$ is invariant for each Hamiltonian flow with respect to the Poisson structure $\mathbb{J}$; such a Poisson manifold is called *uni-modular*.

The generalization of the GENERIC SDE (4.4) to the case of (4.8) is

$$\mathrm{d}Y_t = \left(\mathbb{J}(Y_t)\mathrm{D}\mathcal{E}(Y_t) + \mathbb{K}(Y_t)\mathrm{D}\mathcal{S}(Y_t) + \frac{1}{m(Y_t)}\,\mathrm{div}(m\mathbb{K})(Y_t)\right)\mathrm{d}t + \Sigma(Y_t)\,\mathrm{d}B_t. \tag{4.9}$$

This SDE conserves the measure $\mathrm{e}^{\mathcal{S}(y)}m(y)\,\mathrm{d}y$, as can be verified in the same way as in the proof of Lemma 4.5.

This observation suggests the following interpretation of the interplay between m, $\mathcal{S}$, and the Lebesgue measure. The Poisson structure $\mathbb{J}$ admits an invariant measure $\mu = m\,\mathrm{d}y$; often μ coincides with the Lebesgue measure. The entropy $\mathcal{S}$ has the interpretation of changing the weight of different y-states, thus modifying μ into $\mathrm{e}^{\mathcal{S}}\mu$ (see also Section 4.5). The gradient term $\mathbb{K}\mathrm{D}\mathcal{S}$ and the Itō correction term $m^{-1}\mathrm{div}(m\mathbb{K})$ combine to make the measure $\mathrm{e}^{\mathcal{S}}\mu$ invariant.

The reason that the conserved measure μ often coincides with the Lebesgue measure is related to the use of canonical coordinates in Hamiltonian systems. In canonical coordinates in $\mathbb{R}^{2n}$ the space $\mathbf{Y}$ is the cotangent bundle $T^*\mathcal{M}$ of the manifold $\mathcal{M} = \mathbb{R}^n$, in which case the Poisson structure has the canonical form "$\mathrm{d}p \wedge \mathrm{d}q$" and the Lebesgue measure is invariant.

See also [Ö05, (6.76) and (6.163)] for a different approach to this question. $\qquad\square$

Remark 4.8 (Updated coordinate invariance)**.** Concretely, the coordinate invariance of the modified SDE (4.9) means the following.

If Y_t is a solution of (4.9) in $\mathbf{Y} = \mathbb{R}^n$, and $\phi\colon \mathbb{R}^n \to \mathbb{R}^n$ is a smooth bijection, then $Z_t := \phi(Y_t)$ is a solution of

$$\mathrm{d}Z_t = \left(\widehat{\mathbb{J}}(Z_t)\mathrm{D}_z\widehat{\mathcal{E}}(Z_t) + \widehat{\mathbb{K}}(Z_t)\mathrm{D}_z\widehat{\mathcal{S}}(Z_t) + \frac{1}{\widehat{m}(Z_t)}\,\mathrm{div}_z\left(\widehat{m}\widehat{\mathbb{K}}\right)(Z_t)\right)\mathrm{d}t + \widehat{\Sigma}(Z_t)\,\mathrm{d}B_t. \quad (4.10)$$

Here the components are defined as

$$\begin{aligned}
\widehat{\mathcal{E}}(\phi(y)) &:= \mathcal{E}(y), & \widehat{\mathcal{S}}(\phi(y)) &:= \mathcal{S}(y), \\
\widehat{\mathbb{J}}(\phi(y)) &:= \mathrm{D}\phi(y)\mathbb{J}(y)\mathrm{D}\phi(y)^*, & \widehat{\mathbb{K}}(\phi(y)) &:= \mathrm{D}\phi(y)\mathbb{K}(y)\mathrm{D}\phi(y)^*, & (4.11) \\
\widehat{m}(\phi(y)) &:= \frac{1}{\det \mathrm{D}\phi(y)}m(y), & \text{and} \quad \hat{\Sigma}(\phi(y)) &:= \mathrm{D}\phi(y)\Sigma(y).
\end{aligned}$$

Expressions such as in (4.11) should be read as

$$\widehat{\mathbb{J}}_{ij}(\phi(y)) := \sum_{k,\ell} \partial_{y_k}\phi_i(y)\mathbb{J}_{k\ell}(y)\partial_{y_\ell}\phi_j(y).$$

One can check that

1 $\widehat{m}$ is again stationary in the sense of (4.8), i.e. $\mathrm{div}_z(\widehat{m}\widehat{\mathbb{J}}) = 0$;
2 $\widehat{m}(z)\,\mathrm{d}z$ is the push-forward of the measure $m(y)\,\mathrm{d}y$ under ϕ;
3 The measure $\widehat{\mu}(\mathrm{d}z) := \widehat{m}(z)\mathrm{e}^{\widehat{\mathcal{S}}(z)}\,\mathrm{d}z$ is the push-forward of $\mu(\mathrm{d}y) := m(y)\mathrm{e}^{\mathcal{S}(y)}\,\mathrm{d}y$ under ϕ, and is stationary for (4.10).

$\square$

Remark 4.9 (Reversibility and irreversibility)**.** The terms 'reversible' and 'irreversible' sometimes give rise to confusion. For instance, in the acronym GENERIC (General Equation for the Non-Equilibrium Reversible-Irreversible Coupling) the word 'irreversible' refers to the gradient-flow term $\mathbb{K}\mathrm{D}\mathcal{S}$; this term causes $\mathcal{S}$ to increase along the evolution, and hence generates a form of irreversibility. At the same time, this gradient-flow term is associated with *reversible* stochastic processes (see e.g. [MPR14] and below). In this remark we attempt to resolve this confusion.

A first concept of 'reversibility' comes from the theory of ordinary differential equations. A differential equation $\dot{y} = f(y)$ in $\mathbb{R}^d$ is called *reversible* or *R-reversible* (see [Dev76] or [HLW06, Ch. V]) if there exists a linear involution $R : \mathbb{R}^d \to \mathbb{R}^d$ such that $Rf(Ry) = -f(y)$. With this property, solving the equation forward from y_0 is equivalent to solving it backward from Ry_0. This implies for instance that given the value of $y(t)$ one can retrace the solution back to time $t = 0$ without loss of information; in this sense the forward solution map can be 'reversed'. An important example is that of Hamiltonian systems with Hamiltonians of the form $H(q,p) = \frac{1}{2}|p|^2 + V(q)$ with involution $R : (q,p) \mapsto (q,-p)$. The assumptions of this paper also make Example 1.1 reversible, with involution $R : (q,p,\eta) \mapsto (q,-p,\eta(-\cdot))$.

We now generalise this concept of reversibility by lifting it to measures on path space. A measure P on the path space $\mathrm{C}((-\infty,\infty);\mathbb{R}^d)$ is defined to be *R-reversible* if it is invariant under the combined action of R and time inversion:

$$r_\#P = P, \quad \text{where} \quad r(y)(t) := Ry(-t) \quad \text{for } y \in \mathrm{C}((-\infty,\infty);\mathbb{R}^d) \text{ and } t \in \mathbb{R}.$$

Reversible differential equations, in the first sense above, define reversible path-space measures, provided they are in stationarity, i.e. provided that the single-time marginal distributions $P_t := \operatorname{law} y(t)$ are independent of t. In Example 1.1, this is the case if we start the evolution at any time t_0 with $(q, p, \eta)(t_0)$ is distributed according to the measure μ_β (see Theorem 2.7).

A second important category of reversible path-space measures is generated by stochastic processes. Let μ be an invariant measure of the SDE

$$\mathrm{d}Y_t = \mathbb{K}(Y_t)\mathrm{D}\mathcal{S}(Y_t)\,\mathrm{d}t + \operatorname{div}\mathbb{K}(Y_t)\,\mathrm{d}t + \Sigma(Y_t)\,\mathrm{d}W_t \qquad \text{(i.e. (4.4) without } \mathbb{J}\mathrm{D}\mathcal{E}\text{).} \qquad (4.12)$$

If $\mathbb{K}\mathrm{D}(\mathcal{S} - \log \mathrm{d}\mu/\mathrm{d}\mathscr{L}) = 0$ and $2\mathbb{K} = \Sigma\Sigma^*$ (for instance, $\mu = \mathrm{e}^{\mathcal{S}-\beta\mathcal{E}}$, see Remark 4.6), then this SDE generates a measure P on path space $\mathrm{C}((-\infty, \infty); \mathbb{R}^d)$, that is invariant under time inversion with $R = \mathrm{id}$. (As a general rule, a stationary Markov process with single-time marginal μ generates an R-reversible path-space measure if and only if (a) $R_\#\mu = \mu$ and (b) $\mathcal{L}^*f = (\mathcal{L}(f \circ R)) \circ R$ for any f, where $\mathcal{L}^*$ is the Hilbert adjoint of the generator $\mathcal{L}$ in $L^2(\mu)$.)

The reversibility of the stochastic process (4.12) is generated by the balance of two opposing effects. The two separate equations

$$\mathrm{d}Y_t = \mathbb{K}\mathrm{D}\mathcal{S}(Y_t)\,\mathrm{d}t \qquad \text{and} \qquad \mathrm{d}Y_t = \Sigma\,\mathrm{d}W_t$$

drive Y_t in different directions: the dissipative, 'concentrating' effect of $\mathbb{K}\mathrm{D}\mathcal{S}$ and the 'spreading' effect of $\Sigma\,\mathrm{d}W_t$ together result in stationarity, and because of the fluctuation-dissipation relation (4.5) the resulting path-space measure also is reversible. In other words, the term $\mathbb{K}\mathrm{D}\mathcal{S}$ is at the same time a drift with irreversible effects and one half of a fluctuation-dissipation pair that generates a reversible measure.

In particular, for the multivariate Ornstein-Uhlenbeck process given by

$$\mathrm{d}Y_t = -\mathbb{D}Y_t\,\mathrm{d}t + \Sigma\,\mathrm{d}W \quad \text{with } \Sigma = \left(\frac{1}{\beta}(\mathbb{D}+\mathbb{D}^*)\right)^{1/2}$$

the equilibrium measure P is Gaussian and characterized by the covariance $\mathbb{E}^P(Y_t \times Y_s) = \frac{1}{\beta}\mathrm{e}^{-(t-s)\mathbb{D}}$ for $t \geq s$, we have reversibility if and only if $\mathbb{D} = \mathbb{D}^*$, i.e., $\mathbb{D}_{\mathrm{sym}} = \mathbb{D}$ or $\mathbb{D}_{\mathrm{skw}} = 0$. Thus, from the stochastic point of view we may consider that $\mathbb{D}_{\mathrm{sym}}$ generates the reversible part of the process and $\mathbb{D}_{\mathrm{skw}}$ the irreversible part.

Turning back to the thermodynamical terms 'reversible' and 'irreversible' in the acronym GENERIC, the 'reversibility' of the Hamiltonian term $\mathbb{J}\mathrm{D}\mathcal{E}$ is reversibility in the first sense above, under some involution R. (Note that not all Hamiltonian systems are reversible, and therefore this usage is inspired by those important examples that do have this property). The 'irreversibility' of the term $\mathbb{K}\mathrm{D}\mathcal{S}$ is the thermodynamic irreversibility of the equation $\mathrm{d}Y_t = \mathbb{K}\mathrm{D}\mathcal{S}(Y_t)\,\mathrm{d}t$, which causes the entropy $\mathcal{S}$ to increase.

We recall that the stochastically reversible part $\mathbb{D}_{\mathrm{sym}}$ of $\mathbb{D}$ contributes to the thermodynamically irreversible part by entering in $\mathbb{K}_{\mathrm{GEN}}$. Vice versa, the stochastically irreversible part $\mathbb{D}_{\mathrm{skw}}$ contributes to the thermodynamically reversible part by entering in $\mathbb{J}_{\mathrm{GEN}}$. $\qquad\square$

4.3 Reformulation in GENERIC form

We now re-interpret the ODE (3.2) and the SDE (3.3) as GENERIC equations as introduced in the previous sections; for this we need to enlarge the state space.

We saw above that in GENERIC ODEs and SDEs the energy $\mathcal{E}$ is (almost surely) constant. The total energy $\mathcal{H}_{\text{total}}$ in (2.1) is a natural candidate for such an energy, but it has two drawbacks: first, it depends on η, to which we do not have access after coarse-graining, and secondly, in the case of the SDE the energy $\mathcal{H}_{\text{total}}$ is almost surely infinite (see Remark 2.2).

As described in the introduction, we use the orthogonal split of the heat-bath variable $\eta = \widehat{\mathbb{P}}\eta + \widehat{\mathbb{Q}}\eta = w + \widehat{\mathbb{Q}}\eta$ to split the heat-bath energy $\frac{1}{2}\|\eta\|_{\mathbf{H}}^2$ into two parts $\frac{1}{2}\|w\|_{\mathbf{H}}^2 + \frac{1}{2}\|\widehat{\mathbb{Q}}\eta\|_{\mathbf{H}}^2$. We can then formally write the total energy as

$$\mathcal{H}_{\text{total}}(z,\eta) = \underbrace{\mathcal{H}_{zw}(z,w)}_{\text{visible part}} + \underbrace{\tfrac{1}{2}\|\widehat{\mathbb{Q}}\eta\|_{\mathbf{H}}^2}_{\text{invisible, heat bath part}}, \qquad (4.13)$$

where we set

$$\mathcal{H}_{zw}(z,w) := \mathcal{H}_{\mathcal{A}}(z) + (\mathsf{C}z|w)_{\mathbf{H}} + \tfrac{1}{2}\|w\|_{\mathbf{H}}^2.$$

This split suggests to introduce a new scalar variable $e = e(t) \in \mathbb{R}$ that keeps track of the energy that is exchanged between the macroscopic part and the invisible part of the heat bath:

$$\mathrm{d}e_t = -\mathrm{d}\mathcal{H}_{zw}(z_t, w_t), \qquad \text{and} \qquad e(t=0) = e_0. \qquad (4.14)$$

This setup provides a GENERIC energy $\mathcal{E}_{\text{GEN}} := \mathcal{H}_{zw} + e$ that is constant in time, and also solves the problem of the 'infinitely-large energy' in the heat bath: the new variable e tracks the *changes* in the 'infinitely-large' term $\frac{1}{2}\|\widehat{\mathbb{Q}}\eta\|_{\mathbf{H}}^2$, while being finite itself. (We work out this point of view in more detail in Section 4.6 below.)

Using Itō's lemma to express the right-hand side in (4.14) leads to the following system of equations in the three unknowns (z, w, e). This is one of the main results of this paper.

Theorem 4.10. *Consider the function* $t \mapsto (z_t, w_t)$ *obtained from any one of the three parts of Theorem 3.3, extended by* (4.14) *to* $(z_t, w_t, e_t) \in \mathbf{Z} \times \mathbf{W} \times \mathbb{R}$.

  1 *In the case of part 1 of Theorem 3.3,* (z_t, w_t, e_t) *satisfies the ODE*

$$\dot{z}_t = \mathbb{J}_{\mathcal{A}}(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z_t) + \mathsf{C}^* w_t), \qquad (4.15a)$$

$$\dot{w}_t = -\mathbb{D}(w_t + \mathsf{C}z_t), \qquad (4.15b)$$

$$\dot{e}_t = (\mathbb{D}(w_t + \mathsf{C}z_t)|w_t + \mathsf{C}z_t)_{\mathbf{H}}, \qquad (4.15c)$$

  with initial datum $(z, w, e)(t = 0) = (z_0, w_0, e_0)$. *These equations can be written as the GENERIC ODE*

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} z \\ w \\ e \end{pmatrix} = \mathbb{J}_{\text{GEN}}(z)\mathrm{D}\mathcal{E}_{\text{GEN}}(z, w, e) + \mathbb{K}_{\text{GEN}}(z, w)\mathrm{D}\mathcal{S}_{\text{GEN}}(z, w, e).$$

  2 *In the case of part 2 or 3 of Theorem 3.3,* (z_t, w_t, e_t) *satisfies the SDE*

$$\mathrm{d}z_t = \mathbb{J}_{\mathcal{A}}(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z_t) + \mathsf{C}^* w_t)\mathrm{d}t, \qquad (4.16a)$$

$$\mathrm{d}w_t = -\mathbb{D}(w_t + \mathsf{C}z_t)\mathrm{d}t + \Sigma\,\mathrm{d}B_t, \qquad (4.16b)$$

$$\mathrm{d}e_t = \Big[(\mathbb{D}(w_t + \mathsf{C}z_t)|w_t + \mathsf{C}z_t)_{\mathbf{H}} - \frac{1}{\beta}\,\mathrm{tr}\,\mathbb{D}\Big]\mathrm{d}t - (w_t + \mathsf{C}z_t|\Sigma\,\mathrm{d}B_t)_{\mathbf{H}}, \qquad (4.16c)$$

  with deterministic initial datum $(z, w, e)(t = 0) = (z_0, w_0, e_0)$. *Here* B *is a standard* $\mathbf{W}$-*valued Brownian motion and* $\Sigma\Sigma^* = \beta^{-1}(\mathbb{D} + \mathbb{D}^*)$.

