Quantum Information Geometry and Applications

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Abstract

In the first part of this thesis, we present a brief introduction to quantum information geometry. We start with a discussion of classical information geometry and derive the Fisher-Rao metric. We then proceed to generalize the theory to the quantum setting and derive the Fubini-Study metric. We show how normalized quantum states gain a deeper geometrical meaning through their gauge ambiguity and how this property leads to a phase known as the Berry phase, induced by the Berry connection. Finally, we generalize these results to the mixed state case, deriving the mixed state metric – the Bures metric. In the second part of this thesis, we provide a natural generalization of a Riemannian structure, i.e., a metric, recently introduced by Sjöqvist for the space of non degenerate density matrices, to the degenerate case, i.e., in which the eigenspaces have dimension greater or equal to one. We present a physical interpretation of the metric in terms of an interferometric measurement. We study this metric, physically interpreted as an interferometric susceptibility, to the study of topological phase transitions at finite temperatures for band insulators. We compare the behaviors of this susceptibility and the one coming from the well-known Bures metric, showing them to be dramatically different. While both infer zero temperature phase transitions, only the former predicts finite temperature phase transitions as well. The difference in behaviors can be traced back to a symmetry breaking mechanism, akin to Landau-Ginzburg theory, by which the Uhlmann gauge group is broken down to a subgroup determined by the type of system's density matrix (i.e., the ranks of its spectral projectors).

Keywords: information geometry; geometric phases; phase transitions; susceptibility; interferometric metric.

1. Introduction

Geometry and physics go hand in hand and quantum mechanics is no exception. In the beginning of the 20th century, information geometry was originally motivated by providing a structure to statistical models in order to use geometrical tools and arguments to study and geometrize mathematical statistics. Harold Hotelling [1] was the first to relate the Fisher Information Matrix to a Riemannian metric tensor g and interpreted the parameter space of the probability distribution as a Riemannian manifold $(\mathcal{M}, g)$. Nowadays, the induced Riemannian metric in the space of parametrized probability distributions is called the *Fisher-Rao metric*. Now, quantum mechanics is an intrinsically probabilistic theory, hence one can ask if the same treatment can be applied for the case of quantum states. This has been in fact demonstrated: quantum states may be described by genuine probability distributions [2]. The methods used in classical statistical theory can then be translated into the quantum language when dealing with quantum states. This geometrical picture of quantum mechanics is called *quantum information geometry*.

Recent advances in the area have provided new methods for studying quantum matter and describing macroscopic critical phenomena based on quantum effects. Topological phases of matter are described in terms of *global* topological invariants that are robust against continuous perturbations of the system. An example of these invariants is the Thouless-Kohmoto-Nightingale-den Nihjs (TKNN) invariant, mathematically a Chern number associated to the vector bundle of occupied Bloch states over the Brillouin zone. This invariant captures topological phases of matter that could not be understood previously, such as the case of the anomalous Hall insulator [3], which falls into the class of Chern insulators. The classification of topological phases of gapped free fermions is encoded in the so-called periodic table of topological insulators and superconductors [4]. However, by now we know that these phases of matter were just the tip of the iceberg, see [5–8]. The theory underlying topological phases constitutes a change of paradigm with respect to the Landau theory of phase transitions [9]. The latter is described by means of a *local* order parameter, within the framework of the *symmetry-breaking* mechanism.

One can study phases of matter and the associated phase transitions (in particular topological ones) through a Riemannian metric on the space of quantum states. One such commonly used structure is based on the notion of fidelity, which is an information theoretical quantity that measures the distinguishability between quantum states. It has been widely used in the study of phase transitions [10–20], since its non-analytic behaviour signals phase transitions.

Note that the mentioned topological invariants, being functions of the Hamiltonian only and not the temperature, characterize topological features at zero temperature. Therefore, it is crucial to understand the effect of temperature on topological phase transitions, specially with regards to applications to quantum computers, such as those involving Majorana modes in topological superconductors [21]. To approach this problem, the fidelity and the associated Bures metric and, in addition, the Uhlmann connection, the generalization of the Berry connection to the case of mixed states, have been probed for systems that exhibit zero temperature symmetry protected topological phases [22–26].

