

Theory & Notes

1. SOME TOPOLOGY DEFINITIONS AND RESULTS

First, consider X to be a topological space.

Path-connected. A **path** from a point p to a point q in a topological space X is a continuous function $f : \mathbb{R}_{[0,1]} \rightarrow X$, with $f(0) = p$ and $f(1) = q$. A **path-component** of X is an equivalence class of X under the equivalence relation which makes x equivalent to y if there is a path from x to y . Hence, X is said to be **path-connected** if there is exactly one path component, ie. if there is a path joining any two points X . Some important results regarding path-connectedness are enunciated, as follows.

- Let X and Y be topological spaces and let $f : X \rightarrow Y$ be a continuous function. If X is path-connected then its image $f(X)$ is path-connected as well.
- Every path-connected space is connected
- The closure of a connected subset is connected. Furthermore, any subset between a connected subset and its closure is connected.
- Every product of a family of path-connected spaces is path-connected.
- Every manifold is locally path-connected.

Simply connected. X is **simply connected** (or 1-connected) if it is path-connected and every path between two points can be continuously transformed (intuitively for embedded spaces, staying within the space) into any other such path, while preserving the two endpoints in question. The fundamental group $\pi_1(X)$ is an indicator of the failure of a topological space to be simply connected: a path-connected topological space is simply connected if and only if $\pi_1(X) \simeq \mathbb{Z}$.

An equivalent definition is: X is called simply-connected if

- it is path-connected,
- and any loop in X defined by $f : S^1 \rightarrow X$ can be contracted to a point; ie. $\exists F : D^2 \rightarrow X$ such that $F|_{S^1} = f$, where S^1 denotes the unit circle and D^2 denotes the closed unit disk in the Euclidean plane respectively. In other words, there exists a continuous map from the closed unit disk to X such that F restricted to S^1 is precisely f .

An equivalent formulation is this: X is simply connected if and only if

- it is path-connected,
- and whenever two arbitrary paths (ie. continuous maps) $p : \mathbb{R}_{[0,1]} \rightarrow X$ and $q : \mathbb{R}_{[0,1]} \rightarrow X$ with the same endpoints, $p(0) = q(0)$ and $p(1) = q(1)$, can be continuously deformed into one another. Explicitly, there exists a homotopy $F : \mathbb{R}_{[0,1]} \rightarrow X$ such that $F(x, 0) = p(x)$ and $F(x, 1) = q(x)$.

Equivalently, X is simply connected if and only if X is path-connected and $\pi_1(X) \simeq \mathbb{Z}$ at each point.

Homotopy invariants. Formally, a homotopy between two continuous functions $f, g : X \rightarrow Y$, wherein both X and Y are topological spaces, is defined to be a continuous function $H : X \times \mathbb{R}_{[0,1]} \rightarrow Y$, from the product of the space X with the unit interval to Y , such that

$$H(x, 0) = f(x) \text{ and } H(x, 1) = g(x), \forall x \in X.$$

In particular, a pointed map $f : (X, x_0) \rightarrow (Y, y_0)$ is called **null-homotopic relative to the basepoint** if there is a homotopy $H : X \times \mathbb{R}_{[0,1]} \rightarrow Y$ such that $H(x, 0) = f(x)$ and $H(x, 1) = e_{y_0}$, $\forall x \in X$, with $f(x_0, t) = y_0$.

In practical terms, if H 's second argument is thought of as time, when H describes a continuous deformation of f into g , at time 0 we have the function f and at time 1 we have the function g , in such a way that there is a smooth transition from f to g .

Given two topological spaces X and Y , a homotopy equivalence between X and Y is a pair of continuous maps $f : X \rightarrow Y$ and $g : Y \rightarrow X$, such that $g \circ f$ is homotopic to the identity map on X , id_X and $f \circ g$ is homotopic to the identity map on Y , id_Y . If such a pair exists, then X and Y are homotopy-equivalent, or of the same homotopy type. Intuitively, two space X and Y are homotopy equivalent if they can be transformed into one another by bending, shrinking and expanding operations. Spaces that are homotopy-equivalent to a point are called contractible.

Note that a homeomorphism is a special case of a homotopy equivalence, in which $g \circ f$ is exactly equal to the identity map id_X (not only homotopic to it), and $f \circ g$ is equal to id_Y . Therefore, if X and Y are homeomorphic then they are homotopy-equivalent, but the opposite is not true. Some examples:

- A solid disk is homotopy-equivalent to a single point, since you can deform the disk along radial lines continuously to a single point. However, they are not homeomorphic, since there is no bijection between them (since one is an infinite set, while the other is finite).
- The Möbius strip and an untwisted (closed) strip are homotopy equivalent, since you can deform both strips continuously to a circle. But they are not homeomorphic.

A function f is said to be null-homotopic if it is homotopic to a constant function. (The homotopy from f to a constant function is then sometimes called a null-homotopy.) For example, a map f from the unit circle S^1 to any space X is null-homotopic precisely when it can be continuously extended to a map from the unit disk D^2 to X that agrees with f on the boundary. It follows from these definitions that a space X is contractible if and only if the identity map from X to itself—which is always a homotopy equivalence—is null-homotopic.

In algebraic topology, there are many interesting homotopic invariants. Namely, let X, Y be topological spaces, then

- X is path-connected if and only if Y is.
- X is simply connected if and only if Y is.
- if X and Y are path-connected, then the fundamental groups of X and Y are isomorphic, and so are the higher homotopy groups.

Contractibility. Then, said topological space X is **contractible** if the identity map on X is null-homotopic, ie. if it is homotopic to some constant map. Intuitively, a contractible space is one that can be continously shrunk to a point within that space.

A contractible space is precisely one with the homotopy type of a point. It follows that all the the associated homotopy groups of a contractible space are trivial. Therefore, any space with a non-trivial homotopy group cannot be contractible. There are two non-equivalent definitions for a contractible space:

- Munkres' definition: Let X be a topological space. If the identity map on X , id_X , is null-homotopic, then X is contractible.
- Theodore's definition: Let X be a topological space and let $x_0 \in X$ a point. If there is a continuous map $F : X \times \mathbb{R}_{[0,1]} \rightarrow X$ such that

$$(1) \quad \begin{array}{l} F(x, 0) = x \\ F(x, 1) = x_0 \\ F(x_0, t) = x_0 \end{array} \quad \begin{array}{l} \forall x \in X, \\ \forall t \in \mathbb{R}_{[0,1]} \end{array} \Rightarrow \text{then } X \text{ is contractible.}$$

For a topological space X , the following statements are all equivalent:

- X is contractible (ie. the identity map is null-homotopic).
- X is homotopy-equivalent to a one-point space.
- For any space Y , any two maps $f, g : Y \rightarrow X$ are homotopic.

- For any space Y , any map $f : Y \rightarrow X$ is null-homotopic.
- The cone on a space X is always contractible. Therefore any space can be embedded in a contractible one (which also illustrates that subspaces of contractible spaces need not be contractible themselves).
- X is a contractible if and only if there exists a retraction from the cone of X to X .
- Every contractible space is path-connected and simply connected. Moreover, since all the higher homotopy groups, vanish. Every contractible space is n -connected, for all $n \geq 0$.

Hopf-Rinow theorem. Let (M, g) be a connected Riemannian manifold¹. Then, the following statements are equivalent

- The closed and bounded subsets of M are compact,
- M is a complete metric space,
- M is geodesically complete, that is, $\forall p \in M$, the exponential map \exp_p is defined on the entire tangent space $T_p M$,

Furthermore, any one of the above implies that, given any two points $p, q \in M$, there exists a length-minimizing geodesic connecting these two points.

2. ON THE GEOMETRY OF GAUSSIAN MANIFOLDS

Bosonic and fermionic quantum systems with N modes can be constructed from N creation or annihilation operators,

$$(2) \quad \zeta \stackrel{a, a^\dagger}{=} (a_1, \dots, a_N, a_1^\dagger, \dots, a_N^\dagger), \quad \text{which satisfy the} \quad \begin{aligned} [a_i, a_j] &= [a_i^\dagger, a_j^\dagger] = 0, [a_i, a_j^\dagger] = \delta_{ij}, \text{ for bosons,} \\ \{a_i, a_j\} &= \{a_i^\dagger, a_j^\dagger\} = 0, \{a_i, a_j^\dagger\} = \delta_{ij}, \text{ for fermions.} \end{aligned}$$

In contrast to this set of N creation and annihilation operators, one may choose instead, a basis of $2N$ Hermitian operators, the quadratures, which read

$$(3) \quad \zeta \stackrel{a, a^\dagger}{=} (q_1, \dots, q_N, p_1, \dots, p_N), \quad \text{with} \quad \begin{aligned} a_i &= \frac{q_i + ip_i}{\sqrt{2}} \\ a_i^\dagger &= \frac{q_i - ip_i}{\sqrt{2}} \end{aligned} \quad \text{with} \quad \begin{aligned} [q_i, q_j] &= [p_i, p_j] = 0, [q_i, p_j] = i\delta_{ij} \\ \{q_i, q_j\} &= \{p_i, p_j\} = \delta_{ij}, [q_i, p_j] = 0. \end{aligned}$$

In the fermionic case, these operators are called Majorana modes.