These equations can be written as the GENERIC SDE

$$\mathrm{d}\begin{pmatrix} z \\ w \\ e \end{pmatrix} = \Big[\mathbb{J}_{\mathrm{GEN}}(z)\mathrm{D}\mathcal{E}_{\mathrm{GEN}}(z,w,e) + \mathbb{K}_{\mathrm{GEN}}(z,w)\mathrm{D}\mathcal{S}_{\mathrm{GEN}}(z,w,e) + \mathrm{div}\,\mathbb{K}_{\mathrm{GEN}}(z,w) \Big]\mathrm{d}t$$

$$+ \Sigma_{\mathrm{GEN}}(z,w)\,\mathrm{d}B_t. \quad (4.17)$$

In all cases the various GENERIC components are defined as

$$\mathcal{E}_{\mathrm{GEN}}(z,w,e) = \mathcal{H}_{\mathcal{A}}(z) + \frac{1}{2}\|w\|_{\mathbf{H}}^2 + (\mathsf{C}z|w)_{\mathbf{H}} + e, \quad (4.18a)$$

$$= \mathcal{H}_{zw}(z,w) + e, \quad (4.18b)$$

$$\mathcal{S}_{\mathrm{GEN}}(z,w,e) = \beta e, \quad (4.18c)$$

$$\mathbb{J}_{\mathrm{GEN}}(z) = \begin{pmatrix} \mathbb{J}_{\mathcal{A}}(z) & 0 & 0 \\ 0 & -\mathbb{D}_{\mathrm{skw}} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (4.18d)$$

$$\mathbb{K}_{\mathrm{GEN}}(z,w) = \frac{1}{\beta}\begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbb{D}_{\mathrm{sym}} & -\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}z) \\ 0 & -(\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}z)|\square)_{\mathbf{H}} & (\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}z)|w+\mathsf{C}z)_{\mathbf{H}} \end{pmatrix}, \quad (4.18e)$$

where the operator $\mathbb{D}$ is decomposed into symmetric and skew-symmetric parts:

$$\mathbb{D} = \mathbb{D}_{\mathrm{sym}} + \mathbb{D}_{\mathrm{skw}} \quad \text{with } \mathbb{D}_{\mathrm{sym}} = \frac{1}{2}(\mathbb{D}+\mathbb{D}^*) \text{ and } \mathbb{D}_{\mathrm{skw}} := \frac{1}{2}(\mathbb{D}-\mathbb{D}^*).$$

The noise intensity in (4.17) is given as

$$\Sigma_{\mathrm{GEN}}(z,w) := \begin{pmatrix} 0 \\ \Sigma \\ -(w+\mathsf{C}z|\Sigma\,\square)_{\mathbf{H}} \end{pmatrix},$$

which satisfies the fluctuation-dissipation relation

$$\Sigma_{\mathrm{GEN}}\Sigma_{\mathrm{GEN}}^* = 2\mathbb{K}_{\mathrm{GEN}}. \quad (4.19)$$

Remark 4.11. It is remarkable that the splitting $\mathbb{D} = \mathbb{D}_{\mathrm{sym}} + \mathbb{D}_{\mathrm{skw}}$ is compatible with the non-interaction conditions of GENERIC. Moreover, taking into account the special structure of the differentials $\mathrm{D}\mathcal{H}_{\mathrm{GEN}} = (\mathrm{D}\mathcal{H}_{\mathcal{A}}(z) + \mathsf{C}^*z, w+\mathsf{C}z, 1)^\top$ and $\mathrm{D}\mathcal{S}_{\mathrm{GEN}} = (0,0,\beta)^\top$ and the structure of $\mathbb{K}_{\mathrm{GEN}}$ we see that in the differential equation (4.16b) only the sum $(\mathbb{D}_{\mathrm{sym}}+\mathbb{D}_{\mathrm{skw}})(w+\mathsf{C}z)$ appears. However, in the stochastic forcing we see only the symmetric part $\mathbb{D}_{\mathrm{sym}}$ through

$$\Sigma\Sigma^* = \frac{1}{\beta}\big(\mathbb{D}+\mathbb{D}^*\big) = \frac{2}{\beta}\,\mathbb{D}_{\mathrm{sym}}.$$

$\square$

Example 4.12 (Running example, part 4)**.** For the model in Examples (1.1) and (1.4), where we identify $\mathbf{W}$ with $\mathbb{R}^3$ we obtain a even more specific form of the GENERIC Poisson and Onsager structure in in $\mathbb{R}^{(2n+4)\times(2n+4)}$:

$$\mathbb{J}_{\mathrm{GEN}} = \begin{pmatrix} 0 & \mathbb{I} & 0 & 0 \\ -\mathbb{I} & 0 & 0 & 0 \\ 0 & 0 & -\mathbb{D}_{\mathrm{skw}} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \text{ and } \mathbb{K}_{\mathrm{GEN}} = \frac{1}{\beta}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbb{D}_{\mathrm{sym}} & -\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}q) \\ 0 & 0 & -\big(\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}q)\big)^\top & |w+\mathsf{C}q|_{\mathbb{D}_{\mathrm{sym}}}^2 \end{pmatrix}$$

where $C \in \mathbb{R}^{3 \times n}$ and $\mathbb{D}_{\mathrm{sym}}, \mathbb{D}_{\mathrm{skw}} \in \mathbb{R}^{3 \times 3}$ have the explicit form

$$\mathbb{D}_{\mathrm{skw}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\varsigma \\ 0 & \varsigma & 0 \end{pmatrix}, \quad \mathbb{D}_{\mathrm{sym}} = \begin{pmatrix} \vartheta_1 & 0 & 0 \\ 0 & \vartheta_2 & 0 \\ 0 & 0 & \vartheta_2 \end{pmatrix}, \quad \text{and } |\widehat{w}|_{\mathbb{D}_{\mathrm{sym}}}^2 = \widehat{w} \cdot \mathbb{D}_{\mathrm{sym}} \widehat{w}.$$

Thus, the macroscopic ODE takes the explicit form

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} q \\ p \\ w \\ e \end{pmatrix} = \begin{pmatrix} p \\ -DV(q) - C^*w \\ -\mathbb{D}_{\mathrm{skw}}(w+Cq) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ -\mathbb{D}_{\mathrm{sym}}(w+Cq) \\ |w+Cq|_{\mathbb{D}_{\mathrm{sym}}}^2 \end{pmatrix} = \begin{pmatrix} p \\ -DV(q) - C^*w \\ -\mathbb{D}(w+Cq) \\ |w+Cq|_{\mathbb{D}_{\mathrm{sym}}}^2 \end{pmatrix}.$$

$\square$

4.4 Interpretation of $\mathcal{E}_{\mathrm{GEN}}$, $\mathbb{J}_{\mathrm{GEN}}$, and $\mathbb{K}_{\mathrm{GEN}}$

Interpretation of the energy $\mathcal{E}_{\mathrm{GEN}}$. The discussion in Section 4.3 gives a clear interpretation of the energy

$$\mathcal{E}_{\mathrm{GEN}}(z, w, e) = \mathcal{H}_{\mathcal{A}}(z) + (Cz|w)_{\mathbf{H}} + \frac{1}{2}\|w\|_{\mathbf{H}}^2 + e$$

as a renormalized version of $\mathcal{H}_{\mathrm{total}}$: $\frac{1}{2}\|w\|_{\mathbf{H}}^2$ represents the 'visible' part of the heat-bath energy, e represents changes in the 'invisible' part, and an additional 'infinite but constant' component of the heat-bath energy has been renormalized out. This interpretation also explains why $\mathcal{E}_{\mathrm{GEN}}$ should be preserved by the GENERIC SDE (4.17).

Interpretation of the Poisson operator $\mathbb{J}_{\mathrm{GEN}}$. The Poisson operator $\mathbb{J}_{\mathrm{GEN}}$ is a combination of the symplectic operator $\mathbb{J}_{\mathcal{A}}$ with the skew-symmetric part $\mathbb{D}_{\mathrm{skw}}$ of the compression operator $\mathbb{D}$. This shows how a skew-symmetric component of the compression dynamics should be considered as a conservative (Hamiltonian) component of the evolution. Clearly $\mathbb{J}_{\mathrm{GEN}}(y)$ is skew-symmetric, and it can be easily shown that the Jacobi identity (4.2) holds, because $\mathbb{J}_{\mathcal{A}}$ depends on z but not on (w, e).

It would be interesting to understand in what sense or in which cases the formula (4.18d) for $\mathbb{J}_{\mathrm{GEN}}$ coincides with Öttinger's coarse-graining formula in [Ö05, Eq. (6.67+68)]:

$$\mathbb{J}(z, w, e) = \left\langle D\Pi(z, \eta) \mathbb{J}_{\mathrm{micro}}(z, \eta) D\Pi(z, \eta)^* \right\rangle_{(z, w, e)}, \tag{4.20}$$

where $\langle \cdot \rangle_{(z, w, e)}$ means averaging with respect to the conditional equilibrium measure given the macro-state (z, w, e).

In our case, omitting the energy variable e, the projection mapping reads

$$\begin{pmatrix} z \\ w \end{pmatrix} = \widetilde{\Pi}(z, \eta) = \begin{pmatrix} z \\ \mathbb{P}\eta \end{pmatrix}.$$

Hence, Öttinger's formula would take the form

$$\mathbb{J}_{\mathrm{macro}}(z, w) = \left\langle D\widetilde{\Pi}(z, \eta) \begin{pmatrix} \mathbb{J}_{\mathcal{A}}(z) & 0 \\ 0 & \mathbb{J}_{\mathcal{B}} \end{pmatrix} D\widetilde{\Pi}(z, \eta) \right\rangle_{(z, w)} = \begin{pmatrix} \mathbb{J}_{\mathcal{A}}(z) & 0 \\ 0 & \text{``}\mathbb{P}\mathbb{J}_{\mathcal{B}}\mathbb{P}\text{''} \end{pmatrix}.$$

Here, averaging is not needed, because the integrand is constant. However, as discussed in Remark C.2, the term $\mathbb{P}\,\mathbb{J}_\mathcal{B}\mathbb{P}$ is not well defined, because $\mathbf{W} \cap \mathrm{dom}(\mathbb{J}_\mathcal{B}) = \{0\}$ by construction.

Thus this formula should be considered in a renormalized sense, i.e. be approximating $\mathbb{J}_\mathcal{B}$ suitably. Because of the generator property, we have the approximation property by a symmetric difference of going forward and backward in time (which means extracting irreversible information):

$$\forall\, \eta \in \mathrm{dom}(\mathbb{J}_\mathcal{B}): \quad \frac{1}{2h}\big(\mathrm{e}^{h\mathbb{J}_\mathcal{B}} - \mathrm{e}^{-h\mathbb{J}_\mathcal{B}}\big)\eta = \frac{1}{2h}\big(\mathrm{e}^{h\mathbb{J}_\mathcal{B}} - \mathbb{I}\big)\eta - \frac{1}{2h}\big(\mathrm{e}^{-h\mathbb{J}_\mathcal{B}} - \mathbb{I}\big)\eta \xrightarrow{h\downarrow 0} \mathbb{J}_\mathcal{B}\eta.$$

At the same time, by the Compression Property (1.5) we obtain a different behavior when applying $\mathbb{P}$ from left and right (for $h \searrow 0$):

$$\forall\, v \in \mathbf{W}: \quad \mathbb{P}\frac{1}{2h}\big(\mathrm{e}^{h\mathbb{J}_\mathcal{B}} - \mathrm{e}^{-h\mathbb{J}_\mathcal{B}}\big)\mathbb{P}\,v \stackrel{\mathrm{comp}}{=} \frac{1}{2h}\big(\mathrm{e}^{-h\mathbb{D}} - \mathbb{I}\big)v - \frac{1}{2h}\big(\mathrm{e}^{-h\mathbb{D}^*} - \mathbb{I}\big)v \longrightarrow -\mathbb{D}_{\mathrm{skw}}v.$$

Thus, although this approximation is rather special (because of the symmetry with $\pm h$), we see that it is reasonable to replace the ill-defined expression $\mathbb{P}\,\mathbb{J}_\mathcal{B}\mathbb{P}$ by $-\mathbb{D}_{\mathrm{skw}}$. From this point of view it may be reasonable to interpret the definition (4.18d) of $\mathbb{J}_{\mathrm{GEN}}$ as a version of (4.20).

Interpretation of the Onsager operator $\mathbb{K}_{\mathrm{GEN}}$.   The structure of the Onsager operator $\mathbb{K}_{\mathrm{GEN}}$ can be understood in the following way. To start with, note that in the absence of interaction with z or e, the component $w = \widehat{\mathbb{P}}\eta$ decays as $\mathrm{e}^{-t\mathbb{D}}w$, which implies that the norm $\|w\|_{\mathbf{H}}^2$ then decays with rate $2\mathbb{D}_{\mathrm{sym}}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\|w_t\|_{\mathbf{H}}^2 = (w_t|\mathbb{D}w_t)_{\mathbf{H}} + (\mathbb{D}w_t|w_t)_{\mathbf{H}} = 2\,(w_t|\mathbb{D}_{\mathrm{sym}}w_t)_{\mathbf{H}}.$$

This explains the operator $\mathbb{D}_{\mathrm{sym}}$ in the (w,w)-block of $\mathbb{K}_{\mathrm{GEN}}$. The (w,e)-component of $\mathbb{K}_{\mathrm{GEN}}$ then necessarily has the form $-\mathbb{D}_{\mathrm{sym}}(w+\mathsf{C}z)$ because of the non-interaction condition (4.3), and the remaining components of $\mathbb{K}_{\mathrm{GEN}}$ follow by symmetry.

In fact, in equation (4.16b) the drift term is generated by the (w,e)-component of $\mathbb{K}_{\mathrm{GEN}}$, not the (w,w)-component, since $\mathbb{K}_{\mathrm{GEN}}$ multiplies $\mathrm{D}\mathcal{S}_{\mathrm{GEN}} = (0,0,\beta)^\top$. This does not change the interpretation above, since the non-interaction condition implies that the same drift term also would be generated by an alternative entropy, $(z,w,e) \mapsto -\mathcal{H}_{z,w}(z,w)$. We discuss the role of different entropies in the next section.

4.5   Interpretation of $\mathcal{S}_{\mathrm{GEN}}$

For the interpretation of $\mathcal{S}_{\mathrm{GEN}}$ we start by commenting on the historical development of 'entropy'. Entropy is commonly associated with a description of a system at two levels of aggregation, a 'microscopic' level and a 'macroscopic' level. Different authors, however, have emphasized different ways of placing entropy in this context. Boltzmann's famous postulate

$$\mathcal{S}(x) = k \ln W(x) \tag{4.21}$$

already illustrates this: the symbol $W(x)$ could either represent probability *(Wahrscheinlichkeit)* [Bre75, p. 44], or alternatively 'the number of microstates associated with the macrostate x'. Boltzmann presumably based his discussion on equal probability of microstates, in which case these two interpretations reduce to the same thing.

Einstein [Ein10] postulated that by rewriting (4.21) as

$$\text{Prob}(x) = e^{\frac{1}{k}\mathcal{S}(x)}, \tag{4.22}$$

this expression could be abstracted away from the specific microscopic situation, and could therefore hold also in situations without equal probability of microstates; in fact, the probability distribution over microstates only needs to be stationary under the microscopic dynamics. This approach focuses on an interpretation of entropy as 'logarithm of probabilities' rather than as 'number of microstates'. We take the same view here.

In continuous state spaces an expression such as (4.22) should be interpreted as a density with respect to some fixed measure. We illustrate this on a simple example: in the case of SDEs of the form

$$\mathrm{d}X_t = -K(X_t)\nabla V(X_t)\,\mathrm{d}t + \Sigma(X_t)\,\mathrm{d}B_t, \qquad \Sigma\Sigma^* = 2K,$$

one can consider $-V$ to be an entropy in the sense above, because the flow preserves the measure $e^{-V(x)}\mathrm{d}x$. The appearance of the Lebesgue measure '$\mathrm{d}x$' is explained by observing that this Lebesgue measure is invariant under the Brownian motion B_t, and the function $-V$ converts this invariant measure into $e^{-V(x)}\mathrm{d}x$ through the pair (K, Σ) as described by the Girsanov theorem. In this sense the entropy can be understood as describing an exponential *modification* of an underlying measure, and that is the sense in which (4.22) should be interpreted.

This point of view provides the SDE (3.3) for (z, w) (i.e. before extending with e) with a natural entropy

$$\mathcal{S}(z, w) := \log\frac{\mathrm{d}\nu_\beta}{\mathrm{d}\mathscr{L}_{\mathbf{Z}\times\mathbf{W}}}(z, w) \overset{(3.5)}{=} -\beta\mathcal{H}_{zw}(z, w) + \text{constant}, \tag{4.23}$$

where ν_β is given in (3.5) and $\mathscr{L}_{\mathbf{Z}\times\mathbf{W}}$ is the Lebesgue measure on $\mathbf{Z}\times\mathbf{W}$.

Below we follow this entropy $\mathcal{S}$ as it propagates into the extended system with variables (z, w, e), but that propagation is akin to bookkeeping. The actual appearance of entropy has happened here, at the coarse-graining step from variables (z, η) to variables (z, w).

While (4.23) gives a clear suggestion for an entropy for the variables (z, w), an indeterminacy arises when extending to variables (z, w, e). Indeed, after extension there is a multitude of invariant measures: for instance, if we fix an energy level $\mathcal{E}_0 \in \mathbb{R}$, then under the extension map

$$T^{\mathcal{E}_0} : (z, w) \mapsto \big(z, w, e := \mathcal{E}_0 - \mathcal{H}_{zw}(z, w)\big)$$

the measure ν_β is mapped to the measure

$$\nu_\beta^{\mathcal{E}_0} := T_\#^{\mathcal{E}_0}\nu_\beta,$$

which is concentrated on the '$\mathcal{E}_0$-energy-leaf' $\{(z, w, e) \in \mathbf{Z}\times\mathbf{H}\times\mathbb{R} : \mathcal{E}_{\text{GEN}}(z, w, e) = \mathcal{E}_0\}$. The measure $\nu_\beta^{\mathcal{E}_0}$ is invariant under the flow of the extended SDE (4.16), for each choice of $\mathcal{E}_0$. In fact, for any measure $\zeta \in \mathcal{P}(\mathbb{R})$ on the set of energy values $\mathcal{E}_0$, the compound measure

$$\nu_\beta^\zeta(A) := \int_\mathbb{R} \nu_\beta^{\mathcal{E}_0}(A)\,\zeta(\mathrm{d}\mathcal{E}_0) \qquad \text{for } A \subset \mathbf{Z}\times\mathbf{W}\times\mathbb{R},$$

has energy values $\mathcal{E}_{\text{GEN}}$ distributed according to ζ and is invariant under the SDE (4.16).

An equivalent way of observing the same indeterminacy is the following. If ν_β^ζ is one of the invariant measures that we just constructed, then there is a family of other invariant measures of the form

$$f(\mathcal{E}_{\mathrm{GEN}}(z, w, e))\, \nu_\beta^\zeta(\mathrm{d}z\,\mathrm{d}w\,\mathrm{d}e), \qquad \text{for arbitrary } f\colon \mathbb{R} \to \mathbb{R}. \tag{4.24}$$

Indeed, $f\circ\mathcal{E}_{\mathrm{GEN}}\, \nu_\beta^\zeta = \nu_\beta^{\zeta_f}$ with $\zeta_f(\mathrm{d}\tilde{e}) = f(\tilde{e})\zeta(\mathrm{d}\tilde{e})$.

This non-uniqueness of the invariant measure generates a corresponding non-uniqueness in the entropy. The family (4.24) generates the corresponding family of 'entropies'

$$\mathcal{S}_g(z, w, e) := -\beta\mathcal{H}_{zw}(z, w) + g(\mathcal{E}_{\mathrm{GEN}}(z, w, e)), \quad \text{for arbitrary } g\colon \mathbb{R} \to \mathbb{R}. \tag{4.25}$$

The choice $\mathcal{S}_{\mathrm{GEN}}(z, w, e) := \beta e$ of (4.18c) is one member of this family, corresponding to $g(\tilde{e}) = \beta\tilde{e}$.

Although (4.25) shows that many functions could be called 'entropy', we claim that $\mathcal{S}_{\mathrm{GEN}}(z, w, e) := e$ is the one that should appear in a GENERIC structure, and we give two reasons for this. The first reason is that the GENERIC structure requires $\mathbb{J}_{\mathrm{GEN}}\mathrm{D}\mathcal{S}_{\mathrm{GEN}} = 0$ (see (4.3)); within the family (4.25), only "$\beta e +$ constant" satisfies this. The second reason takes more time to explain, and we do this in the next section.

4.6 Characterization of entropy through finite-dimensional approximations

In this section we give an independent explanation why the expression $\mathcal{S}(z, w, e) = \beta e$ should characterize the entropy in the GENERIC SDE (4.17). The origin of this expression lies in the scaling of 'surface area', and we now describe this in detail.

