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Condensed Matter Theory - Lecture Notes
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Theory & Notes

1. Cuentitas

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 $\mathcal{C}(\mathbb{H})$,

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

where $\mathrm{GL}(N, \mathbb{C})$ 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 $(S, \boldsymbol{S}, \lambda)$ 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

$$\mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N}),\ \text{where } \mathbf{K} \in \mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N}) \text{ if and only if } \begin{array}{c} \mathbf{K} : \mathbb{H}^{\otimes N} \to \mathbb{H}^{\otimes N} \\ \mathbf{K} = \mathbf{K}^\dagger \\ \mathrm{Tr}\,\mathbf{K}^\dagger\mathbf{K} = \mathrm{Tr}\,\mathbf{K^2} < \infty \end{array} \tag{1}$$

We claim the following

Theorem 1. *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* M *is a Riemannian manifold* (M, B)*, where* B *is the Bures metric.*

Proof. In effect, this manifold is path-connected,

$$\forall \rho_1, \rho_2 \in \mathcal{M}, \exists f : \mathbb{R}_{[0,1]} \to \mathcal{M} \text{ and } f(0) = \rho_1, f(1) = \rho_"$$

such that said path always exists. In effect, consider the function

$$\begin{aligned} f &: \mathbb{R}_{[0,1]} \to \mathcal{M} \\ f(x) &= x\rho_1 + (1 - x)\rho_2, \end{aligned}$$

which is continuous for arbitrary density matrices. Thus, according to the Hopf-Rinow theorem, there are a number of inmediate consequences:

- the closed and bounded subsets of $\mathcal{M}$ are compact, ie. for each of these subsets, there always exists a uniformly convergent Cauchy subsequence. [1]
- $\mathcal{M}$ is a complete metric space ie. every Cauchy sequence of points on $\mathcal{M}$ has a limit that is also in $\mathcal{M}$.
- $\mathcal{M}$ is geodesically complete, that is, $\forall \rho \in \mathcal{M}$, the exponential map $\mathfrak{exp}_\rho : T_\rho\mathcal{M} \to \mathcal{M}$ is always well defined and can be defined on the entire tangent space.

In other words, the Hopf-Rinow theorem assures that, given any two arbitrary point $\rho, \sigma \in \mathcal{M}$, there always exists a length-minimizing geodesic connecting these two-points[2].

By construction, it is clear that the natural choice for the tangent space $T_\rho\mathcal{M}$ is $\mathfrak{Hs}^\dagger(\mathbb{H}^{\otimes N})$

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

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

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

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[1] Remember that a set X is compact if every sequence on X has a uniformly convergent subsequence, a subsequence which converges to a point on X.

[2] Note 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 Hilber tspace 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 $\mathbb{H}^{\otimes N}$

Consider the set of all density operators, labelled $\mathcal{C}(\mathbb{H}^{\otimes N})$, we are interested in two subsets of these, the Max-Ent manifolds

By definition, $\mathcal{C}(\mathbb{H}^{\otimes N}) \subset \mathrm{GL}(N, \mathbb{C})$. In particular, we claim that it has the structure of a Riemannian non-convex manifold. All of these density matrices can be written as the exponential of a hermitian $\mathbf{K}$-operator,

$$\mathbf{K} \in \mathrm{End}(\mathcal{C}(\mathbb{H}^{\otimes N})) \text{ and } \mathbf{K}^{\dagger} = \mathbf{K}.$$

If a basis $\mathcal{B}$ of trace-class operators is chosen, then

$$\mathcal{B} = \{\mathbf{O}_i\}_{i=1}^{\dim \mathcal{B}} \Rightarrow \mathbf{K} = \sum_i \alpha_i \mathbf{O}, \alpha_i \in \mathbb{C}$$

so that there exists a mapping from the space of all trace-class endomorphisms to the space of all Max Ent-type density matrices, said mapping being the exponential mapping.

