Tomás Pérez
Condensed Matter Theory - Lecture Notes
August 8, 2022

Theory & Notes

1. Cuentitas

Given a physical system, a density operator for 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

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

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

  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,

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

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

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

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 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[1].

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

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

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

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

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 $\langle \cdot, \cdot \rangle_{\text{HS}}$

[1] 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

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

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

(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 1. *Consider the modified Hilbert-Schmidt product given by*

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

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 hermitian? Yes

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

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

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

quod erat dem■

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.

$$\begin{array}{lll} \mathfrak{Hs}_1(\mathbb{H}) = \{\hat{\mathbf{O}} | \hat{\mathbf{O}} \in \mathcal{B}_1 \wedge ||\mathbf{O}||_{\text{HS}}^{\rho_0} < \infty,\ \forall j \leq N\} & \text{is the space of all one-body operators,} & \text{and where} \\ \mathfrak{Hs}_k(\mathbb{H}) = \{\otimes_{i=1}^k \hat{\mathbf{O}}_i | \hat{\mathbf{O}}_i \in \mathfrak{Hs}_1(\mathbb{H})\ \forall i, k \leq N\} & \text{is the space of all } k\text{-body operators} & \mathfrak{Hs}(\mathbb{H}) = \bigsqcup_{k=1}^N \mathfrak{Hs}_k(\mathbb{H}) \end{array} \tag{3}$$

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

$$\begin{array}{c} \{\mathbf{O}_i^{(1)}\}_{i=1}^{n_1} \in \mathfrak{Hs}_1(\mathbb{H}^{(1)}) \\ \vdots \\ \{\mathbf{O}_i^{(\ell)}\}_{i=1}^{n_\ell} \in \mathfrak{Hs}_1(\mathbb{H}^{(\ell)}) \\ \vdots \\ \{\mathbf{O}_i^{(N)}\}_{i=1}^{n_N} \in \mathfrak{Hs}_1(\mathbb{H}^{(N)}) \end{array}$$

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

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

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

$$\boldsymbol{\mathcal{S}}_{ME,1}(\mathfrak{B}_{ME_1}) = \{\rho \in \mathcal{C}(\mathbb{H}) \mid \exists \{\lambda_k\}_{k=1}^{\dim \mathfrak{B}_{ME_1}} \subset \mathbb{R} \text{ such that } \rho \propto \exp\left(-\sum_i \lambda_i \mathbf{O}_i\right)\}. \tag{4}$$

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

(5)

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

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

$$\mathfrak{c}_{11} = \{\mathbf{O}_i^{(1)}\mathbf{O}_j^{(1)} \otimes_{k=2}^{N} \mathbb{1}^{(k)}\}_{i,j=1}^{\Gamma(n_1,n_1)} \mid \mathbf{O}_i^{(1)} \in \mathfrak{b}_1$$

$$\mathfrak{c}_{12} = \{\mathbf{O}_i^{(1)} \otimes \mathbf{Q}_j^{(2)} \otimes_{k=3}^{N} \mathbb{1}^{(k)}\}_{i,j=1}^{\Gamma(n_1,n_2)} \mid \mathbf{O}_i^{(1)} \in \mathfrak{b}_1, \mathbf{Q}_j^{(2)} \in \mathfrak{b}_2$$

$$\vdots$$

$$\mathfrak{c}_{\ell\ell'} = \{\mathbf{O}_i^{(\ell)} \otimes \mathbf{Q}_j^{(\ell)} \otimes_{\substack{k=1\\ k\neq \ell\ell'}}^{N} \mathbb{1}^{(k)}\}_{i,j=1}^{\Gamma(n_\ell,n_{\ell'})} \mid \mathbf{O}_i^{(1)} \in \mathfrak{b}_\ell, \mathbf{Q}_j^{(2)} \in \mathfrak{b}_{\ell'},$$

$$\vdots$$

$$\mathfrak{c}_{NN} = \{\bigotimes_{k=1}^{N-1} \mathbb{1}^{(k)} \otimes \mathbf{O}_i^{(N)}\mathbf{O}_j^{(N)}\}_{i,j=1}^{\Gamma(n_N,n_N)} \mid \mathbf{O}_i^{(N)} \in \mathfrak{b}_N$$

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,

(6)
$$\Gamma(n_a, n_b) = \begin{cases} n_a^2 & \text{if } n_a = n_b \\ n_b + \frac{n_a(n_b-1)}{2} & \text{otherwise} \end{cases}$$

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

(7)

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

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.