Gaussian states are uniquely specified by their two-point correlation function in the fundamental operators $\delta\zeta$. For any state ρ , the expectation value of an O-operators is given by $\langle O \rangle = \text{Tr } \rho O$. It is useful to separately consider the symmetrized and anti-symmetrized part of these correlations, given by two real bilinear forms

$$(4) \quad \mathcal{G}^{ab} = \langle \zeta^a \zeta^b + \zeta^b \zeta^a \rangle, \quad \Omega^{ab} = -i \langle \zeta^a \zeta^b - \zeta^b \zeta^a \rangle, \quad \text{with } z^a = \langle \zeta^a \rangle = 0.$$

¹Note that a path-connected topological space is connected as well.

Proof: path-connectedness implies connectedness

In effect, if X is a path-connected topological space and assuming (by contradiction) that $X = A \sqcup B$, and $A, B \neq \emptyset$ (ie. X isn't connected). Then, let $a \in A, b \in B$ and let $\gamma : \mathbb{R}_{[0,1]}$ be a path in X such that $\gamma(0) = a, \gamma(1) = b$. Then, given γ 's continuity, there is a decomposition

$$\mathbb{R}_{[0,1]} = \gamma^{-1}(A) \cup \gamma^{-1}(B),$$

which, if true, implies that $\mathbb{R}_{[0,1]}$ is not connected, which is false. Hence, X cannot be path-connected if it isn't connected.

- For bosons, the symplectic form Ω is fixed by canonical commutation relations (CCR), with the positive-definite metric \mathcal{G} containing the physical correlations.
- For fermions, the situation is reversed, with \mathcal{G} fixed by canonical anti-commutation relations (CAR) and Ω describing the physical correlations.

Chain map of the Hierarchical sets.

Here we show the chain map of the Hierarchical sets \mathcal{B}^ℓ and their corresponding Kähler submanifolds \mathcal{V}^ℓ as an almost-commutative diagram

$$\begin{array}{ccccccccc}
 \mathcal{B}^{\ell=0} & \xrightarrow{\subset} & \mathcal{B}^{\ell=1} & \xrightarrow{\subset} & \dots & \xrightarrow{\subset} & \mathcal{B}^{\ell=\gamma-1} & \xrightarrow{\subseteq} & \mathcal{B}^{\ell=\gamma} \\
 \downarrow f_0 & & \downarrow f_1 & & \downarrow f_s & & \downarrow f_{\gamma-1} & & \downarrow f_\gamma \\
 \mathcal{V}^{\ell=0} & \xrightarrow{\subset} & \mathcal{V}^{\ell=1} & \xrightarrow{\subset} & \dots & \xrightarrow{\subset} & \mathcal{V}^{\ell=\gamma-1} & \xrightarrow{\subseteq} & \mathcal{V}^{\ell=\gamma}
 \end{array}$$

where the total length of the bounded chain map is $\gamma + 3$, with $\gamma = \dim G(\mathbb{H})$.

3. CUENTITAS

Density operators can either describe pure or mixed states, which are deffined as follows

- Pure states can be written as an outer product of a vector state with itself, this is

$$\rho \text{ is a pure state if } \exists |\psi\rangle \in \mathbb{H} \mid \rho \propto |\psi\rangle \langle\psi|.$$

In other words, ρ is a rank-one orthogonal projection. Equivalently, a density matrix is a pure state if there exists a unit vector in the Hilbert space such that ρ is the orthogonal projection onto the span of ψ .

Note as well that

$$|\psi\rangle \langle\psi| \in \mathbb{H} \otimes \mathbb{H}^*, \text{ but } \mathbb{H} \otimes \mathbb{H}^* \sim \text{End}(\mathbb{H})$$

ie. the tensor space $\mathbb{H} \otimes \mathbb{H}^*$ is canonically isomorphic to the vector space of endormorphisms in \mathbb{H} , ie. to the space of linear operators from \mathbb{H} to \mathbb{H} . It's important to note that this isomorphism is only strictly valid in finite-dimensional Hilbert spaces, wherein for infinite-dimensional Hilbert spaces, the isomorphism holds as well provided the density operators are redefined as being trace-class.

- Mixed states do not adhere to the previous properties.

Given a physical system, a density operator for it is a positive semi-definite, self-adjoint operator of trace one acting on the system's Hilbert space, denoted by \mathbb{H} . The set of all density operators has the structure of a vector space $\mathcal{C}(\mathbb{H})$,

$$(5) \quad \mathcal{C}(\mathbb{H}) = \{\rho \in \text{GL}(N, \mathbb{C}) \mid \rho^\dagger = \rho, \rho \geq 0, \text{Tr } \rho = 1\},$$

where $\text{GL}(N, \mathbb{C})$ is the general linear group over the complex number field, whose elements are squared matrices of $N \times N$ -dimension. The following statements can then be proved:

- 1) $\mathcal{C}(\mathbb{H})$ is a topological space. This is, this space can be imbued with a topology \mathcal{T} which satisfies a set of axioms.
 - In effect, the desired topology may be chosen to be the trivial topology $\mathcal{T} = \{\emptyset, \mathcal{C}(\mathbb{H})\}$,
 - or it may be chosen out to be the discrete topology, ie. any collection of τ -sets, subsets of $\mathcal{C}(\mathbb{H})$, so that that $\mathcal{T} = \bigcup \tau$ adheres to the topological space's axioms.
 - Another interesting election is to define a metric on this space, allowing for the construction of the metric topology. More on this later.
- 2) $(\mathcal{C}(\mathbb{H}), \mathcal{T})$ is a Hausdorff space, allowing for the distinction of elements via disjoint neighbourhoods,
- 3) $(\mathcal{C}(\mathbb{H}), \mathcal{T})$ is a topological manifold.
- 4) $(\mathcal{C}(\mathbb{H}), \mathcal{T})$ is a differentiable manifold,
- 5) and is a Riemannian non-convex manifold

Let Λ be a d -dimensional quantum spin system, with its lattice being defined as $\mathbb{L} = \mathbb{Z}^d$ so that $\Lambda \subset \mathbb{Z}^d$. Its single-spin space is a probability space $(S, \mathcal{S}, \lambda)$ where $S = \{\pm 1\}$. A spin chain's regular crystalline structure can be viewed as a finite, non-oriented. Let $\mathfrak{Hs}(\mathbb{H}^{\otimes N})$ be the set of all trace-class operators, endomorphisms acting on the N -partite Hilbert space. By construction, this set is, in and on itself, a Hilbert space. In particular, consider the subset of all trace-class hermitian operators, labelled

$$(6) \quad \mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N}), \text{ where } \mathbf{K} \in \mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \text{ if and only if}$$

$$\begin{aligned} \mathbf{K} : \mathbb{H}^{\otimes N} &\rightarrow \mathbb{H}^{\otimes N} \\ \mathbf{K} &\in \text{GL}(N, \mathbb{C}) \\ \mathbf{K} &= \mathbf{K}^\dagger \\ \text{Tr } \mathbf{K}^\dagger \mathbf{K} &= \text{Tr } \mathbf{K}^2 < \infty \end{aligned}$$

We claim the following

Theorem 1. *Consider a finite dimensional system, eg. spin systems, or truncated boson/fermion systems. Then, let $\mathcal{M} = \left\{ \rho \in \mathcal{C}(\mathbb{H}^{\otimes N}) \mid \exists \{\mu\}_{k=1}^\ell \subset \mathbb{R} \wedge \exists \mathbf{K} \in \mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \text{ such that } \rho \propto e^{-\mathbf{K}} \right\}$. Then \mathcal{M} is a Riemannian manifold (\mathcal{M}, B) , where B is the Bures metric.*

Proof. Special care must be taken when dealing with infinite-dimensional systems. We start our proof by concerning ourselves to finite-dimensional physical systems, eg. spins, truncated bosonic and fermionic systems.

