communications in mathematical
match
and in computer chemistry

no. 42, October 2000

ISSN 0340-6253

MATCDY (42) 71-84 (2000)

Geometrical and Operational Aspects of Irreversibility *

P. Busch

Department of Mathematics, University of Hull, Hull HU6 7RX, UK †

Abstract

In the statistical description of dynamical systems, an indication of the irreversibility of a given state change is given geometrically by means of a (pre-)ordering of state pairs. Reversible state changes of classical and quantum systems are shown to be represented by isometric state transformations. An operational distinction between reversible and irreversible dynamics is given and related to the geometric characterisation of the associated state transformations.

KEYWORDS: Dynamical system, statistical state space, irreversibility, measure cone, mixing distance

1 Introduction

In this paper a characterisation of the reversibility or irreversibility of the time evolution of a dynamical system will be given that emphasises the geometric structures underlying any statistical description.

The statistical description of a dynamical system is based on the dual notions of states and observables. The states form a convex set of probability measures (classical system) or density operators (quantum system). These convex sets span in a natural way an ordered real vector space, called *state space.* For a classical system this is the space of bounded (signed) measures on phase space; in the case of a quantum statistical system, the state space is the set of self-adjoint trace class operators over the system's Hilbert space. Observables are then represented as bounded affine functionals on the set of states and hence as bounded linear functionals on state space. This entails the description of observables of a classical system as functions on phase space and of quantum observables as self-adjoint operators on Hilbert space. In turn, a statistical state can be viewed as a linear map on the real vector space of observables, assigning to each observable its statistical average.

A convenient unified statistical description of classical as well as quantum systems is thus given by the structure of a *statistical duality* $\langle V, W\rangle$, where the state space V is

*Dedicated to E. Ruch on his 80th birthday.

†Electronic address: p.busch@maths.hull.ac.uk

taken to be a complete base norm space, with the convex base K of the positive cone V^+ representing the set of states; and the space W of observables is a complete order unit space with closed order unit interval $E = [o, e]$ and such that W can be identified as a $\sigma(V^*, V)$-dense subspace of V^*. The elements of E, called *effects*, correspond to classes of yes-no measurements that are indistinguishable in terms of their statistics. The number $\langle x, f\rangle := f(x)$ is interpreted as the probability for registering a 'yes' outcome in a measurement of the effect $f \in E$ performed on a system described by the state $x \in K$. For a lucid introduction into the structure of a statistical duality, cf. Ref. [1]. Recently the pair $\langle K, E\rangle$ has been the subject of renewed interest and study and is commonly referred to as an instance of a *statistical model*; the set of effects, E, is a realisation of an *effect algebra* [2].
The statistical description of the time evolution of a dynamical system is based on the notion of a *stochastic map* acting on a statistical state space V, that is, a linear map $\Phi : V \to V$ that sends states to states, $\Phi(K) \subseteq K$. A stochastic map Φ is a contraction with respect to the base norm: $||\Phi(z)||_1 \leq ||z||_1$ for all $z \in V$. Hence the norm distance between two different states cannot increase under the action of a stochastic map. This geometric property is taken up here to formulate an operational characterisation for the (ir)reversibility of a given stochastic map. A necessary condition for reversibility is that the stochastic map under consideration must be an isometry. The converse implication is put forward that irreversible dynamics are characterised, on a suitable level of description, in terms of *non-isometric* stochastic maps. This conjecture is explored by means of some case studies of some types of classical and quantum statistical systems. In contrast to the conventional understanding, a reversible state transformation as defined here is not necessarily surjective, though still always injective; but the operational definition of reversible dynamics as a time-parameterised family of reversible stochastic maps will be seen to force surjectivity.
The mathematical structure relevant to the subsequent investigation is primarily that of a base norm space, while little use will be made of the dual order unit space of observables. In a recent related work, a new way of presenting the structure of a statistical state space has been developed which emphasises the essential geometric and measure theoretic aspects of this concept [3]. This reformulation is based on the concepts of *measure cone* (representing the statistical state space), its endomorphisms (which turn out to coincide with the stochastic maps) and, in particular, the *mixing distance*, an ordering relation of state pairs that accounts for the dissimilarity of states. Previous investigations were concerned with the fundamental geometric nature of these concepts [4] and their application in the context of statistical systems [3]. Here the notion of mixing distance will be used to demonstrate the connection between reversibility and isometric stochastic maps.
The present paper being based on [3], notations, terminology and basic facts are only briefly summarised.

2 Statistical Description of Dynamical Systems

2.1 Statistical state space – the measure cone

The first definition describes the basic geometrical features of any probabilistic framework.

Definition 2.1 *A triple (V, V^+, e) is a measure cone if the following postulates are sat-*

isfied:
(a) V is a real vector space with convex, generating cone V^+ ($V = V^+ - V^+$).
(b) $e: V \to \mathbb{R}$ is a linear functional, called charge, *that is strictly positive (on V^+),*

$$z \in V^+ \implies \{e(z) \geq 0, \text{ and } e(z) = 0 \Leftrightarrow z = 0\}. \tag{1}$$

It follows that the charge e admits a decomposition $e = e_+ - e_-$ of e into a difference of nonlinear, positive functionals $e_\pm$, where

$$e_+ \ : \ V \to \mathbb{R}^+, \quad z \mapsto e_+(z) := \inf\left\{e(x) | \ x \in V^+, \ x - z \in V^+\right\}, \tag{2}$$

$$e_- \ : \ V \to \mathbb{R}^+, \quad z \mapsto e_-(z) := \inf\left\{e(y) | \ y \in V^+, \ z + y \in V^+\right\}. \tag{3}$$

Further, it is required that e marks the cone contour:

$$z \in V^+ \iff e(z) = e_+(z). \tag{4}$$

A measure cone (V, V^+, e) is said to be a measure cone with minimal decomposition *if in addition the following postulate is satisfied:*
(c) To any $z \in V$ there exists a decomposition $z = z_+ - z_-$, $z_+, z_- \in V^+$ such that the following holds: $e(z_+) = e_+(z)$, $e(z_-) = e_-(z)$. Any decomposition of z with this property is called a minimal decomposition of z.
A real vector space V equipped with a measure cone (V, V^+, e) (with minimal decomposition) will be called an mc-space (with minimal decomposition).