This interpretation of entropy as 'surface area' can be found in some form or other in many treatments of the connection between statistical mechanics and thermodynamics (see e.g. [Cha87, Sec. 3.2], [Cho94, p. 69], [Ber97, Sec. 1.5], or [FrS01, (2.1.6)]). While the particular dependence of the surface area on n, β, and e given by Lemma 4.13 below must be generally known, we could not find a reference, and therefore we provide the details here. The same holds for the full-space equivalence-of-ensembles result of Lemma 4.14.

We choose $(\Xi_n)_{n\geq 1}$ to be a particular increasing sequence of n-dimensional subspaces of the orthogonal complement $\mathbf{W}^\perp \subset \mathbf{H}$, such that

$$\mathbf{W}^\perp = \overline{\operatorname{span} \bigcup_{n\geq 1} \Xi_n}^{\|\cdot\|_{\mathbf{H}}}.$$

The spaces Ξ_n are in the 'invisible' part of the heat bath, since $\mathbb{P}\Xi_n = 0$ and $\mathbb{Q}\Xi_n = \Xi_n$. We describe this choice in more detail in Appendix B.2.

Fix $\beta > 0$ and $e \in \mathbb{R}$, and for each n let $\zeta_{\beta, n, e}$ be the (non-normalized) measure on Ξ_n defined by

$$\zeta_{\beta, n, e}(\mathrm{d}\xi) := \boldsymbol{\delta}\left[\frac{1}{2}\|\xi\|_{\mathbf{H}}^2 - \frac{n}{2\beta} - e\right](\mathrm{d}\xi), \tag{4.26}$$

where $\boldsymbol{\delta}$ is the measure that is heuristically defined by (see Appendix B.2)

$$\int_{\Xi_n} \varphi(\xi)\boldsymbol{\delta}[f(\xi) - e](\mathrm{d}\xi) := \lim_{h\downarrow 0} \frac{1}{h}\int_{\Xi_n} \varphi(\xi)\mathbb{1}\{e \leq f(\xi) < e + h\}\,\mathrm{d}\xi \qquad \text{for all } \varphi \in C_c(\Xi_n).$$

The total mass of the measure $\boldsymbol{\delta}[f(\xi) - e] = \boldsymbol{\delta}[f(\xi) - e](\mathrm{d}\xi)$ can be interpreted as the area of the surface $f^{-1}(e) \subset \Xi_n$ (weighted by $|\nabla f|$; see Appendix B.2).

In the thermodynamical or statistical-mechanical literature the measure $\zeta_{\beta,n,e}$ would be called 'micro-canonical'. If the expression $\frac{1}{2}\|\xi\|_{\mathbf{H}}^2$ is interpreted as an energy, as in the case of this paper, then this measure is concentrated on an 'energy shell' at energy level $n/2\beta + e$. This particular choice of energy level is geared towards the limit $n \to \infty$: this choice causes each of the n degrees of freedom in Ξ_n to have approximately energy level $1/2\beta$.

The following two properties of this sequence of microcanonical measures probably are known (see e.g. [Cho94, p. 69] for a calculation similar to the first one), but for neither we could find a statement that suits our purposes; for completeness we give a proof in Appendix B.2.

Lemma 4.13. *Fix $\beta > 0$ and $e \in \mathbb{R}$.*

1. *There exists $C(\beta, n)$, converging to ∞ as $n \to \infty$, such that*

$$\mathsf{Z}_{\beta,n,e} := \int_{\Xi_n} \zeta_{\beta,n,e}(\mathrm{d}x)$$

   has the asymptotic behavior

$$\log \mathsf{Z}_{\beta,n,e} - C(\beta,n) \xrightarrow{n\to\infty} \beta e. \tag{4.27}$$

2. *We have the narrow convergence of measures on $\mathbf{X}$*

$$\frac{1}{\mathsf{Z}_{\beta,n,e}} \zeta_{\beta,n,e} \longrightarrow \widehat{\mathbb{Q}}_{\#}\gamma_\beta \qquad \text{as } n \to \infty. \tag{4.28}$$

The first statement above shows that for fixed β and e,

$$\text{surface area scales as} \quad \mathrm{e}^{C(\beta,n)+\beta e} \qquad \text{as } n \to \infty.$$

Note how the largest contribution $C(\beta, n)$ diverges as $n \to \infty$, and the dependence on e remains as an $O(1)$ contribution inside the exponential.

The second statement above is a version of the 'equivalence of ensembles': it can be interpreted as stating that in the large-n limit the microcanonical 'ensemble' $\zeta_{\beta,n,e}$ is similar to the 'canonical ensemble' described by the Gaussian measure $\widehat{\mathbb{Q}}_{\#}\gamma_\beta$ (see Lemma B.3). It differs from the usual treatment of equivalence-of-ensemble results in that it describes the behavior of the whole measure, not of a finite-marginal reduction. Note that under the limit Gaussian measure $\widehat{\mathbb{Q}}_{\#}\gamma_\beta$ each scalar degree of freedom has variance $1/\beta$, or equivalently energy $1/2\beta$, thus matching the scaling choice described above.

For the discussion here it is relevant that the dependence on e in $\zeta_{\beta,n,e}$ is lost in the convergence (4.28) of the measures themselves: the limit is independent of e. At the same time, the value of e *can* be detected by following the e-dependence of the partition function $\mathsf{Z}_{\beta,n,e}$, as described by (4.27).

We now apply this observation to the microscopic system of Section 2. We set $\mathbf{H}_n := \mathbf{W} + \Xi_n$; note that $\mathbb{P}\mathbf{H}_n = \mathbf{W}$ and $\mathbb{Q}\mathbf{H}_n = \Xi_n$.

Similarly to the construction above we fix an 'energy level' $\mathcal{E}_0$ and define the probability measure $\mu_{\beta,n}$ on the subspace $\mathbf{Z} \times \mathbf{H}_n$ by

$$\mu_{\beta,n}(\mathrm{d}z\,\mathrm{d}\eta) := \frac{1}{\mathsf{Z}_{\beta,n,\mathcal{E}_0}} \boldsymbol{\delta}\left[\mathcal{H}_{\mathrm{total}}(z,\eta) - \frac{n}{2\beta} - \mathcal{E}_0\right](\mathrm{d}z\,\mathrm{d}\eta).$$

By extension we can also consider $\mu_{\beta,n}$ as a probability measure on $\mathbf{Z}\times\mathbf{X}$. In contrast to $\zeta_{\beta,n,e}$ above we choose to normalize this measure.

The choice of energy level $n/2\beta + \mathcal{E}_0$ is very similar to the one above: in the limit $n \to \infty$ the bulk of the energy will be located in the n degrees of freedom in the invisible part Ξ_n of the heat bath, with approximately energy $1/2\beta$ per degree of freedom. Indeed, we have an equivalence-of-ensembles statement for the full system that mirrors that of the heat bath in Lemma 4.13:

Lemma 4.14. *As $n \to \infty$ the measure $\mu_{\beta,n}$ converges weakly on $\mathbf{Z}\times\mathbf{X}$ to μ_β.*

Again, only the $O(n)$ scaling of the energy level $\mathcal{E}_0 + n/2\beta$ is visible in the limit μ_β; the $O(1)$ part given by the choice of $\mathcal{E}_0$ can not be recovered from the limit measure μ_β. The proof is given Appendix B.

We next map this microcanonical measure $\mu_{\beta,n}$ to a new state space in which we can track the behavior of z, w, and e independently from the rest of the heat bath. Defining the closure in $\mathbf{X}$ of the Ξ_n as

$$\Xi^{\mathbf{X}} := \overline{\bigcup_{n\geq 1} \Xi_n}^{\|\cdot\|_{\mathbf{X}}},$$

we define the 'decomposition' map

$$T_n \colon \mathbf{Z}\times\mathbf{H}_n \longrightarrow \mathbf{Z}\times\mathbf{W}\times\Xi^{\mathbf{X}}\times\mathbb{R},$$

$$(z, \eta) \longmapsto \left(z,\ w := \mathbb{P}\eta,\ \xi = \mathbb{Q}\eta,\ e := \frac{1}{2}\|\xi\|_{\mathbf{H}}^2 - \frac{n}{2\beta} \right),$$

and the resulting measure on $\mathbf{Z}\times\mathbf{W}\times\Xi^{\mathbf{X}}\times\mathbb{R}$,

$$\mu_{\beta,n,e} := (T_n)_{\#}\mu_{\beta,n}. \tag{4.29}$$

The map T_n makes explicit the orthogonal split $\eta = w + \xi = \mathbb{P}\eta + \mathbb{Q}\eta$, and in addition exposes the renormalized energy variable $\|\xi\|^2/2 - n/2\beta$.

Since for $\eta \in \mathbf{H}_n$ we have

$$\mathcal{H}_{\text{total}}(z, \eta) = \mathcal{H}_{zw}(z, \mathbb{P}\eta) + \frac{1}{2}\|\mathbb{Q}\eta\|_{\mathbf{H}}^2,$$

the properties of the 'delta function' $\boldsymbol{\delta}$ allow us to rewrite $\mu_{\beta,n,e}$ as (see Lemma B.2)

$$\mu_{\beta,n,e}(\mathrm{d}z\,\mathrm{d}w\,\mathrm{d}\xi\,\mathrm{d}e) = \frac{1}{\mathsf{Z}_{\beta,n,\mathcal{E}_0}} \boldsymbol{\delta}\left[\mathcal{H}_{zw}(z, w) - \mathcal{E}_0 + e\right](\mathrm{d}z\,\mathrm{d}w)\,\boldsymbol{\delta}\left[\frac{1}{2}\|\xi\|_{\mathbf{H}}^2 - \frac{n}{2\beta} - e\right](\mathrm{d}\xi)\,\mathrm{d}e. \tag{4.30}$$

By Lemma 4.13 the final $\boldsymbol{\delta}$-measure has the asymptotic behavior

$$\mathrm{e}^{-C(\beta,n)}\boldsymbol{\delta}\left[\frac{1}{2}\|\xi\|_{\mathbf{H}}^2 - \frac{n}{2\beta} - e\right](\mathrm{d}\xi) \longrightarrow \mathrm{e}^{\beta e}\,(\widehat{\mathbb{Q}}_{\#}\gamma_\beta)(\mathrm{d}\xi) \qquad \text{as } n \to \infty.$$

Combining the factor $\mathrm{e}^{-C(\beta,n)}$ with $\mathsf{Z}_{\beta,n,\mathcal{E}_0}$ we thus have proved

Lemma 4.15. *As $n \to \infty$ we have the narrow convergence on $\mathbf{Z}\times\mathbf{W}\times\Xi^{\mathbf{X}}\times\mathbb{R}$,*

$$\mu_{\beta,n,e} \longrightarrow \mu_{\beta,e}, \tag{4.31a}$$

$$\mu_{\beta,e}(\mathrm{d}z\,\mathrm{d}w\,\mathrm{d}\xi\,\mathrm{d}e) := \frac{1}{\mathsf{Z}_{\beta,\mathcal{E}_0}}\,\mathrm{e}^{\beta e}\,\boldsymbol{\delta}\left[\mathcal{H}_{zw}(z, w) - \mathcal{E}_0 + e\right](\mathrm{d}z\,\mathrm{d}w)\,\mathrm{d}e\,(\widehat{\mathbb{Q}}_{\#}\gamma_\beta)(\mathrm{d}\xi). \tag{4.31b}$$

We now use this convergence to understand the interpretation of $\mathcal{S}_{\mathrm{GEN}}(z, w, e) = \beta e + \mathrm{constant}$. The microcanonical measure $\mu_{\beta, n, e}$, written in the form (4.30), can be interpreted as the product of two surface measures, the first for System A and the second one for the heat bath. Each surface measure is calculated at some energy level parametrized by $e \in \mathbb{R}$, but neither are normalized; the normalization happens at the level of the total product, not the individual factors. This gives rise to a trade-off: as a function of e, the surface area of the heat bath at energy level '$c_1 + e$' is multiplied by the surface area of System A at energy level '$c_2 - e$'.

From the discussion above we know that for large n the surface area of the heat bath at energy level $c_1 + e$ has the exponential dependence $\mathrm{e}^{\beta e}$ on e. Therefore higher heat-bath energy levels, which correspond to larger e in (4.30), have a larger contribution in (4.30), and this dependence gives a downward pressure on the energy of System A. This downward pressure can be recognized by integrating $\mu_{\beta, e}$ over both ξ and e; we then obtain

$$
\frac{1}{Z_{\beta, \mathcal{E}_0}} \int_{\mathbb{R}} \mathrm{e}^{\beta e}\, \boldsymbol{\delta}\big[\mathcal{H}_{zw}(z, w) - \mathcal{E}_0 + e\big](B)\,\mathrm{d}e
$$
$$
= \frac{1}{Z_{\beta, \mathcal{E}_0}} \int_B \mathrm{e}^{-\beta \mathcal{H}_{zw}(z, w) + \beta \mathcal{E}_0}\,\mathrm{d}z\,\mathrm{d}w, \qquad \text{for all } B \subset \mathbf{Z} \times \mathbf{W},
$$

or more concisely, as measures on $\mathbf{Z} \times \mathbf{W}$,

$$
\frac{1}{Z_{\beta, \mathcal{E}_0}} \int_{\mathbb{R}} \mathrm{e}^{\beta e}\, \boldsymbol{\delta}\big[\mathcal{H}_{zw}(z, w) - \mathcal{E}_0 + e\big]\,\mathrm{d}e = \frac{1}{Z_{\beta, \mathcal{E}_0}} \mathrm{e}^{-\beta \mathcal{H}_{zw}(z, w) + \beta \mathcal{E}_0}.
$$

(See Definition B.1 for this type of manipulation.) The expression on the right-hand side coincides with (3.5), and shows how the increase in heat-bath surface area with heat-bath energy penalizes energy increases in System A.

Summarizing, the formula $\mathcal{S}_{\mathrm{GEN}}(z, w, e) = \beta e + \mathrm{constant}$ can be interpreted as a characterization of the dependence of microcanonical heat-bath surface area on heat-bath energy, and the discussion above shows how this dependence has a depressing effect on the energy in System A.

5   Conclusion and discussion

While the coarse-graining of Hamiltonian systems is a classical topic, the introduction of the compression hypothesis from dilation theory gives a new type of insight into this question. Specifically, we have shown how the compression hypothesis gives an abstract characterization of heat-bath behaviour that automatically generates two important effects.

First, the existence of a compression means in particular that the Hamiltonian evolution of the coupled system can be projected to the finite-dimensional subspace $\mathbf{Z} \times \mathbf{W}$. Secondly, and just as importantly, the compression property implies that the combination of random heat-bath initial data, Hamiltonian propagation, and projection generates a noise that is memoryless, leading to the Brownian noise terms in the equations (3.3) and (4.16). This is best expressed by Lemma 3.2, and the proof of that lemma clearly shows how the projection and Hamiltonian propagation combine to give the covariance function of an Ornstein-Uhlenbeck process.

In addition, the same compression hypothesis has a clear connection to the GENERIC structure. The operator $\mathbb{D}$ that appears in the compression hypothesis generates terms in both the Poisson operator

$\mathbb{J}_{\mathrm{GEN}}$ and the Onsager operator $\mathbb{K}_{\mathrm{GEN}}$: the skew-symmetric part of $\mathbb{D}$ contributes to $\mathbb{J}_{\mathrm{GEN}}$, and the symmetric part to $\mathbb{K}_{\mathrm{GEN}}$. In this way the compression hypothesis generates new structure in the (formerly) Hamiltonian system, which turns out to be GENERIC structure.

Finally, the fluctuations generated by the noise are linked to the Onsager operator $\mathbb{K}_{\mathrm{GEN}}$ by the fluctuation-dissipation relation (4.19). This puts the GENERIC framework on a firmer footing, and gives modelling insight into the various components of GENERIC.

5.1 Relation with models and results in the literature

Coupled Hamiltonian systems consisting of a fixed system and a 'heat bath' have been studied by many authors. The earliest example that we could find is by Zwanzig [Zwa73a], and similar systems return in [Zwa05, Zwa01b, KS*02b]. In all of these works the heat bath is finite-dimensional; infinite-dimensional heat baths were used in the related work of Jaksic and Pillet [JaP98b] and Rey-Bellet [Rey06].

The fact that a particular tuning of the properties of the heat bath and its projector can lead to Markovianity of the projected subsystem was observed by Ford, Kac, and Mazur [FKM65], and later used by many others [Zwa73b, Zwa05]. Stuart and co-workers [StW99, KS*02b] appear to be the first to give a rigorous convergence statement in the limit of infinite dimensions of the heat bath (and the Compression Property 1.2 is effectively equivalent to the choice of the frequencies of the n oscillators in these two papers).

Very similar ideas were also used to explain dissipation in quantum systems (so-called open quantum systems), in particular in the famous Caldeira-Leggett model [CaL83b, CaL83a], see also [ToH20] where the heat bath is interpreted in terms of a phonon-number representation. The straightforward usage of the classical dilation theory leads to so-called quantum-state diffusion, see e.g. [GiP92], which does not fully account for the true nature of quantum probability. A genuine dilation theory for open quantum system needs a quantum probability theory, see e.g. [AFG84, Mey95].

Remark 5.1. The setup of Jaksic and Pillet [JaP98a] is similar to ours, but their condition (H3) effectively excludes the case of this paper. This is due to the already-remarked fact that $\mathbf{W} \cap \mathrm{dom}(\mathbb{J}_{\mathcal{B}}) = \{0\}$, which is proved in Remark C.2. Jaksic and Pillet find from their (H3) that their equivalent of the process Y_t has C^1 dependence on the initial datum (z_0, η_0) (their Theorem 2.1), while because of the lack of continuity we only obtain measurability. □

The coarse-graining of this paper is closely related to the 'Mori-Zwanzig' reduction method [Mor65, Zwa61, Zwa01a, CHK00, Sch22]. The first step in this method is the expression of the 'hidden' variables in terms of the 'visible' variables. In in this paper equation (2.10) plays the same role. The integral term characterizes the changes in z that are generated by z itself but through the heat bath:

$$\int_0^t \underbrace{\mathsf{C}^* \mathrm{e}^{(t-s)\mathbb{J}_{\mathcal{B}}} \mathsf{C}}_{=:\, K(t-s)} \dot{z}_s \, \mathrm{d}s.$$

The Compression Hypothesis (1.5) amounts to assuming that there exists a finite-dimensional subspace $\mathbf{W}$ with corresponding orthogonal projection $\mathbb{P}\colon \mathbf{H} \to \mathbf{W}$ and a dissipative operator $\mathbb{D}$ on $\mathbf{W}$ such that

$$\text{(a)} \quad \mathsf{C}^* \mathbb{P} = \mathsf{C}^* \quad \text{and} \quad \text{(b)} \quad K(t) = \mathsf{C}^* \mathrm{e}^{-t\mathbb{D}} \mathsf{C} \quad \text{for } t \geq 0. \tag{5.1}$$

Condition (a) means that $\mathbf{W}$ contains all information necessary to characterize the effect of the heat bath on z. Condition (b), on the other hand, amounts to an assumption that K can be written as a finite

sum of exponentials (one for each of the coordinates); this is sometimes used as an approximation in numerical algorithms [Sch22] (see also [StS19]).

