Chaotic and Irreversible Properties of Quantum Scattering Systems

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Recent results for a free particle are generalized to $N$-particle quantum systems. Chaotic and irreversible behavior occurs in scattering states that belong to a certain Hilbert space $K^2$ with a preferred time direction pointing to the future. At positive times the time evolution of positive observables exhibits quantum analogues of sensitive dependence on initial conditions, topological transitivity, and existence of a dense set of periodic points. A mixture of states in $K^2$ can be described in terms of a density operator with thermodynamical entropy that increases to its least upper bound when the time tends to infinity.
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**Chaotic and Irreversible Properties**

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1. Introduction

This paper is devoted to the quantum mechanics of \( N \) particles with two-body inter-
actions that give rise to scattering. The objective is to generalize recent work on entropy
increase \([1]\) and chaotic observables \([2]\) for a free particle. It is shown that chaotic and
irreversible behavior occurs if wave functions belong to a certain Hilbert space \( K^2 \) with a
preferred time direction pointing to the future.

It is assumed that the interaction between any two particles is reasonably smooth and
tends to zero sufficiently fast when the distance between particles tends to infinity. As
a result there are scattering states in which the \( N \)-particle system separates into bound
clusters that eventually move away from one another and in the remote future are infinitely
far apart. Associated with each mode of separation are wave operators that intertwine
between the exact time evolution and the time evolution of bound clusters moving freely
relative to one another. The intertwining property is true for long- as well as for short-
range interactions. It is the feature that enables previous results for free particles to be
generalized. For a function \( f \) to belong to \( K^2 \), it must be a wave function of a scattering
state, hence it must be orthogonal to any bound states of the scattering system. Moreover,
it must satisfy analyticity conditions generalizing the ones in Refs. \([1,2]\).

The wave function for the motion of \( N \) particles relative to their center of mass is
an element of \( L^2(\mathbb{R}^{3N-3}) \). Henceforth we refer to \( L^2 \). There is an orthogonal projection
\( \Pi : L^2 \to \Pi L^2 \) onto scattering states. Let \( H \) be the Hamiltonian of the relative motion. In
the Schrödinger picture the time evolution takes \( f \in L^2 \) into \( f(t) := \exp(-itH)f \). If \( f \in
K^2 \), then \( f(t) \in K^2 \) if \( t \geq 0 \), but not necessarily if \( t < 0 \). This causes a time asymmetry
that is essential in this paper. Unless stated otherwise, it is assumed throughout the
following that \( t \geq 0 \).

The quantities with chaotic properties are operators representing observables in the
Heisenberg picture. Given an operator \( A \) on \( L^2 \), the Heisenberg picture lets

\[
A(t) := \exp(iHt)A \exp(-iHt)
\]
act on time-independent wave functions \( f \). The space \( K^2 \) has a central role in that we focus on positive self-adjoint operators \( A \) on \( \Pi L^2 \) with the property that \( A^{1/2} \) maps \( K^2 \) into \( \Pi L^2 \). Quadratic form techniques developed in Ref. [2] determine a topology for such operators \( A \). The result is a topological space \( X \) with the property that \( A(t) \in X \) if \( A \in X \) and \( t \geq 0 \).

Once a topology is in place, we can formulate conditions for chaos. To this end, we follow Devaney’s definition of chaos in classical dynamical systems [3]. Hence we investigate

\[
\begin{align*}
(S) & \text{ Sensitive dependence on initial conditions,} \\
(T) & \text{ Topological transitivity,} \\
(P) & \text{ Existence of a dense set of periodic points.}
\end{align*}
\]

Precise statements are provided by Theorems S, T, and P in Section 8. Formally, these chaos theorems are the same as in Ref. [2], but they are of wider scope because a more general time evolution is being considered. The proof in the present paper can be reduced to the previous proof. This is an analogue of the fact that chaos in classical dynamical systems is invariant under homeomorphisms [3].

The chaos theorems show that the outcome of experiments is unpredictable, yet retains elements of regularity. As an illustration, let us consider a fixed operator \( A \in X \) and compare this with \( Z \in X \). To do so, we choose finite sets of wave functions \( f_i, g_i \in K^2 (i = 1, 2, ..., j) \), then perform experiments to determine the matrix elements \( \langle f_i | A | g_i \rangle \) and \( \langle f_i | Z | g_i \rangle \). Suppose for each \( i \) the two matrix elements differ by less than the experimental error. We repeat the experiments at a later time with the same \( A, Z \), and \( f_i, g_i \). According to Theorem S, the expectation values \( \langle f_i | A(t) | f_i \rangle \) and \( \langle f_i | Z(t) | f_i \rangle \) may differ by any constant \( \delta \) times \( \| f_i \|^2 \). Given any operator \( B \in X \), Theorem T says that \( \langle f_i | Z(t) | g_i \rangle \) may equal \( \langle f_i | B | g_i \rangle \) within experimental errors, for each \( i (i = 1, 2, ..., j) \). In this sense the space of chaotic operators is indecomposable. The system is not random, however. By Theorem P, the operator \( Z(t) \) may be semiperiodic in the sense that \( \tau \) exists such that \( Z(t + n\tau) = Z(t) \) if \( t \geq 0 \), \( n = 0, 1, 2, ... \). This means that \( \langle f_i | Z(t) | g_i \rangle \) is close to \( \langle f_i | A | g_i \rangle \).
at all times \( t = n\pi \), for every \( i \). The proofs of the theorems show that there are operators \( Z \) with these erratic behaviors in any neighborhood of any operator \( A \in X \).

Chaos as defined in this paper is related to irreversible behavior because either phenomenon occurs if wave functions belong to the space \( K^2 \). First suppose that \( \rho \) is a positive operator in the trace class on \( \Pi L^2 \). To study chaos, we use the Heisenberg picture with time-dependent observables \( A(t) \). Irreversible behavior calls for the Schrödinger picture with time-dependent density operators \( \rho(t) \) determined by

\[
\rho(t) := \exp (-iHt) \rho \exp (iHt). \tag{1.1}
\]

Following von Neumann, we define the quantum-mechanical entropy of \( \rho(t) \) by

\[
S[\rho(t)] := -\text{Tr} \rho(t) \ln \rho(t). \tag{1.2}
\]

Because \( H \) is self-adjoint, the entropy \( S[\rho(t)] \) does not depend on the time \( t \). Hence there is no irreversible behavior at this level.

Now assume that \( t \geq 0 \) and that the range of \( \rho \) belongs to \( K^2 \). The operator \( \rho(t) \) then determines an operator \( \hat{\rho}(t) \) in the trace class on \( K^2 \). The time evolution on \( K^2 \) is represented by a semigroup \( \{ U(t) | 0 \leq t < \infty \} \), not by a unitary group such as \( \{ \exp (-iHt) | -\infty < t < \infty \} \). This eliminates a major paradox of statistical mechanics, but, since \( U(t) \) is an isometry on \( K^2 \), is not sufficient to produce entropy increase.

For further progress, we need to refer to an unbounded positive operator \( J \) introduced in Section 5. A function \( f \in \Pi L^2 \) belongs to \( K^2 \) if and only if \( Jf \in \Pi L^2 \). In terms of the inner product \( \langle \cdot , \cdot \rangle \) on \( \Pi L^2 \), the inner product \( \langle \cdot , \cdot \rangle \) on \( K^2 \) is defined according to

\[
\langle f, g \rangle = \langle f, g \rangle + \langle Jf, Jg \rangle. \tag{1.3}
\]

If \( \text{Tr} \) denotes the trace on \( \Pi L^2 \) and \( \langle \text{Tr} \rangle \) the trace on \( K^2 \),

\[
\langle \text{Tr} \hat{\rho}(t) \rangle = \text{Tr} \rho(t) + \text{Tr} J\rho(t)J. \tag{1.4}
\]

This expression brings to mind a discussion by Mackey [4; 5, Chap. 9] in which he showed that taking a factor of a classical dynamical system with invertible time evolution, may
give rise to a system with increasing entropy. The transformation $\rho(t) \to \sigma(t)$ with

$$\sigma(t) := \rho(t) + J \rho(t) J \quad (t \geq 0)$$ (1.5)

can be viewed as a quantum analogue of taking a factor in the sense of Mackey. It is shown in Section 13 that $S[\sigma(t)]$ is not constant in time and increases to its least upper bound as $t \to \infty$. The irreversible feature at the heart of the proof is easy to visualize by looking at a scattering event. In the distant past the system was separated into clusters that approached the center of mass. In the remote future scattered clusters will move away from it. This history gives rise to Eqs. (13.7) and (13.8), generalizing corresponding relations in Ref. [1]. As a result the proof that $S[\sigma(t)]$ increases is the same as in Ref. [1].

If $\rho$ is of rank 1, it can be shown as in Ref. [1] that the entropy $S[\sigma(t)]$ is a monotone increasing function of $t$. It is an open problem whether $S[\sigma(t)]$ may exhibit fluctuations if $\rho$ is of higher rank. The latter case is difficult to assess due to the fact that there are positive operators in the trace class on $\Pi L^2$ that cannot occur as density operators $\sigma$ because they are not generated by positive operators $\rho$. This problem is discussed in some detail in Ref. [1].

Let us write $\sigma(t) = L \rho(t)$. This defines a linear operator $L$ taking $\rho(t)$ with finite $\langle \text{Tr } \tilde{\rho}(t) \rangle$ into the trace class on $\Pi L^2$. According to Section 14, $L$ is invertible and $L^{-1}$ can be constructed explicitly. Given a bounded operator $T$ on $L^2$, there is an operator $TL^{-1}$ such that

$$\text{Tr } T \rho(t) = \text{Tr } (TL^{-1}) \sigma(t).$$ (1.6)

In combination with the fact that $\text{Tr } \sigma(t)$ does not depend on $t$, Eq. (1.6) indicates that $\sigma(t)$ can be used as a density operator to evaluate expectation values of observables.

The transformation $\rho(t), \quad T \to \sigma(t), \quad TL^{-1}$ can be viewed as a new example of the $\Lambda$-transformation advocated by Prigogine and coworkers [6,7] to show that irreversible behavior originates at the microscopic level. There is an overview of the Prigogine program in Ref. [1]. Further references follow in Section 16.

The next section describes our coordinate systems for $N$-body problems. Section 3
summarizes fundamental concepts in scattering theory. Section 4 is devoted to a Hilbert space of analytic functions that serves as a building block to construct the space of wave functions $K^2$ in Section 5. The topological space $X$ is introduced in Section 6. An essential point about $X$ is that operators $A(t) \in X$ are related to bounded operators $\hat{A}(t)$ on $K^2$. Hence the time evolution on $K^2$ is investigated in Section 7. Devaney’s definition of chaos is reviewed in Section 8. Theorems S,T, and P in Section 8 state that the time evolution of operators $A \in X$ has chaotic properties that can be viewed as quantum transcriptions of Devaney’s chaos conditions for maps on metric spaces. To prove the theorems, one needs to construct nets $\{Z_\tau\} \in X$ ($\tau \geq 0$) that tend to $A \in X$ as $\tau \to \infty$, yet give rise to time evolutions $\{Z_\tau(t)\}$ with erratic behaviors. Section 8 sketches the construction, but formal proofs are omitted because they are the same as in Ref. [2]. The time evolution on $K^2$ is reminiscent of $K$-flows, often quoted as prototypes of chaotic systems. It is discussed in Section 9 how the relation has helped to shape the present paper. Other chaos concepts are mentioned in Section 10, including the notion of quantum chaos.

Comparing the trace classes on $\Pi L^2$ and $K^2$, Section 11 shows how the density operator $\rho$ determines $\hat{\rho}$. Constructing $\sigma$ can be viewed as taking a partial trace of $\hat{\rho}$. It is shown in Section 12 that $\text{Tr} \sigma(t)$ is constant and that $\text{Tr} \sigma^2(t)$ is a decreasing function of $t$, provided $t \geq 0$. The entropy $S[\sigma(t)]$ increases to its least upper bound by Section 13. The proof is the same as in Ref. [1]. Section 14 describes how the usual density operator $\rho$ can be reconstructed when $\sigma$ is known. The density operator $\sigma(t)$ can be used to calculate expectation values of observables according to Section 15. Section 16 relates the transformation $\rho(t) \to \sigma(t)$ to the $\Lambda$-transformation in many papers by Prigogine and coworkers. In certain cases applying $\Lambda$ can be interpreted as taking a factor of a classical dynamical system. That this step may lead to a system with increasing entropy was the reason for us to introduce $\sigma(t)$ and the entropy $S[\sigma(t)]$.

2. Coordinate systems

Consider a system of $n$ particles with masses $m_j$ ($j = 1, 2, \ldots, n$) located at $X_j$.
Suppose the Schrödinger operator has the form
\[
 i \frac{\partial}{\partial t} = -\sum_{j=1}^{n} (2m_j)^{-1} \Delta(X_j) + \sum_{i<j} V_{ij}(X_i - X_j).
\]
It is convenient to introduce a standard notation that separates the relative and center of mass motions.

The total mass of particles 1, 2, ..., \( k \) is \( M_k := \sum_{j=1}^{k} m_j \). The center of mass of this set is located at
\[
\eta_k := (M_k)^{-1} \sum_{j=1}^{k} m_j X_j \quad (k = 1, 2, ..., n).
\]
The vector from \( \eta_k \) to \( X_{k+1} \) is
\[
\xi_k := X_{k+1} - \eta_k = (M_k)^{-1} \sum_{j=1}^{k} m_j (X_{k+1} - X_j) \quad (k = 1, 2, ..., n - 1).
\]
Imagine a particle of mass \( M_k \) at \( \eta_k \) and a particle of mass \( m_{k+1} \) at \( X_{k+1} \). The reduced mass is
\[
\mu_k := (M_{k+1})^{-1} M_k m_{k+1} \quad (k = 1, 2, ..., n - 1).
\]
Hence we define
\[
x_k := (2\mu_k)^{1/2} \xi_k
\]
\[
= (M_k M_{k+1})^{-1/2} (2m_{k+1})^{1/2} \sum_{j=1}^{k} m_j (X_{k+1} - X_j) \quad (k = 1, 2, ..., n - 1),
\]
\[
x_n := (2M_n)^{1/2} \eta_n = (2/M_n)^{1/2} \sum_{j=1}^{n} m_j X_j.
\]
It is easy to verify that
\[
-\sum_{j=1}^{n} (2m_j)^{-1} \Delta(X_j) = -\sum_{j=1}^{n} \Delta(x_j).
\]
\[\text{(2.1)}\]
If there were only \( j \) particles, the system could be described in terms of the coordinates \( x_k \) with \( k = 1, 2, ..., j - 1 \) plus the center-of-mass coordinate \( \eta_j \). If \( i < j \), then \( X_i - X_j \) does not depend on \( \eta_j \). Hence there exist constants \( d_{ij}^k \) such that
\[
V_{ij}(X_i - X_j) = V_{ij} \left( \sum_{k=1}^{j-1} d_{ij}^k x_k \right) \quad (i < j).
\]
Now consider \( n \) multiparticle clusters. Denote the mass of cluster \( c \) by \( N_c \) and assume that the center of mass is located at \( \mathbf{Y}_c \) \( (c = 1, 2, ..., n) \). Introduce internal coordinates in cluster \( c \) as in the previous paragraphs, but denote these by \( \mathbf{y}_c \), where \( c \) is a cluster subscript, not a particle subscript. The interaction within cluster \( c \) depends on \( \mathbf{y}_c \) only. The kinetic energy of cluster \( c \) relative to its center of mass is represented by \( -\Delta(\mathbf{y}_c) \). The total kinetic energy is

\[
- \sum_{c=1}^{n} \Delta(\mathbf{y}_c) - \sum_{c=1}^{n} \left(2N_c\right)^{-1} \Delta(\mathbf{Y}_c).
\]