Within the context of dynamical phase transitions, occurring when one performs a quench on a system, the information geometric methods based on state distinguishability were applied [27]. In particular, for finite temperature studies, besides the standard notion of fidelity induced Loschmidt echo, a notion of *interferometric Loschmidt echo* based on the interferometric phase introduced by Sjöqvist *et al.* in [28], was also considered. With regards to the associated infinitesimal counterparts, i.e., Riemannian metrics, their behaviour is significantly different.

For two-band Chern insulators the fidelity susceptibility, one of the components of the Bures metric, was considered in detail in Ref. [24]. In particular, it was rigorously proven that the thermodynamic and zero temperature limits do not commute — the Bures metric is regular in the thermodynamic limit as one approaches the zero temperature limit.

2. Introduction to quantum information geometry

2.1. Classical information geometry

Let $\sqrt{\boldsymbol{p}} = (\sqrt{p_1}, \sqrt{p_2}, ..., \sqrt{p_n})$ and $\sqrt{\boldsymbol{q}} = (\sqrt{q_1}, \sqrt{q_2}, ..., \sqrt{q_n})$ be two vectors representing two probability distributions, such that $\|\sqrt{p}\| = \|\sqrt{q}\| = 1$, where the norm is induced by the standard scalar product in $\mathbb{R}^n$, with $n \in \mathbb{N}$. Fidelity is an information theoretical quantity that measures the degree of similarity between probability distributions, given by the scalar product between the two probability distribution vectors, i.e.,

$$F(p,q) = \sqrt{\boldsymbol{p}} \cdot \sqrt{\boldsymbol{q}} = \sum_i \sqrt{p_i q_i}\,. \tag{1}$$

It is easy to see that if two states are the same (in other words, indistinguishable), their scalar product is 1 due to the normalization of probability distributions, hence fidelity is 1. If two states are orthogonal, scalar product gives us, by definition, 0 fidelity. Through the mapping: $(p_1, ..., p_n) \mapsto (\sqrt{p_1}, ..., \sqrt{p_n})$, the constraint $\sum_i^n p_i = 1$ defines a portion of the $(n-1) - \text{sphere}\,, \{(p_1, p_2, ..., p_n) \in \mathbb{R}^n : \sum_i (\sqrt{p_i})^2 = 1 \text{ and}\, p_i \geq 0\}$. This means that we can use the induced Fisher-Rao distance, which reads:

$$d_{\text{Fisher-Rao}} = \|\sqrt{p} - \sqrt{q}\| = \sqrt{2(1 - F(p,q))}. \tag{2}$$

The respective infinitesimal version is

$$ds^2_{\text{Fisher-Rao}} = \frac{1}{4}\sum_{i=1}^{n} \frac{dp_i^2}{p_i}. \tag{3}$$

2.2. Pure state geometry

In the context of quantum mechanics, the probability vectors introduced in the previous section are replaced by quantum states: complex vectors that correspond to probability amplitudes. In this context, the fidelity between pure quantum states in an n dimensional Hilbert space is given by

$$F\left(|\psi\rangle, |\phi\rangle\right) = |\langle\psi|\phi\rangle|, \tag{4}$$

where $|\psi\rangle$ and $|\phi\rangle$ are normalized vectors in $\mathcal{H} = \mathbb{C}^n$. The notion of a distance can be defined as

$$d^2(|\psi\rangle, |\phi\rangle) = \ 2\left(1 - |\langle\psi|\phi\rangle|\right). \tag{5}$$

