Tomás Pérez
Condensed Matter Theory - Lecture Notes
August 7, 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 $\mathcal{C}(\mathbb{H})$,

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

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

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,

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

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 $\text{Tr}\, \mathbf{A}^\dagger\mathbf{A} < \infty$. 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[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

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

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

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

[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. A straight-forward modification is to consider instead

$$\begin{aligned}\langle\cdot,\cdot\rangle_{\mathrm{HS}} :\ \mathfrak{Hs}(\mathbb{H}) \times \mathfrak{Hs}(\mathbb{H}) &\to \mathbb{R}\\ \langle\mathbf{A},\mathbf{B}\rangle_{\mathrm{HS}} &= \frac{1}{2}\,\mathrm{Tr}\{\mathbf{A}^{\dagger}\mathbf{B}\}\end{aligned}$$