Now apply to \( N_c, \mathbf{Y}_c \) \( (c = 1, 2, ..., n) \) the coordinate transformation that took \( m_j, \mathbf{X}_j \) \( (j = 1, 2, ..., n) \) into \( \mathbf{x}_k \) \( (k = 1, 2, ..., n) \). Denoting the new variables by \( \mathbf{x}_k \) as before takes the kinetic energy of the relative motion of the clusters into \( -\sum_{j=1}^{n-1} \Delta(\mathbf{x}_j) \). The interaction between clusters \( b \) and \( c \) depends on \( \mathbf{y}_b, \mathbf{y}_c \), and some or all of the \( \mathbf{x}_j \) \( (j = 1, 2, ..., n - 1) \), but not on the overall center-of-mass coordinate \( \mathbf{x}_n \). Thus we find that

\[
i \frac{\partial}{\partial t} = - \sum_{c=1}^{n} \Delta(\mathbf{y}_c) + \sum_{c=1}^{n} V_{cc}(\mathbf{y}_c) - \sum_{j=1}^{n-1} \Delta(\mathbf{x}_j) + \sum_{b < c} V_{bc}(\mathbf{y}_b, \mathbf{y}_c, \mathbf{x}_1, ..., \mathbf{x}_{n-1}) - \Delta(\mathbf{x}_n). \tag{2.2}
\]

In an obvious notation, \( V_{cc} \) and \( V_{bc} \) are interactions within cluster \( c \) and between clusters \( b \) and \( c \), respectively. The operator \( -\Delta(\mathbf{x}_n) \) represents the kinetic energy of the center of mass. To simplify the notation, we combine the vectors \( \mathbf{y}_c \) \( (c = 1, 2, ..., n) \) into a vector \( \mathbf{y} \) and the vectors \( \mathbf{x}_j \) \( (j = 1, 2, ..., n - 1) \) into a vector \( \mathbf{x} \). This takes the relative Hamiltonian for cluster \( c \) into

\[
H_c(\mathbf{y}) := -\Delta(\mathbf{y}_c) + V_{cc}(\mathbf{y}_c).
\]

The relative kinetic energy of the clusters is denoted by

\[
-\Delta(\mathbf{x}) := -\sum_{j=1}^{n-1} \Delta(\mathbf{x}_j).
\]
In this notation the Hamiltonian for the relative motion is

\[ H := \sum_c H_c(y) - \Delta(x) + \sum_{b \neq c} V_{bc}(x, y). \]

There are many ways to separate a system of \( N \) particles into clusters. By Eq. (2.1) all choices transform the kinetic energy into the negative Laplace operator. This indicates that the transformations between various sets of coordinates are orthogonal and allows us to use different coordinates in different parts of the same problem. Moreover, in case there are \( n - 1 \) intercluster coordinates \( x \) as in Eq. (2.2), the transformation from \((2m_j)^{1/2}X_j\) to \( y, x, x_n \) is orthogonal, so that

\[ d^{3N}X = \prod_{j=1}^{N} (2m_j)^{-1/2} d^{3N-3n}y \quad d^{3n-3}x \quad d^3x_n. \]

The mass factor is a constant which should be taken into account if one wishes to calculate actual physical values of matrix elements. In the present context, however, an overall numerical factor is of no consequence. Hence we ignore the mass factor and work with normalized functions of \( y, x, x_n \). In fact, since all cluster decompositions arrive at the same center-of-mass coordinate \( x_n \) equal to \((2/M_N)^{1/2}\sum_j m_jX_j\), the transformations among the relative coordinates \( y, x \) are orthogonal, even if we change cluster decompositions. In studying the relative motion, it is therefore sufficient to work in terms of the usual inner product \( \langle \cdot, \cdot \rangle \) and norm \( \| \cdot \| \) of \( L^2(\mathbb{R}^{3N-3}) \)-functions depending on \( x, y \).

3. Scattering theory

This section reviews concepts from scattering theory [8-10] that are used throughout the paper.

Consider a specific decomposition into \( n \) clusters, hence \((3n - 3)\)-dimensional relative motion \( -\Delta(x) \), and assume that each multiparticle cluster Hamiltonian \( H_c(y) \) has a normalized eigenvector \( \psi_c(y) \) with eigenvalue \( E_c \). Denote the product \( \prod_c \psi_c(y) \) by \( \psi(y) \) and the sum \( \sum_c E_c \) by \( E \). The vector \( y \) must have \( 3N - 3n \) components. Since \( \psi(y) \) is
normalized by assumption, the operator $\Psi$ on $L^2(\mathbb{R}^{3N-3})$ defined by
\[
\Psi f(x, y) := \psi(y) \int f(x, z) \bar{\psi}(z) \, d^{3N-3n} z
\] (3.1)
is an orthogonal projection. If $f \in L^2(\mathbb{R}^{3N-3})$ belongs to the domain of $H$
\[
H \Psi f(x, y) = [E - \Delta(x) + \sum_{b < c} V_{bc}(x, y)] \Psi f(x, y).
\] (3.2)

For a more general notation, we consider all possible cluster decompositions of $N$
particles and in each decomposition allow all possible bound-state wave functions $\psi$.
We refer to the possibilities as scattering channels and label these by a subscript $\alpha$. The
bound-state wave function in channel $\alpha$ is denoted by $\psi_\alpha$. It is a function of $y_\alpha$. Typically,$\psi_\alpha$ is a product of several cluster functions $\psi_c$. The projection operator determined by
$\psi_\alpha$ as in Eq. (3.1) is denoted by $\Psi_\alpha$. The operators $\sum V_{bc}$ and $E - \Delta(x)$ in Eq. (3.2) are
replaced by $V_\alpha$ and
\[
H_\alpha := E_\alpha - \Delta(x_\alpha).
\] (3.3)
Hence
\[
H \Psi_\alpha f = (H_\alpha + V_\alpha) \Psi_\alpha f.
\]
If all interaction terms $V_\alpha$ are of short range, there exist wave operators $\Omega_{\alpha \pm}$ satisfying
\[
\lim_{t \to \pm \infty} \| \exp(iHt) \exp(-iH_\alpha t) \Psi_\alpha f - \Omega_{\alpha \pm} f \| = 0.
\] (3.4)
As a result of this definition, $\Omega_{\alpha \pm}$ annihilates the orthogonal complement of the range of
$\Psi_\alpha$,
\[
\Omega_{\alpha \pm}(1 - \Psi_\alpha) f = 0.
\]
A sufficient condition for $\Omega_{\alpha \pm}$ to exist is that each term $V_{ij}(X_i - X_j)$ in the sum $V_\alpha$
is of the form $V_{ij} = V_2 + V_p$, where $V_2 \in L^2(\mathbb{R}^3)$ and $V_p \in L^p(\mathbb{R}^3)$ with some $p$ satisfying
$2 < p < 3$, see [9, Theorem X1.34]. Another sufficient condition is that $\epsilon > 0$ exists such that
\[
(1 + |X|^2)^{\epsilon+1/2} V_{ij}(X) = V_{3/2} + V_\infty,
\]
where $V_{3/2} \in L^{3/2}(\mathbb{R}^3)$ and $V_{\infty} \in L^\infty(\mathbb{R}^3)$, see [9, Theorem X1.35]. Generally speaking, these conditions are satisfied if $V_{ij}(X)$ does not have serious singularities and at infinity tends to 0 like $|X|^{-1-\delta}$ with some $\delta > 0$.

If $V_{ij}(X)$ behaves at infinity like $|X|^{-\mu}$ with $\mu \leq 1$, the interaction is said to be of long range. In this case the limits in Eq. (3.4) do not exist, but it may be possible to construct modified wave operators provided the factor $\exp(-iH_0 t)$ in Eq. (3.4) is replaced by one that better characterizes the time evolution of scattered clusters at large separations [11]. If $\sqrt{3}-1 < \mu \leq 1$ and $V_{ij}$ satisfies suitable smoothness conditions, modified wave operators exist for any number of particles [10,12]. Even in cases where $\mu \leq \sqrt{3}-1$, there are results for two particles [13]. For such very slowly decaying interactions, modified wave operators have been shown to exist in larger systems [10,12] provided cluster wave functions $\psi(y)$ go to 0 sufficiently rapidly as $|y| \to \infty$.

Whether the interaction is of short or long range, henceforth we simply refer to wave operators and denote these quantities by $\Omega_{\alpha \pm}$. They all satisfy the intertwining relation

$$
\exp(-iHt)\Omega_{\alpha \pm} = \Omega_{\alpha \pm} \exp(-iH_0 t).
$$

(3.5)

Denoting the orthogonal projection onto the range of $\Omega_{\alpha \pm}$ by $\Pi_{\alpha \pm}$, we have

$$
\Omega^*_{\alpha \pm} \Omega_{\alpha \pm} = \Psi_\alpha, \quad \Omega_{\alpha \pm} \Omega^*_{\alpha \pm} = \Pi_{\alpha \pm}.
$$

Since

$$
\Omega^*_{\beta \pm} \Omega_{\alpha \pm} = \delta_{\alpha \beta} \Psi_\alpha,
$$

(3.6)

the projections $\Pi_{\alpha +}$ commute and have mutually orthogonal ranges. The same applies to the projections $\Pi_{\alpha -}$. Summing over channels, we define the projections

$$
\Pi_{\pm} := \sum_{\alpha} \Pi_{\alpha \pm}.
$$

The sum has finitely many terms or converges strongly.

Let $B$ be the projection onto any bound states of the $N$-particle system. If the wave operators exist, $BL^2$ is orthogonal to $\Pi_{\pm}L^2$. If

$$
BL^2 + \Pi_{\pm}L^2 = BL^2 + \Pi_+L^2 = L^2,
$$

(3.7)

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the scattering is said to be asymptotically complete. Under various smoothness assumptions on the interaction, asymptotic completeness has been proved for short-range interactions \([14,15]\) and for long-range interactions \([12]\) with \(\sqrt{3} - 1 < \mu \leq 1\). In two-particle problems asymptotic completeness is even known to be true in cases in which \(\mu \leq \sqrt{3} - 1\) \([13]\). Examples show that the existence of wave operators is not sufficient for asymptotic completeness \([16]\).

The important point in the following is the intertwining relation (3.5). It provides the link between time evolutions with and without interaction. In the present paper we can use operators \(\Omega_{\alpha+}\) throughout. This gives rise to an operator \(J_+\) and space \(K^2_+\). Alternatively, we can use operators \(\Omega_{\alpha-}\) giving rise to \(J_-\) and \(K^2_-\). The restriction \(t \geq 0\) applies in either case. If the projections \(\Pi_+\) and \(\Pi_-\) are equal, the spaces \(K^2_+\) and \(K^2_-\) are isometrically isomorphic, operators \(A_{\alpha+}^{1/2}(t)\) acting on \(K^2_+\) are unitarily equivalent to operators \(A_{\alpha-}^{1/2}(t)\) acting on \(K^2_-\), and each operator \(\sigma_+ (t)\) defined in terms of \(J_+\) by Eq. (1.4) is unitarily equivalent to an operator \(\sigma_- (t)\) defined in terms of \(J_-\). This will become clear once the operators \(J_{\pm}\) are defined in Section 5.

Since the theories with subscripts \(+\) and \(-\) run parallel, we omit the subscripts in the following, writing
\[
\Omega_\alpha \Omega_\alpha^* = \Pi_\alpha, \quad \Pi = \sum_\alpha \Pi_\alpha.
\]
Thus \(\Omega_\alpha\) is either \(\Omega_{\alpha+}\) or \(\Omega_{\alpha-}\), and similarly for the other operators. The projection \(\Pi\) is the projection onto scattering states meant in Section 1. If asymptotic completeness holds, \(\Pi_+ = \Pi_-\), so that \(\Pi\) is uniquely determined.

Recall that \(L^2\) stands for \(L^2(\mathbb{R}^{3N-3})\). If in channel \(\alpha\) the system is separated into \(n\) clusters, a \((3n-3)\)-dimensional coordinate \(x_\alpha\) refers to the relative motion of the clusters. The wave function of the clusters depends on a \((3N-3n)\)-dimensional coordinate \(y_\alpha\). For any \(f \in \Pi L^2\)
\[
\exp (-iHt)f = \exp (-iHt) \sum_\alpha \Omega_\alpha \Omega_\alpha^* f = \sum_\alpha \Omega_\alpha \exp (-iH_\alpha t) \Omega_\alpha^* f. \quad (3.7)
\]
Since $\Omega^*_\alpha f$ belongs to the range of $\Psi_\alpha$, there must be a function $f_\alpha$ such that

$$\Omega^*_\alpha f = \psi_\alpha(y_\alpha) f_\alpha(x_\alpha).$$  \hfill (3.8)

To calculate $f_\alpha$, it suffices to multiply $\Omega^*_\alpha f$ by $\tilde{\psi}(y_\alpha)$ and integrate with respect to $y_\alpha$. Due to Eqs. (3.3) and (3.8)

$$\exp(-i H_\alpha t) \Omega^*_\alpha f = \exp(-i E_\alpha t) \psi_\alpha(y_\alpha) \exp[i \Delta(x_\alpha)t] f_\alpha(x_\alpha).$$

In the following we mainly use the momentum representation. Hence we replace $\exp[i \Delta(x_\alpha)t] f_\alpha(x_\alpha)$ by $\exp(-i k_\alpha^2 t) f_\alpha(k_\alpha)$. For $f$ to belong to $K^2$, the functions $f_\alpha(k_\alpha)$ have to satisfy analyticity conditions introduced in the next section.

4. Analytic functions

This section discusses functions $f(k) \in L^2(\mathbb{R}^\nu)$ that are meant as prototypes of Fourier transforms of functions $f_\alpha(x_\alpha)$ in Eq. (3.8). We follow Ref. [1] closely, but in the process generalize previous results for $L^2(\mathbb{R}^3)$ so that they become valid on $L^2(\mathbb{R}^\nu)$.

Denoting $|k|$ by $k$, we introduce $\nu - 1$ spherical coordinates $\omega$ and replace $f(k)$ by $f(k, \omega)$. Hence $k^{(\nu - 1)/2} f(k, \omega)$ is an element of $L^2(\mathbb{R}^+ \times S^{\nu - 1})$.

The Mellin transform

$$M_\nu f(k, \omega) = f^\#(u, \omega)$$

defined by

$$f^\#(u, \omega) := (2\pi)^{-1/2} \int_0^\infty k^{(\nu - 1)/2} f(k, \omega) k^{iu - 1/2} \, dk$$

is a unitary map taking $L^2(\mathbb{R}^+ \times S^{\nu - 1})$ onto the space $L^2(\mathbb{R} \times S^{\nu - 1})$ consisting of functions $f^\#(u, \omega)$ with inner product

$$(f^\#, g^\#) = \int_{S^{\nu - 1}} \int_{-\infty}^\infty f^\#(u, \omega) \overline{g^\#(u, \omega)} \, du \, d\omega.$$  

The inverse Mellin transform is determined by

$$k^{(\nu - 1)/2} f(k, \omega) = (2\pi)^{-1/2} \int_{-\infty}^\infty f^\#(u, \omega) k^{-iu - 1/2} \, du.$$  

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If we define \( z := \ln k \) and
\[
F(z, \omega) := e^{\nu z/2} f(e^z, \omega),
\]
it follows that
\[
F(z, \omega) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} f^\#(u, \omega) e^{-izu} \, du.
\]
For starters we now assume that \( f^\#(u, \omega) \in C_0^\infty(\mathbb{R} \times S^{\nu-1}) \). This guarantees that \( F \) belongs to the domain of \( \partial/\partial z \). Applying \( i\partial/\partial z \) to \( F \) corresponds to multiplying \( f^\# \) by \( u \). Because \( \partial/\partial z = k \partial/\partial k \),
\[
i \frac{\partial}{\partial z} F(z, \omega) = k^{\nu/2} \left[ i k \frac{\partial}{\partial k} + i \nu/2 \right] f(k, \omega).
\] (4.1)

The operator in square brackets is among our major concepts. To give it a more transparent form, we examine the dilation operator \( D_\nu \), which is the self-adjoint operator on \( L^2(\mathbb{R}^\nu) \) that acts on \( C_0^\infty \)-functions \( f(k) \in L^2(\mathbb{R}^\nu) \) as
\[
D_\nu = i (k \cdot \nabla_k + \nabla_k \cdot k).
\]
The differential operator \( D_\nu \) is equal to \( i k \cdot \nabla_k + i \nu/2 \). The components of \( k \) are of the form \( k_j = k \cos \theta_j(\omega) \), with some set of functions \( \theta_j(\omega) \) \( (j = 1, 2, ..., \nu) \). Hence
\[
k \partial/\partial k = \sum_{j=1}^{\nu} k \frac{\partial k_j}{\partial k} \partial/\partial k_j = \sum_{j=1}^{\nu} k_j \partial/\partial k_j = k \cdot \nabla_k.
\]
It follows that the operator in square brackets in Eq. (4.1) is the dilation operator \( D_\nu \).