Finite dimensional case. Let \mathcal{B} be the set of all operators which are endomorphisms on $\mathcal{C}(\mathbb{H})$, ie.

$$\mathcal{B} = \{ \mathbf{O} \mid \mathbf{O} : \mathcal{C}(\mathbb{H}) \rightarrow \mathcal{C}(\mathbb{H}) \}.$$

Note that, by definition, $\mathcal{C}(\mathbb{H}) \subset \mathcal{B}$. Consider an N -partite physical system, then its associated Hilbert space will have $\mathcal{O}(2^N)$ dimension and its associated density operator space will have $\mathcal{O}(2^{2N})$ dimension. Then, all linear operators acting on $\mathcal{C}(\mathbb{H})$ can be classified as k -body operators, with $k \leq N$. This is, in essence, operators whose action is non-trivial only for a total of k particles. Therefore, the N -partite Hilbert space can be written as

$$\mathbb{H} = \bigotimes_{j=1}^N \mathfrak{H}_j,$$

where \mathfrak{H}_j is the j -th subsystem's Hilbert space. This definition thus allows for systems with different particles species (eg. fermions, bosons, spins etc.). Then,

$$\mathcal{B}_1(\mathbb{H}) = \{ \hat{\mathbf{O}} \mid \hat{\mathbf{O}} : \mathfrak{H}_j \rightarrow \mathfrak{H}_j, \forall j \leq N \}$$

is the space of all one-body operators. Then the space of k -body operators can be recursively defined in terms of this set,

$$\mathcal{B}_k(\mathbb{H}) = \{ \bigotimes_{i=1}^k \mathbf{O}_i \mid \mathbf{O}_i \in \mathcal{B}_1(\mathbb{H}) \}, \text{ where } \mathcal{B}(\mathbb{H}) = \bigsqcup_{i=1}^N \mathcal{B}_i(\mathbb{H}).$$

If \mathbb{H} is a Hilbert space and $A \in \mathcal{B}$ is a non-negative self-adjoint operator on \mathbb{H} , then it can be shown that A has a well-defined, but possible infinite, trace. Now, if \mathbf{A} is a bounded operator, then $\mathbf{A}^\dagger \mathbf{A}$ is self-adjoint and non-negative. An operator \mathbf{A} is said to be Hilbert-Schmidt if $\text{Tr } \mathbf{A}^\dagger \mathbf{A} < \infty$. Naturally, the space of all Hilbert-Schmidt operators form a vector space, labelled by $\mathfrak{Hs}(\mathbb{H})$. Then, the Hilbert Schmidt inner product can be defined as

$$\langle \cdot, \cdot \rangle_{\text{HS}} : \mathfrak{Hs}(\mathbb{H}) \times \mathfrak{Hs}(\mathbb{H}) \rightarrow \mathbb{C}, \text{ where}$$

$$\begin{aligned} \langle \mathbf{A}, \mathbf{B} \rangle_{\text{HS}} &= \text{Tr } \mathbf{A}^\dagger \mathbf{B} \\ ||\mathbf{A}||_{\text{HS}} &= \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{A}}. \end{aligned}$$

If the Hilbert space is finite-dimensional, the trace is well defined and if the Hilbert space is infinite-dimensional, then the trace can be proven to be absolutely convergent and independent of the orthonormal basis choice².

This inner product implies that $(\mathfrak{H}\mathfrak{s}(\mathbb{H}), \langle \cdot, \cdot \rangle_{\text{HS}})$ is a

- inner product space since the norm is the square root of the inner product of a vector and itself ie.

$$\|\mathbf{A}\|_{\text{HS}} = \langle \mathbf{A}, \mathbf{A} \rangle_{\text{HS}} = \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{A}}$$

- and is a normed vector space since the norm is always well defined over $\mathfrak{H}\mathfrak{s}(\mathbb{H})$.

Now, every inner product space is a metric space. In effect, since the function

$$\mathbf{A} \rightarrow \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{A}} \quad \text{then} \quad \mathbf{A}, \mathbf{B} \xrightarrow{d} \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{B}}$$

is a well-defined norm is a well-defined distance

$$d_{\text{HS}}(\cdot, \cdot) : \mathfrak{H}\mathfrak{s}(\mathbb{H}) \times \mathfrak{H}\mathfrak{s}(\mathbb{H}) \rightarrow \mathbb{R}$$

$$d_{\text{HS}}(\mathbf{A}, \mathbf{B}) = \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{B}}$$

With this metric thus defined, then $(\mathfrak{H}\mathfrak{s}(\mathbb{H}), d_{\text{HS}})$ is a metric space. Every metric space can be modified, via the completions of its metric, in such a way that $(\mathfrak{H}\mathfrak{s}(\mathbb{H})^*, d_{\text{HS}}^*)$ is a complete metric space, in the sense of the convergence of Cauchy series, where $\mathfrak{H}\mathfrak{s}(\mathbb{H}) \subset \mathfrak{H}\mathfrak{s}(\mathbb{H})^*$. In this particular case, given that the metric over $\mathfrak{H}\mathfrak{s}(\mathbb{H})$ is always a finite number -having removed those elements with infinite trace-, then it is already complete $\mathfrak{H}\mathfrak{s}(\mathbb{H}) \sim \mathfrak{H}\mathfrak{s}(\mathbb{H})^*$. Therefore, $\mathfrak{H}\mathfrak{s}(\mathbb{H})$ is a Hilbert space with respect to the Hilbert-Schmidt inner product $\langle \cdot, \cdot \rangle_{\text{HS}}$ (or with respect to the Hilbert-Schmidt distance d_{HS}).

Thus defined, the Hilbert-Schmidt inner product is complex-valued, thus not immediately suited for our calculations.

Theorem 2. Consider the modified Hilbert-Schmidt product given by

$$\langle \cdot, \cdot \rangle_{\text{HS}}^{\rho_0} : \mathfrak{H}\mathfrak{s}(\mathbb{H}) \times \mathfrak{H}\mathfrak{s}(\mathbb{H}) \rightarrow \mathbb{R}$$

where $\rho_0 \in \mathcal{C}(\mathbb{H})$.

$$\langle \mathbf{A}, \mathbf{B} \rangle_{\text{HS}}^{\rho_0} = \frac{1}{2} \text{Tr } \rho_0 \{ \mathbf{A}^\dagger, \mathbf{B} \}$$

We claim this is a valid inner product over the space of all linear trace-class endomorphisms on \mathbb{H} , $\mathfrak{H}\mathfrak{s}(\mathbb{H})$.

Proof. In order to prove this is a well-defined inner product over the space of trace-class operators, we must prove that it linear in it second argument and sesquilinear in its first argument, hermitian and positive-defined.

In effect,

1) the linearity and sesquilinearity is self evident.

2) Is it real? Yes

²In effect, given a non-negative, self-adjoint operator, its trace is always invariant under orthogonal change of basis. Should the trace be a finite number, then it is called a trace class. Any given operator $\mathbf{A} \in \mathcal{B}$ is trace-class if the non-negative self-adjoint operator $\sqrt{\mathbf{A}^\dagger \mathbf{A}}$ is trace class as well. Now, given two Hilbert-Schmidt operators $\mathbf{A}, \mathbf{B} \in \mathfrak{H}\mathfrak{s}(\mathbb{H})$, then the new operator $\mathbf{A}^\dagger \mathbf{B}$ is a trace-class operator, meaning that the sum

$$\text{Tr } \mathbf{A}^\dagger \mathbf{B} = \sum_{\lambda \in \Lambda} \langle \mathbf{e}_\lambda, \mathbf{A}^\dagger \mathbf{B} \mathbf{e}_\lambda \rangle$$

is absolutely convergent and the value of the sum is independent of the choice of orthonormal basis $\{\mathbf{e}_\lambda\}_{\lambda \in \Lambda}$.

$$\begin{aligned}
(7) \quad \langle \mathbf{A}, \mathbf{B} \rangle_{\text{HS}}^{\rho_0} &= \frac{1}{2} \text{Tr } \rho_0 \{ \mathbf{A}^\dagger, \mathbf{B} \} = \frac{1}{2} \text{Tr } \rho_0 (\mathbf{A}^\dagger \mathbf{B} + \mathbf{B} \mathbf{A}^\dagger) \\
&= \frac{1}{2} \text{Tr } \rho_0 (\mathbf{B}^\dagger \mathbf{A} + \mathbf{A} \mathbf{B}^\dagger)^\dagger = \frac{1}{2} \text{Tr } \rho_0 \{ \mathbf{B}^\dagger, \mathbf{A} \}^\dagger \\
&= (\langle \mathbf{B}, \mathbf{A} \rangle_{\text{HS}}^{\rho_0})^*
\end{aligned}$$