One can think of the elements of V as (signed) measures over some set, while those of V^+ represent (positive) measures. Physically, a signed measure is the appropriate mathematical representation of a distribution of positive and negative charges in space. In this interpretation, which has been advocated as a valuable heuristic picture by E. Ruch [4], the charge functional measures the overall net charge.
All known physically relevant examples of measure cones are equipped with a minimal decomposition which is even unique. Hence in the sequel the term measure cone shall generally be taken to include the existence of a minimal decomposition.
The set V^+ is a proper (convex) cone so that V becomes an ordered vector space via $z \geq z' \ :\Leftrightarrow \ z - z' \in V^+$. The strict positivity (on V^+) of the charge functional e ensures that the intersection K of the hyperplane $\{z \in V | e(z) = 1\}$ with V^+ is a base of the convex cone V^+. In a measure cone with minimal decomposition the cone contour condition (4) is a consequence of the strict positivity of e. Any vector space V associated with a measure cone can be equipped with a norm. More precisely, a triple (V, V^+, e) consisting of a real vector space V, a convex generating cone $V^+ \subset V$ and a linear functional e is a measure cone if and only if there exists a norm $\|\cdot\|$ marking the cone contour in the following sense:

$$z \in V^+ \iff e(z) = \|z\|. \tag{5}$$

In particular, the following is a norm of this type:

$$\|z\|_1 \ := \ e_+(z) + e_-(z). \tag{6}$$

This norm coincides with the the Minkowski functional of the set $B := \mathrm{co}(K \cup -K)$, the convex hull of $K \cup -K$, which makes V a base norm space (cf. [5]). The norm $\|\cdot\|_1$ is

known as the base norm, but we will referr to it as the 1-norm, thereby making reference to its prime realisation in terms of the space $L^1(\mathbb{R})$ of absolutely integrable functions. More generally, the 1-norm corresponds to the total variation norm in the classical case and the trace norm in the quantum case.
It is worth noting that a decomposition $z = x - y$, $x, y \in V^+$, is a minimal decomposition if and only if $\|x - y\|_1 = \|x + y\|_1 = e(x) + e(y)$.
The use of a measure theoretic terminology can be justified quite generally using the fact that a base norm space $(V, \|\cdot\|_1)$ and its dual order unit space (V^*, e) form a statistical duality. The set of effects $E := [o, e] \subset V^*$ is the partially ordered set of positive linear functionals on V bounded from below by the null functional o on V and bounded from above by the "order unit" functional e (which serves to define the set K of states in V as those elements x of V^+ for which $e(x) = 1$). Two functionals a, b in V^* are said to be ordered, $a \leq b$, if for all $x \in V^+$, $a(x) \leq b(x)$. E is equipped with a complement operation, $a \mapsto a' := e - a$ which induces a kind of weak orthogonality: effects a, b are called *orthogonal* if their sum $a + b$ is an effect again, that is, if $b \leq a'$. The elements x of V^+ (of K), considered as linear functionals on V^* via $x(a) := a(x)$, act as positive, additive $[x(a + b) = x(a) + x(b)$ whenever a, b are orthogonal$]$ (and normalised, $x(e) = 1$) functions on E, representing thus (probability) measures in a generalised sense.

2.2 State transformations – mc-endomorphisms

The dynamics of a physical system is given by a family of state transformations acting on its state space K. In agreement with the statistical ensemble interpretation of the elements of K, a state transformation should not alter the convex composition of a mixed state. Hence a state transformation is an affine map; and as such it extends uniquely to a linear map $\Phi : V \to V$ which is positive ($\Phi(V^+) \subset V^+$) and charge-preserving ($e \circ \Phi = e$). Such maps will be referred to as *mc-endomorphisms* of the mc-space with measure cone (V, V^+, e) generated by K insofar as the geometric aspect is concerned; bearing in mind the physical interpretation, the term *stochastic map* will generally be used.

Proposition 2.1 *Let (V, V^+, e) be a measure cone equipped with the 1-norm.*
(1) A stochastic map is a contraction.
(2) A linear, charge-preserving contraction is positive, hence a stochastic map.

Proof. (1) Let Φ be a stochastic map. Then for $z \in V$, with minimal decomposition $z = z_+ - z_-$,

$$\|\Phi z\|_1 \leq \|\Phi z_+\|_1 + \|\Phi z_-\|_1 = \|z_+\|_1 + \|z_-\|_1 = \|z\|_1 .$$

Hence Φ is a contraction.
(2) Let Φ be linear, charge-preserving and contractive. Let $x \in V^+$. Positive elements z are characterised by the cone contour condition (4); hence we have to show that $\|\Phi x\|_1 = e(\Phi x)$. But we have $\|\Phi x\|_1 \geq e(\Phi x) = e(x) = \|x\|_1 \geq \|\Phi x\|_1$, so that equality must hold.□
The semigroup of stochastic maps induces a pre-ordering on the set of state pairs $K \times K$:

$$(x, y) \sqsupseteq (x', y') \qquad :\Longleftrightarrow \qquad (x', y') = (\Phi x, \Phi y) \quad \text{for some stochastic } \Phi.$$

In subsequent sections we will exhibit conditions under which the sub-semigroup of stochastic isometries induces an equivalence relation on $K \times K$, $(x', y') \equiv (x, y)$ iff

$(x', y') = (\Phi x, \Phi y)$ for some stochastic isometry Φ. Hence an equivalence class contains all state pairs that can be connected among each other by means of some stochastic isometry. Then on the set of these classes the above preordering becomes an ordering relation.