Multiplying Eq. (4.1) by \( k^{-1/2} \) gives
\[
k^{(\nu-1)/2} D_\nu f(k, \omega) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} u f^\#(u, \omega) k^{-i\nu-1/2} \, du.
\]
Following Ref. [1], we now extend multiplication by \( u \) on \( C_0^\infty(\mathbb{R} \times S^{\nu-1}) \) to a self-adjoint operator \( u \) on \( L^2(\mathbb{R} \times S^{\nu-1}) \), then use the operator \( u \) so defined to extend the differential operator \( D_\nu \) to the self-adjoint operator \( D_\nu = M_\nu^{-1} u M_\nu \) on \( L^2(\mathbb{R}^\nu) \). The spectra of \( u \) and \( D_\nu \) are absolutely continuous and run from \(-\infty \) to \( \infty \).

The self-adjoint operator \( D_\nu \) determines \( \exp (\phi D_\nu) \). Taking \( \phi = -\pi/2 \) we define
\[
J_\nu := \exp (-\pi D_\nu/2) = M_\nu^{-1} \exp (-\pi u/2) M_\nu
\] (4.2)
and let the domain of $J_\nu$ be the set of all $f \in L^2(\mathbb{R}^\nu)$ with the property that $f^\#(u, \omega)\exp(-\pi u/2)$ belongs to $L^2(\mathbb{R} \times S^{\nu-1})$. The operator $J_\nu$, so defined is self-adjoint and positive. Henceforth the domain of $J_\nu$ is denoted by $K_\nu^2$. Hence $K_\nu^2$ is the set of all $f \in L^2(\mathbb{R}^\nu)$ with the property that $J_\nu f \in L^2(\mathbb{R}^\nu)$.

Functions in $K_\nu^2$ have certain analyticity properties. This can be seen by examining the set of all functions $f(k e^{i\phi}, \omega)$ which are analytic in the sector $-\pi/2 < \phi < 0$ for almost every $\omega \in S^{\nu-1}$ and have the property that

$$\int_{S^{\nu-1}} \int_0^\infty \left| (k e^{i\phi})^{(\nu-1)/2} f(k e^{i\phi}, \omega) \right|^2 dk \, d\omega$$

is bounded uniformly in the sector $[17,18]$. Functions in this set have mean-square boundary values $f(k, \omega)$ and $f(k e^{-i\pi/2}, \omega)$. Under the inner product

$$\langle f, g \rangle = \int_{S^{\nu-1}} \int_0^\infty [f(k, \omega)\overline{g}(k, \omega) + f(k e^{-i\pi/2}, \omega)\overline{g}(k e^{-i\pi/2}, \omega)] k^{\nu-1} \, dk \, d\omega$$

the set is a Hilbert space which we denote by $G_\nu^2$.

At this point we can adapt the reasoning for $\nu = 3$ in Refs. [1,2] to general $\nu$. On the basis of known properties [17,18] of Mellin transforms of functions in $G_\nu^2$, it can be shown that $f \in L^2(\mathbb{R}^\nu)$ belongs to $K_\nu^2$ if and only if $f(k, \omega)$ is the boundary value at $\phi = 0$ of a function $f(k e^{i\phi}, \omega)$ in $G_\nu^2$. Moreover, for $-\pi/2 \leq \phi \leq 0$

$$e^{i\phi D_\nu} f(k, \omega) = e^{i\pi/2} f(k e^{i\phi}, \omega).$$

We now define an inner product $\langle \cdot, \cdot \rangle$ on $K_\nu^2$ by

$$\langle f, g \rangle := (f, g) + (J_\nu f, J_\nu g)$$

$$= \int_{S^{\nu-1}} \int_{-\infty}^{\infty} (1 + e^{-\pi u}) f^\#(u, \omega)\overline{g^\#}(u, \omega) \, du \, d\omega.$$

The term $(J_\nu f, J_\nu g)$ is equal to the second term on the right in Eq. (4.3). The fact that $G_\nu^2$ is a Hilbert space can now be used to show that $K_\nu^2$ is complete under the inner product $\langle \cdot, \cdot \rangle$, hence a Hilbert space.

If $-\pi/2 < \phi < 0$, then $\exp(-ik^2 e^{2i\phi} t)$ is bounded if and only if $t \geq 0$. Hence $f \in G_\nu^2$ yields $\exp(-ik^2 e^{2i\phi} t)f \in G_\nu^2$ if $t \geq 0$, but not necessarily if $t < 0$. In terms of boundary
values at $\phi = 0$, it follows that $f \in K^2_\nu$ yields $\exp (-i k^2 t) f \in K^2_\nu$ if $t \geq 0$, but not necessarily if $t < 0$. This is the reason why we assume that $t \geq 0$, unless stated otherwise. Due to Eq. (4.4) with $\phi = -\pi/2$

$$J_\nu \exp (-i k^2 t) f(k, \omega) = \exp (i k^2 t) J_\nu f(k, \omega), \quad (4.5)$$

provided $f \in K^2_\nu$ and $t \geq 0$. Taking $\phi = -\pi/4$ gives

$$J^{1/2}_\nu \exp (-i k^2 t) f(k, \omega) = \exp (-k^2 t) J^{1/2}_\nu f(k, \omega). \quad (4.6)$$

5. The space of wave functions

The time evolution of $f \in \Pi L^2$ can be represented by Eq. (3.7). In the momentum representation Eq. (3.8) takes the form

$$\Omega_\alpha^* f = \psi_\alpha(k'_\alpha) f_\alpha(k_\alpha), \quad (5.1)$$

where $k'_\alpha$ and $k_\alpha$ are the variables conjugate to $y_\alpha$ and $x_\alpha$, respectively. If channel $\alpha$ refers to a separation into $n$ clusters, the vector $k_\alpha$ has $3n - 3$ components. We let $3n - 3$ be the number $\nu$ in the previous section and assume that $f_\alpha(k_\alpha)$ belongs to $K^2_\nu$, but we change the notation and now refer to operators $D_\alpha$ and $J_\alpha$ and a space $K^2_\nu$. Using the notation $\| \cdot \|$ for norms on $L^2$-spaces, we denote the norm on $K^2_\nu$ by $\| \| \cdot \| \|$. Thus, if $f_\alpha \in K^2_\nu$, then $\langle f_\alpha, f_\alpha \rangle$ is denoted by $\| f_\alpha \|^2$.

Let $K^2$ be the set of $f \in \Pi L^2$ with the property that $\sum_{\alpha} \| f_\alpha \|^2 < \infty$. If $f \in K^2$, then

$$\| \sum_{\alpha=m}^{n} \Omega_\alpha J_\alpha^* \Omega_\alpha f \| = \sum_{\alpha=m}^{n} \| \psi_\alpha J_\alpha f_\alpha \|^2 \leq \sum_{\alpha=m}^{n} \| f_\alpha \|^2.$$ 

Since $\sum_{\alpha=m}^{n} \| f_\alpha \|^2$ tends to 0 as $m, n \to \infty$, the sum $\sum_{\alpha \leq n} \Omega_\alpha J_\alpha^* f$ tends to a limit as $n \to \infty$. We denote the limit by $J f$. This defines the operator

$$J := \sum_{\alpha} \Omega_\alpha J_\alpha \Omega_\alpha^* \quad (5.2)$$

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on \( \Pi L^2 \) with domain \( K^2 \).

It is easy to verify that \( J \) is symmetric. We claim that the operator \( J \) with domain \( K^2 \) is self-adjoint on \( \Pi L^2 \). To prove this, it is sufficient to show that \((J \pm i)f \) runs through \( \Pi L^2 \) when \( f \) runs through \( K^2 \). By the definition of \( J \)

\[
(J \pm i)f = \sum _\alpha \Omega _\alpha (J_\alpha \pm i)\Omega _\alpha ^* f.
\]

Recall that \( \Omega _\alpha ^* f = \psi _\alpha f_\alpha \), where \( f_\alpha \) belongs to a certain \( L^2(\mathbb{R}^\nu) \)-space. The operator \( J_\alpha \) on \( L^2(\mathbb{R}^\nu) \) is self-adjoint. Its domain is the set \( K^2_\alpha \subseteq L^2(\mathbb{R}^\nu) \). Hence \((J_\alpha \pm i)\psi _\alpha f_\alpha \) runs through \( \psi _\alpha L^2(\mathbb{R}^\nu) \) when \( f_\alpha \) runs through \( K^2_\alpha \). In the process, \( \Omega _\alpha (J_\alpha \pm i)\Omega _\alpha ^* f \) runs through \( \Omega _\alpha \Omega _\alpha ^* L^2 \). When \( f \) runs through \( K^2 \), each \( f_\alpha \) runs through its set \( K^2_\alpha \), hence \((J \pm i)f \) runs through \( \sum _\alpha \Omega _\alpha \Omega _\alpha ^* L^2 \), as we wanted to show.

Now that we know that \( J \) is self-adjoint, we can be more specific about the convergence properties of the sum \( \sum _\alpha \) in Eq. (5.2). If \( f \) runs through \( K^2 \),

\[
\sum _{\alpha \leq n} \Omega _\alpha J_\alpha \Omega _\alpha ^* f \pm i f
\]

runs through a dense set in \( \Pi L^2 \). It follows that \( K^2 \) is a core for \( \sum _{\alpha \leq n} \Omega _\alpha J_\alpha \Omega _\alpha ^* \), for every \( n \). By [19, Theorem VIII.25]

\[
\lim _{n \to \infty} \| \left( \sum _{\alpha \leq n} \Omega _\alpha J_\alpha \Omega _\alpha ^* \pm i \right)^{-1} f - (J \pm i)^{-1} f \| = 0 \tag{5.3}
\]

for every \( f \in \Pi L^2 \). The sets \((J \pm i)^{-1} \Pi L^2 \) are both equal to the domain of \( J \), which can therefore be identified without prior knowledge of \( K^2 \). Instead of looking at \( \sum _\alpha \| f_\alpha \|^2 \) to define \( K^2 \), we can construct \( J \) via Eq. (5.3). Then we can let \( K^2 \) be the set of \( f \in \Pi L^2 \) with the property that \( Jf \in \Pi L^2 \). Either way \( J \) is self-adjoint on \( \Pi L^2 \) with domain \( K^2 \), hence the two definitions of \( K^2 \) are equivalent.

Given \( J \), the relation (1.3) defines an inner product on \( K^2 \). Denoting \( \langle f, f \rangle \) by \( \| f \|^2 \), we proceed to show that the set \( K^2 \) is complete under the \( \| \cdot \| \) norm.
Let \( \{f_n\} \ (n = 1, 2, \ldots) \) be a sequence in \( K^2 \) with the property that \( |||f_m - f_n||| \to 0 \) as \( m,n \to \infty \). Then \( ||f_m - f_n|| \to 0 \) and \( ||Jf_m - Jf_n|| \to 0 \), hence there are elements \( f \) and \( g \) in \( \Pi L^2 \) such that \( ||f_n - f|| \to 0 \) and \( ||Jf_n - g|| \to 0 \). Since \( J \) is self-adjoint, \( J \) is closed. Hence \( f \) must belong to the domain of \( J \) and \( Jf = g \). In other words, \( f \in K^2 \) and

\[
||f_n - f||^2 = ||f_n - f||^2 + ||Jf_n - Jf||^2 \to 0.
\]

This shows that a sequence \( \{f_n\} \) in \( K^2 \) that converges in the \( ||| \cdot ||| \)-norm has a limit \( f \) in \( K^2 \). Equipped with the \( ||| \cdot ||| \) norm, the set \( K^2 \) is a Hilbert space with inner product \( \langle \cdot, \cdot \rangle \). It is easily verified that

\[
\langle f, g \rangle = \langle [1 + J^2]^{1/2} f, [1 + J^2]^{1/2} g \rangle.
\]

The adjoint on \( K^2 \) of an operator \( S : K^2 \to K^2 \) is denoted by \( S^\dagger \). We continue to denote the adjoint on \( L^2 \) of an operator \( T : L^2 \to L^2 \) by \( T^* \). Hence

\[
\langle Sf, g \rangle = \langle f, S^\dagger g \rangle, \quad \langle Tf, g \rangle = \langle f, T^* g \rangle.
\]

The domains of operators \( S \) and \( T \) are denoted by \( \text{Dom} \,(S) \) and \( \text{Dom} \,(T) \), respectively.

If \( f \in K^2 \) and \( t \geq 0 \), then \( \exp(-iHt)f \in K^2 \). Indeed, with Eq. (3.3) for \( H_\alpha \), it follows from the intertwining relation (3.5) and Eq. (5.2) that

\[
J \exp(-iHt)f = \sum_\alpha \Omega_\alpha J_\alpha \exp(-iH_\alpha t)\Omega_\alpha^* f
\]

\[
= \sum_\alpha \Omega_\alpha \exp(iH_\alpha t) \exp(-2iE_\alpha t)J_\alpha \Omega_\alpha^* f
\]

\[
= \exp(iHt) \sum_\alpha \Omega_\alpha \exp(-2iE_\alpha t)J_\alpha \Omega_\alpha^* f.
\]

Defining

\[
W(t) := \sum_\alpha \Omega_\alpha \exp(-2iE_\alpha t)\Omega_\alpha^* \]

gives

\[
J \exp(-iHt)f = \exp(iHt)W(t)Jf.
\]

(5.4)
The operator $W(t)$ is unitary on $\Pi L^2$ and commutes with $\exp(-iHt)$. It follows that $||J \exp(-iHt)f|| = ||Jf||$, hence $||\exp(-iHtf)|| = ||f||$.

In much the same way as we defined the operator $J$, we can introduce the square root

$$J^{1/2} = \sum_{\alpha} \Omega_\alpha J^{1/2}_\alpha \Omega_\alpha^*.$$

If $f \in K^2$, it follows with Eq. (4.6) that

$$J^{1/2} \exp(-iHt)f = W^{1/2}(t) \sum_\alpha \Omega_\alpha \exp(-k^2_\alpha t)J^{1/2}_\alpha \Omega_\alpha^* f. \quad (5.5)$$

The norm of this vector decreases as $t$ increases.

We note for future reference that

$$\langle \exp(-iHt)f, g \rangle = \sum_\alpha \langle \exp(-ik^2_\alpha t - iE_\alpha t)f_\alpha, g_\alpha \rangle, \quad (5.6)$$

where the left side is an inner product on $K^2$, the terms on the right are inner products on spaces $K^2_\alpha$.

Recall that $\Omega_\alpha$ denotes either $\Omega_{\alpha+}$ or $\Omega_{\alpha-}$. Thus Eq. (5.2) actually defines operators

$$J_\pm := \sum \Omega_{\alpha \pm} J_\alpha \Omega_{\alpha \pm}^*$$

giving rise to spaces $K^2_\pm$ with inner products $\langle \cdot, \cdot \rangle_\pm$. Now consider

$$\Theta := \sum_\alpha \Omega_{\alpha-} \Omega_{\alpha+}^*.$$

This operator commutes with $\exp(-iHt)$. Due to Eq. (3.6)

$$\Theta J_+ \Theta^* = J_-,$$

$$\Theta^* J_- \Theta = J_+.$$

If $\Pi_+ = \Pi_- = \Pi$, then $\Theta \Theta^* = \Theta^* \Theta = \Pi$, so that $\Theta$ is a unitary operator on $\Pi L^2$. Under this assumption $\Theta K^2_+ = K^2_-$ and

$$\langle f, g \rangle_+ = (f, g) + (J_+ f, J_+ g)$$

$$= (\Theta f, \Theta g) + (\Theta J_+ \Theta^* \Theta f, \Theta J_+ \Theta^* \Theta g)$$

$$= (\Theta f, \Theta g) + (J_- \Theta f, J_- \Theta g) = \langle \Theta f, \Theta g \rangle_-.$$
Hence $K^2_+$ and $K^2_-$ are isometrically isomorphic. If $f \in K^2_+$ and $A^{1/2}(t)f \in \Pi L^2$, then $\Theta A^{1/2}(t)\Theta^*\Theta f \in \Pi L^2$. Thus if the expectation value of $A(t)$ is chaotic when wave functions belong to $K^2_+$, the expectation value of $\Theta A(t)\Theta^*$ is chaotic when wave functions belong to $K^2_-$. 