3) Is it positive-defined? Yes, in effect,

$$(8) \quad \langle \mathbf{A}, \mathbf{A} \rangle_{\text{HS}}^{\rho_0} = \frac{1}{2} \text{Tr } \rho_0 \{ \mathbf{A}^\dagger, \mathbf{B} \} = \text{Tr } \sqrt{\rho} \frac{\mathbf{A} \mathbf{A}^\dagger + \mathbf{A}^\dagger \mathbf{A}}{2} \sqrt{\rho}$$

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Now, note that the identity map on the Hilbert-Schmidt space is $\text{id}_{\mathfrak{H}\mathfrak{S}^\dagger(\mathbb{H}^{\otimes N})} = \mathbb{1}_N$, which then implies that the identity map on \mathcal{M} is simply $\text{id}_{\mathcal{M}} = \mathbb{1}_N$. We assert that \mathcal{M} is a path-connected topological space. In effect,

$$\forall \rho_1, \rho_2 \in \mathcal{M}, \exists f : \mathbb{R}_{[0,1]} \rightarrow \mathcal{M} \text{ such that } \begin{cases} f(0) = \rho_1 \\ f(1) = \rho_2 \end{cases}$$

$$\text{which always exists } f : \mathbb{R}_{[0,1]} \rightarrow \mathcal{M} \mid f(x) = x\rho_1 + (1-x)\rho_2 \in \mathcal{M}$$

which is continuous for arbitrary density matrices.

Proof: Path-connectedness in the finite-dimensional case.

In effect, let $\rho_1, \rho_2 \in \mathcal{M} \rightarrow \mathbf{K}_1, \mathbf{K}_2 \in \mathfrak{H}\mathfrak{S}^\dagger(\mathbb{H}^{\otimes N}) \mid \rho_1 = e^{-\mathbf{K}_1}, \rho_2 = e^{-\mathbf{K}_2}$, then

$$\begin{aligned}
(9) \quad f(x) &= x\rho_1 + (1-x)\rho_2 = xe^{-\mathbf{K}_1} + (1-x)e^{-\mathbf{K}_2} = e^{-\mathbf{K}} \\
&\Leftrightarrow \mathbf{K} = -\log(xe^{-\mathbf{K}_1} + (1-x)e^{-\mathbf{K}_2}) \in \mathfrak{H}\mathfrak{S}^\dagger(\mathbb{H}^{\otimes N})
\end{aligned}$$

Since path-connectedness implies connectedness, the Hopf-Rinow theorem stands. Therefore, given any two arbitrary points $\rho, \sigma \in \mathcal{M}$, there always exists a length-minimizing geodesic connecting these points³. Moreover, this space is both a complete metric space (hence, a Hilbert space in its own right) and is geodesically complete, with a everywhere well-defined exponential map⁴. By construction, it is clear that the natural choice for the tangent space $T_\rho \mathcal{M}$ is $\mathfrak{H}\mathfrak{S}^\dagger(\mathbb{H}^{\otimes N})$, making this a Hilbert manifold

$$T_\rho \mathcal{M} \simeq \mathfrak{H}\mathfrak{S}^\dagger(\mathbb{H}^{\otimes N}),$$

for all $\rho \in \mathcal{M}$. Therefore, the tangent bundle, a vector bundle made up of copies of $\mathfrak{H}\mathfrak{S}^\dagger(\mathbb{H}^{\otimes N})$, can be written as

³Note that these conclusions only hold for finite dimensional manifolds. The theorem does not hold for infinite dimensional complete Hilbert manifolds. Note that, in our case, the Hilbert space $\mathbb{H}^{\otimes N}$ can be thought of as a Hilbert manifold, with a single global chart given by the identity function $\mathbb{1}_{\mathbb{H}^{\otimes N}}$ on said Hilbert space. Moreover, since by definition a Hilbert space is a vector space, the tangent space $T_\rho \mathcal{M}$ to \mathcal{M} at the point $\rho \in \mathbb{H}^{\otimes}$ is canonically isomorphic to the Hilbert space itself, and thus has a natural inner product, the same as the one defined on the Hilbert space. Thus $\mathbb{H}^{\otimes N}$ can be given the structure of a Riemannian manifold with metric

$$g(v, w)(\rho) = \langle v, w \rangle_{\mathbb{H}^{\otimes N}}, \text{ for } v, w \in T_\rho \mathcal{M}$$

wherein $\langle \cdot, \cdot \rangle_{\mathbb{H}^{\otimes N}}$ denotes the inner product in $\mathbb{H}^{\otimes N}$

⁴Note that "well-defined" in this context means there is a natural isomorphism/diffeomorphism/algo-morphism (????!!) between the manifold itself and its tangent space. Moreover, this is only the case for \mathbb{C} -valued matrices and it is not true for \mathbb{R} -valued matrices.

$$\begin{aligned}
T\mathcal{M} &= \bigsqcup_{\rho \in \mathcal{M}} T_{\rho}\mathcal{M} \\
&= \bigcup_{\rho \in \mathcal{M}} \{\rho\} \times T_{\rho}\mathcal{M} \\
&= \bigcup_{\rho \in \mathcal{M}} \{(\rho, \mathbf{O}) \mid \mathbf{O} \in T_{\rho}\mathcal{M}\} \\
&= \{(\rho, \mathbf{O}) \mid \rho \in \mathcal{M}, \mathbf{O} \in T_{\rho}\mathcal{M}\}
\end{aligned}$$

Moreover, this space is contractible. This is, the identity map on \mathcal{M} is null-homotopic.

Proof of surjectiveness of the exponential map onto the general linear group

It turns out that neither the exponential map $\exp : \mathbb{R}^{N \times N} \rightarrow \text{GL}(N, \mathbb{R})$ nor the exponential map $\exp : \mathbb{R}^{N \times N} \rightarrow \text{GL}^+(N, \mathbb{R})$ are surjective.

Let \mathbf{A} be a linear operator, which should realise in the image of \exp . The vector space may be decomposed as a direct sum of its generalized eigenspaces \mathbb{E}_{λ} as

$$\mathbb{C}^{N \times N} = \bigoplus_{\lambda} \mathbb{E}_{\lambda \in \sigma(\mathbf{A})}, \text{ with } \lambda \neq 0, \forall \lambda \in \sigma(\mathbf{A}).$$

If the restriction of \mathbf{A} to each one of the \mathbb{E}_{λ} lies in the image of \exp applied to the space of linear operators of \mathbb{E}_{λ} , then there exists a choice of pre-images $\mathbf{A}_{\mathbb{E}_{\lambda}}$ to yield \mathbf{A} 's pre-image. In other words, it suffices to consider the case where there is just one generalized eigenspace so that $\mathbf{A} - \lambda \mathbf{1}$ is nilpotent for $\lambda \neq 0$. This is a special case of the Jordan-Chevalley decomposition, wherein any complex-valued matrix X may be decomposed as $X = A + N$, where A is diagonalizable and N is nilpotent with $[A, N] = 0$. Given that $\mathbf{1}$ commutes with everything,

$$\mathbf{A} = \lambda \mathbf{1}(\mathbf{1} - N), \text{ with } N = \lambda^{-1}(\lambda \mathbf{1} - \mathbf{A}).$$

Note that N is nilpotent. Thus, the problem formally reduces to the cases of a nonzero scalar operator $\lambda \mathbf{1}$ on one hand, and that of a unipotent $\mathbf{1} - N$ on the other. For the former case, it suffices to choose a logarithm of the complex number λ and for the latter there is an algebraic formula for its logarithm

$$\log(\mathbf{1} - N) = \sum_{k=1}^{n-1} \frac{N^k}{k}, \text{ with } N^n = 0,$$

which completes the proof.

Alternative proof of surjectiveness of the exponential map onto the general linear group

An equivalent proof is to use \mathbf{A} 's Jordan form. If the underlying field is algebraically closed, then $\mathbf{A} = PJP^{-1}$, where J is \mathbf{A} 's Jordan form. Then,

$$e^{\mathbf{A}} = e^X = Pe^JP^{-1}.$$

Also since,

$$J = \bigoplus_{\lambda_i \in \sigma(\mathbf{A})} J_{a_i}(\lambda_i) \Rightarrow e^J = \exp \left(\bigoplus_{\lambda_i \in \sigma(\mathbf{A})} J_{a_i}(\lambda_i) \right) = \bigoplus_{\lambda_i \in \sigma(\mathbf{A})} \exp(J_{a_i}(\lambda_i))$$

Therefore, the only information needed is the matrix exponential of a Jordan block. But each Jordan block is of the form

$$\begin{aligned}
J_a(\lambda) &= \lambda \mathbf{1} + N \\
\Rightarrow e^{J_a(\lambda)} &= e^{\lambda \mathbf{1} + N} = e^{\lambda} e^N,
\end{aligned}$$

where N is a special nilpotent matrix. The matrix exponential of J is then given by

$$e^J = e^{\lambda_1} e^{N_{a_1}} \oplus e^{\lambda_2} e^{N_{a_2}} \oplus \dots \oplus e^{\lambda_n} e^{N_{a_n}}.$$

Proof of the contractible nature in the finite-dimensional case.