The compression property bypasses the usual solving of the 'hidden-variables' equation, which in the case of this paper would involve the orthogonal component $\xi_t = \widehat{\mathbb{Q}}\eta_t$. The formal generator of this 'orthogonal dynamics' should be either $\mathbb{Q}\mathbb{J}_{\mathcal{B}}$ or $\mathbb{Q}\mathbb{J}_{\mathcal{B}}\mathbb{Q}$, which both are not well defined and tend to be difficult to study, even formally. In the context of the compression property this dynamics is bypassed, and the effect of the hidden variables on the visible ones is instead fully characterized by (5.1).

Mori-Zwanzig reduction schemes come in two forms, depending on whether the split is performed in the state space itself (as in this paper) or in the space of probability measures or 'ensembles' on the state space. The latter approach has the advantage of lifting a nonlinear evolution to a linear one, thereby allowing the application of linear theory such as the Mori-Zwanzig reformulation. In the case of this paper, we can apply the simpler, first type, since the nonlinearity is confined to System A.

5.2   Relation between positive and zero temperature

In the zero-temperature limit, $\beta \to \infty$, the positive-temperature equations (3.3) and (4.16) converge to the corresponding deterministic ODEs (3.2) and (4.15). This can be recognized in the characterization $\Sigma\Sigma^* = \beta^{-1}(\mathbb{D} + \mathbb{D}^*)$ of the noise intensity, which implies that $\Sigma \to 0$ as $\beta \to \infty$.

It is a natural question whether the GENERIC structure itself converges. The answer is that it does not, at least not in this form. The entropy $\mathcal{S}_{\mathrm{GEN}} = \beta e + \text{constant}$ becomes singular as $\beta \to \infty$, and the Onsager operator $\mathbb{K}_{\mathrm{GEN}}$ vanishes. The product $\mathbb{K}_{\mathrm{GEN}}D\mathcal{S}_{\mathrm{GEN}}$, however, is independent of β, and this suggests that in order to study this limit it would make sense to rescale by

$$\mathcal{S}_{\mathrm{GEN}}^{\text{rescaled}} := \frac{1}{\beta}\mathcal{S}_{\mathrm{GEN}}, \qquad \text{and} \qquad \mathbb{K}_{\mathrm{GEN}}^{\text{rescaled}} := \beta\mathbb{K}_{\mathrm{GEN}}.$$

The rescaled objects $\mathcal{S}_{\mathrm{GEN}}^{\text{rescaled}}$ and $\mathbb{K}_{\mathrm{GEN}}^{\text{rescaled}}$ are independent of β, and therefore trivially converge.

As observed in Section 1.4, the deterministic GENERIC evolution, however, is independent of β.

5.3   Well-preparedness of the heat bath at time zero

The central construction of the microscopic evolution in this paper is done in part 3 of Theorem 2.5. There the initial state of the 'visible' part of the heat bath $w_0 = \widehat{\mathbb{P}}\eta_0$ is assumed to be given, while the 'invisible' part $\xi_0 = \widehat{\mathbb{Q}}\eta_0$ is drawn randomly from the corresponding conditioned equilibrium measure $\widehat{\mathbb{Q}}_{\#}\gamma_\beta$ of the heat bath. This randomness then generates the randomness in the SDE (3.3) of the projected system (z, w).

In the philosophical debate about irreversibility and coarse-graining (see e.g. [Rob20]) such a setup has been criticized: it amounts to an assumption that the microscopic state at time $t = 0$ is rather special. This can be recognized in the fact that while the initial hidden variables $\xi = \widehat{\mathbb{Q}}\eta$ have distribution $\widehat{\mathbb{Q}}_{\#}\gamma_\beta$ at time 0, they *will not* have that same distribution at later or earlier times. (The distribution γ_β is invariant under the heat-bath evolution, but $\widehat{\mathbb{Q}}_{\#}\gamma_\beta$ is not.)

In fact, it turns out that the altered distribution of ξ at times different from zero *does not* change the effect of the coarse-graining. To illustrate this, consider starting the heat bath in part 3 of Theorem 2.5 at some time $t_0 \in \mathbb{R}$ with distribution $\xi_{t_0} \sim \widehat{\mathbb{Q}}_{\#}\gamma_\beta$. At time $t = 0$ the corresponding state equals

$\widehat{S}_{-t_0}\xi_{t_0}$. Note that this propagated state is distributed according to $(\widehat{S}_{-t_0}\widehat{\mathbb{Q}})_{\#}\gamma_\beta$, and is not completely hidden ($\widehat{\mathbb{P}}\widehat{S}_{-t_0}\xi_{t_0} \neq 0$). In equation (2.10) describing the evolution of z, only the first term changes:

$$\dot{z}_t = \mathbb{J}_{\mathcal{A}}\mathsf{C}^* Y_{t-t_0}(\xi_{t_0}) + \mathbb{J}_{\mathcal{A}}\big(\mathrm{D}\mathcal{H}_{\mathcal{A}}(z) + \mathsf{C}^*(\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}\mathsf{C}z_0 - \mathsf{C}z_t)\big) + \mathbb{J}_{\mathcal{A}}\int_0^t \mathsf{C}^*\mathrm{e}^{(t-s)\mathbb{J}_{\mathcal{B}}}\mathsf{C}\dot{z}_s\,\mathrm{d}s. \quad (5.2)$$

However, under the compression property by Lemma 2.4 the process $t \mapsto Y_{t-t_0}(\xi_{t_0})$ is again a non-stationary Ornstein-Uhlenbeck process; in other words the *noise* in this process is stationary, even though the state at time $t = 0$ is not in equilibrium. It follows that the noise generated by the heat bath has the same distribution, also if one starts with a hidden variable of the form $\widehat{S}_{-t_0}\xi_{t_0}$, where $\xi_{t_0} \sim \widehat{\mathbb{Q}}_{\#}\gamma_\beta$.

5.4 Other derivations of GENERIC by coarse-graining

Öttinger's coarse-graining of Hamiltonian systems. The closest in spirit to this paper is the coarse-graining approach by Öttinger [Ö05, Ch. 6]. The starting point is again a Hamiltonian system, and a central role is played by a 'coarse-graining map' similar to $\pi_{z,w,e}$ in (1.7). The two approaches differ in the definition of the coarse-grained state: while in this paper we consider $\pi_{z,w,e}(z,\eta)$ itself to be the coarse-grained state (up to renormalization of the infinite energy), in [Ö05, Ch. 6] the coarse-grained state is in effect a *distribution* $\rho_{z,w,e}$ on $\mathbf{Z}\times\mathbf{X}$, parametrized by (z,w,e).

It is tempting to consider Öttinger's distribution $\rho_{z,w,e}$ as an approximation of the conditional distribution of (z,η) given the value of $\pi_{z,w,e}(z,\eta)$. Unfortunately this approach seems to fail: in simple examples one can verify that the *actual* conditional distribution of (z,η) is different from the $\rho_{z,w,e}$ postulated in Öttinger's approach, sufficiently different to make it unclear why $\rho_{z,w,e}$ should be a good approximation for the purpose of coarse-graining. While there are clear parallels between the two approaches, at this stage it is not clear to us whether they should be considered effectively the same or not.

Obtaining GENERIC from large deviations. GENERIC has also been derived from large-deviation principles of stochastic processes. In [DPZ13], Duong and two of us showed how the GENERIC structure of the kinetic Fokker-Planck equation can be recognized in the large-deviations rate functional of a sequence of 'more microscopic' stochastic interacting particle systems. Since a large-deviations principle can also be interpreted as a form of coarse-graining, this gives an independent derivation of the GENERIC structure, but from a process with stochastic forcing and deterministic initial data, the opposite of the setting of this paper. In [KL*18, KL*20] the arguments of [DPZ13] were generalized to a larger class of systems.

A Properties of Gaussian measures

In this appendix we recall a number of properties of Gaussian measures that we use in this paper. We will mostly use the notation and definitions of the book on Gaussian Measures by Bogachev [Bog98].

A.1 Basic setup

In $\mathbb{R}$, a *centered Gaussian random variable* η with variance σ^2, written as $\eta \sim \mathcal{N}(0, \sigma^2)$, has the probability density

$$\mu(\mathrm{d}\eta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\eta^2}{2\sigma^2}\right) \mathrm{d}\eta.$$

Note that such a scalar random variable has the equivalent formulation

$$\text{for all } t \in \mathbb{R}, \quad \mathbb{E}\left[\mathrm{e}^{it\eta}\right] = \mathrm{e}^{-\frac{\sigma^2 t^2}{2}}.$$

Centered Gaussian random variables on $\mathbb{R}^n$ have the probability density

$$\mu(\mathrm{d}\eta) = \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} \exp\left(-\frac{1}{2}\eta^T \Sigma^{-2}\eta\right) \mathrm{d}\eta, \tag{A.1}$$

where Σ is a symmetric positive definite $n \times n$ matrix. We now define the n-dimensional Hilbert space $\mathbf{H}$ to be $\mathbb{R}^n$ with the norm $\|\eta\|_{\mathbf{H}}^2 := \eta^T \Sigma^{-2}\eta$, which implies that the dual norm is $\|f\|_{\mathbf{H}^*} = f^T \Sigma^2 f$. Then the expression above takes the form

$$\mu(\mathrm{d}\eta) = \frac{1}{\mathsf{Z}} \exp\left(-\frac{1}{2}\|\eta\|_{\mathbf{H}}^2\right) \mathrm{d}\eta$$

This leads to the following equivalent characterizations of centered Gaussian measures on any finite-dimensional Hilbert space $\mathbf{H}$.

Lemma A.1. *Let $\mathbf{H}$ be a finite-dimensional real Hilbert space, let $\mu \in \mathcal{P}(\mathbf{H})$, and fix $\beta > 0$. The following are equivalent:*

$$\mu(\mathrm{d}\eta) = \frac{1}{\mathsf{Z}} \exp\left(-\frac{\beta}{2}\|\eta\|_{\mathbf{H}}^2\right) \mathrm{d}\eta; \tag{A.2}$$

$$\textit{For all } f \in \mathbf{H}^*, \, f(\eta) \sim \mathcal{N}_{\mathbb{R}}\left(0, \beta^{-1}\|f\|_{\mathbf{H}^*}^2\right); \tag{A.3}$$

$$\textit{For all } h \in \mathbf{H}, \, (h|\eta)_{\mathbf{H}} \sim \mathcal{N}_{\mathbb{R}}\left(0, \beta^{-1}\|h\|_{\mathbf{H}}^2\right). \tag{A.4}$$

In this case, if $\eta \sim \mu$, then for any bounded linear operator $\mathbb{O} : \mathbf{H} \to \mathbf{H}$, we have

$$\mathbb{E}\,(\mathbb{O}\eta|\eta)_{\mathbf{H}} = \mathrm{tr}_{\mathbf{H}}\,\mathbb{O}. \tag{A.5}$$

Formulations (A.3) and (A.4) above can be interpreted as stating that the covariance structure of the measure μ is given by the norms of $\mathbf{H}$ and $\mathbf{H}^*$, as in (A.1). In this paper we need η to be infinite-dimensional (see for instance Remark C.2), while still having covariance structure determined by $\mathbf{H}$ and $\mathbf{H}^*$. The following lemma allows us to construct such Gaussian measures.

The critical step is that we need to consider larger spaces $\mathbf{X}$, such that $\mathbf{H}$ is Hilbert-Schmidt-embedded into $\mathbf{X}$; the measure is then defined on $\mathbf{X}$, and the random variable η takes values in $\mathbf{X}$.

Lemma A.2. *Let $\mathbf{H}$ and $\mathbf{X}$ be finite- or infinite-dimensional real Hilbert spaces, and let $\mu \in \mathcal{P}(\mathbf{X})$. If the embedding $\mathbf{H} \hookrightarrow \mathbf{X}$ is Hilbert-Schmidt, then there exists a measure $\mu \in \mathcal{P}(\mathbf{X})$ with the properties*

$$\textit{For all } f \in \mathbf{X}^*, \, f(\eta) \sim \mathcal{N}_{\mathbb{R}}\left(0, \beta^{-1}\|f\|_{\mathbf{H}^*}^2\right). \tag{A.6}$$

$$\textit{For all } x \in \mathbf{X}, \, (x|\eta)_{\mathbf{X}} \sim \mathcal{N}_{\mathbb{R}}\left(0, (\mathrm{cov}_\mu\, x|x)_{\mathbf{X}}\right). \tag{A.7}$$

Here cov_μ is a self-adjoint non-negative trace-class operator on $\mathbf{X}$. If $f(\eta) = (x|\eta)_{\mathbf{X}}$ for some $x \in \mathbf{X}$, then $(\mathrm{cov}_\mu\, x|x)_{\mathbf{X}} = \beta^{-1}\|f\|_{\mathbf{H}^*}^2$.

This generalises the finite-dimensional case, where one can take $\mathbf{H} = \mathbf{X}$ and $\mathrm{cov}_\mu = \beta^{-1}\mathrm{id}$, and the properties above reduce to those of Lemma A.1.

Remark A.3 (Definition of infinite-dimensional Gaussian measures)**.** The usual definition of a Gaussian measure on an infinite-dimensional space $\mathbf{X}$ is that for each bounded linear form f on $\mathbf{X}$ the projected measure $f_\#\mu$ is a one-dimensional Gaussian measure (e.g. [Bog98, Def. 2.2.1]); since $\mathbf{X}$ is Hilbert, each such f is an inner product with an $x \in \mathbf{X}$, and this coincides with (A.7). $\qquad\square$

Remark A.4 (Necessity of Hilbert-Schmidt embedding)**.** The formulation of Lemma A.2 suggests that the embedding $\mathbf{H} \hookrightarrow \mathbf{X}$ needs to be Hilbert-Schmidt for the measure μ to exist, and indeed this is necessary. In particular there is no Gaussian measure on an infinite-dimensional space with the identity operator as covariance. $\qquad\square$

The construction above concerns centered Gaussian measures. Non-centered measures are constructed by translating by $a \in \mathbf{X}$, resulting in a random variable with expectation a. We write the corresponding measure as $\mathcal{N}_\mathbf{X}(a, \mathrm{cov})$. Formally, such a measure γ has the form

$$\frac{1}{Z}\mathrm{e}^{-\frac{1}{2}\left(\mathrm{cov}^{-1}(\eta-a)\big|(\eta-a)\right)_\mathbf{X}}\,\mathrm{d}\eta. \tag{A.8}$$

This is the sense in which we construct the 'canonical' Gaussian measure with formal structure (2.6).

Proof of Lemma A.2. Writing id for the embedding $\mathbf{H} \hookrightarrow \mathbf{X}$, the operator $\mathbb{C} := \mathrm{id}\,\mathrm{id}^*$ is a self-adjoint non-negative trace-class operator; by [Bog98, Th. 2.3.1] there exists a Gaussian measure μ with mean zero and covariance operator $\mathrm{cov}_\mu = \beta^{-1}\mathbb{C}$, which therefore satisfies (A.7) by the definition of a Gaussian measure.

From the definition of $\mathrm{id} : \mathbf{H} \hookrightarrow \mathbf{X}$ we have $(x|\eta)_\mathbf{X} = (\mathrm{id}^*x|\eta)_\mathbf{H}$. For $f \in \mathbf{X}^*$ of the form $f(\eta) = (x|\eta)_\mathbf{X} = (\mathrm{id}^*x|\eta)_\mathbf{H}$ for some $x \in \mathbf{X}$, we then calculate

$$\|f\|_{\mathbf{H}^*} = \sup_{\eta\in\mathbf{H}}\frac{f(\eta)}{\|\eta\|_\mathbf{H}} = \sup_{\eta\in\mathbf{H}}\frac{(\mathrm{id}^*x|\eta)_\mathbf{H}}{\|\eta\|_\mathbf{H}} = (\mathrm{id}^*x|\mathrm{id}^*x)_\mathbf{H} = (\mathbb{C}x|x)_\mathbf{X}\,,$$

by which also (A.6) follows from (A.7). $\qquad\square$

A.2   Construction of $\mathbf{X}$ by Gelfand triple

In Section 2.2 we aim to construct a Gaussian measure of the formal structure

$$\mathrm{e}^{-\frac{\beta}{2}\|\eta\|_\mathbf{H}^2}\,\mathrm{d}\eta. \tag{A.9}$$

This expression can be made rigorous as a Gaussian measure on a larger Hilbert space $\mathbf{X}$ with the property that $\mathbf{H}$ admits a Hilbert-Schmidt embedding into $\mathbf{X}$. While essentially 'any' such embedding is possible (see [Bog98, Lemma 3.2.2]), we choose a particular one based on the well-known Gelfand triple. We now describe this setting, which is visualized Fig. A.1.

The space $\mathbf{X}$ is implicitly characterized by the choice of an unbounded, densely defined, self-adjoint linear operator $\mathbb{A} : \mathrm{Dom}(\mathbb{A}) \subset \mathbf{H} \to \mathbf{H}$ with the property that $\mathbb{A}^{-1} : \mathbf{H} \to \mathrm{Dom}(\mathbb{A})$ is well-defined and Hilbert-Schmidt. Given such an operator we construct $\mathbf{X}$ in the following steps.

   1 We define $\mathbf{V} := \mathrm{Dom}(\mathbb{A})$, which is a Hilbert space with norm $\|v\|_\mathbb{V} := \|\mathbb{A}v\|_\mathbf{H}$. This implies that $\mathbf{V} = \mathbb{A}^{-1}\mathbf{H}$.

$$\mathbf{V} \xhookrightarrow{\ \mathbb{A}\ } \mathbf{H} \simeq \mathbf{H}^* \xhookrightarrow{\ \mathbb{A}\ } \mathbf{V}^*$$

$$\mathbf{X}^* \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \quad \| \ \text{definition}$$

$$\mathbf{X}$$

Figure A.1: The Gelfand-triple setup. The top row is the classical Gelfand triple $\mathbf{V} \hookrightarrow \mathbf{H} \simeq \mathbf{H}^* \hookrightarrow \mathbf{V}^*$, and the bottom row connects this triple to the notation of this paper. The space $\mathbf{X}$ is defined as $\mathbf{V}^*$, and $\mathbf{X}^*$ is defined as the space of bounded linear maps on $\mathbf{X}$. The two dotted lines indicate the two Riesz identifications that would be possible in this diagram; because of the risk of confusion we make these identifications explicitly, not implicitly (see (A.11) below).