Following Eq. (1.5) we write

$$\sigma_+(t) = \rho(t) + J_+ \rho(t) J_+.$$ 

If $\Theta$ is unitary, it follows that

$$\Theta \sigma_+(t) \Theta^* = \Theta \rho(t) \Theta^* + J_- \Theta \rho(t) \Theta^* J_-.$$ 

Hence the pair $\rho, J_+$ determines the same entropy as the pair $\Theta \rho \Theta^*, J_-$. 

6. The operator topology

The operator $J$ and the space $K^2$ are important for our purposes because the chaotic and irreversible behavior that we want to discuss, occurs precisely when states belong to $K^2$. The quantities with chaotic time evolution are positive self-adjoint operators $A$ such that $A^{1/2}$ maps $K^2$ into $\Pi L^2$. If $A$ is not bounded, it may happen that $(Af, g)$ is not well defined. Hence for $f, g \in K^2$, matrix elements of $A$ are expressed in the form

$$\langle f | A | g \rangle := \langle A^{1/2}f, A^{1/2}g \rangle.$$ 

(6.1)

These are the quantities meant in Section 1.

Because the operator $J$ and the space $K^2$ have essential properties in common with the corresponding quantities in Refs. [1,2], many previous results can be copied unchanged. In this section we review the steps to construct a topology for the operators $A$ that will later be shown to have chaotic time evolutions. As mentioned before, the domain of an operator $T$ is denoted by $\text{Dom} (T)$. The restriction to $K^2$ of an operator $T : \Pi L^2 \to \Pi L^2$ is denoted by $T \upharpoonright K^2$.

Let $T$ be a positive self-adjoint operator on $\Pi L^2$ such that $\text{Dom} (T^{1/2}) \supseteq K^2$. Consider the quadratic form

$$q[f, g] := \langle T^{1/2}f, T^{1/2}g \rangle$$ 

(6.2)
on $\Pi L^2$ with form domain $\operatorname{Dom}(q) = K^2$.

Since $T^{1/2}\upharpoonright K^2$ is symmetric, the form is closed or closable. Denote the closure by $\bar{q}$ and its form domain by $\operatorname{Dom}(\bar{q})$. The form $\bar{q}$ determines a positive self-adjoint operator $A$ on $\Pi L^2$ with domain $\operatorname{Dom}(A) \subset \operatorname{Dom}(\bar{q})$ and $\operatorname{Dom}(A^{1/2}) = \operatorname{Dom}(\bar{q})$. For every $f, g \in \operatorname{Dom}(\bar{q})$

$$\bar{q}[f, g] = (A^{1/2}f, A^{1/2}g).$$

Since $K^2$ is a core for $\bar{q}$, the set $K^2$ is a core for $A^{1/2}$.

The above propositions follow from two representation theorems for quadratic forms [20, Chap. VI, Section 2]. That $K^2$ is a core for $A^{1/2}$ implies that $A^{1/2} = (A^{1/2}\upharpoonright K^2)^*$.

The theorems depend on the fact that $T^{1/2}\upharpoonright K^2$ is closable, but do not make comparisons between any extensions of $T^{1/2}\upharpoonright K^2$ and $A^{1/2}\upharpoonright K^2$ to domains larger than $K^2$. As long as $f, g \in K^2$,

$$(T^{1/2}f, T^{1/2}g) = (A^{1/2}f, A^{1/2}g).$$

For the purpose of calculating expectation values of observables in states $f, g \in K^2$, all positive self-adjoint operators $T$ with the same $T^{1/2}\upharpoonright K^2$ are equivalent. Henceforth we select the particular operator $A$ that is singled out by the representation theorems. We denote by $\Gamma$ the set of all positive self-adjoint operators $A$ on $\Pi L^2$ with the property that $K^2$ is a core for $A^{1/2}$. On $\Gamma$ one can define a sum as well as multiplication by a positive constant. Hence $\Gamma$ is a cone, which includes all bounded positive operators on $\Pi L^2$.

We now choose $A \in \Gamma$ and focus on the quadratic form

$$q[f, g] := (A^{1/2}f, A^{1/2}g)$$

with form domain $\operatorname{Dom}(q) = K^2$. Since $A$ is a special case of the operator $T$ in Eq. (6.2), the form is closed or closable. It is shown in Ref. [2] that $(1 + J^2)^{-1/2}A^{1/2}$ is a bounded linear operator on $K^2$. Hence the operator $\tilde{A}$ defined by

$$\tilde{A} := [(1 + J^2)^{-1/2}A^{1/2}]^\dagger (1 + J^2)^{-1/2}A^{1/2}$$

(6.3)
is a bounded positive operator on $K^2$ satisfying

$$ (A^{1/2}f, A^{1/2}g) = \langle \tilde{A}f, g \rangle \quad (6.4) $$

for every $f, g \in K^2$.

Let us denote by $\Gamma_q$ the set of positive closable forms on $\Pi L^2$ with form domain $K^2$. The representation theorems do not require that $q \in \Gamma_q$ be given in terms of an operator $T^{1/2}$ as in Eq. (6.2). Any $q \in \Gamma_q$ determines $A \in \Gamma$ and $A \in \Gamma$ determines $\tilde{A}$. Hence $q \in \Gamma_q$ is of the form $\langle \tilde{A}f, g \rangle$ with some $\tilde{A}$.

Now consider a positive operator $\tilde{T}$ on $K^2$ with the property that the form $\langle \tilde{T}f, g \rangle$ on $\Pi L^2$ with form domain $K^2$ is closable. Since $\langle \tilde{T}f, g \rangle$ must exist for every $f, g \in K^2$, the operator $\tilde{T}$ must be bounded on $K^2$. The form $\langle \tilde{T}f, g \rangle$ determines $A$ and $A$ determines the bounded linear operator $\tilde{A}$ on $K^2$ satisfying

$$ \langle \tilde{T}f, g \rangle = \langle \tilde{A}f, g \rangle $$

for every $f, g \in K^2$. This requires that $\tilde{T} = \tilde{A}$. Hence the set $\Gamma_q$ is associated with a set $\tilde{\Gamma}$ consisting of uniquely determined operators $\tilde{A}$. There is an invertible function $A = \gamma(\tilde{A})$ mapping $\tilde{\Gamma}$ onto $\Gamma$.

In order that we can define chaos, we need a topology on $\Gamma$. We begin with the topology on $\tilde{\Gamma}$ induced by the weak topology for bounded linear operators on $K^2$. This turns $\tilde{\Gamma}$ into a topology space $\tilde{X}$ with the property that a net $\{\tilde{Z}_\tau\} \in \tilde{X} (\tau \geq 0)$ tends to $\tilde{A} \in \tilde{X}$ as $\tau \to \infty$ if and only if $\langle \tilde{Z}_\tau f, g \rangle$ tends to $\langle \tilde{A}f, g \rangle$ for every fixed $f, g \in K^2$. Via the map $\gamma$, it follows that

$$ \lim_{\tau \to \infty} (Z_{\tau}^{1/2}f, Z_{\tau}^{1/2}g) = (A^{1/2}f, A^{1/2}g), \quad (6.5) $$

Conversely, if Eq. (6.5) is true for every $f, g \in K^2$, then $\tilde{Z}_\tau$ tends to $\tilde{A}$ in $\tilde{X}$.

Since Eq. (6.5) says that the expectation value of $Z_{\tau}$ tends to the expectation value of $A$ as $\tau \to \infty$, it represents a convergence concept that is suitable for our purpose. It implies that both $\gamma$ and its inverse $\gamma^{-1}$ are continuous. Given the topology of $\tilde{X}$ and the
fact that $\gamma$ maps $\tilde{\Gamma}$ onto $\Gamma$, there is one and only one topology on $\Gamma$ that makes $\gamma$ and $\gamma^{-1}$ continuous. Details about the open sets that determine this topology are in Ref. [2].

With the topology that recognizes Eq. (6.5) as convergence on $\Gamma$, the set $\Gamma$ becomes a topological space denoted by $X$. This is our space of observables $A$.

By a transcription of Eq. (6.5), a net $\{Z_\tau\} \in X$ tends to $A \in X$ as $\tau \to \infty$ if and only if $f, g \in K^2$ and $\epsilon > 0$ determine $T > 0$ such that

$$|(A^{1/2}f, A^{1/2}g) - (Z_t^{1/2}f, Z_t^{1/2}g)| < \epsilon \text{ if } \tau > T.$$ 

We denote this relation by $\lim_{\tau \to \infty} Z_\tau = A$.

7. The time evolution

Given an operator $A \in X$, our goal is to show that there exist nets $\{Z_\tau\} (\tau \geq 0)$ that tend to $A$ as $\tau \to \infty$ while the $Z_\tau(t)$ with $t > 0$ have the special properties required by the chaos theorems $S, T,$ and $P$ in Section 8. For the proof we construct nets $\{\tilde{Z}_\tau\}$ that tend to $\tilde{A}$. These determine $Z_\tau = \gamma(\tilde{Z}_\tau)$ as desired. To control $\tilde{Z}_\tau(t)$, we need to know how the time evolution acts on $K^2$. To simplify the notation, we denote $\exp(-iHt)$ by $U(t)$. Wherever $f$ is viewed as an element of $\Pi L^2$ or $K^2$, the time evolution takes $f$ into $f(t) = U(t)f$. The adjoint of $U(t)$ on $\Pi L^2$ is denoted by $U^*(t)$. It acts as $\exp(iHt)$. The adjoint of $U(t)$ on $K^2$ is denoted by $U^\dagger(t)$. This operator differs from $U^*(t)$. Due to Eq. (5.4)

$$\langle U(t)f, U(t)g \rangle = \langle f, g \rangle,$$

so that $U(t)$ is an isometry on $K^2$. As a result the set $U(t)K^2$ is a subspace of $K^2$ which is closed in the $K^2$-norm. If $Q(t)$ denotes the orthogonal projection of $K^2$ onto $U(t)K^2$, it follows from general properties of isometries [20, Chap. V, Section 2] that

$$U(t)U^\dagger(t) = Q(t).$$

To investigate $U^\dagger(t)$ and the projection $Q(t)$, we decompose $U(t)$ according to Eq. (3.7) and take advantage of the close connection between the space $G^2_{\nu}$ and the Hardy
space $H^2$ of the lower half-plane [17]. When $k e^{i \phi}$ varies in the sector $-\pi/2 < \phi < 0$, then $(k e^{i \phi})^2$ runs through the lower half-plane. Hence we define

$$v + i w := k^2 e^{2i \phi}, \quad F(v + i w, \omega) := 2^{1/2} (k e^{i \phi})^{(\nu - 2)/2} f_\nu(k e^{i \phi}, \omega),$$

and similarly for $G(v + i w, \omega)$ in terms of $g_\nu$. If $f_\nu, g_\nu \in G^2_\nu$,

$$\langle f_\nu, g_\nu \rangle = \int_{S^\nu - 1} \int_{-\infty}^\infty F(v - i 0, \omega) \tilde{G}(v - i 0, \omega) \, dv \, d\omega.$$

The Fourier transform of $F$ is

$$\hat{f}_\nu(s, \omega) = (2\pi)^{-1/2} \int_{-\infty}^\infty \exp(i sv) F(v - i 0, \omega) \, dv.$$

The function $F(v + i w, \omega)$ belongs to the space $H^2$ of the $(v + i w)$-variable if and only if $f_\nu \in G^2_\nu$. By the Paley-Wiener theorem [21] $\hat{f}_\nu(s, \omega) = 0$ if $s < 0$, for almost every $\omega \in S^{\nu - 1}$.

Since the Fourier transform is unitary,

$$\langle f_\nu, g_\nu \rangle = \int_{S^\nu - 1} \int_0^\infty \hat{f}_\nu(s, \omega) \tilde{g}_\nu(s, \omega) \, ds \, d\omega. \quad (7.3)$$

We derived this relation assuming that $f_\nu, g_\nu \in G^2_\nu$. Now recall that $f_\nu(k, \omega) \in K^2_\nu$ if and only if $f_\nu(k, \omega)$ is the boundary value of $f_\nu(k e^{i \phi}, \omega) \in G^2_\nu$. Whether $f_\nu$ and $g_\nu$ are viewed as elements of $G^2_\nu$ or $K^2_\nu$, the inner product $\langle f_\nu, g_\nu \rangle$ is the same. Hence there is a unitary map taking $f_\nu(k, \omega) \in K^2_\nu$ into $\hat{f}_\nu(s, \omega) \in L^2(\mathbb{R}^+ \times S^{\nu - 1})$ and Eq. (7.3) applies whenever $f_\nu, g_\nu \in K^2_\nu$.

The time evolution multiplies $f_\nu \in K^2_\nu$ by $\exp(-i k^2 t)$ and $f_\nu(k e^{i \phi}, \omega) \in G^2_\nu$ by $\exp(-i k^2 e^{2i \phi} t)$. In the process $F(v + i 0, \omega)$ is multiplied by $\exp(-i v t)$, taking $\hat{f}_\nu(s, \omega)$ into

$$(2\pi)^{-1/2} \int_{-\infty}^\infty \exp(ivs - ivt) F(v - i 0, \omega) \, dv = \hat{f}_\nu(s - t, \omega).$$

It follows that

$$\langle \exp(-i k^2 t) f_\nu, g_\nu \rangle = \int_{S^\nu - 1} \int_0^\infty \hat{f}_\nu(s - t, \omega) \tilde{g}_\nu(s, \omega) \, ds \, d\omega,$$

$$= \langle f_\nu, [\exp(-i k^2 t)]^t g_\nu \rangle = \int_{S^\nu - 1} \int_0^\infty \hat{f}_\nu(s, \omega) \tilde{g}_\nu(s + t, \omega) \, ds \, d\omega. \quad (7.4)$$

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Replacing $\nu$ by the appropriate channel subscript $\alpha$, we may use Eq. (5.6) on the right in Eq. (7.4). For $f, g \in K^2$ it follows that

$$
\langle U(t)f, g \rangle = \sum_\alpha \int_{S_\alpha} \int_0^t \int_0^\infty \exp \left(-i E_\alpha t \hat{f}_\alpha (s - t, \omega) \tilde{g}_\alpha (s, \omega) \right) ds \, d\omega
$$

$$
= \langle f, U^\dagger(t)g \rangle = \sum_\alpha \int_{S_\alpha} \int_0^\infty \hat{f}_\alpha (s, \omega) \exp \left(-i E_\alpha t \right) \tilde{g}_\alpha (s + t, \omega) ds \, d\omega.
$$

(7.5)

Replacing $f$ by $U^\dagger(t)f$ gives

$$
\langle Q(t)f, g \rangle = \sum_\alpha \int_{S_\alpha} \int_t^\infty \hat{f}_\alpha (s, \omega) \tilde{g}_\alpha (s, \omega) ds \, d\omega.
$$

Since $Q(t)$ is an orthogonal projection

$$
|||Q(t)f|||^2 = \sum_\alpha \int_{S_\alpha} \int_t^\infty |\hat{f}_\alpha (s, \omega)|^2 ds \, d\omega.
$$

This is a non-increasing function of $t$ which tends to 0 as $t \to \infty$.