2.3 Dissimilarity of states – mixing distance

The contractive nature of a stochastic map Φ leads to decreasing distances (with respect to any mc-norm) between pairs of states from K under the action of Φ. More specifically, the action of Φ leads to decreasing *mixing distance*.
The *mixing distance* of $x \in V^+ \setminus \{0\}$ from $y \in V^+ \setminus \{0\}$ is defined as the map

$$d[x/y] : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+, \quad (\alpha, \beta) \mapsto \|\alpha x_0 - \beta y_0\|_1 \tag{7}$$

($x_0 := x/\|x\|_1$, etc.). Two pairs (x, y) and $x', y')$ in $V^+ \times V^+$ are called norm-equivalent if $d[x/y] = d[x'/y']$. Thus the mixing distance induces an ordering on the classes of norm-equivalent pairs from $V^+ \times V^+$ via

$$d[x/y] \succ d[x'/y'] \;:\Longleftrightarrow\; \forall \alpha, \beta \in \mathbb{R}^+ : \|\alpha x_0 - \beta y_0\|_1 \geq \|\alpha x_0' - \beta y_0'\|_1 . \tag{8}$$

This concept is found to possess a canonical geometric interpretation in terms of the direction distance, a norm-specific metric of angles in affine spaces associated with a normed real vector space [4]. The ensuing ordering of angles suggests among others a notion of orthogonality which (in the case of state pairs) corresponds to the idea of maximal mixing distance: $x, y \in K$ are called *orthogonal*, $x \perp_1 y$, if the following condition is satisfied:

$$\|\alpha x_0 - \beta y_0\|_1 \;=\; \|\alpha x_0 + \beta y_0\|_1 \qquad \forall \alpha, \beta \in \mathbb{R}^+ . \tag{9}$$

If $z = x - y$ is a minimal decomposition, then $x \perp_1 y$; and conversely, if $x \perp_1 y$ for $x, y \in V^+$, then $z = x - y$ is a minimal decomposition of z ([3], Proposition 2.3).

Proposition 2.2 *Let (V, V^+, e) be a measure cone.*
(1) Any stochastic map Φ leads to decreasing mixing distance on $K \times K$:

$$d[\Phi x/\Phi y] \prec d[x/y] \qquad \text{for} \qquad x, y \in K.$$

Hence, $(x, y) \sqsupseteq (x', y') \Rightarrow d[x/y] \succ d[x'/y']$.
(2) A stochastic map Φ is an isometry (hence preserving the mixing distance) if and only if Φ is orthogonality-preserving:

$$\begin{aligned} \|\Phi z\|_1 = \|z\|_1 \qquad \forall z \in V \qquad &\Longleftrightarrow \qquad d[\Phi x/\Phi y] = d[x/y] \qquad \forall x, y \in K \\ &\Longleftrightarrow \qquad (x \perp_1 y \Rightarrow \Phi x \perp_1 \Phi y)\, \forall x, y \in K. \end{aligned}$$

Proof. (1) This is an immediate consequence of the fact that Φ is a contraction.
(2) Let Φ be an orthogonality-preserving stochastic map. Then

$$\begin{aligned} \|\Phi z\|_1 &= e(\Phi z_+) + e(\Phi z_-) \qquad [\Phi \text{ positive, orthogonality} - \text{preserving}] \\ &= e(z_+) + e(z_-) \qquad [\Phi \text{ charge} - \text{preserving}] \\ &= \|z\|_1 . \end{aligned}$$

Conversely, assume Φ to be a stochastic isometry; then for the minimal decomposition of $z \in V$, $z = z_+ - z_-$ one has

$$e(\Phi z_+) + e(\Phi z_-) = e(z_+) + e(z_-) = \|z_+ - z_-\|_1 = \|\Phi z_+ - \Phi z_-\|_1 ,$$

so that $\Phi z = \Phi(z_+) - \Phi(z_-)$ is a minimal decomposition as well and therefore orthogonal. Thus if $z = x - y$ for any orthogonal pair $x, y \in V^+$, then $\Phi x, \Phi y$ is an orthogonal pair. □
Statement (1) describes the crucial role of the mixing distance as an indicator of irreversibility: if the mixing distance decreases under a stochastic map Φ, then Φ cannot be an isometry, so that there is no stochastic map that would reverse the action of Φ. In this sense the mixing distance has the same function as the (relative) entropy. However, it is known that under certain conditions (though not in general) the converse of statement to (1) holds, thus showing that the mixing distance is superior to entropy insofar as its decrease between two state pairs is even sufficient to ensure the existence of: a state transformation that connects the pair.

Theorem 2.3 *Let the measure cone (V, V^+, e) be given by $V = L^1(\Omega, \Sigma, \mu)$, with (Ω, Σ, μ) a separable, σ-finite measure space. The following is true: given two pairs of states x, y and x', y' such that $d[x'/y'] \prec d[x/y]$, then there exists a stochastic map which transforms x into x' and y into y'. That is:*

$$(x, y) \sqsupseteq (x', y') \Leftrightarrow d[x/y] \succ d[x'/y'].$$

In this form the theorem has been proved in [8]. The theorem was initially found in a more specific form as a generalisation of a theorem due to Hardy, Littlewood and Polya on doubly stochastic matrices[7]. Recently this result has been exhaustively generalised by Ruch and Stulpe to cover all conceivable "classical" spaces of measures [9].

3 Irreversibility

The convex semigroup of stochastic maps acts transitively on the set K. Hence any transition $x \to x'$ is physically realisable in the sense that there exists a stochastic map Φ such that $x' = \Phi x$. As a consequence, the phenomenon of irreversibility can manifest itself only if at least pairs of states and their transitions are taken into consideration [4]. According to Proposition 2.2, decreasing mixing distance is a necessary condition for the possibility of transforming x, y into x', y' by means of one and the same stochastic map. Thus, if $d[\Phi x/\Phi y] \neq d[x/y]$, then there is no stochastic map transforming both x', y' back into x, y. In this sense, strict decrease of the mixing distance between two state pairs is an indicator of the irreversibility of the stochastic map Φ.