$$\begin{aligned}
&\mathfrak{exp} : T_{\alpha}\mathcal{M} \to \mathcal{M} \\
&\mathfrak{exp}(\mathbf{K}) \to e^{\mathbf{K}} \text{ so long as } \mathbf{K} \in \mathrm{End}(\mathcal{C}(\mathbb{H}^{\otimes N})) \text{ and } \mathbf{K} = \mathbf{K}^{\dagger}
\end{aligned}$$

The exponential mapping is well defined for all trace-class hermitian operators since the manifold is path-connected. In effect,

$$\forall \rho_1, \rho_2 \in \mathbf{S}_{\mathrm{ME2}} \tag{2}$$

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

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

  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

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

  ie. the tensor space $\mathbb{H} \otimes \mathbb{H}^\star$ 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.

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

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

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 subsytem's Hilbert space. This definition thus allows for systems with different particles species (eg. fermions, bosons, spins etc.). Then,

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

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

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

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

$$\langle \cdot, \cdot \rangle_{\text{HS}} : \mathfrak{Hs}(\mathbb{H}) \times \mathfrak{Hs}(\mathbb{H}) \to \mathbb{C}, \text{ where } \quad \begin{array}{l} \langle \mathbf{A}, \mathbf{B} \rangle_{\text{HS}} = \text{Tr } \mathbf{A}^\dagger \mathbf{B} \\ ||\mathbf{A}||_{\text{HS}} = \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{A}}. \end{array}$$

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 choice[3].

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

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[3] In 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 $\mathbf{A}, \mathbf{B} \in \mathfrak{Hs}(\mathbb{H})$, then the new operator $\mathbf{A}^\dagger \mathbf{B}$ is a trace-class operator, meaning that the sum

- 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 $\mathfrak{hs}(\mathbb{H})$.

Acá va un comentario "importante": no tiene sentido que dos vectores estén infinitamente lejos, no? entónces tengo que definir esto producto interno y métrico solo en HS(H) y no sobre B(H)

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

$$\begin{array}{c} \mathbf{A} \to \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{A}} \\ \text{is a well-defined norm} \end{array} \quad \text{then} \quad \begin{array}{c} \mathbf{A}, \mathbf{B} \xrightarrow{d} \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{B}} \\ \text{is a well-defined distance} \end{array}$$

$$\begin{aligned} d_{\text{HS}}(\cdot, \cdot) :\ & \mathfrak{Hs}(\mathbb{H}) \times \mathfrak{Hs}(\mathbb{H}) \to \mathbb{R} \\ & d_{\text{HS}}(\mathbf{A}, \mathbf{B}) = \sqrt{\text{Tr } \mathbf{A}^\dagger \mathbf{B}} \end{aligned}$$

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

$$\begin{aligned} \langle \cdot, \cdot \rangle^{\rho_0}_{\text{HS}} :\ & \mathfrak{Hs}(\mathbb{H}) \times \mathfrak{Hs}(\mathbb{H}) \to \mathbb{R} \\ & \langle \mathbf{A}, \mathbf{B} \rangle^{\rho_0}_{\text{HS}} = \tfrac{1}{2} \text{Tr } \rho_0 \{\mathbf{A}^\dagger, \mathbf{B}\} \end{aligned} \quad \text{where } \rho_0 \in \mathcal{C}(\mathbb{H}).$$

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

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

$$\begin{aligned} \langle \mathbf{A}, \mathbf{B} \rangle^{\rho_0}_{\text{HS}} &= \frac{1}{2} \text{Tr } \rho_0 \{\mathbf{A}^\dagger, \mathbf{B}\} = \frac{1}{2} \text{Tr } \rho_0 \left(\mathbf{A}^\dagger \mathbf{B} + \mathbf{B} \mathbf{A}^\dagger \right) \\ &= \frac{1}{2} \text{Tr } \rho_0 \left(\mathbf{B}^\dagger \mathbf{A} + \mathbf{A} \mathbf{B}^\dagger \right)^\dagger = \frac{1}{2} \text{Tr } \rho_0 \{\mathbf{B}^\dagger, \mathbf{A}\}^\dagger \\ &= (\langle \mathbf{B}, \mathbf{A} \rangle^{\rho_0}_{\text{HS}})^* \end{aligned} \tag{3}$$