The family \{\langle U(t) \mid 0 \leq t < \infty \} is a semigroup of operators on $K^2$. As in Ref. [2], it follows from the semigroup property and Eq. (7.2) that

$$
Q(s)U(t) = \begin{cases} 
U(t) & \text{if } 0 \leq s \leq t, \\
U(t)Q(s-t) & \text{if } 0 \leq t < s
\end{cases}
$$

(7.6)

$$
Q(s)Q(t) = Q(\max s, t).
$$

(7.7)

If $A \in \Gamma$, it can be shown as in Ref. [2] that the quadratic form

$$
q_t[f, g] := (A^{1/2}U(t)f, A^{1/2}U(t)g) = \langle U^\dagger(t)A^\dagger U(t)f, g \rangle
$$

with form domain $K^2$ is closable, hence determines an operator $A_t \in \Gamma$. Moreover, $A_t$ is equal to the self-adjoint operator $U^\dagger(t)AU(t)$ with domain $U^\dagger(t)\text{Dom}(A)$. It follow that $U^\dagger(t)AU(t) \in \Gamma$. We denote this operator by $A(t)$. It represents the observable $A$ in the Heisenberg picture. Given a form $q[f, g] \in \Gamma_q$, we can extract $A \in \Gamma$, then construct $A(t) \in \Gamma$. Or we can replace $f, g$ by $U(t)f, U(t)g$ to find $q_t$, then determine $A_t \in \Gamma$. Since
the two procedures give the same result, the Heisenberg picture can be used without ambiguity. The operator in \( \tilde{\Gamma} \) determined by \( A(t) \in \Gamma \) is
\[
\tilde{A}(t) := U(t)A(t)U(t)^\dagger.
\]

The set \( \Gamma \) contains unbounded operators such as \( J \). In particular, the operators \( Z_r \) in the proofs of the chaos theorems are not bounded. It may happen that the domain of \( A \in \Gamma \) is a proper subset of \( K^2 \) and that the domain of \( A(t) \) depends on \( t \). In that case the intersection \( \cap_{t \geq 0} \text{Dom} [A(t)] \) could be very small, so that there would be few vectors \( f \) allowing \( (A(t)f, g) \) to be followed over the entire interval \( 0 \leq t < \infty \). On the other hand, the operator \( [A(t)]^{1/2} \) can be applied to every \( f \in K^2 \) at all times \( t \geq 0 \). Hence the notation of Eq. (6.1) can be used at all positive times, expressing the matrix elements of \( A(t) \in \Gamma \) in the form
\[
\langle f | A(t) | g \rangle = \langle [A(t)]^{1/2}f, [A(t)]^{1/2}g \rangle.
\]

8. Chaotic observables

The previous sections provide the framework to show that the time evolution of a large class of observables in quantum mechanics exhibits chaos in the spirit of Devaney’s definition of chaos in classical dynamical systems [3]. Among the three components of chaos listed in Section 1, properties (T) and (P) are strictly topological. According to Devaney [3], a map \( F : X \to X \) on a topological space \( X \) is topologically transitive if for any pair of open sets \( V, W \subseteq X \) there exists \( n > 0 \) such that \( F^n(V) \cap W \neq 0 \). We replace points \( x \in X \) by operators \( A \in X \). The iterated map \( x \to F^n(x) \) is replaced by the time evolution \( A \to A(t) \). Our results on topological transitivity and periodic points are as follows.

**Theorem T.** (Topological transitivity) Given \( A, B \in X \), there is a net \( \{Z_r\} \in X \ (\tau \geq 0) \) such that
\[
\lim_{\tau \to \infty} Z_r = A, \quad \lim_{\tau \to \infty} Z_r(\tau) = B.
\]
The interpretation is that the time evolution takes \(Z_r\) in a neighborhood \(V\) of \(A\) into \(Z_r(\tau)\) in a neighborhood \(W\) of \(B\).

**Theorem P.** (Existence of a dense set of periodic points) Given \(A \in X\), there is a net \(\{Z_r\} \subset X \quad (\tau \geq 0)\) such that

\[
\lim_{\tau \to \infty} Z_r = A,
\]

\[
Z_r(t + n\tau) = Z_r(t) \quad \text{if} \quad t \geq 0, \quad n = 0, 1, 2, ...
\]

This theorem states that there is an operator \(Z_r \in X\) with semiperiodic \(Z_r(t)\) in any neighborhood of any \(A \in X\).

According to Devaney [3] a map \(F : X \to X\) on a metric space \(X\) has sensitive dependence on initial conditions if there exists \(\delta > 0\) such that, for any \(x \in X\) and any neighborhood \(V\) of \(x\), there exists \(y \in V\) and \(n \geq 0\) such that \(|F^{[n]}(x) - F^{[n]}(y)| > \delta\). Given \(x, y \in X\) and the map \(F^{[n]}\), the distance \(|F^{[n]}(x) - F^{[n]}(y)|\) is determined by the metric that defines the topology of Devaney’s \(X\). Typical examples allow scaling, so that the actual magnitude of \(\delta\) is not important. In our transcription \(\delta\) may be any positive number. Because our \(X\) is not a metric space, we have to introduce a distance between operators as an additional quantity. Since one would like the distance between \(A \in X\) and \(B \in X\) to be large when the difference between expectation values is large, regardless of the wave function \(f \in K^2\), we define

\[
|A - B| := \inf_{f \in K^2} \|f\|^{-2} \left| \|A^{1/2}f\|^2 - \|B^{1/2}f\|^2 \right|.
\]

Notice that \(|A - B|\) does not satisfy the triangle inequality, hence does not determine a metric.

**Theorem S.** (Sensitive dependence on initial conditions) Given \(A \in X\) and \(\delta > 0\), there is a net \(\{Z_{\delta r}\} \subset X \quad (\tau \geq 0)\) such that

\[
\lim_{\tau \to \infty} Z_{\delta r} = A,
\]

\[
\|A^{1/2}(t)f\|^2 - \|Z_{\delta r}^{1/2}(t)f\|^2 > \delta \|f\|^2 \quad \text{if} \quad t \geq \tau, \quad \text{for all} \quad f \in K^2.
\]
Assuming that $\tau$ and $\delta$ are sufficiently large, Theorem S says that the expectation values of $A(t)$ and $Z_{\delta \tau}(t)$ are very close at time $t = 0$, yet very different at times $t \geq \tau$.

According to Devaney’s definition, a map $F: X \rightarrow X$ is chaotic on $X$ if $F$ has sensitive dependence on initial conditions, is topologically transitive, and has a dense set of periodic points. Due to Theorems S, T, and P, the time evolution of operators $A(t) \in X$ is chaotic in the sense of Devaney.

Among Devaney’s conditions for chaos, sensitive dependence is probably best known, suggesting that it is the most important concept. In actual fact, if the map $F$ is continuous and $X$ is a metric space, the two topological conditions imply sensitive dependence [22]. Alternative definitions of chaos have been proposed by several authors. As shown in a recent review with comparison table [23], various definitions are not equivalent. On the other hand, all definitions are meant to capture the same set of essential features, and these have been retained in Theorems S, T, and P.

The wording of Theorems S, T, and P is the same as in Ref. [2], only the space $X$ and the time evolution $U(t)$ are different. The proofs in Ref. [2] construct operators $\tilde{Z}_\tau$ with suitable properties, then invoke the map $\gamma$ to find operators $Z_\tau$ that satisfy the theorems. The sole relation used in the construction of $\tilde{Z}_\tau$ is the counterpart in Ref. [2] of Eqs. (7.6) and (7.7) for the time evolution. Because this counterpart is the same as the current equations, the proofs in Ref. [2] may be copied unchanged. To illustrate how the theorems work, we quote the respective operators $\tilde{Z}_\tau$. Further details are in Ref. [2].

The proof of Theorem S uses

$$\tilde{Z}_{\delta \tau} := \tilde{A} + (1 + \tau)^{-1} + \delta Q(\tau).$$

The term $(1 + \tau)^{-1}$ guarantees that the form $\langle \tilde{Z}_{\delta \tau} f, g \rangle$ on $\Pi L^2$ with form domain $K^2$ is closed for every $\delta, \tau$. When $\tau$ is sufficiently large and $f$ is fixed, $\|Q(\tau)f\|$ is small so that $\langle \tilde{Z}_{\delta \tau} f, g \rangle$ is close to $\langle \tilde{A} f, g \rangle$. At time $t \geq \tau$ we have to examine $U^t Z_{\delta \tau} U(t)$. By Eqs. (7.1) and (7.6)

$$U^t(t) Q(\tau) U(t) = \begin{cases} Q(\tau - t) & \text{if } 0 \leq t \leq \tau \\ I & \text{if } 0 \leq \tau \leq t \end{cases}$$

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where $I$ is the identity operator. Hence
\[
|\langle \hat{A}(t)f, f \rangle - \langle \hat{Z}_\tau(t)f, f \rangle| > \delta \|f\|^2 \geq \delta \|f\|^2
\]
if $t \geq \tau$, for all $f \in K^2$.

Theorem S now follows easily. Moreover, we see that the error term $\delta \langle \hat{U}^\dagger(t)Q(\tau)U(t)f, f \rangle$ is a non-decreasing function of $t \geq 0$ which reaches its maximum $\delta \|f\|^2$ at time $t = \tau$.

The proof of Theorem T uses
\[
\hat{Z}_\tau := [1 - Q(\tau)]\hat{A}[1 - Q(\tau)] + U(\tau)\hat{B}U^\dagger(\tau) + (1 + \tau)^{-1}.
\]
Since $\|\|U^\dagger(\tau)f\|\| = \|\|Q(\tau)f\|\|$, the matrix element $\langle \hat{Z}_\tau f, g \rangle$ is close to $\langle \hat{A}f, g \rangle$ if $\tau$ is large.

On the other hand, at time $t = \tau$ the operator $\hat{A}$ acts on $[1 - Q(\tau)]U(\tau) = 0$ while $\hat{B}$ acts on $U^\dagger(\tau)U(\tau) = I$. As a result $\langle \hat{Z}_\tau(\tau)f, g \rangle$ is close to $\langle \hat{B}f, g \rangle$.

The proof of Theorem P uses
\[
\hat{Z}_\tau = \sum_{n=0}^{\infty} U(n\tau)[1 - Q(\tau)]\hat{A}[1 - Q(\tau)]U^\dagger(n\tau) + (1 + \tau)^{-1}.
\]
Write this in the form $\hat{Z}_\tau = \sum_{n=0}^{\infty} \hat{Z}_{\tau n} + (1 + \tau)^{-1}$. The sum converges in the strong operator topology. Since
\[
Q(\tau)U(n\tau) = U(n\tau) \quad \text{if } n \geq 1,
\]
the terms $\hat{Z}_{\tau n}$ with $n \geq 1$ are equal to $Q(\tau)\hat{Z}_{\tau n}Q(\tau)$, hence tend strongly to 0 if $\tau \to \infty$.

For any fixed $f$ and sufficiently large $\tau$ the norm $\|\|\hat{Z}_\tau f - \hat{Z}_{\tau 0} f\|\|$ is close to 0. Hence $\langle \hat{Z}_\tau f, g \rangle$ is close to $\langle \hat{A}f, g \rangle$.

Now examine $\sum_{n=0}^{n=\infty} U^\dagger(\tau)\hat{Z}_{\tau n}U(\tau)$. The term with $n = 0$ contains a factor $[1 - Q(\tau)]U(\tau)$.

Since this vanishes $\hat{Z}_{\tau 0}(\tau) = 0$. In the term with $n = 1$ the operator $\hat{A}$ acts on
\[
[1 - Q(\tau)]U^\dagger(\tau)U(\tau) = 1 - Q(\tau).
\]

Hence $\hat{Z}_{\tau 1}(\tau) = \hat{Z}_{\tau 0}$. By a similar reasoning $\hat{Z}_{\tau n}(\tau) = \hat{Z}_{\tau n-1}$ $(n = 1, 2, \ldots)$. Also $U^\dagger(\tau)(1 + \tau)^{-1}U(\tau) = (1 + \tau)^{-1}$. It follows that $\hat{Z}_\tau(\tau) = \hat{Z}_\tau$. The argument can be
repeated to show that $\tilde{Z}_r(t + m\tau) = \tilde{Z}_r(t)$ if $t \geq 0$ and $m = 0, 1, 2, \ldots$ Hence the operator $\tilde{Z}_r(t)$ is semiperiodic.

9. Notes and remarks

The chaos concept in this paper was developed with the idea in mind that $K$-maps and $K$-flows are classical dynamical systems with chaotic properties that are well understood. The proofs of Theorems S,T, and P are inspired by the symbolic dynamics used in chaos proofs for Bernoulli systems and other $K$-maps in which the dynamics can be represented by a shift on sequences of symbols [24-28]. Wave functions in this paper are assumed to belong to the space $K^2$ because the time evolution $\{U(t) \mid 0 \leq t < \infty\}$ on $K^2$ is unitarily equivalent to a semigroup of shift operators, as shown by Eq. (7.5). The semigroup on $K^2$ is probably our best substitute for a $K$-flow. By a result due to Sinai [29] the non-equilibrium part of a $K$-flow can be represented in terms of Hilbert spaces $N$ and $L^2(\mathbb{R}) \otimes N$ and a unitary group $\{V(t) \mid -\infty < t < \infty\}$ such that $\hat{g}(s) \in L^2(\mathbb{R}) \otimes N$ transforms according to

$$(V(t)\hat{g})(s) = \hat{g}(s - t). \quad (9.1)$$

The same canonical form is used extensively in the Lax-Phillips scattering theory for the wave equation [30].

The group \{V(t)\} in Eq. (9.1) has self-adjoint generator $-id/ds$ with spectrum $(-\infty, \infty)$. We want to contrast this with the semigroup \{U(t)\} on $K^2$ generated by $H$. To this end, we apply the reasoning developed in Ref. [2] to the resolvent $(H - \lambda)^{-1}$. By Eq. (5.6)

$$\langle (H - \lambda)^{-1}f, g \rangle = \sum_\alpha \langle k_\alpha^2 + E_\alpha - \lambda\rangle^{-1}f_\alpha, g_\alpha \rangle. \quad (9.2)$$

A function $(k_\alpha^2 + E_\alpha - \lambda)^{-1}f_\alpha$ belongs to $K^2_\alpha$ if and only if it has a square-integrable analytic continuation taking the $k_\alpha^2$-variable into the lower half-plane. It follows that each operator $(k_\alpha^2 + E_\alpha - \lambda)^{-1}$ on the right in Eq. (9.2) is bounded if and only if Im $\lambda > 0$. Hence $(H - \lambda)^{-1}$ is bounded if and only if Im $\lambda > 0$. The spectrum of $H$ on $K^2$ is the half-plane Im $\lambda \leq 0$. 

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The foregoing implies that $H$ cannot represent the energy on $K^2$. If there is an energy operator $\tilde{H}$ on $K^2$, it must have the same spectrum as $H$ on $\Pi L^2$. To identify $\tilde{H}$, we examine the form

$$q[f, g] := (H f, g) = \langle (1 + J^2)^{-1} H f, g \rangle$$

as a quadratic form on $K^2$ with form domain $\text{Dom} \ (q)$ consisting of all $f \in K^2$ with the property that $H f \in \Pi L^2$. Since $\text{Dom} \ (q)$ contains all $f \in K^2$ that can be written as

$$\sum_{\alpha} \Omega_{\alpha} \psi_{\alpha} f_{\alpha}$$

with functions $f_{\alpha}(k_{\alpha}, \omega) \in K^2_{\alpha}$ such that $k_{\alpha}^2 f_{\alpha}(k_{\alpha}, \omega) \in L^2(R^\nu)$, properties of the spaces $K^2_{\alpha}$ can be used to show that $\text{Dom} \ (q)$ is dense in $K^2$. Now consider the operator $(1 + J^2)^{-1} H$ on $K^2$ with domain $\text{Dom} \ (q)$. This operator is symmetric and bounded below, due to properties of $H$ on $\Pi L^2$. Hence the form $q$ has a well-defined closure $\tilde{q}$ [20, Chap. VI, Section 1]. The closed from $\tilde{q}$ determines a self-adjoint operator $\tilde{H}$ on $K^2$ satisfying

$$\tilde{q}[f, g] = \langle \tilde{H} f, g \rangle$$

for every $f \in \text{Dom} \ (\tilde{H}) \subset \text{Dom} \ (\tilde{q})$ and $g \in \text{Dom} \ (\tilde{q})$. The operator $\tilde{H}$ is the Friedrichs extension of $(1 + J^2)^{-1} H$, see [20, Chap. VI, Section 2]. Since $\tilde{H}$ is an extension, $\text{Dom}(\tilde{H}) \supset \text{Dom} \ (q)$. For $f, g \in \text{Dom} \ (q)$

$$(H f, g) = \langle \tilde{H} f, g \rangle.$$  

It is a significant property of the space $K^2$ that it gives rise to a time evolution whose generator $H$ differs from the energy operator $\tilde{H}$.