Definition 3.1 *A stochastic map Φ acting on an mc-space is irreversible if and only if there is a pair $(x, y) \in K \times K$ such that $(\Phi x, \Phi y)$ cannot be transformed back into (x, y), i.e., $(\Phi x, \Phi y) \not\sqsupseteq (x, y)$.*

In general a physical "reversal of motion" involves a time-inversion operation Θ, represented as a positive surjective isometry on V. Thus irreversibility as defined above is equivalent to $(\Theta\Phi x, \Theta\Phi y) \not\sqsupseteq (\Theta x, \Theta y)$, as it should.
An immediate consequence of Proposition 2.1 is the following.

Proposition 3.1 *A reversible stochastic map on an mc-space is an isometry.*

In cases where Theorem 2.3 is valid it follows that a stochastic map Φ is reversible whenever for arbitrary state pairs $x, y \in K$ one has $d[x/y] \prec d[\Phi x/\Phi y]$. But this amounts to saying that Φ is an isometry. Hence, one has the following result.

Theorem 3.2 *Let V be an mc-space equipped with the 1-norm in which the statement of Theorem 2.3 holds. Then a stochastic map Φ on V is reversible if and only if it is an isometry. This is the case exactly when the mixing distance is invariant under Φ.*

Within the domain of validity of this theorem, the symmetry of the relation $(x', y') \equiv (x, y)$ defined at the end of subsection 2.2 is thus established, so that this relation is an equivalence relation.

Definition 3.1 constitutes what we referred to as an operational characterisation of the irreversibility of state changes. Theorems 2.3 and 3.2 provide the foundation for the geometric indication of irreversibility via strictly decreasing mixing distance. Theorem 2.3 also gives a sufficient criterion for the operational realisability (existence of a stochastic map) of certain changes (jointly sending state pair x, y to state pair x', y'). The question arises whether strictly decreasing mixing distance under the action of a stochastic map Φ, or equivalently, lack of the isometric property of Φ, fully captures the physical content of the notion of irreversibility. The study of irreversibility is primarily concerned with dynamical processes taking place over a period of time rather than for a single time step. Thus reversibility or irreversibility is to be regarded as a property of a (statistical) dynamical system, represented as a time-parameterised family of stochastic maps, $(\Phi_t)_{t\in T}$, with $T = [0, \infty)$ or $T = \mathbb{R}$. (For simplicity we assume homogeneity of time and allow for time to extend to the infinite future (and past); hence for any time t_0, the transition to t_0+t is given by Φ_t). Moreover, it is important to bear in mind that the irreversible behaviour of a dynamical system emerges at a certain level of description, usually referred to as macroscopic or thermodynamic. This has led to the well-known problem of reconciling the omnipresence of a time arrow in large-scale phenomena with the microscopic description of the world which is usually taken to be based on the fundamentally reversible dynamical laws (of Newtonian mechanics or quantum mechanics). Without going into further detail, we recall that the statistical description ((quantum) statistical mechanics) was introduced as a basis for any attempt to formulate a consistent bridge between the two (microscopic and macroscopic) levels of description. In fact, statistical models as defined in Section 2 can be viewed as a convenient unified framework for formalising all kinds of coarse-grainings used to reflect the coarseness of macroscopic observations as well as the tracing out of unobservable degrees of freedom.

The fact that in the modelling of real physical systems there is usually a hierarchy of levels of descriptions shows that a characterisation of the irreversibility or reversibility of the observed dynamics must depend on the level of description appropriate to the feasible observations. Thus the formal definitions of (ir)reversibility for (a) a single stochastic map and (b) for a statistical dynamical system $(\Phi_t)_{t\in T}$ are not in themselves sufficient to characterise the irreversible behaviour of a physical system but they must be supplemented with a specification of the appropriate level of description to which they pertain. We believe the following definition captures those features that are commonly accepted as characteristic of irreversible physical processes. To formulate the notion of a reversed process, one must postulate the existence of a stochastic map Θ which represents the action of time inversion, or more precisely, motion reversal. As a double application of Θ should restore the original state of motion, Θ must equal its own inverse and thus is a bijective stochastic isometry.

Definition 3.2 *A dynamical system $(\Phi_t)_{t\in T}$ on a statistical state space V, with time inversion operation Θ, is* reversible *if for all t,*

$$\Theta^{-1}\Phi_t\Theta \mid_{\Phi(V)}= \Phi_t^{-1}. \tag{10}$$

Note that this concept does not stipulate the state transformation to be surjective. It thus represents exactly the idea of reversing a given state change, by means of the *same* dynamics, without changes in the environment. Usually the condition of time reflection symmetry, $\Phi_t^{-1} = \Phi_{-t}$, is taken to be part of the concept of reversibility, so that a semigroup $(\Phi_t)_{t\in T}$ actually would have to extend to a group in order to be reversible. These considerations will be illustrated with a number of case studies.

4 Case Studies

4.1 Classical Dynamical Systems

In this section (Ω, Σ, μ) denotes a separable, σ-finite measure space and $V = V_c$ the "classical" mc-space corresponding to the real-valued, bounded, σ-additive set functions on (Ω, Σ) which are absolutely continuous with respect to μ. Hence, V_c is isomorphic to the Banach space $L^1(\Omega, \Sigma, \mu)$. In this situation Theorem 2.3 can be used to obtain a characterisation of reversible state transformations which is based on the existence of an inverse map. In general it need not be true that the inverse of a stochastic map Φ (if it exists) can be extended from the range of Φ to all of V_c, nor that it is positive itself; a non-positive inverse, or one that cannot be extended, does not have a physical interpretation as a state transformation.