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

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

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

$$\langle \mathbf{A}, \mathbf{A} \rangle_{\text{HS}}^{\rho_0} = \frac{1}{2}\text{Tr}\,\rho_0\{\mathbf{A}^\dagger, \mathbf{B}\} = \text{Tr}\,\sqrt{\rho}\frac{\mathbf{A}\mathbf{A}^\dagger + \mathbf{A}^\dagger\mathbf{A}}{2}\sqrt{\rho} \tag{4}$$

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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.

(5)

$\mathfrak{Hs}_1(\mathbb{H}) = \{\hat{\mathbf{O}} | \hat{\mathbf{O}} \in \mathcal{B}_1 \wedge ||\mathbf{O}||_{\text{HS}}^{\rho_0} < \infty,\ \forall j \leq N\}$ is the space of all one-body operators, and where

$\mathfrak{Hs}_k(\mathbb{H}) = \{\otimes_{i=1}^{k} \hat{\mathbf{O}}_i | \hat{\mathbf{O}}_i \in \mathfrak{Hs}_1(\mathbb{H})\ \forall i, k \leq N\}$ is the space of all k-body operators $\quad \mathfrak{Hs}(\mathbb{H}) = \bigsqcup_{k=1}^{N} \mathfrak{Hs}_k(\mathbb{H})$

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

$$\begin{array}{ccc}
\{\mathbf{O}_i^{(1)}\}_{i=1}^{n_1} \in \mathfrak{Hs}_1(\mathbb{H}^{(1)}) & & \mathfrak{b}_1 = \{\mathbf{O}_i^{(1)} \otimes \bigotimes_{k=2}^{N} \mathbb{1}^{(k)}\}_{i=1}^{n_1} \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N}) \\
\vdots & \text{The operators are then} & \vdots \\
\{\mathbf{O}_i^{(\ell)}\}_{i=1}^{n_\ell} \in \mathfrak{Hs}_1(\mathbb{H}^{(\ell)}) & \text{redefined so that they act on the global} & \mathfrak{b}_\ell = \{\otimes_{k=1}^{\ell} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(\ell)} \otimes_{k'=\ell+1}^{N} \mathbb{1}^{(k')}\}_{i=1}^{n_\ell} \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N}) \\
\vdots & \text{Hilbert space } \mathbb{H}^{\otimes N} & \vdots \\
\{\mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \in \mathfrak{Hs}_1(\mathbb{H}^{(N)}) & & \mathfrak{b}_N = \{\bigotimes_{k=1}^{N-1} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N})
\end{array}$$

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

$$\boldsymbol{\mathcal{S}}_{ME,1}(\mathfrak{B}_{ME_1}) = \{\rho \in \mathcal{C}(\mathbb{H}) \mid \exists \{\lambda_k\}_{k=1}^{\dim \mathfrak{B}_{ME_1}} \subset \mathbb{R} \text{ such that } \rho \propto \exp\Big(-\sum_i \lambda_i \mathbf{O}_i\Big)\}. \tag{6}$$

Näive two-body Max-Ent

Here, similarly to the näive 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