This is known as the *Fubini-Study distance* between states $|\psi\rangle$ and $|\phi\rangle$. States in quantum mechanics are *rays*, that is, any state $|\psi\rangle$ represents the same physical state as $|\phi\rangle = \lambda|\psi\rangle$, with $\lambda \in \mathbb{C}\setminus\{0\}$, which forms an equivalence class of states $[|\psi\rangle] = \{\lambda|\psi\rangle : \lambda \in \mathbb{C}\}$. Therefore, the space of states of a given quantum system is the space of *rays* in $\mathcal{H}$

$$\mathbb{P}(\mathcal{H}) = \{[|\psi\rangle] : |\psi\rangle \in \mathcal{H}\} \tag{6}$$

known as the *projective Hilbert space*. Usually, one restricts themselves to normalized states, i.e., $S(\mathcal{H}) = \{|\psi\rangle \in \mathcal{H} : \langle\psi|\psi\rangle = 1\}$. Under this restriction, the equivalence relation is simply multiplication by a phase. Hence, from a physical standpoint, two states are equivalent if they differ by a phase $\lambda = e^{i\phi}$. In other words, normalized states have a U(1)-gauge freedom and the projective Hilbert space is $\mathbb{P}(\mathcal{H}) = \mathcal{S}(\mathcal{H})/U(1)$. When $\mathcal{H} = \mathbb{C}^N$, the space is also known as the *complex projective space* $\mathbb{C}P^n \cong S^{2n+1}/U(1)$, where S^{2n+1} is the $(2n+1)$-sphere. We can then define a projection $\pi : \mathcal{S}(\mathcal{H}) \mapsto \mathbb{P}(\mathcal{H})$ explicitly realized as

$$\pi : |\psi\rangle \longmapsto P_\psi = |\psi\rangle\langle\psi| = e^{i\phi}|\psi\rangle\langle\psi|\, e^{-i\phi}. \tag{7}$$

Note that, unlike the vector representatives of quantum states, the orthogonal projector is gauge invariant, i.e., there is no phase ambiguity in its definition. So there is, indeed, a one-to-one correspondence $[|\psi\rangle] \leftrightarrow P_\psi = |\psi\rangle\langle\psi|$. This construction defines a prin-

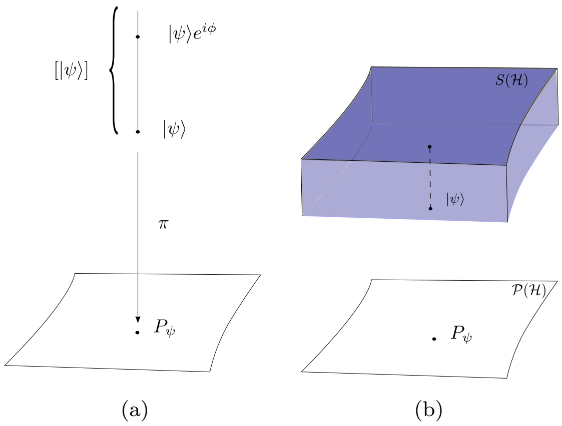


Figure 1: (a) Representation of a fiber: There is an equivalence class of states separated by a phase $e^{i\phi}$ that all project onto the same projector P_ψ. (b) Representation of a fiber bundle: there is a fiber for each point in the space of projectors $\mathbb{P}(\mathcal{H})$. This construction, along with the projection π defines a fiber bundle over the base space $\mathbb{P}(\mathcal{H})$

cipal bundle over $\mathbb{P}(\mathcal{H})$, which, for each projector P_ψ, has a collection of equivalent states that differ by a phase – the fiber. The principal bundle space can then be split into two subspaces: a vertical subspace attributed to variations along the fiber and a horizontal subspace which we define as the orthogonal complement of the vertical space. The unitary gauge ambiguity in specifying a state leads to a gauge field given by the 1-form

$$A = \langle\psi|d|\psi\rangle. \tag{8}$$

This is known as the *Berry connection.*

Taking a curve in the space of quantum states and computing the distance between two infinitesimally close points yields the Fubini-Study metric

$$d^2(P_{\psi(t)}, P_{\psi(t+\delta t)}) = ds^2_{\mathrm{FS}} = \langle\dot{\psi}|(1-|\psi\rangle\langle\psi|)|\dot{\psi}\rangle\delta t^2, \tag{9}$$