Proposition 4.1 *A stochastic map $\Phi : V_c \to \Phi(V_c)$ is reversible if and only if there exists an inverse map $\Phi^{-1} : \Phi(V_c) \to V_c$ which is positive.*

Proof. Let Φ be reversible and therefore, by Theorem 3.2, an isometry. The range $\Phi(V_c)$ is a closed subspace of V_c, thus a base norm space itself. Due to the injectivity of Φ the inverse Φ^{-1} exists on $\Phi(V_c)$ and is a charge-preserving contraction (in fact, an isometry). Φ^{-1} is positive; otherwise there were an element z with minimal decomposition $z = z_+ - z_-$, $z_\pm \in V_c^+ \setminus \{0\}$ such that $\Phi z \in V_c^+$, in contradiction to the fact that $\Phi z_- \neq 0$ (note that Φ is orthogonality-preserving).
Conversely, if the inverse $\Phi^{-1} : \Phi(V_c) \to V_c$ exists and is positive (it is automatically charge-preserving), then Φ is necessarily an isometry, hence, by Theorem 3.2, reversible. □
As noted above, the reversibility of a dynamical system is sometimes defined by means of the group property of the respective family of state transformations. We have introduced a general (statistical) dynamical system as a semigroup $(\Phi_t)_{t\geq 0}$ of stochastic maps acting on V_c. More specifically, given a measure space (Ω, Σ, μ), we will now consider dynamical

systems defined as a semigroup $(S_t)_{t\geq 0}$ of measurable maps $S_t : \Omega \to \Omega$ which leave μ invariant. Then the associated semigroup of stochastic maps is determined via

$$\int_\Delta \Phi_t \rho d\mu := \int_{S_t^{-1}(\Delta)} \rho d\mu, \qquad \rho \in V_c,\ \Delta \in \Sigma.$$

In the case of a normalised measure space ($\mu(\Omega) = 1$), the uniform distribution $\rho_u = 1_\Omega$ is a fixed point of all Φ_t, $t \geq 0$. In accordance with Definition 3.1 a semigroup $(\Phi_t)_{t\geq 0}$ of stochastic maps shall be called reversible if all Φ_t are reversible. While the group property is sufficient to ensure reversibility in the sense of Definition 3.1, it is not in general a necessary condition as will be shown by means of an example below. However, for a fairly general class of dynamical systems the group property is necessary and sufficient for reversibility. The following result is due to R. Quadt and the author and was originally published in [10].

Proposition 4.2 *Let $(\Omega, \mathcal{B}(\Omega), \mu)$ be a normalised measure space, with $(\Omega, \mathcal{B}(\Omega))$ a standard Borel space. Let $(S_t)_{t\geq 0}$ be a dynamical system, with induced semigroup $(\Phi_t)_{t\geq 0}$ and time inversion operation Θ. $(\Phi_t)_{t\geq 0}$ of stochastic maps is reversible if and only if it can be extended to a group via $\Theta^{-1}\Phi_t\Theta =: \Phi_{-t}$.*

Proof. That the group property is sufficient for reversibility is clear from Proposition 4.1. Conversely, let $(\Phi_t)_{t\geq 0}$ be reversible. By Theorem 3.2 all the Φ_t are isometries. To ensure the group extension, one shows that the Φ_t are surjective. To this end one constructs a family $\gamma_t : \Omega \to \Omega$ of measurable, μ-preserving, surjective point maps such that $\Phi_t\rho(x) = \rho \circ \gamma_t(x)$ (μ-almost everywhere) for $\rho \in V_c$. The maps γ_t will turn out to be uniquely determined up to Borel sets of measure zero. It then follows that an inverse map Φ_t^{-1} is defined on all of V_c via $\int_\Delta \Phi_t^{-1}\rho d\mu := \int_{\gamma_t^{-1}(\Delta)} \rho d\mu$. Then $\Phi_{-t} = \Phi_t^{-1}$, and the group property is established. To find γ_t, note that since $(\Omega, \mathcal{B}(\Omega))$, is a standard Borel space, there exists a measurable, bijective map $\psi : \Omega \to [0,1]$ which induces a bijective isometry $j : V_c \to L^1([0,1], \mathcal{B}([0,1]), \nu)$ via $\int_{\tilde{\Delta}} j\rho d\nu := \int_{\psi^{-1}(\tilde{\Delta})} \rho d\mu$ and $\nu(\tilde{\Delta}) := \mu\left(\psi^{-1}(\tilde{\Delta})\right)$. Here $([0,1], \mathcal{B}([0,1]), \nu)$ is a normalised, separable measure space. It follows that the map $\tilde{\Phi}_t := j \circ \Phi_t \circ j^{-1}$ is an isometry on $L^1([0,1], \mathcal{B}([0,1]), \nu)$. By Lamperti's theorem [11], there exists a measurable, surjective map $\varphi_t : [0,1] \to [0,1]$ (unique up to Borel sets of ν−measure zero) such that $\tilde{\Phi}_t f = \tilde{\Phi}_t 1_{[0,1]} \cdot f \circ \varphi_t$ and $\int_{\varphi_t^{-1}(\tilde{\Delta})} \tilde{\Phi}_t 1_{[0,1]} d\nu = \int_{\tilde{\Delta}} d\nu$. Since $\tilde{\Phi}_t 1_{[0,1]} = 1_{[0,1]}$, it follows that φ_t is measure-preserving. Now, using the equation $j\rho(x) = \rho \circ \psi^{-1}(x)$ (valid almost everywhere), one obtains the desired result: $\Phi_t\rho(x) = \left(j^{-1} \circ \tilde{\Phi}_t \circ j\rho\right)(x) = \rho \circ \psi^{-1} \circ \varphi_t \circ \psi(x) =: \rho \circ \gamma_t(x)$ (valid almost everywhere). □