In effect, since \mathcal{M} is a subset of $\mathrm{GL}(N, \mathbb{C})$, \mathcal{M} is trivially contractible. This is, the identity map on \mathcal{M} , $\mathrm{id}_{\mathcal{M}} = \mathbb{1}_N$ is null-homotopic. In effect, let $H : \mathcal{M} \times \mathbb{R}_{[0,1]} \rightarrow \mathcal{M}$ given by

$$H(\mathbf{A}, t) = (1 - t)\mathbf{A} \in \mathcal{M}, (\mathbf{A}, t) \in \mathcal{M} \times \mathbb{R}_{[0,1]}.$$

Therefore, this implies that \mathcal{M} 's first homotopy group $\pi^1(\mathcal{M}) = \mathbb{Z}$.

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In our context, since the calculations are to be computed via the (modified) Hilbert-Schmidt inner product and metric, only trace-class operators are allowed. Therefore, some redefinitions are needed.

$$\begin{aligned}
 (10) \quad \mathfrak{H}\mathfrak{s}_1(\mathbb{H}) &= \{\hat{\mathbf{O}} | \hat{\mathbf{O}} \in \mathcal{B}_1 \wedge \|\hat{\mathbf{O}}\|_{\text{HS}}^{\rho_0} < \infty, \forall j \leq N\} && \text{is the space of all one-body operators,} && \text{and where} \\
 \mathfrak{H}\mathfrak{s}_k(\mathbb{H}) &= \{\otimes_{i=1}^k \hat{\mathbf{O}}_i | \hat{\mathbf{O}}_i \in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}) \forall i, k \leq N\} && \text{is the space of all } k\text{-body operators} && \mathfrak{H}\mathfrak{s}(\mathbb{H}) = \bigsqcup_{k=1}^N \mathfrak{H}\mathfrak{s}_k(\mathbb{H})
 \end{aligned}$$

Consider now an N -body quantum system, where correlations, entanglements, and interactions are present. Different particle species are allowed. The One-body and Two-body Max-Ent frameworks are defined as follows

Näive one-body Max-Ent

In the Näive one-body Max-Ent framework, there are N sets of one-body operators, each one corresponding to one the N subsystems, which are assumed to be the local basis. These operators must be local operators, acting non-trivially in only one Hilbert subspace, and must be trace-class. The framework thus allows for interactions between different particle species since the basis may have different dimension, this is

$$\begin{aligned}
 \{\mathbf{O}_i^{(1)}\}_{i=1}^{n_1} &\in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}^{(1)}) && \mathfrak{b}_1 = \{\mathbf{O}_i^{(1)} \otimes \otimes_{k=2}^N \mathbb{1}^{(k)}\}_{i=1}^{n_1} \subset \mathfrak{H}\mathfrak{s}(\mathbb{H}^{\otimes N}) \\
 &\vdots && \vdots \\
 \{\mathbf{O}_i^{(\ell)}\}_{i=1}^{n_\ell} &\in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}^{(\ell)}) && \mathfrak{b}_\ell = \{\otimes_{k=1}^\ell \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(\ell)} \otimes_{k'=\ell+1}^N \mathbb{1}^{(k')}\}_{i=1}^{n_\ell} \subset \mathfrak{H}\mathfrak{s}(\mathbb{H}^{\otimes N}) \\
 &\vdots && \vdots \\
 \{\mathbf{O}_i^{(N)}\}_{i=1}^{n_N} &\in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}^{(N)}) && \mathfrak{b}_N = \{\otimes_{k=1}^{N-1} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \subset \mathfrak{H}\mathfrak{s}(\mathbb{H}^{\otimes N})
 \end{aligned}$$

The operators are then redefined so that they act on the global Hilbert space $\mathbb{H}^{\otimes N}$

Then, the one-body Max-Ent basis \mathfrak{B}_{ME_1} is defined as the union of these sets

$$\mathfrak{B}_{ME_1} = \bigsqcup_{k=1}^N \mathfrak{b}_k,$$

whose dimension is given by the sum of the \mathfrak{b} -basis dimensions ie. $\dim(\mathfrak{B}_{ME_1}) = \sum_{k=1}^N \dim(\mathfrak{b}_k) \sim \mathcal{N}$. Then, the one-body Max-Ent states are given by

$$(11) \quad \mathcal{S}_{ME,1}(\mathfrak{B}_{ME_1}) = \{\rho \in \mathcal{C}(\mathbb{H}) \mid \exists \{\lambda_k\}_{k=1}^{\dim \mathfrak{B}_{ME_1}} \subset \mathbb{R} \text{ such that } \rho \propto \exp\left(-\sum_i \lambda_i \mathbf{O}_i\right)\}.$$

Näive two-body Max-Ent

Here, similarly to the naïve one-body Max-Ent framework, we have N sets of local one-body operators at our disposal, which must be trace-class and must only non-trivially act in only one Hilbert subspace. If the one-body local operators are

$$(12) \quad \begin{aligned} & \{\mathbf{O}_i^{(1)}\}_{i=1}^{n_1} \in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}^{(1)}) & \mathfrak{b}_1 = \{\mathbf{O}_i^{(1)} \otimes \bigotimes_{k=2}^N \mathbb{1}^{(k)}\}_{i=1}^{n_1} \subset \mathfrak{H}\mathfrak{s}(\mathbb{H}^{\otimes N}) \\ & \vdots & \vdots \\ & \{\mathbf{O}_i^{(\ell)}\}_{i=1}^{n_\ell} \in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}^{(\ell)}) & \text{then the global one-body operators are } \mathfrak{b}_\ell = \{\bigotimes_{k=1}^\ell \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(\ell)} \otimes \bigotimes_{k'=\ell+1}^N \mathbb{1}^{(k')}\}_{i=1}^{n_\ell} \subset \mathfrak{H}\mathfrak{s}(\mathbb{H}^{\otimes N}) \\ & \vdots & \vdots \\ & \{\mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}^{(N)}) & \mathfrak{b}_N = \{\bigotimes_{k=1}^{N-1} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \subset \mathfrak{H}\mathfrak{s}(\mathbb{H}^{\otimes N}) \end{aligned}$$

However, unlike the previous case, we now allow for two-body operators to be included. These new sets of two-body operators may be defined as follows

$$\begin{aligned} \mathfrak{c}_{11} &= \{\mathbf{O}_i^{(1)} \mathbf{O}_j^{(1)} \bigotimes_{k=2}^N \mathbb{1}^{(k)}\}_{i,j=1}^{\Gamma(n_1, n_1)} \mid \mathbf{O}_i^{(1)} \in \mathfrak{b}_1 \\ \mathfrak{c}_{12} &= \{\mathbf{O}_i^{(1)} \otimes \mathbf{Q}_j^{(2)} \bigotimes_{k=3}^N \mathbb{1}^{(k)}\}_{i,j=1}^{\Gamma(n_1, n_2)} \mid \mathbf{O}_i^{(1)} \in \mathfrak{b}_1, \mathbf{Q}_j^{(2)} \in \mathfrak{b}_2 \\ & \vdots \\ \mathfrak{c}_{\ell\ell'} &= \{\mathbf{O}_i^{(\ell)} \otimes \mathbf{Q}_j^{(\ell')} \bigotimes_{\substack{k=1 \\ k \neq \ell, \ell'}}^N \mathbb{1}^{(k)}\}_{i,j=1}^{\Gamma(n_\ell, n_{\ell'})} \mid \mathbf{O}_i^{(\ell)} \in \mathfrak{b}_\ell, \mathbf{Q}_j^{(\ell')} \in \mathfrak{b}_{\ell'}, \\ & \vdots \\ \mathfrak{c}_{NN} &= \{\bigotimes_{k=1}^{N-1} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(N)} \mathbf{O}_j^{(N)}\}_{i,j=1}^{\Gamma(n_N, n_N)} \mid \mathbf{O}_i^{(N)} \in \mathfrak{b}_N \end{aligned}$$

where $\Gamma(n_a, n_b)$ counts all the possible, non-repeating, order notwithstanding, pair combinations of elements from a n_a -cardinality set with elements from a n_b -cardinality set. In other words,

$$(13) \quad \Gamma(n_a, n_b) = n_a + n_b + \frac{n_a(n_b - 1)}{2}$$

Then, the two-body Max-Ent basis is

$$\mathfrak{B}_{ME_2} = \bigsqcup_{k=1}^N \mathfrak{b}_k \cup \bigsqcup_{k,k'=1}^N \mathfrak{c}_{kk'},$$

from which the two-body Max-Ent states are given by

$$(14) \quad \mathcal{S}_{ME,2}(\mathfrak{B}_{ME_2}) = \{\rho \in \mathcal{C}(\mathbb{H}) \mid \exists \{\lambda_k\}_{k=1}^{\ell \leq N}, \{\gamma_{mn}\}_{\substack{m,n=1 \\ m < n}}^{\ell \leq N} \subset \mathbb{R} \text{ such that } \rho \propto \exp\left(-\sum_{i,j} \lambda_i \mathbf{O}_i - \gamma_{ij} \mathbf{O}_i \mathbf{O}_j\right)\}.$$