(7)
$$\begin{array}{ccc}
\{\mathbf{O}_i^{(1)}\}_{i=1}^{n_1} \in \mathfrak{Hs}_1(\mathbb{H}^{(1)}) & & \mathfrak{b}_1 = \{\mathbf{O}_i^{(1)} \otimes \bigotimes_{k=2}^{N} \mathbb{1}^{(k)}\}_{i=1}^{n_1} \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N}) \\
\vdots & & \vdots \\
\{\mathbf{O}_i^{(\ell)}\}_{i=1}^{n_\ell} \in \mathfrak{Hs}_1(\mathbb{H}^{(\ell)}) \quad , & \begin{array}{c}\text{then the global} \\ \text{one-body operators are}\end{array} & \mathfrak{b}_\ell = \{\otimes_{k=1}^{\ell} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(\ell)} \otimes_{k'=\ell+1}^{N} \mathbb{1}^{(k')}\}_{i=1}^{n_\ell} \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N}) \\
\vdots & & \vdots \\
\{\mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \in \mathfrak{Hs}_1(\mathbb{H}^{(N)}) & & \mathfrak{b}_N = \{\bigotimes_{k=1}^{N-1} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \subset \mathfrak{Hs}(\mathbb{H}^{\otimes N})
\end{array}$$

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

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

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,

$$\Gamma(n_a, n_b) = n_a + n_b + \frac{n_a(n_b - 1)}{2} \tag{8}$$

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

(9)
$$\boldsymbol{\mathcal{S}}_{ME,2}(\mathfrak{B}_{ME_2}) = \{\rho \in \mathcal{C}(\mathbb{H}) \mid \exists \{\lambda_k\}_{k=1}^{\ell\leq N}, \{\gamma_{mn}\}_{\substack{m,n=1 \\ m<n}}^{\ell\leq N} \subset \mathbb{R} \text{ such that } \rho \propto \exp\left(-\sum_{i,j} \lambda_i \mathbf{O}_i - \gamma_{ij}\mathbf{O}_i\mathbf{O}_j\right)\}.$$

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

$$\rho_0 = e^{-\mathbf{K}} \quad \begin{array}{c} \text{where } \rho_0 \in \mathcal{C}(\mathbb{H}^{\otimes N})) \\ \text{and with } \mathbf{K} \in \mathfrak{Hs}(\mathbb{H}^{\otimes N}) \Longleftrightarrow \mathbf{K} = -\log \rho \end{array}$$

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

$$\rho \in \boldsymbol{\mathcal{S}}_{ME,1}(\mathfrak{B}_{ME_1}) \quad \begin{array}{c} \text{which in turn implies that the } \mathbf{K}\text{-operator} \\ \text{can be uniquely decomposed,} \\ \text{upto phase factors, as} \end{array} \quad \mathbf{K} = \sum_{\mu}^{\ell} \phi^{\mu}(t) \boldsymbol{\mathcal{O}}_{\mu}, \tag{10}$$

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

$$\begin{aligned} \rho &= \mathbb{1} - \mathbf{K} + \frac{1}{2}\mathbf{K}^2 - \frac{1}{3!}\mathbf{K}^3 + \cdots \\ d\rho &= 0 - d\mathbf{K} + \frac{1}{2}\Big(d\mathbf{K}\mathbf{K} + \mathbf{K}d\mathbf{K}\Big) - \frac{1}{3!}\Big((d\mathbf{K})\mathbf{K}^2 + \mathbf{K}(d\mathbf{K})\mathbf{K} + \mathbf{K}^2(d\mathbf{K})\Big) + \cdots \end{aligned} \tag{11}$$

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

$$\begin{aligned} d\rho &= 0 - d\mathbf{K} + \frac{1}{2}\Big(d\mathbf{K}\mathbf{K} + \mathbf{K}d\mathbf{K}\Big) - \frac{1}{3!}\Big((d\mathbf{K})\mathbf{K}^2 + \mathbf{K}(d\mathbf{K})\mathbf{K} + \mathbf{K}^2(d\mathbf{K})\Big) + \cdots \\ &= -d\mathbf{K} + \mathbf{K}d\mathbf{K} - \frac{1}{2}\mathbf{K}^2 d\mathbf{K} + \cdots \\ &= -\Big(\mathbb{1} - \mathbf{K} + \frac{1}{2}\mathbf{K}^2 + \cdots\Big)d\mathbf{K} = -e^{-\mathbf{K}}d\mathbf{K} \\ &\Rightarrow \frac{d\rho}{dt} = -e^{-\mathbf{K}}\frac{d\mathbf{K}}{dt}, \end{aligned} \tag{12}$$