There exist semigroups of reversible stochastic maps which do not admit an extension to a group. As an example, let $(\mathbb{R}, \mathcal{B}(\mathbb{R}), \mu_{\mathcal{L}})$ be the Borel-Lebesgue measure space. It is easy to construct a measurable bijection $\gamma : \mathbb{R} \to (0, \infty)$ which, together with its inverse $\gamma^{-1} : (0, \infty) \to \mathbb{R}$, is measure-preserving. For example, consider a partitioning of the real line into intervals of the form $(n, n+1]$, n integer. If the label n is even (odd), call the corresponding interval even (odd). Now the map γ may be defined by shifting the positive (negative) intervals one by one with increasing $|n|$ onto the positive even (odd) intervals with correspondingly increasing labels. With $\gamma_n := \gamma^n$ one defines a (discrete) semigroup of transformations on $\mathbb{R}$ such that the induced family of linear operators (Φ_n), $\Phi_n\rho := \rho \circ \gamma_n$ on V_c is a semigroup of isometric stochastic maps. By Theorem 3.2 the stochastic maps Φ_n are reversible; but $(\Phi_n)_{n\in\mathbb{N}_0}$ does not have an extension to a group since the Φ_n^{-1} cannot be extended to isometries on V_c. So if one could construct a bijective stochastic isometry Θ such that $\Theta^{-1}\Phi_1\Theta = \Phi_1^{-1}$, one would have found an example of a reversible dynamical semigroup which does *not* admit a group extension. The crucial point of this example is that the underlying measure space is not finite, so that proper subsets of Ω are measure theoretically equivalent to Ω itself. Redistribution operations such as γ can be applied, for instance, as a coding of the set $\mathbb{R}$ into $(0, \infty)$.

4.2 Damped Motion

As an example of a deterministic dynamical system that is not measure preserving we consider the simple case of linearly damped motion of a particle in one dimension. Thus the state of the particle at any time t is given by its position $X(t)$ and velocity $\dot{X}(t)$, that is, $\omega = \left(X, \dot{X}\right) \in \Omega = \mathbb{R}^2$. The dynamics is determined by the equation of motion $\ddot{X} = -\kappa\dot{X}$, $\kappa > 0$, which is solved by

$$S_t : \left(X(0), \dot{X}(0)\right) \mapsto \left(X(t), \dot{X}(t)\right) = \left(X(0) + \tfrac{1}{\kappa}\dot{X}(0)\left(1 - e^{-\kappa t}\right), \dot{X}(0)\, e^{-\kappa t}\right).$$

It is easy to verify that $S_t^{-1} = S_{-t}$, so that $(S_t)_{t\in\mathbb{R}}$ is a group. But the latter maps, S_{-t}, are seen to solve the anti-damping equation $\ddot{X} = +\kappa\dot{X}$, which is obtained from the previous one by application of the time inversion map $\theta : \left(X, \dot{X}\right) \mapsto \left(X, -\dot{X}\right)$. Accordingly, we find that $\theta^{-1}S_t\theta \neq S_t^{-1}$, which carries over in the corresponding inequality $\Theta^{-1}\Phi_t\Theta \neq \Phi_t^{-1}$ for the induced stochastic semigroup, with all Φ_t surjective stochastic isometries on $L^1(\Omega, \mathcal{B}(\otimes))$. This confirms that the damped motion is irreversible, despite the fact that a formal extension to a group is possible. A natural indicator of the irreversibility (Lyapunov variable) is given by the magnitude of the velocity, $\left|\dot{X}(t)\right| = \left|\dot{X}(0)\right| e^{-\kappa t}$, which tends monotonically to 0 as t increases.

Damped motion of a particle can be viewed as a reduced description of a system consisting of a very massive body suspended in a medium (gas or fluid) of molecules with which it interacts via collisions. Despite the presence of the environment, the body performs a deterministic motion whereas its energy is dissipated into the degrees of freedom represented by the molecules of the medium (as well as increase of internal heat of the body). The next example of Brownian motion belongs to the same physical class but the body suspended in the medium is not as massive so that its motion is randomised due to unobservable collisions with the surrounding molecules.

4.3 Brownian Motion

The random collisions determining the motion of a Brownian particle are modelled by means of a stochastic differential equation for its position, $X(t)$:

$$\dot{X} = b(X) + \sigma(X)\xi.$$

Here $b(X)$ describes a deterministic influence while the white noise term $\xi = \dot{w}$ is given as the time derivative of a Wiener process; $\sigma(X)$ is the amplitude of the stochastic perturbation. As is well known, this stochastic process can be represented in terms of an associated Fokker-Planck (or Kolmogorov) equation for density functions $\rho_t(X)$,

$$\frac{\partial \rho_t}{\partial t} = -\frac{\partial \left[b(X)\rho_t\right]}{\partial X} + \frac{1}{2}\frac{\partial^2 \left[\sigma^2(X)\,\rho_t\right]}{\partial X^2},$$

the solution of which (for sufficiently regular amplitude $\sigma(X)$) is given by an *exact* semigroup $(\Phi_t)_{t\geq 0}$; exactness meaning that $\Phi_t\rho$ converges in 1-norm to a unique stationary distribution ρ^* [12]. This process is thus characterised by decreasing mixing distance between any density ρ_t and ρ^*, in agreement with the fact that there exist Lyapunov variables indicating the irreversibility.

4.4 Instability

The preceding examples display irreversible behaviour of a system due to its interaction with a (stationary) environment. An alternative type of situation is given by *closed* deterministic systems which are characterised by a degree of intrinsic *instability*. Thus it is known that for the so-called *K-systems* there are dynamics-dependent coarse grainings under which the *observable* motion is described by a semigroup of strictly contractive stochastic maps (e.g., [13]). Alternatively, a dynamical system $(S_t)_{t\in\mathbb{R}}$ is called *intrinsically random* if its associated group of stochastic isometries $(\Phi_t)_{t\in\mathbb{R}}$ is similar to a semigroup of strictly contractive stochastic maps $\left(\tilde{\Phi}_t\right)_{t\geq 0}$; this means that there is an invertible stochastic map W whose inverse has dense domain and is *not* positive such that $\tilde{\Phi}_t = W\Phi_t W^{-1}$. It has been shown that K-systems possess this property of intrinsic randomness and that for them the irreversibility of the stochastic semigroup $\left(\tilde{\Phi}_t\right)_{t\geq 0}$ can be indicated by some Lyapunov variables [13, 14].