Note that $\dim \mathfrak{B}_{ME_2} = \sum_{k=1}^N \dim(\mathfrak{b}_k) + \sum_{i,j=1}^N \dim(\mathfrak{c}_{ij}) \sim \mathcal{O}(N^2)$

Both of these techniques require substantially fewer parameters than the exact dynamics, which requires $\mathcal{O}(2^{2N})$ complex-valued entries (or alternatively $\mathcal{O}(2^{2N+1})$ real-valued parameters).

Consider a closed quantum many-body system described by a Hamiltonian \mathbf{H} and with its initial state, ρ_0 , given by

$$\begin{aligned} & \text{where } \rho_0 \in \mathcal{C}(\mathbb{H}^{\otimes N}) \\ \rho_0 &= e^{-\mathbf{K}} \\ & \text{and with } \mathbf{K} \in \mathfrak{H}(\mathbb{H}^{\otimes N}) \iff \mathbf{K} = -\log \rho \end{aligned}$$

The system's time evolution of course governed by the Schrödinger equation.

$$i \frac{d\rho(t)}{dt} = [\mathbf{H}, \rho]$$

For the time being, consider ρ_0 as a one-body Max-Ent state, with respect to some general Max-Ent 1 basis composed of a collection of one-body local operators

$$(15) \quad \rho \in \mathcal{S}_{ME,1}(\mathfrak{B}_{ME_1}) \quad \begin{array}{l} \text{which in turn implies that the } \mathbf{K}\text{-operator} \\ \text{can be uniquely decomposed,} \\ \text{upto phase factors, as} \end{array} \quad \mathbf{K} = \sum_{\mu}^{\ell} \phi^{\mu}(t) \mathcal{O}_{\mu},$$

where we have chosen the Schrodinger picture for the operators. Now we claim the following

Theorem 3. *Since $\rho = e^{-\mathbf{K}}$ is a well-defined density operator $\rho_0 \in \mathcal{C}(\mathbb{H}^{\otimes N})$, the \mathbf{K} -operator's time evolution is governed by a Schrödinger equation as well, this is*

$$i \frac{d\mathbf{K}}{dt} = [\mathbf{K}, \rho].$$

Proof. If $\rho = e^{-\mathbf{K}}$ then, by definition

$$(16) \quad \begin{aligned} \rho &= \mathbb{1} - \mathbf{K} + \frac{1}{2}\mathbf{K}^2 - \frac{1}{3!}\mathbf{K}^3 + \dots \\ d\rho &= 0 - d\mathbf{K} + \frac{1}{2}(d\mathbf{K}\mathbf{K} + \mathbf{K}d\mathbf{K}) - \frac{1}{3!}((d\mathbf{K})\mathbf{K}^2 + \mathbf{K}(d\mathbf{K})\mathbf{K} + \mathbf{K}^2(d\mathbf{K})) + \dots \end{aligned}$$

which, if we are willing to assume that $[\mathbf{K}, d\mathbf{K}] = 0$, yields

$$(17) \quad \begin{aligned} d\rho &= 0 - d\mathbf{K} + \frac{1}{2}(d\mathbf{K}\mathbf{K} + \mathbf{K}d\mathbf{K}) - \frac{1}{3!}((d\mathbf{K})\mathbf{K}^2 + \mathbf{K}(d\mathbf{K})\mathbf{K} + \mathbf{K}^2(d\mathbf{K})) + \dots \\ &= -d\mathbf{K} + \mathbf{K}d\mathbf{K} - \frac{1}{2}\mathbf{K}^2d\mathbf{K} + \dots \\ &= -\left(\mathbb{1} - \mathbf{K} + \frac{1}{2}\mathbf{K}^2 + \dots\right)d\mathbf{K} = -e^{-\mathbf{K}}d\mathbf{K} \\ &\Rightarrow \frac{d\rho}{dt} = -e^{-\mathbf{K}}\frac{d\mathbf{K}}{dt}, \end{aligned}$$

and given that ρ 's time evolution is governed by the Schrödinger equation, this yields

$$(18) \quad \begin{aligned} i \frac{d\rho}{dt} &= [\mathbf{H}, \rho] \\ i e^{-\mathbf{K}} \frac{d\mathbf{K}}{dt} &= [\mathbf{H}, e^{-\mathbf{K}}] \end{aligned}$$

[Comentario FTBP: Acá algunas cosas me hacen ruido. Primero, la identidad $\frac{d\rho}{dt} = -e^{-\mathbf{K}}\frac{d\mathbf{K}}{dt}$ se mantiene sí y solo sí asumo que $d\mathbf{K}$ y \mathbf{K} conmutan, lo cual en general no es el caso. Por otro lado, si intento hacer la cuenta por el lado de la derivada del logaritmo tengo que $d \log \rho / dt = \rho^{-1} d\rho / dt$]

$$\begin{aligned}
\frac{d}{dt} \log \rho(t) &= \lim_{\Delta t \rightarrow 0} \frac{\log[\rho + \rho' \Delta t] - \log \rho}{\Delta t} \\
&= \lim_{\Delta t \rightarrow 0} \frac{\log[\rho \rho^{-1} + \rho' \rho^{-1} \Delta t]}{\Delta t} \\
&= \lim_{\Delta t \rightarrow 0} \frac{\log[\mathbb{1} + \rho' \rho^{-1} \Delta t]}{\Delta t} \\
&= \lim_{\Delta t \rightarrow 0} \log \left([\mathbb{1} + \rho' \rho^{-1} \Delta t] \right)^{\frac{1}{\Delta t}} \\
&= \lim_{\sigma \rightarrow 0} \log \left([\mathbb{1} + \sigma] \right)^{\rho' \rho^{-1} \sigma^{-1}} \quad \text{where } \sigma = \rho' \rho^{-1} \Delta t \\
&= \rho' \rho^{-1} \lim_{\sigma \rightarrow 0} \log \left([\mathbb{1} + \sigma] \right)^{\sigma^{-1}} \\
&= \rho' \rho^{-1} \lim_{\sigma \rightarrow 0} \log e \\
&= \rho' \rho^{-1}
\end{aligned}$$

[Comentario FTBP: pero lo que no me gusta de acá es que es que usé que $\log AB^{-1} = \log A - \log B$, que vale solo si conmutan y si $\rho' \rho^{-1}$ conmutan dentro del límite. Me hace ruido]

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Theorem 4. Consider an N -particle closed quantum system and consider an $\ell + \ell'$ -dimensional basis of Hilbert-Schmidt operators, which includes upto two-body operators, ie.

$$\mathfrak{B} = \{\mathbf{O}_i\}_{i=1}^{\ell} \cup \{\mathbf{O}_i \mathbf{O}_j\}_{i=1}^{\ell'} \text{ with } O_i \in \mathfrak{H}\mathfrak{s}_1(\mathbb{H}^{(\ell)}) \forall i \text{ and } \mathfrak{B} \subset \mathfrak{H}\mathfrak{s}_2(\mathbb{H}^{(\ell)}).$$

We then claim that the system's time evolution can then be approximated as

$$\rho(t) = e^{\mathfrak{K}} \text{ where } \mathfrak{K} = \sum_{\mu} \phi^{\mu}(t) \mathbf{O}_{\mu} + \sum_{\mu\nu} \gamma^{\mu\nu}(t) \mathbf{O}_{\mu} \mathbf{O}_{\nu} \text{ for some } \{\phi^{\mu}\}_{\mu}, \{\gamma^{\mu\nu}\}_{\mu,\nu} \subset C^{\infty}(\mathbb{R}) \text{ such that } \rho \in \mathcal{C}(\mathbb{H}), \forall t.$$