If $A \in X$ is a bounded operator on $\Pi L^2$, then $\tilde{A}$ defined by Eq. (6.3) equals $(1 + J^2)^{-1} A$. By the same token, if $\tilde{A} \in \tilde{X}$ is the identity operator on $K^2$, then $A^{1/2}$ equals $(1 + J^2)^{1/2}$, so that $A \in X$ equals $1 + J^2$. It follows that the terms $(1 + \tau)^{-1}$ in the operators $\tilde{Z}_r$ make unbounded contributions to the corresponding $Z_r$ on $\Pi L^2$. The terms in question are included to guarantee that the form $\langle \tilde{Z}_r f, g \rangle$ on $\Pi L^2$ with form domain $K^2$ is closed. It appears that we cannot avoid unbounded operators on $\Pi L^2$. To take advantage of the special properties of the space $K^2$, we have to allow operators such as $J$ whose domains are no larger than $K^2$. Such operators are not bounded on $\Pi L^2$. 

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10. Other chaos concepts

Since operators in $X$ have to be positive and are not necessarily bounded on $\Pi L^2$, the elements of $X$ do not give rise to an algebra. Hence the set of operators in this paper differs substantially from the operator algebras used by several authors to define non-commutative $K$-systems [31-34]. In an algebraic $K$-system [31,32,34] a sequence of operator-subalgebras replaces the $\sigma$-subalgebras of measurable sets that determine a classical $K$-system. An entropic $K$-system [33] is characterized in terms of its quantum dynamical entropy [35]. While these definitions are not equivalent [36], all authors report mixing behavior characteristic of chaos [31,32,37-42]. In cases where spectral properties were investigated [31,32,39,41] there was agreement with Eq. (9.1).

Examples include a quantum version of the Arnold cat map [39-42]. Several statistical-mechanics models were shown [43] to be entropic $K$-systems. Because classically the Kolmogorov-Sinai entropy being positive indicates chaos, it was proposed [44] that quantum chaos is related to a positive quantum dynamical entropy. It was found, however [44], that the quantum dynamical entropy vanishes in the case of a system of finitely many particles described by a density matrix with unitary time evolution. Such a system is therefore not chaotic from the dynamical-entropy point of view.

In typical papers on quantum chaos the question is not whether a system is chaotic in the sense of a mathematical definition. Starting from a chaotic classical system, one constructs a quantum counterpart and looks for characteristic features that would be different if the underlying classical system were integrable [45-49]. The distribution of energy-level spacings is an example. Computer calculations [50,51] show that the energy levels of a classically chaotic quantum billiard agree with a level-spacing distribution that is well established in nuclear physics [52] and in that context can be derived from random matrix theory [53]. If the billiard is classically integrable, a Poisson distribution applies [54]. That the classically chaotic case agrees with the predictions of random matrix theory has been explained [55] with the help of semiclassical path integrals that relate periodic orbits of a classical system to spectral properties of its quantum counterpart [46]. A more
recent argument [56] arrives at the same conclusion on the basis of a supersymmetric field theory [57].

Since a particle on a quantum billiard is confined to a bounded region in space, its energy spectrum is purely discrete. To investigate continuous spectra, several authors have developed scattering theories for classically chaotic systems in unbounded regions [58-62]. In this context random matrix theory was shown to apply to statistical properties of scattering amplitudes. These investigations are of practical interest because billiards with external leads are used as models for mesoscopic semiconductor devices [49,63].

Since there is strong evidence that random matrix theory applies to nuclear physics [52] it might apply as well to a system of \( N \) distinguishable particles. One would like to know whether the results of this paper can be related to quantum chaos as studied in the literature.

11. Density operators

Whether chaos is related to irreversible behavior is a question with a long history. Boltzmann [64] implicitly invoked the assumption of molecular chaos in the 1872 proof of his \( H \)-theorem. Since \( K \)-systems are both chaotic and reversible, it is clear that chaos is not sufficient for irreversible behavior, yet many authors believe that chaos at the microscopic level promotes macroscopic irreversibility. Essentially, however, this is an open problem.

It is shown in the following sections that states in the space \( K^2 \) give rise to irreversible behavior that can be characterized in terms of an increasing entropy. Although chaos as such does not play a role in the proof, there is a connection in that the space \( K^2 \) provides the framework to describe chaotic as well as irreversible properties of scattering systems.

Let \( \rho \) be a positive operator in the trace class on \( \mathbb{H} L^2 \) with time evolution \( \rho(t) \) defined by Eq. (1.1). Since the entropy \( S[\rho(t)] \) does not depend on \( t \), we want to replace \( \rho(t) \) by the density operator \( \sigma(t) \) defined by Eq. (1.5) and show that \( S[\sigma(t)] \) increases. With this objective in mind, we first examine the set of all positive operators \( R \) in the trace class
on $\Pi L^2$. Any $R$ in this set acts on $f \in \Pi L^2$ according to

$$Rf = \sum_n \mu_n \phi_n(f, \phi_n),$$

where $\{\phi_n\}$ is an orthonormal set on $\Pi L^2$ and the $\mu_n$ are positive numbers satisfying $\text{Tr } R = \sum_n \mu_n < \infty$.

Given the set $\{\phi_n\}$ on $\Pi L^2$, the set $\{(1 + J^2)^{-1/2} \phi_n\}$ is orthonormal on $K^2$. Hence $\tilde{\rho}$ acting on $f \in K^2$ as

$$\tilde{\rho} f = \sum_n \mu_n (1 + J^2)^{-1/2} \phi_n(f, (1 + J^2)^{-1/2} \phi_n)$$

(11.1)

belongs to the trace class on $K^2$, satisfying

$$\langle \text{Tr } \tilde{\rho} \rangle = \text{Tr } R.$$  (11.2)

Given $R$ and $\tilde{\rho}$, we now consider $\rho$ acting on $f \in \Pi L^2$ as

$$\rho f = \sum_n \mu_n (1 + J^2)^{-1/2} \phi_n(f, [1 + J^2]^{-1/2} \phi_n).$$  (11.3)

This operator satisfies

$$\rho = (1 + J^2)^{-1/2} R (1 + J^2)^{-1/2}.$$  (11.4)

It can be shown as in Ref. [1] that a density operator $\rho$ on $\Pi L^2$ is of the form (11.4) with some positive operator $R$ in the trace class if and only if $\rho$ and $J \rho$ belong to the trace class and $\rho J$ and $J \rho J$ have closures in the trace class. The operator $R$ is the closure of $(1 + J^2)^{1/2} \rho (1 + J^2)^{1/2}$, and

$$\text{Tr } R = \text{Tr } \rho + \text{Tr } J \rho J.$$  (11.5)

The relation (1.4) follows from Eqs. (11.2) and (11.5). Henceforth we simply refer to $J \rho J$ when we actually mean its closure, and similarly for operators such as $\rho J$ and $\rho (1 + J^2)^{1/2}$.

If $A$ is an operator in $\Gamma$, then $A^{1/2} (1 + J^2)^{-1/2}$ is bounded. Assuming that $\rho$ is of the form (11.4) we examine the operator

$$T := A^{1/2} (1 + J^2)^{-1/2} R [A^{1/2} (1 + J^2)^{-1/2}]^*.$$
Since $R$ belongs to the trace class, so does $T$. When applied to an element of $K^2$, the
operator $T$ acts as $A^{1/2} \rho A^{1/2}$. Hence $A^{1/2} \rho A^{1/2}$ is closable with closure $T$. In the following
we simply write $A^{1/2} \rho A^{1/2}$ when the closure is meant.

If $\rho$ is normalized so that $\text{Tr} \rho = 1$, then $\text{Tr} (A^{1/2} \rho A^{1/2})$ is the expectation value of the
observable $A$ in the state $\rho$. To show this, we assume that $\rho$ has orthonormal eigenvectors
$r_n$ with eigenvalues $\lambda_n$. If $\rho$ is of the form (11.4) each $r_n$ belongs to $K^2$. Hence for any
$f \in \Pi L^2$

\[ A^{1/2} \rho A^{1/2} f = \sum_n \lambda_n A^{1/2} r_n (f, A^{1/2} r_n). \]

It follows easily that

\[ \text{Tr} (A^{1/2} \rho A^{1/2}) = \sum_n \lambda_n (A^{1/2} r_n, A^{1/2} r_n). \]

The eigenvalue $\lambda_n$ is the probability that the system is in the state $r_n$. The expectation
value of $A$ in this state is $(A^{1/2} r_n, A^{1/2} r_n)$. Hence $\text{Tr} (A^{1/2} \rho A^{1/2})$ can be interpreted as
the expectation value of $A$ in the mixed state $\rho$.

Let $\{\chi_m\}$ be a complete orthonormal set on $\Pi L^2$. If we expand $\rho$ as in Eq. (11.3), the
expectation value of $A$ takes the form

\[ \text{Tr} (A^{1/2} \rho A^{1/2}) = \sum_m (A^{1/2} \rho A^{1/2} \chi_m, \chi_m) \]
\[ = \sum_m \sum_n \mu_n |(A^{1/2}[1 + J^2]^{-1/2} \phi_n, \chi_m)|^2 \]
\[ = \sum_n \mu_n ||A^{1/2}(1 + J^2)^{-1/2} \phi_n||^2 \]
\[ = \sum_n \mu_n ||(1 + J^2)^{-1/2} A^{1/2}(1 + J^2)^{-1/2} \phi_n||^2 \]
\[ = \sum_n \mu_n \langle A(1 + J^2)^{-1/2} \phi_n, (1 + J^2)^{-1/2} \phi_n \rangle = \langle \text{Tr} \tilde{A} \rho \rangle. \]

This generalized Eq. (6.4) and indicates that $\tilde{\rho}$ is the density operator on $K^2$ that matches
$\rho$ of the form (11.4) on $\Pi L^2$.

Our problem is that the entropy $S[\rho(t)]$ does not depend on $t$ if $\rho$ is a density operator
on $\Pi L^2$. The time evolution on $K^2$ replaces $(1 + J^2)^{-1/2} \phi_n$ by $U(t)(1 + J^2)^{-1/2} \phi_n$. As
a result \( \hat{\rho} \) is replaced by \( U(t)\hat{\rho}U^\dagger(t) \). Since \( U(t) \) is an isometry on \( K^2 \), the entropy
\(-\langle \text{Tr} \hat{\rho}(t) \ln \hat{\rho}(t) \rangle\) does not depend on \( t \geq 0 \) either. In the next section we therefore take a partial trace of \( \hat{\rho} \) as in Eq. (1.5). This defines the density operator \( \sigma(t) \) with increasing entropy \( S[\sigma(t)] \).

12. The density operator \( \sigma \)

If \( \rho \) is of the form (11.4) and \( t > 0 \), there is an operator \( R(t) \) in the trace class on \( \Pi L^2 \) such that \( \rho(t) \) satisfies Eq. (11.4) with \( R(t) \) instead of \( R \). Moreover,

\[
J \rho(t) J = \exp (i H t) W(t) J \rho J W^* (t) \exp (-i H t). \tag{12.1}
\]

These properties follow from Eq. (5.4). A formal proof with attention to all domain questions can be conducted as in Ref. [1]. Since \( W(t) \) is unitary, \( \text{Tr} J \rho(t) J \) does not depend on \( t \). Hence \( \text{Tr} \sigma(t) \) does not depend on \( t \).

While \( \text{Tr} \rho^2(t) \) does not depend on \( t \) either, \( \text{Tr} \sigma^2(t) \) is a decreasing function of \( t \geq 0 \),

\[
\text{Tr} \sigma^2(s) > \text{Tr} \sigma^2(t) \quad \text{if} \quad 0 \leq s < t. \tag{12.2}
\]

To show this, we deduce from Eq. (5.5) that

\[
\Omega_\alpha \Omega^*_\alpha J^{1/2} \exp (-i H t) f = W^{1/2}(t) \Omega_\alpha \exp (-k^2_\alpha t) J^{1/2} \Omega^*_\alpha f,
\]

for every \( f \in K^2 \). This relation can be used to prove that

\[
\Omega_\alpha \Omega^*_\alpha J^{1/2} \rho(t) J^{1/2} \Omega_\beta \Omega^*_\beta
\]

\[
= W^{1/2}(t) \Omega_\alpha \exp (-k^2_\alpha t) T_{\alpha \beta} \exp (-k^2_\beta) \Omega^*_\beta [W^{1/2}(t)]^*,
\]

where we have used the abbreviation

\[
T_{\alpha \beta} := J^{1/2} \Omega^*_\alpha \rho \Omega_\beta J^{1/2}.
\]

As in Ref. [1]

\[
\text{Tr} \rho(t) J \rho(t) J = \text{Tr} [J^{1/2} \rho(t) J^{1/2}] [J^{1/2} \rho(t) J^{1/2}]. \tag{12.3}
\]

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Let us define
\[ \Pi_n := \sum_{\alpha \leq n} \Omega_\alpha \Omega_\alpha^*. \] (12.4)

Even if the number of channels is not finite, \( \Pi_n \) tends strongly to the identity operator on \( \Pi L^2 \) as \( n \to \infty \). Hence it follows from known properties of the trace class [65, Chap. III, Theorem 6.3] that
\[ \text{Tr} \, \Pi_n [J^{1/2} \rho(t) J^{1/2}] \Pi_n [J^{1/2} \rho(t) J^{1/2}] \Pi_n \] (12.5)
tends to the right-hand side of Eq. (12.3) when \( n \to \infty \). We want to prove that \( \text{Tr} \, \rho(t) J \rho(t) J \) is a decreasing function of \( t \). For this it is sufficient to show that
\[ \text{Tr} \, \Omega_\alpha \exp (-k^2_\alpha t) T_{\alpha \beta} \exp (-k^2_\beta t) \Omega_\beta^* \Omega_\beta \exp (-k^2_\beta t) T_{\beta \alpha} \exp (-k^2_\alpha t) \Omega_\alpha^* \] (12.6)
is decreasing for every fixed \( \alpha, \beta \).

The projection operator \( \Omega_\beta^* \Omega_\beta \) commutes with \( \exp (-k^2_\beta t) \) and with the operator \( J^{1/2} \_ \beta \) included in \( T_{\beta \alpha} \). Hence it can be absorbed in \( T_{\beta \alpha} \). With a similar procedure for \( \Omega_\alpha^* \Omega_\alpha \), it follows that expression (12.6) is equal to
\[ \text{Tr} \, \exp (-k^2_\alpha t) T_{\alpha \beta} \exp (-2k^2_\beta t) T_{\beta \alpha} \exp (-k^2_\alpha t). \]

In an obvious notation, we denote this quantity by \( \text{Tr} \, \Theta_{\alpha \beta \alpha}(t) \). It is equal to \( \text{Tr} \, \Theta_{\beta \alpha \beta}(t) \).