4.5 Quantum Mechanics

One may consider the conjecture that the assertion made in Theorem 3.2 remains true even beyond the scope of Theorem 2.3. This question shall be investigated in the context of quantum mechanical measure cones for which Theorem 2.3 is known to be violated unless the underlying Hilbert space is two-dimensional [15], see also the corresponding remarks in [3]. One can construct quantum mechanical stochastic maps that are isometric and reversible without being surjective but such that their inverse maps can be extended to stochastic maps.

Let $\mathcal{H}$ denote a separable complex Hilbert space (with inner product $\langle\cdot|\cdot\rangle$ associated to a quantum mechanical system. The ensuing mc-space $V = V_q$ is given by the Banach space of selfadjoint trace class operators, with $K = K_q$ representing the set of density operators. The charge functional and 1-norm are given by the trace and trace norm, respectively. The surjective isometries among the stochastic operators possess a particularly simple structure.

Proposition 4.3 *Let V_q be the mc-space associated with a separable complex Hilbert space $\mathcal{H}$. A surjective stochastic map $\Phi : V_q \to V_q$ is an isometry if and only if it is induced by a linear or antilinear isometry $U : \mathcal{H} \to \mathcal{H}$ such $\Phi(z) = UzU^*$ for $z \in V_q$.*

This fact follows readily from the Wigner–Kadison characterisation of the automorphisms of states or observables [16, 17]. We present a concise proof that makes use of a result of Davies [18].

Proof. First, any Φ defined as above in terms of some unitary or antiunitary U is a positive, trace-preserving map on V_q. This follows from the fact that $U^*U = I$: $e(UzU^*) = e(U^*Uz) = e(z)$, the first equality being due to the invariance of the trace under cyclic permutations of the factors in its argument. Let $z \in V_q^+$, then $\langle\varphi|UzU^*\varphi\rangle = \langle U^*\varphi|zU^*\varphi\rangle \geq 0$ for all $\varphi \in \mathcal{H}$; hence, $\Phi(z)$ is positive, too. To verify the isometric nature of Φ, let $z = z_+ - z_-$ be a minimal decomposition. It follows that $z_+ \cdot z_- = 0$ and therefore $Uz_+U^* \cdot Uz_-U^* = U(z_+ \cdot z_-)U^* = 0$. Thus, $\Phi(z_+)$ and $\Phi(z_-)$ are orthogonal so that $\Phi(z) = \Phi(z_+) - \Phi(z_-)$ is a minimal decomposition. Since Φ is trace-preserving it follows that $\|\Phi(z)\|_1 = e(z_+) + e(z_-) = \|z\|_1$.
Next, let Φ be a surjective isometric stochastic map. Then it is also injective. It follows that Φ is a *pure* map sending pure (extremal) states to pure states: indeed, assume $x \in K_q$ is pure, let $\Phi(x) = \lambda y_1 + (1-\lambda)y_2$ for some $y_1, y_2 \in K_q$ and $0 < \lambda < 1$. Since Φ is surjective there exist $x_1, x_2 \in K_q$ such that $\Phi(x_1) = y_1$, $\Phi(x_2) = y_2$. By the injectivity of Φ, $x = \lambda x_1 + (1-\lambda)x_2$, and due to the purity of x, $x_1 = x_2 = x$; therefore $y_1 = y_2 = y$, that is, $y = \Phi(x)$ is pure, too. According to Theorem 2.3.1 of [18], Φ is induced by a unitary or antiunitary operator. □
If in the case of an infinite-dimensional Hilbert space the assumption of surjectivity is dropped, then there exists a class of non-pure stochastic isometries which can be constructed as follows.

Proposition 4.4 *Let $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_n$ be a direct sum decomposition of $\mathcal{H}$ such that* $\dim\mathcal{H}_k = \infty$, $k = 1, 2, \cdots, n$, $2 \leq n \leq \infty$. *Let $U_k : \mathcal{H} \to \mathcal{H}_k$ be linear or antilinear isometries, $0 \leq w_k \leq 1$, $\sum w_k = 1$. Then*

$$\Phi : V_q \to V_q, \quad z \mapsto \Phi(z) := \sum w_k U_k z U_k^*, \tag{11}$$

is an isometric stochastic map. Moreover, the following is a stochastic map whose restriction to the range of Φ coincides with the inverse of Φ: Let P_0, $P_k = U_k U_k^*$ denote the orthogonal projections associated to the subspaces $\mathcal{H}_0$, $\mathcal{H}_k$, respectively.

$$\Psi : V_q \to V_q, \quad z \mapsto \Psi(z) := \sum_{k=1}^{n} U_k^* P_k z P_k U_k + P_0 z P_0. \tag{12}$$

Proof. It is obvious that Φ is a stochastic map. The isometric nature follows from the fact that all the $U_k(z_\pm)$, $U_l(z_\pm)$ (for minimal decompositions $z = z_+ - z_-$ and $k \neq l$) are mutually orthogonal, so that $\|\sum w_k U_k z U_k^*\|_1 = \sum w_k \|U_k z U_k^*\|_1 = \sum w_k \|z\|_1$.
The positivity of Ψ is obvious. It follows from $\sum_{k=0}^n P_k = I$ that Ψ is trace-preserving. Finally, for any element $\Phi(z)$ one has $P_k\Phi(z)P_k = w_k U_k z U_k^*$ and $P_0\Phi(z)P_0 = 0$. This immediately yields $\Psi(\Phi(z)) = \sum w_k z = z$.□
The last result shows that isometric state transformations of the form (11) are indeed reversible. It is known that all isometric stochastic maps on V_q are of this form [19].
While the statement of Theorem 2.3 does not in general hold in quantum mechanics, the last result entails that for pairs of quantum states, the relation $(x', y') \equiv (x, y)$ (subsection 2.2) is again symmetric. Hence it is an equivalence relation and renders the relation $\sqsupseteq$ a partial ordering on the ensuing equivalence classes. These classes contain as a subclass those state pairs that can be connected with a *surjective* stochastic isometry. In the above quantum mechanical example it becomes apparent that this specific subclass is strictly smaller than the original equivalence class. In fact, the surjective stochastic isometries are

those induced by either unitary or antiunitary maps and hence always send pure states to pure states. By contrast, the map (11) sends pure states to mixed states whenever it is not surjective. Thus a pair of image states cannot be sent to a pair of pure states by means of a surjective stochastic isometry. The implication of this observation is that non-surjective maps of the form (11) cannot be interpreted as (discrete-time) reversible dynamics: the maps (12) are not stochastic isometries themselves, so that requirement (10) of Definition 3.2 cannot be satisfied for a statistical dynamical system consisting solely of stochastic isometries.