Proof. In effect, the closed evolution is governed by the Schrodinger equation on the density matrix,

$$\frac{d\rho}{dt} = \frac{[\mathbf{H}, \rho]}{i},$$

If the density operator can be written as the exponential of a positive-defined operator \mathfrak{K} , the previous equation naturally induces a Schrodinger equation on the \mathfrak{K} -operator, as follows

$$\frac{d\mathfrak{K}}{dt} = \frac{[\mathbf{H}, \mathfrak{K}]}{i}.$$

Which entails,

$$\begin{aligned}
(19) \quad & \sum_{\mu} \frac{d\phi^{\mu}}{dt} \mathbf{O}_{\mu} + \sum_{\mu\nu} \frac{d\gamma^{\mu\nu}}{dt} \mathbf{O}_{\mu} \mathbf{O}_{\nu} = \left[\mathbf{H}, \sum_{\mu} \phi^{\mu}(t) \mathbf{O}_{\mu} + \sum_{\mu\nu} \gamma^{\mu\nu}(t) \mathbf{O}_{\mu} \mathbf{O}_{\nu} \right] \\
& \sum_{\mu} \frac{d\phi^{\mu}}{dt} \mathbf{O}_{\mu} + \sum_{\mu\nu} \frac{d\gamma^{\mu\nu}}{dt} \mathbf{O}_{\mu} \mathbf{O}_{\nu} = \sum_{\mu} \phi^{\mu}(t) [\mathbf{H}, \mathbf{O}_{\mu}] + \sum_{\mu\nu} \gamma^{\mu\nu}(t) [\mathbf{H}, \mathbf{O}_{\mu} \mathbf{O}_{\nu}]
\end{aligned}$$

(20)

$$\begin{aligned} &\Rightarrow \left(\mathbf{O}_\alpha, \sum_\mu \frac{d\phi^\mu}{dt} \mathbf{O}_\mu + \sum_{\mu\nu} \frac{d\gamma^{\mu\nu}}{dt} \mathbf{O}_\mu \mathbf{O}_\nu\right) = \left(\mathbf{O}_\alpha, \sum_\mu \phi^\mu(t) [\mathbf{H}, \mathbf{O}_\mu] + \sum_{\mu\nu} \gamma^{\mu\nu}(t) [\mathbf{H}, \mathbf{O}_\mu \mathbf{O}_\nu]\right) \\ &\sum_\mu \frac{d\phi^\mu}{dt} (\mathbf{O}_\alpha, \mathbf{O}_\mu) + \sum_{\mu\nu} \frac{d\gamma^{\mu\nu}}{dt} (\mathbf{O}_\alpha, \mathbf{O}_\mu \mathbf{O}_\nu) \overset{\delta_{\alpha\mu}}{\overset{0}{=}} \left(\sum_\mu \phi^\mu(t) (\mathbf{O}_\alpha, [\mathbf{H}, \mathbf{O}_\mu]) + \sum_{\mu\nu} \gamma^{\mu\nu}(t) (\mathbf{O}_\alpha, [\mathbf{H}, \mathbf{O}_\mu \mathbf{O}_\nu])\right) \\ &\frac{d\phi^\alpha}{dt} = \left(\sum_\mu \phi^\mu(t) (\mathbf{O}_\alpha, [\mathbf{H}, \mathbf{O}_\mu]) + \sum_{\mu\nu} \gamma^{\mu\nu}(t) (\mathbf{O}_\alpha, [\mathbf{H}, \mathbf{O}_\mu \mathbf{O}_\nu])\right) \end{aligned}$$

$$\frac{d\phi^\alpha}{d\alpha} = \sum_\mu \mathcal{H} \phi^\mu,$$

where

$$\begin{aligned} \mathcal{H} : \mathfrak{Hs}(\mathbb{H}^{\otimes N}) \times \mathfrak{Hs}(\mathbb{H}^{\otimes N}) &\rightarrow \mathbb{C}^{\dim \times \dim} \\ (\mathcal{H})_{\mu\nu} &= (\mathbf{O}_\nu, [\mathbf{H}, \mathbf{O}_\nu]) \end{aligned}$$

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4. RESÚMEN

Sea $\mathcal{C}(\mathbb{H}) = \{\rho \in \text{GL}(N, \mathbb{C}) \mid \rho^\dagger = \rho, \rho \geq 0, \text{Tr } \rho = 1\}$, el conjunto de todas las matrices densidad. Este espacio tiene la estructura de una variedad de Kahler $(\mathcal{C}(\mathbb{H}), g, J)$, donde tanto g como J deben ser evaluadas localmente. Resolver el problema

$$\frac{d\rho}{dt} = [\mathbf{H}, \rho(t)] \Big|_{\rho(t) \in \mathcal{C}(\mathbb{H}), \forall t},$$

es un problema NP-hard, intractable para un espacio de Hilbert con dimensión mayor a 2^N , $N = 15$ configuraciones. Una forma de obtener soluciones aproximadas a la dinámica es considerar estados gaussianos.

Sea un sistema dinámico cuántico cerrado (sin interacciones con el exterior) cuyo estado inicial es

$$\rho_0 = e^{-\mathbf{K}} \text{ con } \mathbf{K} \in \mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \iff \mathbf{K} = -\log \rho$$

donde $\mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N})$ es el conjunto de todos los operadores Hilbert-Schmidt, i.e. de traza finita, que sean hermíticos; dicho espacio imbuído con el producto interno de Hilbert-Schmidt $\langle A, B \rangle_{\text{HS}} = \text{Tr } A^\dagger B$. En tales condiciones, la ecuación diferencial sobre ρ se convierte en una ecuación diferencial sobre \mathbf{K} mismo.

$$i \frac{d\mathbf{K}}{dt} = [\mathbf{K}, \rho]$$

Luego, si se considera una base, ortonormal respecto a este producto interno, ℓ -dimensional de operadores \mathfrak{B}_{ME} , la exponencial de combinaciones lineales de estos operadores da origen a una variedad gaussiana denotada por $\mathcal{S}_{ME}(\mathfrak{B}_{ME})$

$$(21) \quad \rho(t) \in \mathcal{S}_{ME}(\mathfrak{B}_{ME}) \quad \text{which in turn implies that the } \mathbf{K}\text{-operator} \\ \text{can be uniquely decomposed,} \quad \mathbf{K} = \sum_{\mu}^{\ell} \phi^{\mu}(t) \mathcal{O}_{\mu}, \\ \text{upto phase factors, as}$$

Luego de algunas cuentas, resulta que la evolución puede ser reescrita como

$$(22) \quad \frac{d\phi^{\alpha}}{dt} = \sum_{\mu} \mathcal{H}_{\alpha\mu} \phi^{\mu},$$

donde $\mathcal{H}_{\alpha\mu} = (\mathbf{O}_{\alpha}, [\mathbf{H}, \mathbf{O}_{\mu}])$ y tal que

$$\mathcal{H} : \mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \times \mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \rightarrow \mathbb{C}^{\dim \times \dim} \\ (\mathcal{H})_{\mu\nu} = (\mathbf{O}_{\nu}, [\mathbf{H}, \mathbf{O}_{\mu}]).$$

La solución a (19) es simple pues esta matriz \mathcal{H} es constante

$$\phi^{\alpha}(t) = \sum_{\beta} (e^{\mathcal{H}t})_{\alpha\beta} \phi_0^{\beta} \Rightarrow \rho(t) = e^{\sum_{\alpha} \phi(t)_{\alpha} \mathbf{O}^{\alpha}}$$

La gracia del método que innovamos con Mauricio es que no necesito todos los operadores de la base enorme, puedo poner algunos y obtener buenos resultados. Un método muy eficiente de construir una base es a partir de un operador semilla \mathbf{O} y sus conmutadores

$$\mathfrak{B}_{ME} = \{\mathbf{O}, [\mathbf{H}, \mathbf{O}], [\mathbf{H}, [\mathbf{H}, \mathbf{O}]] \cdot \dots, [\mathbf{H}, \dots [\mathbf{O}] \dots]\} = \{[\mathbf{H}, \mathbf{O}]^{\wedge n}\}_{n=0}^{\ell},$$

es decir esta base la armo con el operador semilla, el primer conmutador con el Hamiltoniano del sistema, el segundo conmutador y así sucesivamente todo lo que yo quiera. Y esta base la puedo calcular muy rápidamente con el algoritmo de Strassen para sistemas de mucha dimensión, ya que al fin y al cabo es multiplicar matrices.