Now suppose \( 0 \leq s < t \) and examine
\[ \text{Tr} \, \Theta_{\alpha \beta \alpha}(s) + \text{Tr} \, \Theta_{\beta \alpha \beta}(s) - \text{Tr} \, \Theta_{\alpha \beta \alpha}(t) - \text{Tr} \, \Theta_{\beta \alpha \beta}(t) \]
\[ = \text{Tr} \, \exp (-k^2_\alpha s) T_{\alpha \beta} [\exp (-2k^2_\beta s) - \exp (-2k^2_\alpha s)] T_{\beta \alpha} \exp (-k^2_\alpha s) \]
\[ + \text{Tr} \, \exp (-k^2_\beta s) T_{\beta \alpha} [\exp (-2k^2_\alpha s) - \exp (-2k^2_\alpha s)] T_{\alpha \beta} \exp (-k^2_\beta s) \] (12.7)
\[ + \text{Tr} \, \exp (-k^2_\alpha t) T_{\alpha \beta} [\exp (-2k^2_\beta s) - \exp (-2k^2_\beta s)] T_{\beta \alpha} \exp (-k^2_\alpha t) \]
\[ + \text{Tr} \, \exp (-k^2_\beta t) T_{\beta \alpha} [\exp (-2k^2_\alpha s) - \exp (-2k^2_\alpha s)] T_{\alpha \beta} \exp (-k^2_\beta t). \]

If \( s < t \), the operators \( \exp (-2k^2_\beta s) - \exp (-2k^2_\beta s) \) and \( \exp (-2k^2_\alpha s) - \exp (-2k^2_\alpha s) \) are strictly positive. Since \( T_{\beta \alpha} = T_{\alpha \beta}^* \), expression (12.7) vanishes if and only if \( T_{\alpha \beta} = 0 \). If
$T_{\alpha \beta} \neq 0$, the traces in Eq. (12.7) are positive. Repeating this reasoning for all $\alpha, \beta$, we see that expression (12.5) is a decreasing function of $t$ unless $T_{\alpha \beta} = 0$ for all $\alpha, \beta \leq n$. Since any positive $\rho$ gives rise to some non-vanishing operators $T_{\alpha \beta}$, it follows with Eq. (12.3) that

$$\text{Tr} \rho(s) J \rho(s) J > \text{Tr} \rho(t) J \rho(t) J \quad \text{if} \quad 0 \leq s < t,$$

whenever $\rho$ is of the form (11.4) with a positive trace-class operator $R$.

By Eq. (12.1) $\text{Tr} [J \rho(t) J] [J \rho(t) J]$ does not depend on $t$. Hence

$$\text{Tr} \sigma^2(t) = \text{Tr} \rho^2 + \text{Tr} \rho(t) J \rho(t) J + \text{Tr} J \rho(t) J \rho(t) + \text{Tr} (J \rho J)(J \rho J).$$

Two terms on the right do not depend on $t$ while the remaining two are decreasing. Hence $\text{Tr} \sigma^2(t)$ is decreasing, as we wanted to show.

Let $\nu(t)$ be a positive operator satisfying $\text{Tr} \nu(t) = 1$. The quantities

$$S_\alpha[\nu(t)] := (1 - \alpha)^{-1} \ln \text{Tr} [\nu(t)]^\alpha \quad (\alpha > 0; \alpha \neq 1)$$

are called Rényi entropies or $\alpha$-entropies [66, Definition 2.2.2, Remark 2.2.5; 67, Eq. (7.14)]. Taking $\alpha = 2$ and $\nu(t) = \sigma(t)/\text{Tr} \sigma(t)$, we have an increasing Rényi entropy $S_2[\sigma(t)/\text{Tr} \sigma(t)]$.

13. The entropy

If $T$ is any positive compact operator, we denote by $\gamma_n(T)$ the $n$th largest eigenvalue of $T$, counting multiplicity. If $\rho$ and $J \rho J$ belong to the trace class

$$\sum_n \gamma_n(\rho) < \infty, \quad \sum_n \gamma_n(J \rho J) < \infty. \quad (13.1)$$

With a view to the entropy, we define

$$s(\gamma) := \begin{cases} -\gamma \ln \gamma & \text{if } \gamma > 0 \\ 0 & \text{if } \gamma = 0 \end{cases}$$

and assume

$$S(\rho) := \sum_n s[\gamma_n(\rho)] < \infty, \quad S(J \rho J) := \sum_n s[\gamma_n(J \rho J)] < \infty. \quad (13.2)$$

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Due to Eq. (5.4) and the fact that \( \exp (i H t) \) and \( W(t) \) are unitary, \( S[\rho(t)] \) and \( S[J \rho(t) J] \) do not depend on \( t \).

By general entropy inequalities \( [68] \)

\[
S[\sigma(t)] \leq S[\rho(t)] + S[J \rho(t) J]
\]

with equality if and only if

\[
\rho(t) J \rho(t) J = 0, \quad J \rho(t) J = 0.
\]

The sum \( S(\rho) + S(J \rho J) \) is finite by Eq. (13.2). It is an upper bound for \( S[\sigma(t)] \) by Eq. (13.3). We claim that

\[
\lim_{t \to \infty} S[\sigma(t)] = S(\rho) + S(J \rho J).
\]

Typically, \( \rho J \rho J \neq 0 \), hence \( S[\sigma(t)] \) has to increase, approaching its least upper bound as \( t \to \infty \).

The relations (13.3) and (13.4) are compatible due to the fact that \( \rho(t) J \rho(t) J \) and its adjoint \( J \rho(t) J \rho(t) \) tend to 0 in the trace norm as \( t \to \infty \). To show this, we denote the trace norm of an operator \( T \) in the trace class by \( ||T||_1 \). By Eq. (5.4)

\[
||J \rho(t) J [\Pi_n \rho(t) - \rho(t)]||_1
= ||\exp (i H t) W(t) J \rho J W^*(t) \exp (-2i H t) (\Pi_n \rho - \rho) \exp (i H t)||_1
\leq ||J \rho J|| ||\Pi_n \rho - \rho||_1,
\]

where \( \Pi_n \) is the projection defined by Eq. (12.4). Since the right-hand side tends to 0 as \( n \to \infty \), uniformly in \( t \), it is sufficient to show that \( J \rho(t) J \Omega_\alpha \Omega^*_\alpha \rho(t) \) tends to 0 in the trace norm as \( t \to \infty \), for every fixed \( \alpha \). Since \( J^{1/2} \) commutes with \( \Omega_\alpha \Omega^*_\alpha \), it follows with Eq. (5.5) that

\[
J \rho(t) J \Omega_\alpha \Omega^*_\alpha \rho(t) = J \rho(t) J^{1/2} \Omega_\alpha \Omega^*_\alpha J^{1/2} \rho(t)
= \exp (i H t) W(t) J \rho \Omega_\alpha J^{1/2} \exp (-2k^2_\alpha t) \Omega^*_\alpha \rho \exp (i H t)
= \exp (i H t) W(t) J \rho J^{1/2} \Omega_\alpha \exp (-2k^2_\alpha t) \Omega^*_\alpha J^{1/2} \rho \exp (i H t).
\]

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The operator \( \exp\left(-2i\alpha^2 t\right) \) tends strongly to 0 as \( t \to \infty \). Since \( \Omega^*_\alpha J^{1/2} \rho \) belongs to the trace class and \( J\rho J^{1/2}\Omega^*_\alpha \) is bounded, the expression on the right in Eq. (13.5) tends to 0 in the trace norm, as we wanted to show.

The proof of Eq. (13.4) rests on a fundamental concept of physics. To explain this, we have to go back to the dilation operator \( D_\nu \) of Section 4. Let \( P_{\nu+} \) and \( P_{\nu-} \) be the spectral projections onto the subspaces of \( L^2(\mathbb{R}^\nu) \) in which \( D_\nu \) is positive and negative, respectively. The important equations are [69]

\[
\lim_{t \to \infty} \|P_{\nu-} \exp\left(-i k^2 t\right) f\| = 0,
\]

\[
\lim_{t \to -\infty} \|P_{\nu+} \exp\left(-i k^2 t\right) f\| = 0
\]

for every \( f(k) \in L^2(\mathbb{R}^\nu) \). If \( f \in K^2_\nu \), it follows with Eq. (4.5) that

\[
\lim_{t \to \infty} \|P_{\nu+} J_\nu \exp\left(-i k^2 t\right) f\| = 0.
\]

Hence \( \exp\left(-i k^2 t\right) f \) and \( J_\nu \exp\left(-i k^2 t\right) f \) become mutually orthogonal as \( t \to \infty \).

The dilation operator is the quantum analogue of \( \mathbf{x} \cdot \mathbf{k} \), where \( \mathbf{x} \) represents the position relative to the center of mass and \( \mathbf{k} \) is proportional to the momentum of a multiparticle system. One expects that \( \mathbf{x} \cdot \mathbf{k} \) was negative in the distant past and will be positive in the remote future. This is confirmed by Eq. (13.6). It is the irreversible aspect of the time evolution that causes \( S[\sigma(t)] \) to tend to its least upper bound.

The generalization to a scattering system goes as follows. Depending on the channel being considered, \( D_\nu \) is denoted by \( D_\alpha \), giving rise to the generalized dilation operator

\[
D := \sum_\alpha \Omega_\alpha D_\alpha \Omega^*_\alpha.
\]

For any \( f \in K^2 \), it is easy to show that \( Jf = \exp\left(-\pi D/2\right) f \). The projection operators \( P_{\nu \pm} \) are denoted by \( P_{\alpha \pm} \). They determine orthogonal projections

\[
P_{\pm} := \sum_\alpha \Omega_\alpha P_{\alpha \pm} \Omega^*_\alpha.
\]

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satisfying \( P_+ + P_- = \sum_\alpha \Omega_\alpha \Omega_\alpha^* = \Pi \). By Eq. (5.1) and the intertwining relation (3.5), any \( f \in \Pi L^2 \) satisfies

\[
\lim_{t \to \infty} \| P_- \exp (-iHt) f \| = 0,
\]

(13.7)

\[
\lim_{t \to -\infty} \| P_+ \exp (-iHt) f \| = 0.
\]

If \( f \in K^2 \), it follows from Eq. (5.4) that

\[
\lim_{t \to \infty} \| P_+ J \exp (-iHt) f \| = 0.
\]

(13.8)

Given the interpretation of the dilation operators \( D_\alpha \), Eq. (13.7) expresses the fact that clusters in a scattering experiment moved in the direction of the center of mass in the distant past and will move away from the center of mass in the remote future.

The above relations are the key ingredients in proving Eq. (13.4). Since the proof is the same as in Ref. [1], we sketch the general idea, referring to Ref. [1] for details.

The first step defines

\[
\pi_+(t) := P_+ \rho(t) P_+, \quad \pi_-(t) := P_- J \rho(t) J P_-
\]

and shows that

\[
\lim_{t \to \infty} \| \pi_+(t) + \pi_-(t) - \sigma(t) \|_1 = 0.
\]

It follows that

\[
\lim_{t \to \infty} \gamma_k [\pi_+(t) + \pi_-(t)] = \lim_{t \to \infty} \gamma_k [\sigma(t)].
\]

By a separate argument

\[
\lim_{t \to \infty} \gamma_k [\pi_+(t) + \pi_-(t)] = \lambda_k,
\]

where \( \lambda_k (k = 1, 2, \ldots) \) is the \( k \)th largest number, counting multiplicity, in the set consisting of all non-vanishing eigenvalues \( \gamma_n (\rho) \) and \( \gamma_m (J \rho J) \) \((m, n = 1, 2, \ldots)\).

We want to compare the entropies

\[
S(\rho) + S(J \rho J) = \sum_k s(\lambda_k) = \sum_k \lim_{t \to \infty} s(\gamma_k [\sigma(t)])
\]

(13.9)

and

\[
\lim_{t \to \infty} S[\sigma(t)] = \lim_{t \to \infty} \sum_k s(\gamma_k [\sigma(t)]).
\]

(13.10)
To prove that $S[\sigma(t)]$ tends to $S(\rho) + S(J\rho J)$, it is sufficient to show that the limit and the summation in Eq. (13.10) may be interchanged. In this context, it can be shown that

$$0 \leq s \{ \gamma_{k+1}[\sigma(t)] \} \leq s(2\lambda_k)$$

whenever $2\lambda_k \leq 1/e$. Since $\sum_k s(2\lambda_k)$ converges absolutely by Eqs. (13.1) and (13.2), the right-hand sides of Eqs. (13.9) and (13.10) are equal by the dominated convergence theorem. This completes the proof of Eq. (13.4). The result is summarized in the following theorem.

**Theorem E.** (Entropy increase) If $\rho$ is of the form (11.4), $\sigma(t)$ and $S[\sigma(t)]$ are defined by Eqs. (1.5) and (1.2), and Eq. (13.2) is satisfied, the entropy $S[\sigma(t)]$ tends to its maximum possible value $S(\rho) + S(J\rho J)$ as $t \to \infty$.

### 14. Reconstructing the density operator $\rho$

With the help of the Mellin transform, it is possible to recover $\rho$ when $\sigma$ is known. For the reconstruction procedure to be meaningful, $\sigma$ has to be of the form $\rho + J\rho J$ with a positive trace-class operator $\rho$ satisfying Eq. (11.4). It was shown in Ref. [1] that not all positive operators in the trace class satisfy the conditions on $\sigma$. In particular, there are examples of positive $\tau$ in the trace class that would yield non-positive $\rho$. This paper is not meant for such operators $\tau$. They cannot occur as operators $\sigma$.

Given $\rho$, let us first examine $\Omega_\alpha^* \rho \Omega_\beta$. Since $\rho$ belongs to the trace class on $\Pi L^2$, both $\rho$ and $\Omega_\alpha^* \rho \Omega_\beta$ are integral operators. In the notation of Eq. (5.1), the integral kernel of $\Omega_\alpha^* \rho \Omega_\beta$ is of the form

$$\psi_\alpha(k'_\alpha) \rho_{\alpha\beta}(k_\alpha; l_\beta) \tilde{\psi}_\beta(l'_\beta).$$

It is convenient to write $\Omega_\alpha^* \rho \Omega_\beta = \psi_\alpha \rho_{\alpha\beta} \tilde{\psi}_\beta$. Expressing $k_\alpha, l_\beta$ in terms of spherical polar coordinates replaces $\rho_{\alpha\beta}(k_\alpha; l_\beta)$ by $\rho_{\alpha\beta}(k_\alpha, \omega_\alpha; l_\beta, \omega'_\beta)$. The Mellin transform $M_\alpha$ acting on $k_\alpha$ commutes with $\tilde{\psi}_\alpha(k'_\alpha)$. Henceforth we omit the variable $k'_\alpha$. Thus

$$M_\alpha \Omega_\alpha^* \rho \Omega_\beta M_\beta^{-1} = \psi_\alpha M_\alpha \rho_{\alpha\beta} M_\beta^{-1} \tilde{\psi}_\beta = \psi_\alpha \rho_{\alpha\beta} \tilde{\psi}_\beta$$

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has integral kernel
\[
\psi_\alpha \rho^\#_{\alpha \beta}(u, \omega_\alpha; v, \omega'_\beta) \tilde{\psi}_\beta. \tag{14.1}
\]
By Eq. (4.2) \( M_\alpha J_\alpha M_\alpha^{-1} \) acts as multiplication by \( \exp(-\pi u/2) \). Hence \( M_\alpha J_\alpha \Omega_\alpha^* \rho \Omega_\beta J_\beta M_\beta^{-1} \) has integral kernel
\[
\psi_\alpha \exp \left(-\pi u/2\right) \rho^\#_{\alpha \beta}(u, \omega_\alpha; v, \omega'_\beta) \exp \left(-\pi v/2\right) \tilde{\psi}_\beta. \tag{14.2}
\]
Adding expressions (14.1) and (14.2) shows that \( M_\alpha \Omega_\alpha^* \sigma \Omega_\beta M_\beta^{-1} \) has integral kernel
\[
\psi_\alpha \left[1 + \exp \left[-\pi(u + v)/2\right]\right] \rho^\#_{\alpha \beta}(u, \omega_\alpha; v, \omega'_\beta) \tilde{\psi}_\beta. \tag{14.3}
\]
Conversely, suppose \( \sigma \) is known. Construct the integral operator \( M_\alpha \Omega_\alpha^* \sigma \Omega_\beta M_\beta^{-1} \). By the reasoning for \( \rho \), the integral kernel is of the form
\[
\psi_\alpha \sigma^\#_{\alpha \beta}(u, \omega_\alpha; v, \omega'_\beta) \tilde{\psi}_\beta.
\]
This quantity must be equal to expression (14.3). Hence
\[
\rho^\#_{\alpha \beta}(u, \omega_\alpha; v, \omega'_\beta) = \left[1 + \exp \left[-\pi(u + v)/2\right]\right]^{-1} \sigma^\#_{\alpha \beta}(u, \omega_\alpha; v, \omega'_\beta), \tag{14.4}
\]
showing that there is a bounded transformation taking \( \sigma^\#_{\alpha \beta} \) into \( \rho^\#_{\alpha \beta} \).