where $|\dot{\psi}\rangle$ is the first order time derivative of $|\psi\rangle$. In terms of more general parameters $\theta^\mu(t)$ one can write

$$ds^2_{\mathrm{FS}} = \langle\partial_\mu\psi|\left(I-|\psi\rangle\langle\psi|\right)|\partial_\nu\psi\rangle d\theta^\mu d\theta^\nu, \tag{10}$$

where $Q_{\mu\nu} = \langle\partial_\mu\psi|\left(I-|\psi\rangle\langle\psi|\right)|\partial_\nu\psi\rangle$ is the Hermitian *quantum geometric tensor.*

2.3. Mixed state geometry

Mixed state systems are fully characterized by their density matrix ρ which contains the full information about the ensemble. A mixed quantum state is a probabilistic mixture of ℓ pure states $|\varphi_j\rangle$ weighed by the relative proportions $q_j > 0$. With this in mind, the operator that fully describes this mixture is the *density operator* $\rho \in \mathbb{C}^{n\times n}$ defined by

$$\rho = \sum_{j=1}^{\ell} q_j |\varphi_j\rangle\langle\varphi_j|. \tag{11}$$

Their degree of mixture is directly correlated with the entropy of the system, which, as formulated by von Neumann, is given by

$$S = -\operatorname{Tr}(\rho\ln\rho). \tag{12}$$

Note that ρ is a trace 1, Hermitian operator, hence, it can be written as

$$\rho = \sum_{i=1}^{k} p_i P_i, \tag{13}$$

where $p_i > 0$ with $i = 1, ..., k \leq \ell$ satisfying $\sum_{i=1}^{k} p_i r_i = 1$, with the r_i's being the ranks of the orthogonal projectors P_i's. The total rank of ρ is then $r = \sum_{i=1}^{k} r_i$.

Considering that the space of pure states is $\mathbb{C}^n$, one can introduced matrices w called *amplitudes* of ρ, with $w \in \mathbb{C}^{n\times r}$, such that we can restate the density matrix as

$$\rho = ww^\dagger. \tag{14}$$

In order to define a distance, an Hermitian form can be defined by the formula

$$\langle w, v\rangle := \operatorname{Re}\operatorname{Tr}\left(w^\dagger v\right), \tag{15}$$

where v is the amplitude associated with density matrix σ, such that $\sigma = vv^\dagger$. We can define a notion of distance between states ρ and σ as

$$d_B^2(\rho,\sigma) = \inf_{\{w,v\}} ||w-v||^2 = 2 - \sup_{\{w,v\}} \operatorname{Tr}\left[w^\dagger v + v^\dagger w\right], \tag{16}$$

where $||\cdot||$ is the Hilbert Schmidt scalar product on the space $\mathbb{C}^{n\times r}$. By choosing amplitudes given by $w = \sqrt{\rho}$ and $v = \sqrt{\sigma}$, we have

$$d_B^2(\rho,\sigma) = 2\left(1 - F(\rho,\sigma)\right), \tag{17}$$

where we have defined a mixed state fidelity counterpart, given by

$$F(\rho,\sigma) = \operatorname{Tr}\sqrt{\sqrt{\rho}\,\sigma\sqrt{\rho}}, \tag{18}$$

and $F(\rho,\sigma) = \operatorname{Tr}\mathcal{F}(\rho,\sigma)$. Eq.(17) is the mixed state counterpart of the Fubini-Study distance in Eq. (5). Consider now the space $\mathcal{B}$ of rank r density matrices. Then, the corresponding amplitudes w belong to $\mathbb{C}^{n\times r}$. We can define a projection from the space of amplitudes w to the space of density matrices ρ, denoted P_{Ulh}, by

$$\begin{aligned} \pi : P_{\mathrm{Ulh}} &\to B \\ w &\mapsto \rho = ww^\dagger. \end{aligned} \tag{19}$$