Las dos preguntas no triviales que me surgieron que pueden ser tratadas con el análisis matricial son:

- 1) Primero estimar el error en la aproximación. Claramente si elijo una base a partir de cierto operador semilla y agarro la misma base con más elementos, voy a obtener mejores resultados. Pero me gustaría ver si es posible estimar el error y la rapidez de convergencia, capaz a partir de estudiar los autovalores de \mathcal{H} .
- 2) La otra es elaborar un criterio para elegir el operador semilla inicial. Por ejemplo, en algunos casos simples he visto, heurísticamente, que si agarro un operador A con n conmutadores y agarro otro operador B con m conmutadores, de forma tal que $m < n$, sucede que (dependiendo de la elección de los operadores semilla), la base que tiene menos operadores puede dar mejores resultados que la otra; lo cual me pareció muy interesante.

5. RESULTADOS DEL ALGORITMO

Longitud de la cadena variable.

- First case

Consider the XX-Heisenberg Hamiltonian. At $T_{\rho_{\text{ref}}} = 2T_{\rho_0} = 2 \times 10^{-1}K$, with a basis, reference state and occupation list given by

$$(23) \quad \mathfrak{B} = [\text{id}, \mathbf{H}, [\mathbf{H}, \cdot]^{\wedge s=4}(\mathbf{S}_1)]$$

$$(24) \quad \rho_r ef = e^{-\beta_{\text{ref}} \mathbf{S}_1^x}$$

$$(25) \quad (\mathbf{K}_0)_i = [0, 0, .5, 0, 0, 0].$$



FIGURE 1. Averages for a variable-length spin chain.

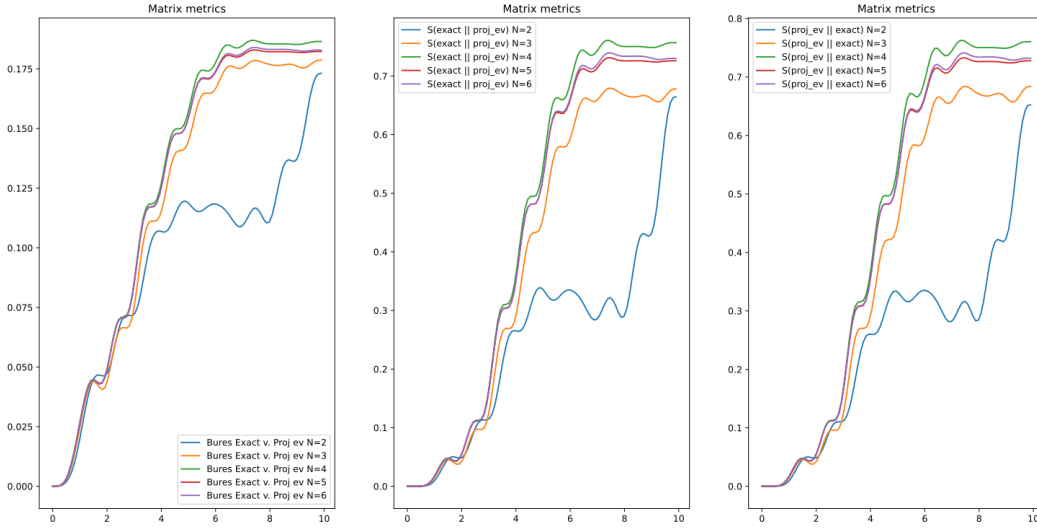


FIGURE 2. Metrics for a variable-length spin chain.

Temperatura de referencia variable. For a spin chain of length $N = 2$, with a basis, reference state and occupation list given by

$$(26) \quad \mathfrak{B} = [\mathfrak{i}\partial, \mathbf{H}, [\mathbf{H}, \cdot]^{\wedge s=4}(\mathbf{S}_1)]$$

$$(27) \quad \rho_{\text{ref}} = e^{-\beta_{\text{ref}} \mathbf{S}_1^x}$$

$$(28) \quad (\mathbf{K}_0)_i = [0, 0, .5, 0, 0, 0].$$

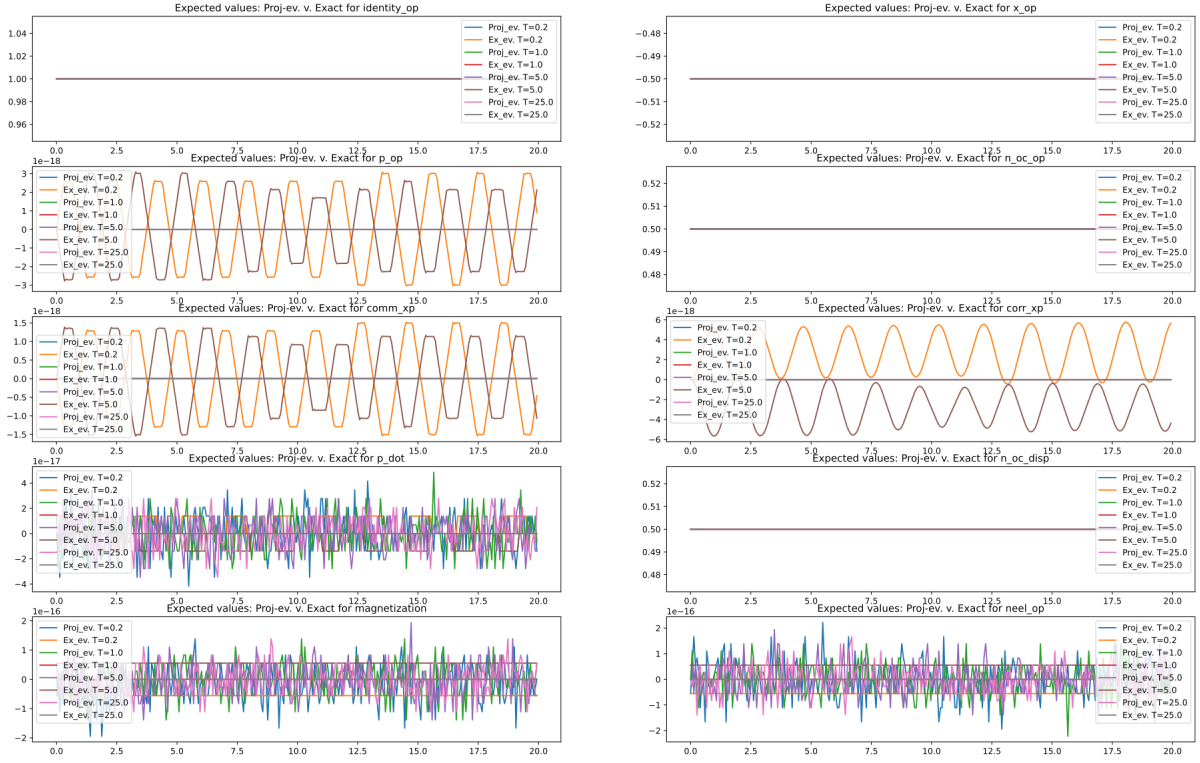


FIGURE 3. Avgs

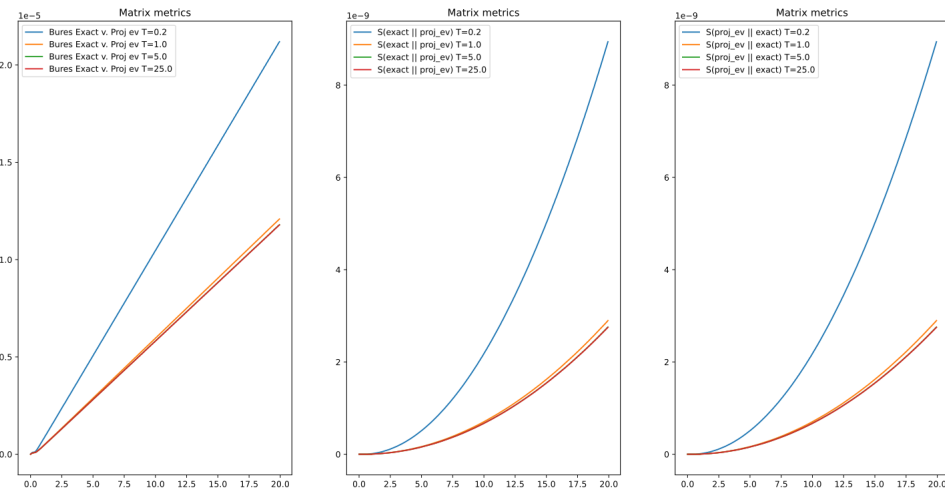


FIGURE 4. Caption