2 We identify $\mathbf{H}^*$ with $\mathbf{H}$ and define the norm $\|\cdot\|_{\mathbf{V}^*}$ on $\mathbf{H}$ by

$$\frac{1}{2}\|h\|_{\mathbf{V}^*}^2 := \sup_{v \in \mathbf{V}} (h|v)_{\mathbf{H}} - \frac{1}{2}\|v\|_{\mathbf{V}}^2 \qquad \text{for } h \in \mathbf{H}.$$

We then define $\mathbf{V}^*$ as the closure of $\mathbf{H}$ in the norm $\|\cdot\|_{\mathbf{V}^*}$. By construction the elements of $\mathbf{V}^*$ are in duality with $\mathbf{V}$, and we write ${}_{\mathbf{V}^*}\langle \xi, v \rangle_{\mathbf{V}}$ for the dual product. We then also have $\mathbf{H} \hookrightarrow \mathbf{V}^*$, in the sense that any $h \in \mathbf{H}$ is a bounded linear form on $\mathbf{V}$ by

$$_{\mathbf{V}^*}\langle h, v \rangle_{\mathbf{V}} := (h|v)_{\mathbf{H}} \qquad \text{for all } v \in \mathbf{V}.$$

3 We extend $\mathbb{A}^{-1}$ as an operator $\mathbf{V}^* \to \mathbf{H}$ by setting for any $\xi \in \mathbf{V}^*$

$$\left(\mathbb{A}^{-1}\xi\big|h\right)_{\mathbf{H}} := {}_{\mathbf{V}^*}\big\langle \xi, \mathbb{A}^{-1}h \big\rangle_{\mathbf{V}} \qquad \text{for all } h \in \mathbf{H}.$$

We can then write

$$\|\xi\|_{\mathbf{V}^*} = \|\mathbb{A}^{-1}\xi\|_{\mathbf{H}} \qquad \text{for all } \xi \in \mathbf{V}^*. \tag{A.10}$$

The extension is also a symmetric operator in $\mathbf{V}^*$, since for $h_1, h_2 \in \mathbf{H}$ we have

$$\left(\mathbb{A}^{-1}h_1\big|h_2\right)_{\mathbf{V}^*} = \left(h_1\big|\mathbb{A}^{-1}h_2\right)_{\mathbf{H}} = \left(h_1\big|\mathbb{A}^{-1}h_2\right)_{\mathbf{V}^*}.$$

We similarly extend $\mathbb{A}$ as an operator $\mathbf{H} \to \mathbf{V}^*$.

4 We define $\mathbf{X} := \mathbf{V}^*$. The space $\mathbf{X}$ is a Hilbert space with norm $\|\xi\|_{\mathbf{X}} = \|\mathbb{A}^{-1}\xi\|_{\mathbf{H}}$ for all $\xi \in \mathbf{X}$. We have $\mathbf{H} \hookrightarrow \mathbf{X}$ as mentioned above, with $\|h\|_{\mathbf{X}} = \|\mathbb{A}^{-1}h\|_{\mathbf{H}}$; this shows that the embedding $\mathbf{H} \hookrightarrow \mathbf{X}$ is Hilbert-Schmidt.

5 We characterize elements of the dual space

$$\mathbf{X}^* := \{f \colon \mathbf{X} \to \mathbb{R} \text{ linear and bounded }\}$$

in two different ways, by applying Riesz representation on either $\mathbf{X}$ or $\mathbf{H}$, leading to an element $x_f \in \mathbf{X}$ or equivalently an element $v_f \in \mathbf{V}$:

$$\begin{aligned}
f(\xi) &= (\xi|x_f)_{\mathbf{X}} & &\text{for all } \xi \in \mathbf{X}, & \text{(A.11a)} \\
&= {}_{\mathbf{V}^*}\langle \xi, v_f \rangle_{\mathbf{V}} & &\text{for all } \xi \in \mathbf{X}, & \text{(A.11b)} \\
&= (\xi|v_f)_{\mathbf{H}} & &\text{whenever } \xi \in \mathbf{H}. & \text{(A.11c)}
\end{aligned}$$

We have $x_f = \mathbb{A}^2 v_f$ and $\|f\|_{\mathbf{X}^*} = \|x_f\|_{\mathbf{X}} = \|v_f\|_{\mathbf{V}}$.

The setup above defines the space $\mathbf{X}$. In order to define the measure (A.9) we define the trace-class operator

$$\mathbb{C} := \mathbb{A}^{-2} \colon \mathbf{X} \to \mathbf{X} \qquad \text{or equivalently} \qquad (\mathbb{C}\xi|\xi)_{\mathbf{X}} := \|\mathbb{A}^{-1}\xi\|_{\mathbf{X}}^2 \text{ for } \xi \in \mathbf{X}.$$

We then set, for $\beta > 0$, γ_β to be the Gaussian measure on $\mathbf{X}$

$$\gamma_\beta = \mathcal{N}_{\mathbf{X}}(0, \beta^{-1}\mathbb{C}).$$

This can be considered a rigorous version of (A.9), because from $\|\eta\|_{\mathbf{X}} = \|\mathbb{A}^{-1}\eta\|_{\mathbf{H}}$ we deduce that

$$\mathrm{e}^{-\frac{\beta}{2}\|\eta\|_{\mathbf{H}}^2} = \mathrm{e}^{-\frac{\beta}{2}\|\mathbb{A}\eta\|_{\mathbf{X}}^2} = \mathrm{e}^{-\frac{\beta}{2}\left(\mathbb{A}^2\eta|\eta\right)_{\mathbf{X}}} = \mathrm{e}^{-\frac{\beta}{2}\left(\mathbb{C}^{-1}\eta|\eta\right)_{\mathbf{X}}},$$

which matches with (A.8).

Note that $\mathbb{C}$ also is trace-class as a map $\mathbf{H} \to \mathbf{H}$, since in terms of an orthonormal basis e_k of $\mathbf{H}$ we can write

$$\mathrm{tr}_{\mathbf{H}}\,\mathbb{C} = \sum_{k=1}^{\infty}(\mathbb{C}e_k|e_k)_{\mathbf{H}} = \sum_{k=1}^{\infty}\|\mathbb{A}^{-1}e_k\|_{\mathbf{H}}^2,$$

and $\mathbb{A}^{-1}$ is Hilbert-Schmidt on $\mathbf{H}$.

Remark A.5 (Positive temperature implies infinite energy)**.** A well-known property of infinite-dimensional Gaussian measures such as γ_β is that for any $\beta > 0$, $\gamma_\beta(\mathbf{H}) = 0$. This shows that if η is distributed according to γ_β, then the natural energy $\frac{1}{2}\|\eta\|_{\mathbf{H}}^2$ is almost surely infinite. See e.g. [Rey06, Sec. 2.1] or [Bog98, Rem. 2.2.3] for a discussion of this property. $\qquad\qquad\square$

To facilitate applying the theorems of [Bog98] we make explicit the relationship between the objects of this paper and the notation of [Bog98]. The covariance bilinear form R_{γ_β} is given by

$$R_{\gamma_\beta}(f)(f) = \frac{1}{\beta}\left(\mathbb{C}x_f|x_f\right)_{\mathbf{X}} \qquad \text{for } f \in \mathbf{X}^* \text{ and for } x_f \text{ given by (A.11b),} \qquad \text{(A.12)}$$

and the Cameron-Martin Hilbert space $H(\gamma_\beta)$ coincides with $\mathbf{H}$, up to a scaling of the norm:

$$\|h\|_{H(\gamma_\beta)}^2 = \beta\|h\|_{\mathbf{H}}^2 \qquad \text{for all } h \in \mathbf{H}. \qquad \text{(A.13)}$$

A.3 Measurable extensions of linear maps

In Section 2 we constructed several extensions of linear operators on $\mathbf{H}$ to $\mathbf{X}$. In this section we give the details of these extensions.

Definition A.6 (Measurable linear extensions of [Bog98, Def. 2.10.1+3.7.1])**.** *Let $\mathbf{Y}$ be a normed linear space, and let $f\colon \mathbf{H} \to \mathbf{Y}$ be given. If there exists a subspace $\mathbf{L}$ with $\mathbf{H} \subset \mathbf{L} \subset \mathbf{X}$ and $\gamma_\beta(\mathbf{L}) = 1$ and a linear map $\widehat{f}\colon \mathbf{L} \to \mathbf{Y}$, measurable with respect to $(\mathcal{B}(\mathbf{X})_{\gamma_\beta}, \mathcal{B}(\mathbf{Y}))$, such that $\widehat{f}$ coincides with f on $\mathbf{L}$, then we call $\widehat{f}$ a measurable linear extension of f.*

Such an extension is characterized γ_β-a.e. by its values on $\mathbf{H}$ [Bog98, Cor. 2.10.8], and therefore can be considered γ_β-unique.

Note that if $\eta \sim \gamma_\beta$ and g is a measurable map from $\mathbf{X}$ to $\mathbf{Y}$, then $g(\eta)$ has distribution $g_\#\gamma_\beta$, the push-forward measure of γ_β under g, defined by

$$\int_{\mathbf{Y}} \varphi(\xi)(g_\#\gamma_\beta)(\mathrm{d}\xi) = \int_{\mathbf{X}} \varphi(g(\eta))\gamma_\beta(\mathrm{d}\eta) \qquad \text{for all } \varphi \in C_b(\mathbf{Y}).$$

Lemma A.7 (Extensions of bounded linear operators on $\mathbf{H}$). *Let η have distribution γ_β.*

1 *If $h \in \mathbf{H}$, then the bounded linear map $f_h \colon \mathbf{H} \ni \eta \mapsto (h|\eta)_{\mathbf{H}} \in \mathbb{R}$ can be extended to a measurable linear map $\widehat{f}_h$, and we have for all $h_1, h_2 \in \mathbf{H}$*

$$\mathbb{E}\left[\widehat{f}_{h_1}(\eta)\,\widehat{f}_{h_2}(\eta)\right] = \text{``}\mathbb{E}\left[(h_1|\eta)_{\mathbf{H}}\,(h_2|\eta)_{\mathbf{H}}\right]\text{''} = \frac{1}{\beta}\,(h_1|h_2)_{\mathbf{H}}. \tag{A.14}$$

2 *If $\mathbb{O} \colon \mathbf{H} \to \mathbf{H}$ is a bounded linear operator on $\mathbf{H}$, then there exists a measurable extension $\widehat{\mathbb{O}}$. Then $\widehat{\mathbb{O}}\eta$ is an $\mathbf{X}$-valued Gaussian random variable with covariance $\beta^{-1}\mathbb{C}_{\mathbb{O}}$ defined by*

$$\frac{1}{\beta}\,(\mathbb{C}_{\mathbb{O}}x|x)_{\mathbf{X}} := \frac{1}{\beta}\|\mathbb{O}^*\mathbb{C}x\|^2_{\mathbf{H}}, \qquad x \in \mathbf{X}, \tag{A.15}$$

where $\mathbb{O}^*$ is the adjoint of $\mathbb{O}$ in $\mathbf{H}$.
If in addition $\mathbb{O}$ has finite rank, then $\widehat{\mathbb{O}}\eta$ is an $\mathbf{H}$-valued Gaussian random variable with covariance $\beta^{-1}\mathbb{O}\mathbb{O}^*$ on $\mathbf{H}$. In particular, $\widehat{\mathbb{O}}\eta$ has finite $\mathbf{H}$-variance given by

$$\mathbb{E}\big\|\widehat{\mathbb{O}}\eta\big\|^2_{\mathbf{H}} = \frac{1}{\beta}\,\text{tr}_{\mathbf{H}}(\mathbb{O}\mathbb{O}^*). \tag{A.16}$$

3 *Let $\mathbb{P}$ be an orthogonal projection on $\mathbf{H}$ and $\mathbb{Q} := I - \mathbb{P}$ the complementary projection. Let $X \sim \widehat{\mathbb{P}}_{\#}\gamma_\beta$ and $Y \sim \widehat{\mathbb{Q}}_{\#}\gamma_\beta$ be independent random variables. Then $X + Y$ is distributed according to γ_β.*

In addition, in order to recognize a probability measure $\zeta \in \mathcal{P}(\mathbf{X})$ as $\widehat{\mathbb{Q}}_{\#}\gamma_\beta$ it is sufficient that there exists a subspace $\widetilde{\mathbf{V}} \subset \mathbf{V}$, dense in $\mathbf{H}$ in the $\mathbf{H}$-norm, such that for all $h \in \widetilde{\mathbf{V}}$

$$\int_{\mathbf{X}} e^{i(h|\xi)_{\mathbf{H}}}\zeta(\mathrm{d}\xi) = \exp\left(-\frac{1}{2\beta}\|\mathbb{Q}h\|^2_{\mathbf{H}}\right). \tag{A.17}$$

Remark A.8. Part 2 above implies in particular that if $\mathbb{O}$ is a unitary operator on $\mathbf{H}$, then $\widehat{\mathbb{O}}\eta$ has the same covariance as η. $\qquad\square$

Proof. Part 1 is [Bog98, Th. 2.10.11] in combination with (A.13). In part 2, the general case is [Bog98, Th. 3.7.6]. To calculate the covariance, first note that since measurable linear extensions are characterized by their values on $\mathbf{H}$, the two linear extensions $\widehat{f}_1$ and $\widehat{f}_2$ of

$$f_1(\xi) := \left(h\big|\widehat{\mathbb{O}}\xi\right)_{\mathbf{H}} \qquad \text{and} \qquad f_2(\xi) := (\mathbb{O}^*h|\xi)_{\mathbf{H}}$$

are γ_β-a.e. equal. It follows that

$$\mathbb{E}|f_1(\eta)|^2 = \mathbb{E}|f_2(\eta)|^2 \stackrel{(\text{A.14})}{=} \frac{1}{\beta}\|\mathbb{O}^*h\|^2_{\mathbf{H}}.$$

The characterization (A.15) follows by remarking that for $x \in \mathbf{X}$, $(x|\xi)_{\mathbf{X}} = (\mathbb{C}x|\xi)_{\mathbf{H}}$, so that f_1 equals $(x|\xi)_{\mathbf{X}}$ whenever $h = \mathbb{C}x$.

The case of finite rank follows from part 1, by choosing orthonormal bases $\{e_k\}_{k=1}^{\infty}$ and $\{f_k\}_{k=1}^{\infty}$ of $\mathbf{H}$ such that that $\text{Range}(\mathbb{O}) \subset \text{span}\big(\{e_k\}_{k=1}^d\big)$ and $\text{Ker}(\mathbb{O})^{\perp} \subset \text{span}\big(\{f_k\}_{k=1}^d\big)$, and expanding the squared norm (see also [Bog98, Ex. 3.7.14]).

In part 3 the distribution of $X + Y$ is given by [Bog98, Lemma 3.11.25]. The characterization $\zeta = \widehat{\mathbb{Q}}_\# \gamma_\beta$ can be obtained as follows. By [Bog98, Cor. A.3.13], the identity (A.17) for all elements of $\widetilde{\mathbf{V}}$ uniquely identifies ζ as a centered Gaussian measure on $\mathbf{X}$. Writing for $h = \mathbb{C}x$ the exponent as

$$(h|\xi)_{\mathbf{H}} = (\mathbb{C}x|\xi)_{\mathbf{H}} = (x|\xi)_{\mathbf{X}},$$

we observe that ζ has covariance operator

$$\frac{1}{\beta}\left(\mathbb{C}_\zeta x|x\right)_{\mathbf{X}} := \frac{1}{\beta}\|\mathbb{Q}h\|_{\mathbf{H}}^2 = \frac{1}{\beta}\|\mathbb{Q}\mathbb{C}x\|_{\mathbf{H}}^2.$$

Using part 2 we recognize this Gaussian measure as the law of $\widehat{\mathbb{Q}}\eta$ where $\eta \sim \gamma_\beta$. □

An important consequence of the above extension results is that the extended group $(\widehat{S}_t)_{t\in\mathbb{R}}$ on $\mathbf{X}$ preserves the measure γ_β.

Lemma A.9 (Invariance of the Gaussian measure)**.** *The extension $\widehat{S}_t : \mathbf{X} \to \mathbf{X}$ of $\mathrm{e}^{t\mathbb{J}\mathcal{B}} : \mathbf{H} \to \mathbf{H}$ (see Assumption 2.3) leaves the Gaussian measure γ_β invariant.*

Proof. We apply Part 2 of Lemma A.7 with the unitary operator $\mathbb{O} = \mathrm{e}^{t\mathbb{J}\mathcal{B}}$ and its extension $\widehat{\mathbb{O}} = \widehat{S}_t$. Hence, starting from $\eta \sim \gamma_\beta$ we see that the random variable $\widehat{\mathbb{O}}\eta = \widehat{S}_t\eta$ is a centered Gaussian in $\mathbf{X}$ with covariance $\beta^{-1}\mathbb{C}_t$ characterized by

$$\frac{1}{\beta}\left(\mathbb{C}_t x|x\right)_{\mathbf{X}} = \frac{1}{\beta}\|\mathrm{e}^{-t\mathbb{J}\mathcal{B}}\mathbb{C}x\|_{\mathbf{H}}^2 = \frac{1}{\beta}\|\mathbb{C}x\|_{\mathbf{H}}^2.$$

In particular, this means $\beta^{-1}\mathbb{C}_t = \beta^{-1}\mathbb{C}$; hence $\widehat{S}_t\eta$ has the same distribution γ_β. □

Remark A.10 (Invariance of γ_β via inner products)**.** The invariance of γ_β can also be shown by working in $\mathbf{X}$ rather than in $\mathbf{X}^*$ as in the above proof. We do not have the commutation property $\mathbb{C}\widehat{S}_t = \widehat{S}_t\mathbb{C}$ but we have the invariance property

$$\widehat{S}_t^*\mathbb{C}\widehat{S}_t = \mathbb{C}, \tag{A.18}$$

which implies $\left(\mathbb{C}\widehat{S}_t\eta \big| \widehat{S}_t\eta\right) = \left(\widehat{S}_t^*\mathbb{C}\widehat{S}_t\eta \big| \eta\right) = (\mathbb{C}\eta|\eta)$.

To see the validity of (A.18), we need to calculate the Hilbert-space adjoint $\widehat{S}_t^*$ of $\widehat{S}_t$. For an operator $A: \mathbf{U} \to \mathbf{V}$ denote the Banach-space adjoint by $A^\top : \mathbf{V}^* \to \mathbf{U}^*$, which is defined via $\langle A^\top\nu, u\rangle_{\mathbf{U}} = \langle \nu, Au\rangle_{\mathbf{V}}$. Using the dual space $\mathbf{X}^*$ satisfying $\mathbf{X}^* \subset \mathbf{H} \subset \mathbf{X}$ and the duality isomorphism $\mathbb{C}: \mathbf{X} \to \mathbf{X}^*$ we have the relation $\widehat{S}_t^* = \mathbb{C}\,\widehat{S}_t^\top\,\mathbb{C}^{-1}$, where $\widehat{S}_t^\top : \mathbf{X}^* \to \mathbf{X}^*$. As $\widehat{S}_t$ is the extension of $\mathrm{e}^{t\mathbb{J}\mathcal{B}}$ from $\mathbf{H}$ to $\mathbf{X}$, the Banach-space adjoint is simply the restriction $\mathrm{e}^{t\mathbb{J}\mathcal{B}}|_{\mathbf{X}^*}$. Together with $(\mathrm{e}^{t\mathbb{J}\mathcal{B}})^\top = \mathrm{e}^{-t\mathbb{J}\mathcal{B}}$ in $\mathbf{H}$, we found the representation $\widehat{S}_t^* = \mathbb{C}\,\mathrm{e}^{-t\mathbb{J}\mathcal{B}}|_{\mathbf{X}^*}\,\mathbb{C}^{-1}$, and the desired identity (A.18) follows. □

B   Delayed proofs

B.1   Section 2: Microscopic setup

Proof of Lemma 2.4. Part 1 follows from the assumption that $\mathrm{e}^{t\mathbb{J}\mathcal{B}}$ is a strongly continuous group on $\mathbf{H}$ and from the fact that on $\mathbf{H}$ the operator $\widehat{\mathbb{P}}$ reduces to the bounded linear operator $\mathbb{P}$.