We must remind ourselves that each amplitude has an $U(r)$ gauge freedom, so that $(\pi, P_{\text{Ulh}}, B, U(r))$ define a principal $U(r)$-bundle. Once again, we define horizontal tangent directions orthogonal to the vertical, i.e., gauge transformation geometry directions and hence find a geometry for mixed states. In this case, the connection is defined again by the horizontality condition, given by

$$\langle \dot{w}, \dot{w}' \rangle = 0, \tag{20}$$

where $\dot{w}$ is a tangent vector under consideration and $\dot{w}'$ is an arbitrary vertical tangent vector.

The metric can also be stated in terms of tangent vectors as $g(\widetilde{v}, \widetilde{v}) = \langle \widetilde{v}^H, \widetilde{v}^H \rangle$ and we claim that a horizontal vector can be written as $\widetilde{v}^H = Gw$, where G is Hermitian. Through this, the metric can be shown to give

$$g(v, v) = \operatorname{Tr} \rho G^2. \tag{21}$$

This is the so-called *Bures metric* for quantum mixed states. A more useful formula can be reached by taking a diagonalization of $\rho = \sum_i p_i |i\rangle\langle i|$. This leads to the explicit form of the Bures metric

$$g_\rho = \frac{1}{4} \sum_i \frac{dp_i^2}{p_i} + \sum_{i \neq j} p_i \frac{(p_i - pj)^2}{(p_i + p_j)^2} |\langle i|dj\rangle|^2. \tag{22}$$

It can be shown that this metric reduces to the Fubini-Study metric when considering a single state.

2.4. The geometry of the Sjöqvist metric

In Ref. [29], Sjövist considers a smooth path $t \mapsto \rho(t)$ of non-degenerate density operators with a fixed rank N and respective elements of the principal bundle given by

$$\{\sqrt{p_j(t)} e^{if_j(t)} |n_j(t)\rangle\}_{j=1}^N, \tag{23}$$

that project to the density matrix through π, i.e.,

$$\begin{aligned} \pi\left(\sqrt{p_j(t)} e^{if_j(t)} |n_j(t)\rangle\right) &= \sum_{j=1}^N \sqrt{p_j(t)} \sqrt{p_j(t)} \\ &\quad e^{if_j(t)} |n_j(t)\rangle\langle n_j(t)| e^{-if_j(t)} \\ &= \sum_{j=1}^N p_j |n_j(t)\rangle\langle n_j(t)|. \end{aligned} \tag{24}$$

Computing the minimum of the distance between two infinitesimally close elements of the principal bundle yields the *Sjöqvist metric* for a non-degenerate density matrix

$$ds^2 = \frac{1}{4} \sum_k \frac{dp_k^2}{p_k} + \sum_k p_k \langle dn_k| \left(1 - |n_k\rangle\langle n_k|\right) |dn_k\rangle. \tag{25}$$

This metric has a special property, not featured in the Bures case. From Eq. (25) we see that the Sjöqvist metric can be separated into the classical Fisher-Rao metric of Eq. (3) and a quantum contribution. This quantum part paints quite the intuitive picture different from the Bures metric case: it is itself segmented into Fubini-Study metrics for each state $|n_k\rangle$ of the non-degenerate density matrix ρ, such that the mixed system contribution is really the sum of the metrics of pure quantum states weighed by their respetive probabilities p_k.

The aim of this thesis is to generalize this result to accomodate degenerate density matrices into the theory.