Once \( \rho^\#_{\alpha \beta} \) is known, the inverse Mellin transform determines \( M_\alpha^{-1} \rho^\#_{\alpha \beta} M_\beta = \rho_{\alpha \beta} \), hence \( \Omega_\alpha^* \rho \Omega_\beta \). Denoting \( \sum_{\alpha \leq n} \Omega_\alpha^* \Omega_\alpha \) by \( \Pi_n \) as in Eq. (12.4), we can find \( \Pi_n \rho \Pi_n \). This quantity tends to \( \rho \) in the trace norm as \( n \to \infty \) [65, Chap. III, Theorem 6.3]. Hence, even if the number of channels is infinite, \( \sigma \) completely determines \( \rho \).

If \( \rho \) is of the form (11.4) then \( \rho(t) \) is of this form for all \( t \geq 0 \). Since neither the transformation taking \( \rho \) into \( \sigma \), nor the Mellin transform depends on \( t \), the reasoning that proved Eq. (14.4) can be repeated for every \( t > 0 \). Summarizing, we have a linear transformation \( L : \sigma(t) = L \rho(t) \) whose domain consists of all operators \( \rho \) of the form (11.4). This operator is invertible. Defined on the range of \( L \), the inverse is a linear operator \( L^{-1} : \rho(t) = L^{-1} \sigma(t) \).
15. Observables in the $\sigma$-representation

If $T$ is a bounded self-adjoint operator, its expectation value is $\text{Tr} T \rho(t)$. In this section we construct a set of operators $(TL^{-1})_{\beta\alpha}$ with the property that

$$\lim_{n \to \infty} \sum_{\alpha, \beta \leq n} \text{Tr} \Omega_{\beta}(TL^{-1})_{\beta\alpha} \Omega^*_\alpha \sigma(t) = \text{Tr} T \rho(t), \quad (15.1)$$

provided $\sigma(t)$ is of the form (1.5). This result means that $\sigma(t)$ can be used as a density operator to calculate expectation values of bounded observables.

We first consider

$$(M_{\beta} \Omega_{\beta}^* T \Omega_{\alpha} M_{\alpha}^{-1})(M_{\alpha} \Omega_{\alpha}^* \rho \Omega_{\beta} M_{\beta}^{-1})$$

$$= (M_{\beta} \Omega_{\beta}^* T \Omega_{\alpha} M_{\alpha}^{-1}) (\psi_{\alpha}^{\#} \tilde{\psi}_{\beta})$$

$$= (M_{\beta} \Omega_{\beta}^* T \Omega_{\alpha} M_{\alpha}^{-1}) \{1 + \exp \left[ -\pi (u + v)/2 \right] \}^{-1} \psi_{\alpha}^{\#} \tilde{\sigma}_{\alpha\beta} \psi_{\beta}, \quad (15.2)$$

where $u$ and $v$ are variables in the integral kernel of $\tilde{\sigma}_{\alpha\beta}$, as in Eq. (14.4). Now we define

$$(TL^{-1})^{\#}_{\beta\alpha} := (M_{\beta} \Omega_{\beta}^* T \Omega_{\alpha} M_{\alpha}^{-1}) \{1 + \exp \left[ -\pi (u + v)/2 \right] \}^{-1}. \quad (15.3)$$

This is an operator that acts on trace-class operators with kernels $\psi_{\alpha} \tilde{\sigma}_{\alpha\beta}(u, \omega_{\alpha}; v, \omega_{\beta}) \tilde{\psi}_{\beta}$.

It cannot act on elements of $\Pi L^2$. We can define

$$(TL^{-1})_{\beta\alpha} := M_{\beta}^{-1} (TL^{-1})^{\#}_{\beta\alpha} M_{\alpha}. \quad (15.4)$$

This operator acts on trace-class operators

$$M_{\alpha}^{-1} \psi_{\alpha} \tilde{\sigma}_{\alpha\beta} \tilde{\psi}_{\beta} M_{\beta} = \psi_{\alpha} \sigma_{\alpha\beta} \tilde{\psi}_{\beta} = \Omega_{\alpha}^* \sigma \Omega_{\beta}. \quad (15.4')$$

Due to Eqs. (15.2)-(15.4)

$$(TL^{-1})_{\beta\alpha} \Omega_{\alpha}^* \sigma \Omega_{\beta} = \Omega_{\beta}^* T \Omega_{\alpha} \Omega_{\alpha}^* \rho \Omega_{\beta}. \quad (15.5)$$

Hence

$$\text{Tr} \Omega_{\beta} (TL^{-1})_{\beta\alpha} \Omega_{\alpha}^* \sigma = \text{Tr} \Omega_{\beta} \Omega_{\alpha}^* T \Omega_{\alpha} \Omega_{\alpha}^* \rho.$$
Summing over $\alpha, \beta \leq n$ on the right gives $\text{Tr} \Pi_n T \Pi_n \rho$. In terms of the trace norm

$$||\Pi_n T \Pi_n \rho - T \rho||_1 = ||\Pi_n T \Pi_n \rho - \Pi_n T \rho + \Pi_n T \rho - T \rho||_1$$

$$\leq ||T|| ||\Pi_n \rho - \rho||_1 + ||\Pi_n T \rho - T \rho||_1.$$ 

Since $\Pi_n$ tends strongly to the identity on $\Pi L^2$ as $n \to \infty$, each term on the right tends to 0 as $n \to \infty$. Hence

$$\lim_{n \to \infty} |\text{Tr} \Pi_n T \Pi_n \rho - \text{Tr} T \rho| \leq \lim_{n \to \infty} ||\Pi_n T \Pi_n \rho - T \rho||_1 = 0.$$

This proves Eq. (15.1) at time $t = 0$. The proof can be repeated at all later times.

The foregoing can be generalized to unbounded operators $A \in \Gamma$ by taking advantage of the fact that $A^{1/2}(1 + J^2)^{-1/2}$ is bounded. Instead of $\text{Tr} T \rho$ we consider $\text{Tr} (A^{1/2} \rho A^{1/2})$. If $\rho$ is of the form (11.4) it is not difficult to prove that

$$\sum_{\alpha, \beta \leq n} \text{Tr} A^{1/2}(1 + J^2)^{-1/2} \Omega_\alpha \Omega^*_\beta R \Omega_\alpha \Omega^*_\beta [A^{1/2}(1 + J^2)^{-1/2}]^*$$

(15.5) 

tends to $\text{Tr} (A^{1/2} \rho A^{1/2})$ as $n \to \infty$. We want to express this quantity in terms of $\sigma$ instead of $R$ or $\rho$.

It is easy to see that

$$(1 + J^2)^{-1/2} \Omega_\alpha \Omega^*_\alpha = \Omega_\alpha \Omega^*_\alpha (1 + J^2)^{-1/2} = \Omega_\alpha (1 + J^2)^{-1/2} \Omega^*_\alpha.$$ 

Hence define

$$(AL^{-1})^{1/2}_\alpha := A^{1/2} \Omega_\alpha M^{-1}_\alpha \{1 + \exp[-\pi(u + v)/2]\}^{-1/2} M_\alpha.$$ 

This operator is not bounded, but the range of $\Omega^*_\alpha \sigma \Omega_\beta$ is in its domain. The closure of

$$(AL^{-1})^{1/2}_\alpha \Omega^*_\alpha \sigma \Omega_\beta [AL^{-1})^{1/2}_\beta]^*$$

is equal to the operator in expression (15.5). Taking the trace and summing over $\alpha, \beta$ gives $\text{Tr} (A^{1/2} \rho A^{1/2})$ as desired.
16. The Prigogine program

It has long been advocated by Prigogine and coworkers [6,7] that irreversible behavior originates at the microscopic level. Their strategy for proving this calls for a transformation $\Lambda$ that breaks the time-reversal symmetry in the sense that $\Lambda \rho(t)$ is defined only for $t \geq 0$ and evolves in time according to a semigroup. In quantum mechanics the quantity

$$\Omega(t) := \text{Tr} \rho^*(t) \Lambda^* \Lambda \rho(t) \quad (t \geq 0)$$

should be a decreasing function of $t$. The classical counterpart of $\Omega(t)$ is obtained if the trace in Eq. (16.1) is replaced by integration over the phase space.

It was predicted early on that any $\Lambda$-operator in quantum mechanics would have to act on operators and could not act on the elements of the Hilbert space on which $\rho$ operates [70]. The authors referred to a superoperator. They also observed that one would have to introduce a time evolution that is not generated by the Hamiltonian [70]. Our transformation $\rho(t) \rightarrow L \rho(t) = \sigma(t)$ agrees with the above requirements. The operator $\sigma(t)$ is defined for $t \geq 0$ only. Due to Eq. (1.1) for $\rho(t)$ and Eq. (12.1) for $J \rho(t) J$, the time evolution of $\sigma(t)$ is described by a semigroup. To define $\sigma$, we have to start from an operator $\rho$ on $\Pi L^2$, an element $f \in \Pi L^2$ will not do. This is the superoperator aspect. According to Eq. (12.2) $\text{Tr} \sigma^2(t)$ is a monotone decreasing function of $t$, as is $\Omega(t)$ in Eq. (16.1). Since $\text{Tr} \sigma(t)$ is the same as $\langle \text{Tr} \tilde{\rho}(t) \rangle$, the Prigogine observation about the time evolution agrees with the discussion in Section 9, which shows that the time evolution of $\tilde{\rho}(t)$ on $K^2$ is not generated by the Hamiltonian $\tilde{H}$ on $K^2$.

In the early years of the Prigogine program, $\Lambda$-operators were constructed explicitly for several classical dynamical systems, including the baker map [71] and other Bernoulli systems [72], as well as $K$-flows [73]. The focus has since shifted to large non-integrable Hamiltonian systems with many resonances. Since this part of the program is not directly related to the present paper, we merely refer to recent papers on classical [74] and quantum systems [75]. A brief overview of earlier work by Prigogine and coworkers can be found in Ref. [1]. There are no previous results on $\Lambda$-operators for $N$-particle quantum systems.
The classical dynamical systems for which \( \Lambda \)-operators were constructed have a compact phase space and a uniform equilibrium density \( \rho_0 = 1 \). The norm \( \| \Lambda \rho(t) - 1 \| \) is a monotone decreasing function of \( t \) which tends to 0 as \( t \to \infty \), for all initial densities \( \rho(0) \neq 1 \). This is necessary and sufficient in order that the entropy associated with \( \Lambda \rho(t) \) is a non-decreasing function of \( t \) that tends to its maximal value of 0 as \( t \to \infty \) [4; 5, Corollary 7.8].

If a classical dynamical system allows an invertible \( \Lambda \)-operator, it has to be mixing [76]. If \( \Lambda \) is a projection and \( \| \Lambda \rho(t) - 1 \| \) is monotone decreasing to 0, it is necessary [77,78] and sufficient [79] that the underlying invertible system is a \( K \)-system.

The inverse problem of finding the \( K \)-system when \( \Lambda \rho(t) \) is known, was investigated in recent papers [80-82]. With a slight change of notation, the authors considered measure preserving Markov semigroups \( \{ M_t | 0 \leq t < \infty \} \) satisfying \( \| M_t \rho - 1 \| \to 0 \) as \( t \to \infty \), with the understanding that \( M_t \Lambda \rho = \Lambda \rho(t) \) in our earlier notation. Their question was whether the semigroup \( \{ M_t \} \) can be lifted to an invertible time evolution. Assuming that \( \Lambda \) was a projection [80], they showed that the semigroup \( \{ M_t \} \) is the Frobenius-Perron semigroup of an exact dynamical system. Let this be \( \{ S_t \} \) with phase space \( Y \). By a result due to Rohlin [83], the system \( \{ S_t \} \) is a factor of a \( K \)-system \( \{ K_t \} \) with phase space \( X \). This means that there is a transformation \( F : X \to Y \) such that \( S_t \circ F = F \circ K_t \).

The Rohlin theory provides a natural extension mechanism by which the \( K \)-system \( \{ K_t \} \) was constructed explicitly [80].

Since the \( \Lambda \)-operators referred to above [71-73] are invertible, the assumption that \( \Lambda \) is a projection does not cover all possibilities. With more general methods than used in Ref. [80] it was shown [81,82] that any measure preserving Markov semigroup can arise as a projection of a \( K \)-system, be it that the projection is not necessarily the \( \Lambda \)-operator that was used to find the Markov semigroup in the first place.

The prevalence of \( K \)-systems in the foregoing suggest, that a \( \Lambda \)-operator for a classical dynamical system is most likely to exist when the time evolution can be represented by a group of shift operators \( \{ V(t) | -\infty < t < \infty \} \) as in Eq. (9.1). In quantum mechanics
the semigroup \( \{U(t) | 0 \leq t < \infty\} \) is our best analogue of \( \{V(t)\} \). Although the Rohlin theory does not apply to this situation, it suggests the following point of view.

Given \( \rho \) and \( \tilde{\rho} \) satisfying Eqs. (11.3) and (11.1), and \( f, g \in K^2 \),

\[
\langle \tilde{\rho} f, g \rangle = (\rho f, g) + (\rho J^2 f, g) + (J \rho f, J g) + (J \rho J^2 f, J g).
\]

To express this equation in a different form, we define the two-component vector \( \tilde{f} \) with components \( \tilde{f}_0 := f, \tilde{f}_1 := Jf \), and inner product

\[
\sum_{i=0,1} (\tilde{f}_i, \tilde{g}_i) = \langle f, g \rangle.
\]

Next, we define the \( 2 \times 2 \) matrix \( \tilde{\rho} \) with elements

\[
\tilde{\rho}_{00} := \rho, \quad \tilde{\rho}_{01} := \rho J, \\
\tilde{\rho}_{10} := J \rho, \quad \tilde{\rho}_{11} := J \rho J.
\]

It follows that

\[
\sum_{i,j} (\tilde{\rho}_{ij} \tilde{f}_j, \tilde{g}_i) = \langle \tilde{\rho} f, g \rangle.
\]

Now we take the trace of the \( 2 \times 2 \) matrix \( \tilde{\rho} \) and let this operation be the transformation \( F \),

\[
F \rho := \sum_{i=0,1} \tilde{\rho}_{ii} = \sigma.
\]

Hence \( F \) is the operator that was denoted by \( L \) before. The time evolution takes \( \rho \) into \( \rho(t) \) and \( \tilde{\rho} \) into \( \tilde{\rho}(t) \). This replaces the Rohlin transformation \( K_t \). Instead of \( F \circ K_t \) we consider \( \rho \to \rho(t) \to \sigma(t) \). Alternatively, we first take the step \( \rho \to \sigma \). The time evolution \( \sigma \to \sigma(t) \) replaces \( S_t \). Instead of \( S_t \circ F \) we find \( \rho \to \sigma \to \sigma(t) \), producing the same net result as \( \rho \to \rho(t) \to \sigma(t) \). In this sense, replacing \( \rho \to \rho(t) \) by \( \sigma \to \sigma(t) \) is like taking a factor of a classical dynamical system.

The idea to introduce \( \sigma(t) \) came from publications by Mackey [4, 5, Chap. 9] in which he pointed out that taking a factor of a classical dynamical system with constant entropy, may give rise to an entropy that increases. Quoting the Rohlin theorem [83], Mackey
referred to papers on $\Lambda$-operators [71,79] as an illustration. If $\Lambda$ is a projection, it is an example of a transformation $F$ that yields a factor with increasing entropy. In Mackey’s terminology, a factor is a specific type of trace. This suggested taking the sum of the diagonal elements of the matrix $\hat{\rho}$. Since the transformation $\rho(t) \rightarrow \sigma(t)$ is invertible, it is not a projection, yet it does have the property of leading to an increasing entropy $S[\sigma(t)]$. 
REFERENCES


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