For part 2, first note that $Y(\eta_0)$ is stationary since γ_β is invariant under $\widehat{S}_t$. We next show that both processes are measurable with respect to the product σ-algebra $\mathcal{B}(\mathbb{R}) \times \mathcal{B}(\mathbf{X})_{\gamma_\beta}$. The following decomposition shows that $Y_t(\eta_0)$ is a measurable function of (t, η_0), with each arrow a measurable map between the two σ-algebras:

$$
\begin{array}{ccccc}
(t, \eta_0) & \mapsto & \widehat{S}_t \eta_0 & \mapsto & \widehat{\mathbb{P}} \widehat{S}_t \eta_0 \\
\mathcal{B}(\mathbb{R}) \times \mathcal{B}(\mathbf{X})_{\gamma_\beta} & & \mathcal{B}(\mathbf{X})_{\gamma_\beta} & & \mathcal{B}(\mathbf{W})
\end{array}
$$

The first arrow is measurable by the continuity given by Assumption 2.3, and the second by the measurability of $\widehat{\mathbb{P}}$ as a map from $(\mathbf{X}, \mathcal{B}(\mathbf{X})_{\gamma_\beta})$ to $(\mathbf{W}, \mathcal{B}(\mathbf{W}))$ (Lemma A.7).

To show that $Y = Y(\widehat{\mathbb{Q}}\eta_0)$ similarly is measurable we decompose it as

$$
Y_t(\widehat{\mathbb{Q}}\eta_0) = \widehat{\mathbb{P}}\widehat{S}_t\widehat{\mathbb{Q}}\eta_0 = \widehat{\mathbb{P}}\widehat{S}_t\eta_0 - \widehat{\mathbb{P}}\widehat{S}_t\widehat{\mathbb{P}}\eta_0.
$$

We just showed that the first term is measurable from $\mathcal{B}(\mathbb{R}) \times \mathcal{B}(\mathbf{X})_{\gamma_\beta}$ to $\mathcal{B}(\mathbf{W})$. The measurability of the second follows from remarking that $\widehat{\mathbb{P}}\widehat{S}_t\widehat{\mathbb{P}}\eta_0 = \mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\widehat{\mathbb{P}}\eta_0$, since the range of $\widehat{\mathbb{P}}$ is included in $\mathbf{W} \subset \mathbf{H}$. With this we then have

$$
\begin{array}{ccccccc}
(t, \eta_0) & \mapsto & (t, \widehat{\mathbb{P}}\eta_0) & \mapsto & \mathrm{e}^{t\mathbb{J}_\mathcal{B}}\widehat{\mathbb{P}}\eta_0 & \mapsto & \mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\widehat{\mathbb{P}}\eta_0. \\
\mathcal{B}(\mathbb{R}) \times \mathcal{B}(\mathbf{X})_{\gamma_\beta} & & \mathcal{B}(\mathbb{R}) \times \mathcal{B}(\mathbf{W}) & & \mathcal{B}(\mathbf{H}) & & \mathcal{B}(\mathbf{W})
\end{array}
$$

Here the first arrow is measurable again by the construction of $\widehat{\mathbb{P}}$ (Lemma A.7), the second by the strong continuity of $\mathrm{e}^{t\mathbb{J}_\mathcal{B}}$ on $\mathbf{H}$, and the third by the continuity of $\mathbb{P}$ on $\mathbf{H}$.

Finally, to show that $Y(\eta_0)$ and $Y(\widehat{\mathbb{Q}}\eta_0)$ have sample paths in L^2_{loc}, we calculate for $t \in \mathbb{R}$ that

$$
\mathbb{E}_{\eta_0 \sim \gamma_\beta} \|Y_t(\eta_0)\|_{\mathbf{H}}^2 = \mathbb{E}_{\eta_0} \|\widehat{\mathbb{P}}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\eta_0\|_{\mathbf{H}}^2 \overset{\text{(A.16)}}{=} \frac{1}{\beta} \mathrm{tr}_{\mathbf{H}}\big(\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\big(\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\big)^*\big) = \frac{1}{\beta} \mathrm{tr}_{\mathbf{H}} \mathbb{P} = \frac{\dim \mathbf{W}}{\beta}.
$$

The measurability allows us to apply Fubini and calculate for $-\infty < a < b < \infty$

$$
\mathbb{E}_{\eta_0 \sim \gamma_\beta} \int_a^b \|Y_t(\eta_0)\|_{\mathbf{H}}^2 \, \mathrm{d}t = \int_a^b \mathbb{E}_{\eta_0} \|Y_t(\eta_0)\|_{\mathbf{H}}^2 = (b-a) \frac{\dim \mathbf{W}}{\beta}.
$$

This shows that almost surely $Y(\eta_0)$ is an element of $L^2_{\mathrm{loc}}(\mathbb{R}; \mathbf{W})$.

To show the analogous result for $Y(\widehat{\mathbb{Q}}\eta_0)$, we similarly obtain

$$
\mathbb{E}_{\eta_0 \sim \gamma_\beta} \int_a^b \big\|Y_t(\widehat{\mathbb{Q}}\eta_0)\big\|_{\mathbf{H}}^2 \mathrm{d}t = \frac{1}{\beta}(b-a) \, \mathrm{tr}_{\mathbf{H}}(\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\mathbb{Q}^2\mathrm{e}^{-t\mathbb{J}_\mathcal{B}}\mathbb{P}).
$$

To estimate the trace we choose an orthonormal basis $(e_k)_{k=1}^d$ of $\mathbf{W}$ of size $d = \dim \mathbf{W}$, and calculate

$$
\mathrm{tr}_{\mathbf{H}}(\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\mathbb{Q}^2\mathrm{e}^{-t\mathbb{J}_\mathcal{B}}\mathbb{P}) = \sum_{k=1}^d \big|\big(\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\mathbb{Q}^2\mathrm{e}^{-t\mathbb{J}_\mathcal{B}}\mathbb{P}e_k\big|e_k\big)_{\mathbf{H}}\big| \le \sum_{k=1}^d \big\|\mathbb{P}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}\mathbb{Q}^2\mathrm{e}^{-t\mathbb{J}_\mathcal{B}}\mathbb{P}e_k\big\|_{\mathbf{H}} \|e_k\|_{\mathbf{H}}
$$

$$
\le \sum_{k=1}^d \|e_k\|_{\mathbf{H}}^2 = d.
$$

Again it follows that $Y(\widehat{\mathbb{Q}}\eta_0)$ is almost surely in $L^2_{\mathrm{loc}}(\mathbb{R}; \mathbf{W})$. $\qquad \square$

B.2 Microcanonical measures and Section 3.2

In the physics literature it is common to define 'microcanonical ensembles', which effectively are measures on the set of possible states. A useful tool for this is the following delta-function-like object.

Let $f\colon \mathbb{R}^n \to \mathbb{R}$ be continuous. For $a \in \mathbb{R}$ the non-negative measure $\mu \in \mathcal{M}(\mathbb{R}^n)$

$$\mu(\mathrm{d}x) := \boldsymbol{\delta}[f(x) - a](\mathrm{d}x)$$

is defined by the property

$$\mu(A) = \lim_{h \downarrow 0} \frac{1}{h} \int_A \mathbb{1}\big\{a \le f(x) < a + h\big\}\,\mathrm{d}x \in [0, \infty] \qquad \text{for all } A \subset \mathbb{R}^n,$$

whenever this definition makes sense.

One way of making this definition rigorous is by integration against test functions:

Definition B.1 ([LRS10, (1.25)])**.** *The measure* $\boldsymbol{\delta}[f(x) - a]$ *on* $\mathbb{R}^n$ *is defined by the property that for all* $F \in C_c(\mathbb{R}^n)$ *and* $G \in C(\mathbb{R})$,

$$\int_{\mathbb{R}} G(a) \int_{\mathbb{R}^n} F(x)\boldsymbol{\delta}[f(x) - a](\mathrm{d}x)\,\mathrm{d}a = \int_{\mathbb{R}^n} G(f(x))F(x)\,\mathrm{d}x. \tag{B.1}$$

The right-hand side above is finite for all $F \in C_c(\mathbb{R}^n)$ and $G \in C(\mathbb{R})$, since $\operatorname{supp} F$ is compact and $G \circ f$ therefore is bounded on this support. This implies that $\boldsymbol{\delta}[f(x) - a](\mathrm{d}x)\,\mathrm{d}a$ can be considered a locally finite non-negative measure on $(x, a) \in \mathbb{R}^n \times \mathbb{R}$. For almost all $a \in \mathbb{R}$ the disintegration $\boldsymbol{\delta}[f(x) - a](\mathrm{d}x)$ is then a locally finite non-negative measure on $\mathbb{R}^n$.

By the co-area formula (see, e.g., [LRS10, Sec. 3.2.1]) this measure can also be expressed with help of the $(n-1)$-dimensional Hausdorff measure $\mathcal{H}^{n-1}$ on the set $S_a := \{x \in \mathbb{R}^n : f(x) = a\}$ as

$$\boldsymbol{\delta}[f(x) - a](\mathrm{d}x) = \frac{1}{|\nabla f(x)|}\mathcal{H}^{n-1}\big|_{S_a}(\mathrm{d}x). \tag{B.2}$$

In Section 4.6 we made use of the following property, which allows us to write a microcanonical measure on a product space as the product of two such measures on the individual spaces. The crucial element is the fact that the 'energy' function has the additive structure $(x, y) \mapsto f(x) + g(y)$.

Lemma B.2. *Let* X *and* Y *be finite-dimensional spaces, and let* $f\colon X \to \mathbb{R}$ *and* $g\colon Y \to \mathbb{R}$ *be continuous. Set*

$$T\colon X \times Y \to X \times Y \times \mathbb{R}, \qquad (x, y) \mapsto (x, y, e := g(y)).$$

For Lebesgue almost all $a \in \mathbb{R}$ *we then have*

$$\Big(T_\# \boldsymbol{\delta}[f(x) + g(y) - a]\Big)(\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}e) = \boldsymbol{\delta}[f(x) - a + e](\mathrm{d}x)\boldsymbol{\delta}[g(y) - e](\mathrm{d}y)\,\mathrm{d}e.$$

Proof. By the definition of the push-forward $T_\# \boldsymbol{\delta}$ we need to show that for all $\varphi \in C_c(X \times Y \times \mathbb{R})$ we have for almost all $a \in \mathbb{R}$

$$\int_{X \times Y} \varphi(x, y, g(y))\boldsymbol{\delta}[f(x) + g(y) - a](\mathrm{d}x\,\mathrm{d}y)$$

$$= \int_{X \times Y \times \mathbb{R}} \varphi(x, y, e)\boldsymbol{\delta}[f(x) - a + e](\mathrm{d}x)\boldsymbol{\delta}[g(y) - e](\mathrm{d}y)\,\mathrm{d}e.$$

Since in the right-hand integral we can replace $\varphi(x, y, e)$ by $\varphi(x, y, g(y))$, it is sufficient to show that for almost all $a \in \mathbb{R}$ and for all measurable $A \subset X$, $B \subset Y$

$$\boldsymbol{\delta}[f(x) + g(y) - a](A \times B) = \int_{\mathbb{R}} \boldsymbol{\delta}[f(x) + e - a](A)\boldsymbol{\delta}[g(y) - e](B) \, \mathrm{d}e. \tag{B.3}$$

To prove this identity we take $G \in C(\mathbb{R})$ and $F \in C_c(X \times Y)$ and rewrite the left-hand side of (B.3) using (B.1),

$$\int_{\mathbb{R}} G(a) \int_{X \times Y} F(x, y)\boldsymbol{\delta}[f(x) + g(y) - a](\mathrm{d}x \, \mathrm{d}y) \, \mathrm{d}a$$

$$\overset{\text{(B.1)}}{=} \int_{X \times Y} G(\underbrace{f(x) + g(y)}_{=:g_x(y)})F(x, y) \, \mathrm{d}y \, \mathrm{d}x$$

$$\overset{\text{(B.1)}}{=} \int_X \int_{\mathbb{R}} G(\tilde{e}) \int_Y F(x, y)\boldsymbol{\delta}[g_x(y) - \tilde{e}](\mathrm{d}y) \, \mathrm{d}\tilde{e} \, \mathrm{d}x$$

$$\overset{\tilde{e}=e+f(x)}{=} \int_X \int_{\mathbb{R}} G(e + f(x)) \underbrace{\int_Y F(x, y)\boldsymbol{\delta}[g(y) - e](\mathrm{d}y)}_{=:\tilde{F}_e(x)} \, \mathrm{d}e \, \mathrm{d}x$$

$$= \int_{\mathbb{R}} \int_X G(e + f(x))\tilde{F}_e(x) \, \mathrm{d}x \, \mathrm{d}e$$

$$\overset{\text{(B.1)}}{=} \int_{\mathbb{R}} \int_{\mathbb{R}} G(a) \int_X \tilde{F}_e(x)\boldsymbol{\delta}[e + f(x) - a](\mathrm{d}x) \, \mathrm{d}a \, \mathrm{d}e$$

$$= \int_{\mathbb{R}} G(a) \int_{X \times Y \times \mathbb{R}} F(x, y)\boldsymbol{\delta}[f(x) + e - a](\mathrm{d}x)\boldsymbol{\delta}[g(y) - e](\mathrm{d}y) \, \mathrm{d}e \, \mathrm{d}a.$$

It follows that for almost all $a \in \mathbb{R}$ the identity (B.3) holds. $\qquad\square$

For the next two lemmas we adopt the setting of Section 4.6. Since the aim is to illustrate the interpretation of the formula $\mathcal{S} = \beta e$, we simplify by assuming that $\mathbf{W} \subset \mathbf{V}$. We then can choose an orthonormal basis $\{e_k\}_{k \geq 1}$ of both $\mathbf{W}$ and $\mathbf{H}$ consisting of elements of $\mathbf{V}$ (see [Bog98, Cor. 2.10.10]). The benefit of choosing the basis in $\mathbf{V}$ is that the basis vectors can be interpreted as elements of $\mathbf{X}^*$, allowing us to apply existing density results.

Letting $\mathbf{W}$ be $\mathrm{span}\{e_k\}_{k=1}^d$, we then construct an increasing sequence of n-dimensional subspaces Ξ_n of the complement $\mathbf{W}^\perp$,

$$\Xi_n := \mathrm{span}\{e_k\}_{k=d+1}^{d+n}.$$

We then define the microcanonical probability measure of radius $\sqrt{R}$:

$$\nu_{n,R}(\mathrm{d}\xi) := \frac{1}{Z_{n,R}} \boldsymbol{\delta}\left[\frac{1}{2}\|\xi\|_\mathbf{H}^2 - \frac{nR}{2}\right]\Big|_{\Xi_n} (\mathrm{d}\xi). \tag{B.4}$$

This measure is a normalized version of the measure $\zeta_{n,\beta,e}$ in (4.26) for the choice $R = \beta^{-1} + 2e/n$.

The first result is the 'equivalence of ensembles', also known as 'Boltzmann's equivalence principle' or 'Poincaré's Lemma' (see [DiF87, Sec. 6] for a discussion of the history). This result states that if X_n is distributed according to $\nu_{n,R}$, then the first k coordinates resemble a Gaussian random variable in the limit $n \to \infty$:

Lemma B.3 (Equivalence of ensembles; e.g. [DiF87]). *Let $\{e_k\}_{k=1}^\infty$ be an orthonormal basis of $\mathbf{H}$ such that $\{e_k\}_{k=1}^n$ is a basis of Ξ_n. Let $R_n \to R > 0$ and let X_n have law ν_{n,R_n}. Fix $k \geq 1$. As $n \to \infty$, the first k coordinates*

$$\big((X_n|e_1)_\mathbf{H}, \ldots, (X_n|e_k)_\mathbf{H}\big)$$

converge in distribution to a centered Gaussian random variable in $\mathbb{R}^k$ with covariance $R\, I_k$.

The second result is a variance bound for $\nu_{n,R}$, which probably is standard, but for which we could not find a convenient reference. Note that it does not follow from equivalence-of-ensemble results such as Lemma B.3 since it concerns the variance of the full random variable, not a finite-dimensional marginal.

Lemma B.4 (Variance bound for microcanonical measures). *Let Y_n have distribution $\nu_{n,R}$, and let $\mathbb{T}$ be a symmetric non-negative trace-class operator on $\mathbf{H}$. Then there exists $C > 0$, independent of R and $\mathbb{T}$, such that*

$$\mathbb{E}\|\mathbb{T}^{1/2}Y_n\|_\mathbf{H}^2 \leq CR\operatorname{tr}_\mathbf{H}\mathbb{T} \qquad \text{for all } n \geq 1.$$

In particular,

$$\mathbb{E}\|Y_n\|_\mathbf{X}^2 = \mathbb{E}\|\mathbb{C}^{1/2}Y_n\|_\mathbf{H}^2 \leq CR\operatorname{tr}_\mathbf{H}\mathbb{C} \qquad \text{for all } n \geq 1.$$

Proof. Let X_n be a standard normal random variable in Ξ_n; then $Y_n \stackrel{\text{dist}}{=} \sqrt{R}\, X_n/\|X_n\|_\mathbf{H}$, and therefore

$$\mathbb{E}\|\mathbb{T}^{1/2}Y_n\|_\mathbf{H}^2 = R\, \mathbb{E}\frac{\|\mathbb{T}^{1/2}X_n\|_\mathbf{H}^2}{\|X_n\|_\mathbf{H}^2}.$$

The random variable $\|X_n\|_\mathbf{H}^2$ is $\chi^2(n)$-distributed, and therefore $\|X_n\|_\mathbf{H}^2/n$ concentrates onto 1; it follows that there exists $r_n \to 0$ such that

$$\mathbb{E}\|\mathbb{T}^{1/2}Y_n\|_\mathbf{H}^2 \leq R(1+r_n)\mathbb{E}\|\mathbb{T}^{1/2}X_n\|_\mathbf{H}^2 \stackrel{\text{(A.5)}}{=} R(1+r_n)\operatorname{tr}_{\Xi_n}\mathbb{T},$$

where $\operatorname{tr}_{\Xi_n}\mathbb{T} = \operatorname{tr}_\mathbf{H}\mathcal{P}_n\mathbb{T}\mathcal{P}_n$ in terms of the orthogonal projection $\mathcal{P}_n$ in $\mathbf{H}$ onto Ξ_n. Since $\operatorname{tr}_{\Xi_n}\mathbb{T} \leq \operatorname{tr}_\mathbf{H}\mathbb{T}$, the result follows. $\square$

We conclude by giving the proofs of Lemmas 4.13 and 4.14.