3. Interferometric geometry from symmetry-broken Uhlmann gauge group and applications to topological phase transitions

3.1. The geometry of the Sjöqvist metric and natural generalisations to degenerate cases

Consider a quantum system with the corresponding n-dimensional Hilbert space $\mathcal{H}$. Its general mixed state (density matrix) ρ can be, using the spectral decomposition, written as

$$\rho = \sum_{i=0}^k p_i P_i, \tag{26}$$

where the real eigenvalues satisfy $p_0 = 0$ and $(i \neq j \Rightarrow p_i \neq p_j)$, while the orthogonal projectors satisfy $(i > 0 \Rightarrow \operatorname{Tr} P_i \equiv r_i > 0)$, and $\sum_{i=1}^k r_i = r$. We call $r \in \{1, \ldots, n\}$ the *rank* of the state. Note that we do not require for the kernel of ρ to be nontrivial (i.e., $r_0 \equiv \operatorname{Tr} P_0 \geq 0$), while all other eigenspaces, $\mathcal{H}_i$, are at least one-dimensional (such that $\mathcal{H} = \oplus_{i=0}^k \mathcal{H}_i$). We call the k-tuple $\tau \equiv (r_1, r_2, \ldots r_k) \in \mathcal{T}$, with $k \in \{1, \ldots, n\}$ and $(1 \leq r_1 \leq r_2 \leq \cdots \leq r_k)$, the *type* of the state ρ, where $\mathcal{T}$ is the set of all possible types. Note that as a consequence of the normalization of density matrices we have the additional constraint

$$\sum_{i=1}^k r_i p_i = 1. \tag{27}$$

Consider the set of all density operators of type τ, denoted by B_τ. The union, over the types $\tau \in \mathcal{T}$, of all sets B_τ forms the set of all possible states of a given system,

$$\begin{aligned} B &= \bigcup_{\tau \in \mathcal{T}} B_\tau \\ &= \{\rho \in \mathcal{H} \otimes \mathcal{H}^* : \rho^\dagger = \rho \text{ and } \rho \geq 0 \text{ and } \operatorname{Tr} \rho = 1\}. \end{aligned} \tag{28}$$

We would like to analyse the geometry of the B_τ's, and see whether it is possible to induce a Riemannian metric on them along the lines of the metric introduced by Sjöqvist [29], for the case of type $\tau = (1, 1, ..., 1)$, for some $r = k$. We will do so by introducing gauge invariant Riemannian metrics and associated Ehresmann connections in suitably chosen principal bundles P_τ with corresponding base spaces B_τ. Observe that every state ρ is completely specified in terms of its *"classical part"*, the vector of probabilities $\sqrt{\mathbf{p}} = (\sqrt{p_1}, \sqrt{p_2}, \dots, \sqrt{p_k})$ satisfying the normalization constraint (27), and its *"quantum part"*, the mutually orthogonal projectors $P_1, P_2, \dots, P_k$ (note that P_0 is then determined unambiguously, $P_0 = I - \sum_{i=1}^{k} P_i$), which we compactly denote by $\mathbf{P} = (P_1, P_2, \dots, P_k)$. We will explore a particular gauge degree of freedom in describing the quantum part in our construction. Namely, each eigenspace projector P_i is uniquely specified by an orthonormal basis $\beta_i = \{|e_{i,j}\rangle : j = 1, \dots r_i\}$. However, the basis β_i itself is not uniquely determined by P_i. Indeed, every basis $U\beta_i = \{U|e_{i,j}\rangle : j = 1, ..., r_i\}$ with U a unitary that acts non-trivially only on the image of P_i, the subspace $\mathcal{H}_i$, defines the same projector P_i.

We then define (the total space of) a principal bundle P_τ as the set of all k-tuples of pairs $p_\tau = \big((p_i, \beta_i)\big)_{i=1}^{k}$, such that $(\sqrt{\mathbf{p}}, \mathbf{P})$ give rise to well-defined type τ density operators (observe that $p_i \neq p_j$ for all $i \neq j$). This space comes equipped with an obvious projection to the base space B_τ is given by

$$\pi_\tau(p_\tau) \equiv \sum_{i=1}^{k} p_i P_i = \rho, \tag{29}$$

with the fibers being isomorphic to the product of the corresponding unitary groups in the type τ,

$$G_\tau \equiv \prod_{i=1}^{k} \mathrm{U}(r_i). \tag{30}$$

The group G_τ acts on the right in the obvious way, for $U_i \in \mathrm{U}(r_i)$, we write $U_i = [(U_i)^{j'}_{j}]_{1 \le j, j' \le r_i} \in \mathrm{U}(r_i)$ and then $\beta_i \cdot U_i$ is given by

$$|e_{i,j}\rangle \mapsto \sum_{j'=1}^{r_i} |e_{i,j'}\rangle (U_i)^{j'}_{j}, \;\; j = 1, ..., r_i. \tag{31}$$