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

$$\begin{aligned} i\frac{d\rho}{dt} &= [\mathbf{H}, \rho] \\ ie^{-\mathbf{K}}\frac{d\mathbf{K}}{dt} &= [\mathbf{H}, e^{-\mathbf{K}}] \end{aligned} \tag{13}$$

[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 dK y 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 $d\log\rho/dt = \rho^{-1}d\rho/dt$]

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

[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]

quod erat dem■

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.*

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

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,

$$
\begin{aligned}
\sum_{\mu}\frac{d\phi^{\mu}}{dt}\mathbf{O}_{\mu}+\sum_{\mu\nu}\frac{d\gamma^{\mu\nu}}{dt}\mathbf{O}_{\mu}\mathbf{O}_{\nu} &= \Big[\mathbf{H},\sum_{\mu}\phi^{\mu}(t)\mathbf{O}_{\mu}+\sum_{\mu\nu}\gamma^{\mu\nu}(t)\mathbf{O}_{\mu}\mathbf{O}_{\nu}\Big]\\
\sum_{\mu}\frac{d\phi^{\mu}}{dt}\mathbf{O}_{\mu}+\sum_{\mu\nu}\frac{d\gamma^{\mu\nu}}{dt}\mathbf{O}_{\mu}\mathbf{O}_{\nu} &= \sum_{\mu}\phi^{\mu}(t)[\mathbf{H},\mathbf{O}_{\mu}]+\sum_{\mu\nu}\gamma^{\mu\nu}(t)[\mathbf{H},\mathbf{O}_{\mu}\mathbf{O}_{\nu}]
\end{aligned}
\tag{14}
$$

$$
\begin{aligned}
&\Rightarrow \left(\mathbf{O}_\alpha, \sum_\mu \frac{d\phi^\mu}{dt}\mathbf{O}_\mu + \sum_{\mu\nu}\frac{d\gamma^{\mu\nu}}{dt}\mathbf{O}_\mu\mathbf{O}_\nu\right) = \left(\mathbf{O}_\alpha, \sum_\mu \phi^\mu(t)[\mathbf{H},\mathbf{O}_\mu] + \sum_{\mu\nu}\gamma^{\mu\nu}(t)[\mathbf{H},\mathbf{O}_\mu\mathbf{O}_\nu]\right)\\
&\sum_\mu \frac{d\phi^\mu}{dt}\cancelto{\delta_{\alpha\mu}}{(\mathbf{O}_\alpha,\mathbf{O}_\mu)} + \cancelto{0}{\sum_{\mu\nu}\frac{d\gamma^{\mu\nu}}{dt}(\mathbf{O}_\alpha,\mathbf{O}_\mu\mathbf{O}_\nu)} = \left(\sum_\mu \phi^\mu(t)(\mathbf{O}_\alpha,[\mathbf{H},\mathbf{O}_\mu]) + \sum_{\mu\nu}\gamma^{\mu\nu}(t)(\mathbf{O}_\alpha,[\mathbf{H},\mathbf{O}_\mu\mathbf{O}_\nu])\right)\\
&\frac{d\phi^\alpha}{dt} = \left(\sum_\mu \phi^\mu(t)(\mathbf{O}_\alpha,[\mathbf{H},\mathbf{O}_\mu]) + \sum_{\mu\nu}\gamma^{\mu\nu}(t)(\mathbf{O}_\alpha,[\mathbf{H},\mathbf{O}_\mu\mathbf{O}_\nu])\right)
\end{aligned}
\tag{15}
$$

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

where

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

quod erat dem ■