Proof of Lemma 4.13. To prove part 1, remark that $\operatorname{supp}\zeta_{n,\beta,e}$ is an n-dimensional sphere of radius $r = \sqrt{2e + n/\beta}$; using the co-area formula (B.2) we find

$$\mathsf{Z}_{\beta,n,e} := \int_{\Xi_n} \boldsymbol{\delta}\left[\frac{1}{2}\|\xi\|_\mathbf{H}^2 - \frac{n}{2\beta} - e\right]\mathrm{d}\xi = r^{-1}\underbrace{n\omega_n r^{n-1}}_{\text{area of sphere of radius } r},$$

so that

$$\log \mathsf{Z}_{\beta,n,e} = \log n\omega_n + \frac{n-2}{2}\log\left(\frac{n}{\beta} + 2e\right)$$

$$= \underbrace{\log n\omega_n + \frac{n-2}{2}\log\frac{n}{\beta}}_{=:\, C(\beta,n)} + \frac{n-2}{2}\log\left(1 + \frac{2\beta e}{n}\right),$$

and the convergence (4.27) follows from a Taylor development of the final term.

To prove part 2, first note that the sequence $Z_{\beta,n,e}^{-1}\zeta_{\beta,n,e}$ of probability measures is not tight on $\mathbf{H}$ (in fact its support tends to infinity in the $\mathbf{H}$-norm). However, applying the variance bound of Lemma B.4 we observe that

$$\frac{1}{Z_{\beta,n,e}}\int_{\Xi_n}\|\xi\|_{\mathbf{X}}^2\zeta_{\beta,n,e}(\mathrm{d}\xi)=\mathbb{E}_{\nu_{n,R_n}}\|\mathbb{C}^{1/2}\xi\|_{\mathbf{H}}^2\leq C\frac{1}{\beta}\operatorname{tr}_{\mathbf{H}}\mathbb{C},$$

where we set $R_n:=\beta^{-1}+2e/n\to\beta^{-1}$. Therefore the sequence is tight when considered as probability measures on $\mathbf{X}$, and along a subsequence the sequence converges narrowly to a probability measure ζ_β on $\mathbf{X}$ (e.g. [Bog18, Th. 2.3.4]).

To characterize the limit, note that for any $h\in\Xi_k$ the equivalence-of-ensemble result of Lemma B.3 implies that

$$\int_{\Xi_n}\mathrm{e}^{i(h|\xi)_{\mathbf{H}}}\zeta_{\beta,n,e}(\mathrm{d}\xi)\overset{n\to\infty}{\longrightarrow}\exp\left(-\frac{1}{2\beta}\|h\|_{\mathbf{H}}^2\right).$$

Taking elements h of the form

$$h=h_k+h^\perp\in\left(\bigcup_{k\geq1}\Xi_k\right)\oplus(\Xi^{\mathbf{H}})^\perp,\tag{B.5}$$

we note that $h_k=\mathcal{Q}h$, and since $h^\perp$ vanishes on each Ξ_n we find

$$\int_{\Xi_n}\mathrm{e}^{i(h|\xi)_{\mathbf{H}}}\zeta_{\beta,n,e}(\mathrm{d}\xi)=\int_{\Xi_n}\mathrm{e}^{i(h_k|\xi)_{\mathbf{H}}}\zeta_{\beta,n,e}(\mathrm{d}\xi)\overset{n\to\infty}{\longrightarrow}\exp\left(-\frac{1}{2\beta}\|\mathcal{Q}h\|_{\mathbf{H}}^2\right).$$

Since the space in (B.5) is a subspace of $\mathbf{V}$ and is dense in $\mathbf{H}$, by part 3 of Lemma A.7 we recognize the limit ζ_β as the push-forward measure $\widehat{\mathcal{Q}}_\#\gamma_\beta$. This also implies that the whole sequence converges. $\square$

Proof of Lemma 4.14. The assertion of Lemma 4.14 follows from that of Lemma 4.15 by integration: for any $\varphi\in\mathrm{C}_{\mathrm{b}}(\mathbf{Z}\times\mathbf{X})$ we have

$$\int_{\mathbf{Z}\times\mathbf{X}}\varphi(z,\eta)\,\mu_{\beta,n}(\mathrm{d}z\,\mathrm{d}\eta)\overset{(4.29)}{=}\int_{\mathbf{Z}\times\mathbf{W}\times\Xi^{\mathbf{X}}\times\mathbb{R}}\varphi(z,w+\xi)\,\mu_{\beta,n,e}(\mathrm{d}z\,\mathrm{d}w\,\mathrm{d}\xi\,\mathrm{d}e)$$

$$\overset{n\to\infty}{\longrightarrow}\frac{1}{Z_{\beta,\mathcal{E}_0}}\int_{\mathbf{Z}\times\mathbf{W}\times\Xi^{\mathbf{X}}\times\mathbb{R}}\varphi(z,w+\xi)\,\mathrm{e}^{\beta e}\,\boldsymbol{\delta}\big[\mathcal{H}_{zw}(z,w)-\mathcal{E}_0+e\big](\mathrm{d}z\,\mathrm{d}w)\,(\widehat{\mathbb{Q}}_\#\gamma_\beta)(\mathrm{d}\xi)\,\mathrm{d}e$$

$$\overset{(B.1)}{=}\frac{1}{Z_{\beta,\mathcal{E}_0}}\int_{\mathbf{Z}\times\mathbf{W}\times\Xi^{\mathbf{X}}}\varphi(z,w+\xi)\,\mathrm{e}^{-\beta\mathcal{H}_{zw}(z,w)+\beta\mathcal{E}_0}\,(\widehat{\mathbb{Q}}_\#\gamma_\beta)(\mathrm{d}\xi)\,\mathrm{d}z\,\mathrm{d}w$$

$$=\frac{1}{\widetilde{Z}_\beta}\int_{\mathbf{Z}\times\mathbf{W}\times\Xi^{\mathbf{X}}}\varphi(z,w+\xi)\,\mathrm{e}^{-\beta\mathcal{H}_{zw}(z,w)}(\widehat{\mathbb{Q}}_\#\gamma_\beta)(\mathrm{d}\xi)\,\mathrm{d}z\,\mathrm{d}w$$

$$\overset{(4.13)}{=}\int_{\mathbf{Z}\times\mathbf{X}}\varphi(z,\eta)\mu_\beta(\mathrm{d}z\,\mathrm{d}\eta).\qquad\square$$

C Dilations

The notion of dilations and compressions was introduced in Section 3.1. We now recall the existence of dilations.

Theorem C.1 ([SzF70, Thm. 8.1])**.** *Every strongly continuous contraction semigroup $(C_t)_{t \geq 0}$ on a Hilbert space $\mathbf{G}$ admits a dilation $(S_t)_{t \in \mathbb{R}}$ on a Hilbert space $\mathbf{H} \supset \mathbf{G}$.*

Moreover, there is a minimal dilation in the sense that

$$\operatorname{span}\Big(\bigcup\nolimits_{t \in \mathbb{R}} S_t \mathbf{G} \Big) \text{ is dense in } \mathbf{H}.$$

Any two minimal dilations $\big(\mathbf{H}, (S_t)_{t \in \mathbb{R}} \big)$ and $\big(\widetilde{\mathbf{H}}, (\widetilde{S}_t)_{t \in \mathbb{R}} \big)$ are isormorphic in the sense that there exists a Hilbert-space isomorphism $\Psi \colon \mathbf{H} \to \widetilde{\mathbf{H}}$ such that $\widetilde{S}_t = \Psi S_t \Psi^{-1}$ for all $t \in \mathbb{R}$.

It turns out that even for finite-dimensional $\mathbf{G}$ the dilation space $\mathbf{H}$ will be infinite-dimensional as soon as $(C_t)_{t \geq 0}$ is not unitary, i.e., as soon as C_t is a non-trivial contraction. Moreover, the subspace $\mathbf{G}$ cannot be contained in the domain of the generator of the unitary group $(S_t)_{t \in \mathbb{R}}$, as we now show.

Remark C.2 (Domains of the generators)**.** The unitary group has a densely-defined generator $\mathbb{J} \colon \operatorname{dom}(\mathbb{J}) \subset \mathbf{H} \to \mathbf{H}$ which is skew-adjoint, i.e., $\mathbb{J}^* = -\mathbb{J}$. For $h_0 \in \operatorname{dom}(\mathbb{J})$ the function $h(t) = S_t h_0 = \mathrm{e}^{t\mathbb{J}} h_0$ is differentiable and satisfies $\dot{h}(t) = \mathbb{J} h(t)$.

The contraction semigroup can be written as $C_t = \mathrm{e}^{-t\mathbb{D}}$ for a generator $\mathbb{D}$ satisfying $\mathbb{D} + \mathbb{D}^* \geq 0$. If C_t is not unitary, then $\mathbb{D}$ is not skew-adjoint and there exists a $g \in \mathbf{G}$ such that $\gamma := (g | \mathbb{D}g)_{\mathbf{G}} > 0$. We set $p(t) = \|\mathrm{e}^{-t\mathbb{D}} g\|^2$ and find $\lim_{t \to 0^+} \dot{p}(t) = -2\gamma$. Assuming $g \in \operatorname{dom}(\mathbb{J})$, the dilation property gives $\dot{p}(0) = \frac{\mathrm{d}}{\mathrm{d}t} \|\mathbb{P} \mathrm{e}^{t\mathbb{J}} g\|^2 \big|_{t=0} = 2 \, (\mathbb{P}g | \mathbb{P} \mathbb{J} g)_{\mathbf{H}} = 2 \, (g | \mathbb{J}g)_{\mathbf{H}} = 0$. This is a contradiction, and we conclude $g \notin \operatorname{dom}(\mathbb{J})$.

Hence, $\mathbb{J}$ is an unbounded operator, and $\mathbf{H}$ is infinite-dimensional. If $(g | \mathbb{D}g)_{\mathbf{G}} > 0$ for every $g \neq 0$, then we even have $\operatorname{dom}(\mathbb{J}) \cap \mathbf{G} = \{0\}$. □

In the context of this paper, it is advantageous to generalize the notion of dilation slightly.

Definition C.3 (Generalized dilation)**.** *A triple $\big(\mathbf{H}, \Phi, (S_t)_{t \in \mathbb{R}} \big)$ is called a* generalized dilation *of the contraction semigroup $\big(\mathbf{W}, (\widehat{C}_t)_{t \geq 0} \big)$ if $(S_t)_{t \in \mathbb{R}}$ is a strongly continuous unitary group on $\mathbf{H}$ and the linear map $\Phi \colon \mathbf{W} \to \mathbf{H}$ satisfies*

$$\Phi^* \Phi = \operatorname{id}_{\mathbf{W}} \quad \text{and} \quad \Phi^* S_t \Phi = \widehat{C}_t \in \operatorname{Lin}(\mathbf{W}; \mathbf{W}) \text{ for all } t \geq 0.$$

Note that from this definition we see that $\mathbb{P} = \Phi \Phi^* \colon \mathbf{H} \to \mathbf{H}$ is an orthogonal projection onto $\mathbf{G} = \Phi \mathbf{W} \subset \mathbf{H}$. In particular, setting $C_t = \Phi \widehat{C}_t \Phi^* |_{\mathbf{G}}$ the unitary group $\big(\mathbf{H}, (S_t)_{t \in \mathbb{R}} \big)$ is a dilation of $\big(\mathbf{G}, (C_t)_{t \geq 0} \big)$ in the sense of Definition 3.1. However, since $\Phi \colon \mathbf{W} \to \mathbf{G}$ is an isometry with inverse $\Phi^* |_{\mathbf{G}}$, the two contraction semigroups $(C_t)_{t \geq 0}$ and $(\widehat{C}_t)_{t \geq 0}$ are isomorphic. As a consequence, all minimal dilations are isomorphic to any minimal generalized dilation, which is defined via the minimality condition that $\bigcup_{t \in \mathbb{R}} \Phi \big(C_t \mathbf{W} \big)$ is dense in $\mathbf{H}$.

C.1 An explicit construction of a generalized dilation

Here we repeat the explicit construction of a generalized dilation from [LaS89, Thm. 2.1] or [KüS84, Sec. 1.2.3] and give the full proofs because of its importance of compressions and dilations for our analysis.

We now write the contraction semigroup $\big(\mathbf{W}, (C_t)_{t\geq 0}\big)$ in the form $C_t = \mathrm{e}^{-t\mathbb{D}}$. Moreover, we follow our assumptions in Section 2 and assume

$$\dim(\mathbf{W}) < \infty \quad \text{and} \quad \exists\, \delta > 0 :\ \|\mathrm{e}^{-t\mathbb{D}}\| \leq \mathrm{e}^{-\delta t} \text{ for all } t \geq 0. \tag{C.1}$$

To construct a generalized dilation we define

$$\overline{\mathbf{H}} := \mathrm{L}^2(\mathbb{R}; \mathbf{W}) \text{ with } \|f\|_{\overline{\mathbf{H}}}^2 = \int_{\mathbb{R}} \|f(y)\|_{\mathbf{W}}^2 \,\mathrm{d}y \quad \text{and} \quad \mathbf{G} := \big\{\, \Phi v \in \overline{\mathbf{H}} \,\big|\, v \in \mathbf{W} \,\big\},$$

where the bounded linear operator $\Phi \colon \mathbf{W} \to \mathbf{G} \subset \overline{\mathbf{H}}$ is given by

$$(\Phi w)(y) := \Sigma_{\mathbb{D}}\, \mathrm{e}^{y\mathbb{D}} w\, \mathbf{1}_{]-\infty,0]}(y), \quad \text{with } \Sigma_{\mathbb{D}} := (\mathbb{D}+\mathbb{D}^*)^{1/2}, \tag{C.2}$$

with adjoint operator $\Phi^* \colon \overline{\mathbf{H}} \to \mathbf{W}$, $\Phi^* f = \int_{-\infty}^0 \mathrm{e}^{y\mathbb{D}^*} \Sigma_{\mathbb{D}} f(s) \,\mathrm{d}y$.

In contrast to [LaS89, KüS84], we included the factor $\Sigma_{\mathbb{D}}$ into the mapping Φ to obtain a isometry in the given norm. For the convenience of the reader we provide the full proof that $\big(\overline{\mathbf{H}}, \Phi, (\mathbb{S}_t)_{t\in\mathbb{R}}\big)$ is a generalized dilation for $\big(\mathbf{W}, (\mathrm{e}^{-t\mathbb{D}})_{t\geq 0}\big)$.

Proposition C.4 (Explicit dilation)**.** *Assume that* $\big(\mathbf{W}, (\mathrm{e}^{-t\mathbb{D}})_{t\geq 0}\big)$ *satisfies* (C.1)*, define* $\overline{\mathbf{H}}$, $\mathbf{G}$*, and* $\Phi \colon \mathbf{W} \to \mathbf{G} \subset \mathbf{G}$ *as above, and set* $\mathbb{P} = \Phi\Phi^* \colon \overline{\mathbf{H}} \to \mathbf{G} \subset \overline{\mathbf{H}}$.

1. *We have* $\Phi^*\Phi = \mathbb{I}_{\mathbf{W}}$, $\quad \mathbb{P} = \mathbb{P}^2 = \mathbb{P}^*$, $\quad \mathrm{range}\,\mathbb{P} = \mathbf{G}$.
   In particular, $\Phi \colon \mathbf{W} \to \overline{\mathbf{H}}$ *is an isometry and* $\Phi \colon \mathbf{W} \to \mathbf{G}$ *is unitary with inverse* $\Phi^*|_{\mathbf{G}}$. *Moreover,* $\mathbb{P}$ *is the orthogonal projector from* $\overline{\mathbf{H}}$ *onto* $\mathbf{G}$.
2. *Defining the strongly continuous unitary shift group* $(\mathbb{S}_t)_{t\in\mathbb{R}}$ *on* $\overline{\mathbf{H}} = \mathrm{L}^2(\mathbb{R}; \mathbf{W})$ *via* $\mathbb{S}_t f = f(\cdot - t)$ *the semigroup* $\big(\mathbf{W}, (\mathrm{e}^{-t\mathbb{D}})_{t\geq 0}\big)$ *has the generalized dilation* $\big(\overline{\mathbf{H}}, \Phi, (\mathbb{S}_t)_{t\in\mathbb{R}}\big)$. *Moreover, for all* $t \in \mathbb{R}$ *and* $g \in \mathbf{G} = \Phi\mathbf{W}$ *we have the relation*

$$\mathbb{P}\,\mathbb{S}_t g = \mathbf{R}(t) g, \quad \text{where } \mathbf{R}(t) = \begin{cases} \Phi\, \mathrm{e}^{-t\mathbb{D}}\, \Phi^* & \text{for } t \geq 0, \\ \Phi\, \mathrm{e}^{t\,\mathbb{D}^*}\, \Phi^* & \text{for } t \leq 0. \end{cases} \tag{C.3}$$

Proof. Part 1. The property of an isometry is based on the standard relation

$$\int_{-\infty}^0 \big(\Sigma_{\mathbb{D}} \mathrm{e}^{y\mathbb{D}}\big)^* \Sigma_{\mathbb{D}} \mathrm{e}^{y\mathbb{D}} \,\mathrm{d}y = \int_{-\infty}^0 \mathrm{e}^{y\mathbb{D}^*} (\mathbb{D}^*+\mathbb{D})\, \mathrm{e}^{y\mathbb{D}} \,\mathrm{d}y = \int_{-\infty}^0 \frac{\mathrm{d}}{\mathrm{d}y}\big(\mathrm{e}^{y\mathbb{D}^*} \mathrm{e}^{y\mathbb{D}}\big) \,\mathrm{d}y = \mathbb{I}_{\mathbf{W}}. \tag{C.4}$$

To establish $\Phi^*\Phi = \mathbb{I}_{\mathbf{W}}$ we simply calculate, for $w_1, w_2 \in \mathbf{W}$,

$$(\Phi w_1|\Phi w_2)_{\mathbf{H}} = \int_{-\infty}^0 \big(\Sigma_{\mathbb{D}}\mathrm{e}^{y\mathbb{D}} w_1\big|\Sigma_{\mathbb{D}}\mathrm{e}^{y\mathbb{D}} w_2\big)_{\mathbf{W}} \,\mathrm{d}y = \int_{-\infty}^0 \big(\mathrm{e}^{y\mathbb{D}^*} \Sigma_{\mathbb{D}}^2 \mathrm{e}^{y\mathbb{D}} w_1\big|w_2\big)_{\mathbf{W}} \,\mathrm{d}y \overset{\text{(C.4)}}{=} (w_1|w_2)_{\mathbf{W}}.$$

With this and $\mathbb{P} = \Phi\Phi^*$ the identities $\mathbb{P}^2 = \mathbb{P}$ and $\mathbb{P} = \mathbb{P}^*$ follow immediately, i.e., $\mathbb{P}$ is an orthogonal projector. Moreover, $\mathbb{P}f = \Phi(\Phi^* f)$ implies $\mathrm{range}\,\mathbb{P} \subset \mathrm{range}\,\Phi = \mathbf{G}$, whereas $\mathbb{P}\Phi v = \Phi\Phi^*\Phi w = \Phi w$ shows $\mathrm{range}\,\mathbb{P} \supset \mathrm{range}\,\Phi = \mathbf{G}$.