By introducing *generalized amplitudes* $w_i \in \mathbb{C}^{n \times r_i}$ as matrices whose columns are vectors $|e_{i,j}\rangle \in \mathbb{C}^n$, $j = 1, ..., r_i$, i.e., $w_i \equiv \big(|e_{i,1}\rangle \; |e_{i,2}\rangle \dots |e_{i,r_i}\rangle\big)$, $i = 1, ..., k$, we can see P_τ as

$$\begin{aligned} P_\tau = \{ & \big((p_i, w_i)\big)_{i=1}^{k} : \sum_{i=1}^{k} p_i \; w_i w_i^\dagger \in B_\tau \\ & \text{and } w_i^\dagger w_i = I_{r_i}, \text{ for all } i = 1, ..., k, \\ & \text{and } p_i \neq p_j, \text{ for all } i \neq j \}, \end{aligned} \tag{32}$$

and the right action of the gauge group is given by $w_i \mapsto w_i \cdot U_i$, with $U_i \in \mathrm{U}(r_i)$. With this notation, we finally introduce a suitable "Hermitian form" (note that it is not a scalar product, as P_τ is not a linear space), that will define Horizontal subspaces, by the formula

$$\begin{aligned} \langle p_\tau, p'_\tau \rangle_\tau &\equiv \sum_{i=1}^{k} \sqrt{p_i p'_i} \, \mathrm{Tr}(w_i^\dagger w'_i) \\ &= \sum_{i=1}^{k} \mathrm{Tr}[(\sqrt{p_i} w_i^\dagger)(\sqrt{p'_i} w'_i)]. \end{aligned} \tag{33}$$

Observe that it is clear that this pairing arises from the restriction of the usual Hermitian inner product in $\bigoplus_{i=1}^{k} \mathbb{C}^{n \times r_i} \cong \mathbb{C}^{n \times r}$.

Additionally, this allows for a convenient comparison with the Uhlmann principal bundle

$$\begin{aligned} P_r^{\mathrm{Uh}} = \{ & w \in \mathbb{C}^{n \times r} : \pi(w) \equiv w w^\dagger = \rho \in B, \\ & \text{with } \mathrm{rank}(\rho) = r \}, \end{aligned} \tag{34}$$

where the typical fibre is $\mathrm{U}(r) \subset \mathbb{C}^{r \times r}$, whose elements act from the right ($w \mapsto w \cdot U$), and the Hermitian form, induced by the Hilbert-Schmidt scalar product on the space of linear operators from $\mathbb{C}^{r \times r}$, is

$$\langle w, w' \rangle = \mathrm{Tr}(w^\dagger w'). \tag{35}$$

Note that the base space for the Uhlmann bundle is the set of density matrices with rank r, which is the union of all B_τ sharing the same rank. Observe that for one such τ, P_τ can be identified as a subset of P_r^{Uhlmann}. This follows from the map

$$P_\tau \ni \big((p_i, w_i)\big)_{i=1}^{k} \mapsto (\sqrt{p_1} w_1, ..., \sqrt{p_k} w_k) \in \bigoplus_{i=1}^{k} \mathbb{C}^{n \times r_i}, \tag{36}$$