5 Conclusion

In this work we have reviewed the operational characterisation of irreversible dynamical processes and have explored the possibility of an intrinisically geometrical indication of reversibility or irreversibility, based on the fundamental concept of mixing distance introduced by E. Ruch. We have reviewed this concept in the abstract language of statistical dualities which provides a unified framework for classical and quantum statistical theories and moreover brings out the essential geometric features.

Irreversibility of a *single* statistical state transformation is defined as the impossibility of undoing the change of some pairs of states by application of another state transformation. It follows that a reversible stochastic map is necessarily an isometry. On the other hand, stochastic isometries which are surjective are reversible. The conjecture is proposed that all stochastic isometries are reversible. On the basis of the principle of decreasing mixing distance (Theorem 2.3) this conjecture is verified for certain classical cases. An explicit classification of quantum mechanical stochastic isometries yields the same result for quantum statistical systems. Hence reversible state transformations are necessarily isometric, that is, they leave the mixing distance for state pairs invariant; but they are *not* necessarily surjective.

The full physical content of the notion of reversibility cannot solely be represented as a metric property involving the mixing distance; in addition one needs to make explicit the notion of motion reversal, which involves a bijective isometric stochastic time inversion map Θ. Physically, reversibility means that it is the *same* dynamical map Φ_t that leads back to the initial state if applied to the motion-reverted final state:

$$x \to \Phi_t x \to \Theta\Phi_t x \to \Phi_t\Theta\Phi_t x \to \Theta^{-1}\Phi_t\Theta\Phi_t x = x.$$

This again entails that the inverse to Φ_t is positive and charge-preserving on its domain and hence a stochastic map; thus any reversible statistical dynamical system (Φ_t) must be composed of isometric stochastic maps. The possibility remains that reversible dynamics may not in every case be given by surjective stochastic isometries. To summarise, invariance of mixing distance is necessary for reversibility and decrease of mixing distance is an indication of irreversibility. The power of the concept of mixing distance in the context of classical statistical systems lies in the fact that its decrease provides a sufficient criterion for the physical realisability of joint changes of state pairs as expressed in Theorem 2.3.

References

[1] W. Stulpe: Conditional Expectations, Conditional Distributions, and A Posteriori

Ensembles in Generalized Probability Theory. *Int. J. Theor. Phys.* **27** (1988) 587–611.

[2] E. Beltrametti, S. Bugajski: Effect algebras and statistical physical theories. *J. Math. Phys.* **38** (1997) 3020–3030.

[3] P. Busch, E. Ruch: The Measure Cone – Irreversibility as a Geometrical Phenomenon. *Int. J. Quant. Chem.* **41** (1992) 163–185.

[4] E. Ruch: Der Richtungsabstand. *Acta Applic. Math.* **30** (1992) 67–93.

[5] E. M. Alfsen: *Compact Convex Sets and Boundary Integrals.* Springer, Berlin, 1971.

[6] P. Busch: Orthogonality and Disjointness in Spaces of Measures. *Lett. Math. Phys.* **44** (1998) 215-224.

[7] E. Ruch, R. Schranner, T. H. Seligman: Generalization of a Theorem by Hardy, Littlewood, and Polya. *J. Math. Anal. and Appl.* **76** (1980) 222–229.

[8] P. Busch, R. Quadt: On Ruch's Principle of Decreasing Mixing Distance in Classical Statistical Physics. *J. Stat. Phys.* **61** (1990) 311–328.

[9] E. Ruch, W. Stulpe: The Proof of the Mixing Theorem for Statistical Systems in Classical Physics. *Acta Applic. Math.* **53** (1998) 329-352.

[10] R. Quadt: *Verallgemeinerte Entropiekonzepte und Anwendungen in der Theorie dynamischer Systeme und in der Informationstheorie.* Doctoral Dissertation, Cologne, 1992, Verlag Shaker, Aachen, ISBN 3-86111-183-7.

[11] H.L. Royden: *Real Analysis.* Macmillan, New York, 2nd ed., 1968.

[12] M.C. Mackey: *Time's Arrow: The Origins of Thermodynamic Behavior.* Springer-Verlag, New York, 1992.

[13] S. Goldstein, B. Misra, M. Courbage: On Intrinsic Randomness of Dynamical Systems. *J. Stat. Phys.* **25** (1981) 111-126.

[14] B. Misra, I. Prigogine, M. Courbage: From Deterministic Dynamics to Probabilistic Descriptions. *Physica* **98A** (1979) 1-26.

[15] P.M. Alberti, A. Uhlmann: A Problem Relating to Positive Linear Maps on Matrix Algebras. *Rep. Math. Phys.* **18** (1980) 163–176.

[16] V. Bargmann: Notes on Wigner's theorem on symmetry operations. *J. Math. Phys.* **5** (1964) 862-868.

[17] R.V. Kadison: Transformations of states in operator theory and dynamics. *Topology* **2** (1965) 177-198.

[18] E.B. Davies: *Quantum Theory of Open Systems.* Academic Press, New York, 1976.

[19] P. Busch: Stochastic Isometries in Quantum Mechanics. *Math. Phys., Analysis and Geom.* **2** (1999) 83-106.