Part 2. Now we consider $t \geq 0$ and $v \in \mathbf{W}$ and obtain

$$\Phi^*\big(\mathbb{S}_t \Phi w\big) = \int_{-\infty}^0 \mathrm{e}^{s\mathbb{D}^*} \Sigma_{\mathbb{D}} \big(\Phi w\big)(s{-}t) \,\mathrm{d}s = \int_{-\infty}^0 \mathrm{e}^{s\mathbb{D}^*} \Sigma_{\mathbb{D}}^2\, \mathrm{e}^{(s-t)\mathbb{D}} w\, \mathbf{1}_{]-\infty,0]}(s{-}t) \,\mathrm{d}s$$

$$= \int_{-\infty}^0 \mathrm{e}^{s\mathbb{D}^*} \Sigma_{\mathbb{D}}^2\, \mathrm{e}^{s\mathbb{D}} \,\mathrm{d}s\, \mathrm{e}^{-t\mathbb{D}} w \overset{\text{(C.4)}}{=} \mathrm{e}^{-t\mathbb{D}} w.$$

Hence, $\big(\overline{\mathbf{H}}, \Phi, (\mathbb{S}_t)_{t\in\mathbb{R}}\big)$ is a generalized dilation in the sense of Definition C.3.

For $t \leq 0$ we have $\mathbf{1}_{]-\infty,0]}(s-t) = 0$ for $s > t$ and obtain

$$\Phi^*\big(\mathbb{S}_t\Phi w\big) = \int_{-\infty}^{t} \mathrm{e}^{s\mathbb{D}^*}\Sigma_{\mathbb{D}}^2 \mathrm{e}^{(s-t)\mathbb{D}} w \, \mathrm{d}s = \int_{-\infty}^{0} \mathrm{e}^{t\mathbb{D}^*}\mathrm{e}^{r\mathbb{D}^*}\Sigma_{\mathbb{D}}^2 \, \mathrm{e}^{r\mathbb{D}} w \, \mathrm{d}s = \mathrm{e}^{t\mathbb{D}^*} w.$$

Applying the operator Φ to the two relations for $\Phi^*\big(\mathbb{S}_t\Phi w\big)$ (for $t \geq 0$ and $t \leq 0$, respectively) and replacing Φw by $g = \Phi w$ such that $w = \Phi^* g$, we find the final relation (C.3). $\qquad\square$

The major advantage of this explicit generalized dilation is that it introduces, in a very natural way, the time shift $\mathbb{S}_t$ on the Hilbert space $\overline{\mathbf{H}} = \mathrm{L}^2(\mathbb{R}; \mathbf{W})$ which will take over the place of the linear evolution $\mathrm{e}^{t\mathbb{J}_{\mathcal{B}}}$. The specification to the time shift is advantageous as the time shift is also the natural variable in the random processes $(Y_t)_{t\in\mathbb{R}}$.

Remark C.5 (Minimality)**.** The above construction of a generalized dilation also allows us to show that the dilation is minimal. For this we have to show that

$$\mathfrak{G} := \mathrm{span}\big\{\, \mathbb{S}_t g \,\big|\, t \in \mathbb{R}, \; g \in \mathbf{G} \,\big\} = \mathrm{span}\big\{\, \mathbb{S}_t(\Phi w) \,\big|\, t \in \mathbb{R}, \; w \in \mathbf{W} \,\big\}$$

is dense in $\overline{\mathbf{H}} = \mathrm{L}^2(\mathbb{R}; \mathbf{W})$. For $h \in\,]0, 1[$ and $w \in \mathbf{W}$, we define the functions

$$\Psi_{h,w} := \mathbb{S}_h\big(\Phi w\big) - \Phi w : \; y \mapsto \begin{cases} 0 & \text{for } y > h, \\ \Sigma_{\mathbb{D}}\mathrm{e}^{(y-h)\mathbb{D}}w & \text{for } y \in\,]0, h], \\ \Sigma_{\mathbb{D}}\mathrm{e}^{y\mathbb{D}}\big(\mathrm{e}^{-h\mathbb{D}} - \mathbb{I}\big)w & \text{for } y \leq 0. \end{cases}$$

Clearly, $\Psi_{h,w} \in \mathfrak{G}$. Using $\dim(\mathbf{W}) < \infty$ we have $\|\mathrm{e}^{-h\mathbb{D}} - \mathbb{I}\| \leq Ch$ for $h \in [0, 1]$ and obtain

$$\big\|\Psi_{h,w} - w\mathbf{1}_{[0,h[}\big\|_{\mathrm{L}^2(\mathbb{R};\mathbf{W})} \leq C_* h \|w\|_{\mathbf{W}},$$

with a constant C_* depending only on $\mathbb{D}$.

To show that $f \in \mathrm{L}^2(\mathbb{R}; \mathbf{W})$ can be approximated by linear combinations of $\mathbb{S}_t\Psi_{h,w}$, we fix $\varepsilon > 0$ and find a piecewise constant $\overline{f}_N \in \mathrm{L}^2(\mathbb{R}; \mathbf{W})$ such that

$$\big\|f - \overline{f}_N\big\|_{\mathrm{L}^2(\mathbb{R};\mathbf{W})} < \varepsilon/2 \quad \text{and} \quad \overline{f}_N = \sum_{j=-N^2}^{N^2} w_j^N \mathbf{1}_{[j/N,(j+1)/N[} \; \text{with } N \in \mathbb{N} \text{ and } w_j^N \in \mathbf{W}.$$

Here N can be made as large as desired, by refining the partition. We now approximate $\overline{f}$ by $\widehat{f}_N = \sum_{-N^2}^{N^2} \mathbb{S}_{j/N}\Psi_{1/N,w_j^N}$, which clearly lies in $\mathfrak{G}$, and obtain

$$\big\|\overline{f}_N - \widehat{f}_N\big\|_{\mathrm{L}^2(\mathbb{R};\mathbf{W})}^2 = \sum_{j=-N^2}^{N^2} \big\|w_j^N \mathbf{1}_{[j/N,(j+1)/N[} - \overline{\mathbb{S}}_{j/n}\Psi_{1/N,w_j^N}\big\|_{\mathrm{L}^2(\mathbb{R};\mathbf{W})}^2$$
$$\leq \sum_{j=-N^2}^{N^2} C_*^2(1/N)^2\|w_j^N\|_{\mathbf{W}}^2 \; = \; \frac{C_*}{N}\big\|\overline{f}_N\big\|_{\mathrm{L}^2(\mathbb{R};\mathbf{W})}^2 \; \leq \; \frac{C_*}{N}\big(\|f\|_{\mathrm{L}^2(\mathbb{R};\mathbf{W})}^2 + \tfrac{\varepsilon}{2}\big)^2.$$

Choosing $N \in \mathbb{N}$ sufficiently big, the last term is less than $\varepsilon^2/4$, and thus we conclude $\|f - \widehat{f}_N\|_{\mathrm{L}^2(\mathbb{R};\mathbf{W})} < \varepsilon$ as desired. Hence, $\mathfrak{G}$ is dense in $\overline{\mathbf{H}} = \mathrm{L}^2(\mathbb{R}; \mathbf{W})$. $\qquad\square$

C.2 Continuous extension of the group $(\mathrm{e}^{t\mathbb{J}_\mathcal{B}})_{t\in\mathbb{R}}$ from $\mathbf{H}$ to $\mathbf{X}$

In Assumption 2.3 we assumed that the unitary group $\big(\mathbf{H}, (\mathrm{e}^{t\mathbb{J}_\mathcal{B}})_{t\in\mathbb{R}}\big)$ describing the heat bath can be extended to a strongly continuous group on the larger space $\mathbf{X}$, on which we are able to realize the Gaussian measure γ_β for the finite-temperature heat bath. We will show in Proposition C.6 that this assumption is already a consequence of the dilation property from Assumption 1.2.

As a first step we construct the Gaussian measure $\overline{\gamma}_\beta$ on an extension $\overline{\mathbf{X}}$ of the special space $\overline{\mathbf{H}} = \mathrm{L}^2(\mathbb{R}; \mathbf{W})$. This leads to a classical white noise process, but now taking values in the finite-dimensional Hilbert space $\mathbf{W}$. While translations $\mathbb{S}_t$ can easily defined for the white noise process, we have to be more careful and construct a Hilbert space $\overline{\mathbf{X}}$ on which we can extend the unitary group $\big(\overline{\mathbf{H}}, (\mathbb{S}_t)_{t\in\mathbb{R}}\big)$ to a strongly continuous group $\big(\overline{\mathbf{X}}, (\mathbb{S}_t^{\mathbf{X}})_{t\in\mathbb{R}}\big)$, which will be no longer unitary. If $\mathbb{N}\colon \overline{\mathbf{H}} \to \overline{\mathbf{X}}$ is the embedding operator, then the extension property means

$$\forall\, t \in \mathbb{R} \ \ \forall\, h \in \overline{\mathbf{H}}\colon \quad \mathbb{S}_t^{\mathbf{X}}\mathbb{N}h = \mathbb{N}\mathbb{S}_t h. \tag{C.5}$$

As explained in Section 2.2 we further need that $\mathbb{C} = \mathbb{N}\mathbb{N}^*\colon \overline{\mathbf{X}} \to \overline{\mathbf{X}}$ is trace class.

We give an explicit construction following the ideas in [Rey06]. We define the self-adjoint operator $\mathbb{A}\colon \mathrm{Dom}(\mathbb{A}) \subset \overline{\mathbf{H}} \to \overline{\mathbf{H}}$ via

$$\mathrm{Dom}(\mathbb{A}) = \big\{\, u \in \mathrm{H}^2(\mathbb{R}; \mathbf{W}) \,\big|\, t \mapsto (1{+}t^2)u(t) \in \mathrm{L}^2(\mathbb{R}; \mathbf{W}) \,\big\},$$
$$(\mathbb{A}u)(t) = -\frac{1}{2}u''(t) + \frac{t^2}{2}\,u(t).$$

Here $\mathrm{H}^2(\mathbb{R}; \mathbf{W})$ is the Sobolev space of measurable L^2-functions $u\colon \mathbb{R} \to \mathbf{W}$ with two weak derivatives in L^2. This is a $\mathbf{W}$-valued version of the quantum harmonic oscillator, and hence is self-adjoint with the discrete spectrum $\big\{\, n{-}1/2 \,\big|\, n \in \mathbb{N} \,\big\} \subset [1/2, \infty)$, where all eigenvalues have multiplicity $\dim(\mathbf{W}) < \infty$. Consequently $\mathbb{A}$ is an invertible operator, and its inverse $\mathbb{A}^{-1}$ is a Hilbert-Schmidt operator. This implies that $\mathbb{A}$ satisfies the assumptions for the construction in Section A.2, i.e. we can define

$$\overline{\mathbf{V}} = \mathrm{Dom}(\mathbb{A}) = \mathrm{H}^2(\mathbb{R}; \mathbf{W}) \cap \mathrm{L}^2_{(2)}(\mathbb{R}; \mathbf{W}) \quad\text{and}\quad \overline{\mathbf{X}} = \overline{\mathbf{V}}^* = \mathrm{H}^{-2}(\mathbb{R}; \mathbf{W}) + \mathrm{L}^2_{(-2)}(\mathbb{R}; \mathbf{W}),$$

where the subscripts "$_{(m)}$" denote the L^2 space with measure $(1{+}t^2)^m \mathrm{d}t$. In $\overline{\mathbf{V}}$ we choose the graph norm $\|u\|_{\overline{\mathbf{V}}} = \|\mathbb{A}u\|_{\overline{\mathbf{H}}}$.

Concerning the shift group $\big(\overline{\mathbf{H}}, \mathbb{S}_t\big)_{t\in\mathbb{R}}$ we observe that it can be restricted to $\overline{\mathbf{V}}$, since $u \in \overline{\mathbf{V}}$ implies $\mathbb{S}_t u \in \overline{\mathbf{V}}$ for all t. Setting $\mathbb{S}_t^{\mathbf{V}} = \mathbb{S}_t|_{\overline{\mathbf{V}}}\colon \overline{\mathbf{V}} \to \overline{\mathbf{V}}$ we have

$$\begin{aligned}
\|\mathbb{S}_t^{\mathbf{V}} u\|_{\overline{\mathbf{V}}} &\le C\big(\|(\mathbb{S}_t u)''\|_{\mathrm{L}^2} + \|(1{+}s^2)(\mathbb{S}_t u)(s)\|_{\mathrm{L}^2}\big) \\
&\le 2C\big(\|u''\|_{\mathrm{L}^2} + (1{+}t^2)\|(1{+}r^2)u(r)\|_{\mathrm{L}^2}\big) \le (1{+}t^2)C\|u\|_{\overline{\mathbf{V}}}.
\end{aligned}$$

Hence, $\big(\overline{\mathbf{V}}, (\mathbb{S}_t^{\mathbf{V}})_{t\in\mathbb{R}}\big)$ forms a strongly continuous group of shift operators. By dualization (with respect to the duality in $\overline{\mathbf{H}}$) we can define the extension

$$\mathbb{S}_t^{\mathbf{X}}\colon \overline{\mathbf{X}} \to \overline{\mathbf{X}}; \ \ \mathbb{S}_t^{\mathbf{X}} = \big(\mathbb{S}_{-t}^{\mathbf{V}}\big)^*$$

which provides the strongly continuous group $\big(\overline{\mathbf{X}}, (\mathbb{S}_t^{\mathbf{X}})_{t\in\mathbb{R}}\big)$ satisfying $\|\mathbb{S}_t^{\mathbf{X}}\|_{\overline{\mathbf{X}}} \le C^2(1{+}t^2)$.

Proposition C.6 (Assumption 2.3 holds). *If the contraction semigroup $\big(\mathbf{G}, (\mathrm{e}^{-t\mathbb{D}})_{t\geq 0}\big)$ satisfies* (C.1) *and* $\big(\mathbf{H}, (\mathrm{e}^{t\mathbb{J}_\mathcal{B}})_{t\in\mathbb{R}}\big)$ *is an arbitrary minimal dilation, then there exists a larger space* $\mathbf{X}$ *with embedding* $\mathbb{N} : \mathbf{H} \to \mathbf{X}$ *and a strongly continuous group* $(\widehat{S}_t)_{t\in\mathbb{R}}$ *such*

$$\mathbb{N}\mathbb{N}^* : \mathbf{X} \to \mathbf{X} \quad \textit{is trace class}$$

$$\forall\, t \in \mathbb{R}\; \forall\, h \in \mathbf{H} : \quad \widehat{S}_t\mathbb{N}h = \mathbb{N}\mathrm{e}^{t\mathbb{J}_\mathcal{B}}h.$$

Proof. We use the explicit construction of the generalized dilation $\big(\overline{\mathbf{H}}, (\mathbb{S}_t)_{t\in\mathbb{R}}\big)$ and of the explicit extension to $\big(\overline{\mathbf{X}}, (\mathbb{S}_t^{\mathbf{X}})_{t\in\mathbb{R}}\big)$.

By Theorem C.1 the two dilations are unitarily equivalent by a unitary map $U : \mathbf{H} \to \overline{\mathbf{H}}$. If $\overline{\mathbb{N}}$ is the embedding of $\overline{\mathbf{H}}$ into $\overline{\mathbf{X}}$, then we can define

$$\mathbf{X} := \overline{\mathbf{X}}, \quad \mathbb{N} := \overline{\mathbb{N}}\,U, \quad \widehat{S}_t = \mathbb{S}_t^{\mathbf{X}}.$$

Clearly, $\mathbb{N}\mathbb{N}^* = \overline{\mathbb{N}}\,U\,U^*\overline{\mathbb{N}}^* = \overline{\mathbb{N}}\,\overline{\mathbb{N}}^*$ is trace class by the explicit construction. Moreover,

$$\widehat{S}_t\mathbb{N}h = \mathbb{S}_t^{\mathbf{X}}\overline{\mathbb{N}}Uh \overset{(1)}{=} \overline{\mathbb{N}}\mathbb{S}_tUh = \overline{\mathbb{N}}\,UU^{-1}\mathbb{S}_tUh \overset{(2)}{=} \mathbb{N}\,\mathrm{e}^{t\mathbb{J}_\mathcal{B}}h$$

holds for all $h \in \mathbf{H}$. In $\overset{(1)}{=}$ we used the explicit extension of $\mathbb{S}_t^{\mathbf{X}}$ of $\mathbb{S}_t$ with embedding $\overline{\mathbb{N}}$, and in $\overset{(2)}{=}$ we used the definition of $\mathbb{N}$ and that the two dilations are equivalent via the unitary operator U. □

The advantage of using the explicit generalized dilation involving $\overline{\mathbf{H}} = \mathrm{L}^2(\mathbb{R}; \mathbf{W})$ becomes even more apparent if we use the structure of the mapping $\Phi : \mathbf{W} \to \mathbf{G} \subset \overline{\mathbf{H}}$ and $\Phi^* : \overline{\mathbf{H}} \to \mathbf{W}$. Combining Φ^* and the shift $\mathbb{S}_t$ we obtain the mapping

$$\mathcal{U} : \overline{\mathbf{H}} \to \overline{\mathbf{H}}; \quad (\mathcal{U}f)(t) := \Phi^*\big(\mathbb{S}_tf\big).$$

This corresponds to the mapping $t \mapsto Y_t(\eta_0) := \widehat{\mathbb{P}}\widehat{S}_t\eta_0$ from Lemma 2.4. We simply "dropped" the Hilbert-space isomorphism $\Phi : \mathbf{W} \xleftrightarrow{\text{1-1}} \mathbf{G}$.

We now show that $\mathcal{U}$ has a bounded linear extension $\widehat{\mathcal{U}} : \overline{\mathbf{X}} \to \overline{\mathbf{X}}$ that is consistent with Y_t in Lemma 2.4 and is defined everywhere, i.e., we do not need the measurable extension $\widehat{\mathbb{P}}$ defined γ_β a.e. For this we observe that

$$\big(\mathcal{U}f\big)(t) = \int_{-\infty}^0 \Sigma_\mathbb{D}\, \mathrm{e}^{s\mathbb{D}^*}f(s{-}t)\,\mathrm{d}s.$$

Thus, $\mathcal{U}$ is realized by convolution with the kernel $s \mapsto \Sigma_\mathbb{D}\,\mathrm{e}^{s\mathbb{D}^*}\mathbf{1}_{]-\infty,0]}$. In Fourier space the convolution is realized by the multiplication with the Fourier multiplier

$$\mathbb{R} \ni \sigma \mapsto M(\sigma)^* := \Sigma_\mathbb{D}\big(\mathbb{D}^* - \mathrm{i}\sigma\mathbb{I}\big)^{-1}$$

which is smooth and bounded. As the operator $\mathbb{A}$ stays invariant (up to changing constants) under Fourier transform $\mathfrak{F}$, we also see that $\mathfrak{F}$ maps $\mathbf{V}$ into itself, and hence by duality also $\mathbf{X}$ into $\mathbf{X}$. Clearly, multiplying by M defines a bounded linear operator in $\mathbf{V}$, because M lies in $\mathrm{C}_{\mathrm{b}}^2\big(\mathbb{R}; \mathrm{Lin}(\mathbf{W})\big)$. By duality the multiplication multiplying by M^* defines a bounded linear operator in $\mathbf{X} = \mathbf{V}^*$. This shows that there is a bounded linear extension $\widehat{\mathcal{U}} : \mathbf{X} \to \mathbf{X}$ of $\mathcal{U} : \mathbf{H} \to \mathbf{H}$.

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