being an embedding of P_τ. Moreover, once we identify $\bigoplus_{i=1}^{k} \mathbb{C}^{n \times r_i} \cong \mathbb{C}^{n \times r}$, the image sits precisely in P_{Uhl}. In other words $P_\tau \subset P_{\mathrm{Uhl}}$ and also π_τ equals the restriction of the projection of the Uhlmann bundle to P_τ ($p_i \neq p_j$, for all $i \neq j$, guarantees this), the image being precisely B_τ. We remark that the gauge group of the Uhlmann bundle is far larger than the one for the principal bundle $P_\tau \to B_\tau$. By passing to a preferred type, we performed a symmetry breaking operation from $\mathrm{U}(r)$ to $G_\tau = \prod_{i=1}^{k} \mathrm{U}(r_i) \subset \mathrm{U}(r)$. This is another way to see why interferometric-like quantities, like the interferometric Loschmidt echo, in certain applications develop non-analyticities, while the ones based on the fidelity do not (see for example [30] and the references therein): the former have smaller space to "go through", while the latter can, following the "broader" Uhlmann connection, instead of the interferometric ones, avoid possible sources of non-analyticities.

3.2. Distance measures and Riemannian metrics

Consider now two points, $p_\tau = \big((p_i, w_i)\big)_{i=1}^{k}$ and $q_\tau = \big((q_i, v_i)\big)_{i=1}^{k} \in P_\tau$. By making use of Eq. (33) one can define a distance between elements p_τ and q_τ in the total space of the principal bundle given by

$$
\begin{aligned}
d_\tau^2(p_\tau, q_\tau) &= 2\Big(1 - \mathrm{Re}\left(\langle p_\tau, q_\tau\rangle_\tau\right)\Big) \\
&= 2\left(1 - \sum_{i=1}^{k} \sqrt{p_i q_i}\ \mathrm{Re}\left(\mathrm{Tr}(w_i^\dagger v_i)\right)\right). \quad (37)
\end{aligned}
$$

The fact that d_τ is a distance follows from the fact that it is the restriction of the usual distance in $\oplus_{i=1}^{k}\mathbb{C}^{n\times r_i}$, where we see P_τ as a subset of this space through the map of Eq. (36). One can use this distance to define a distance on B_τ, through the formula:

$$
\begin{aligned}
d_I^2(\rho, \sigma) = \inf\{d_\tau^2(p_\tau, q_\tau) : \pi(p_\tau) = \rho \quad (38)\\
\text{and } \pi(q_\tau) = \sigma,\ \text{for } p_\tau, q_\tau \in P_\tau\}.
\end{aligned}
$$

The associated infinitesimal counterparts of the distances defined above are Riemannian metrics on P_τ and B_τ, respectively. The Riemannian metric on P_τ, which is gauge invariant, allows for the definition of what is called an Ehresmann connection over P_τ and this, in turn, defines a metric downstairs over the base space B_τ.

Another way to see that $d_\tau^2(p_\tau, q_\tau)$ is indeed a metric is through what we call *"generalised purifications"*. Let us introduce *"ancilla"* amplitudes $\mathrm{w}_i \in \mathbb{C}^{k\times 1}$, with $i = 1, 2, \dots k$, such that $\mathrm{w}_i \mathrm{w}_i^\dagger = \mathrm{P}_i \in \mathbb{C}^{n\times n}$ are *fixed* orthogonal projectors of rank 1 (i.,e., P_i do not depend on the choice of the state), satisfying $\mathrm{P}_i \mathrm{P}_j = \delta_{ij} I_k$ and $\sum_{i=1}^{k} \mathrm{P}_i = I_k$. Define a generalised purification of state ρ, associated to the corresponding p_τ, as

$$
|p_\tau\rangle = \sum_{i=1}^{k} \sqrt{p_i} w_i \otimes \mathrm{w}_i. \quad (39)
$$

Then, we have that the scalar product between $|p_\tau\rangle$ and $|q_\tau\rangle$, induced by the Hilbert-Schmidt scalar product in the corresponding factor spaces, is

$$
\begin{aligned}
\langle p_\tau, q_\tau\rangle &= \sum_{i,j=1}^{k} \sqrt{p_i q_j} \langle w_i, v_j\rangle \langle \mathrm{w}_i, \mathrm{w}_j\rangle \\
&= \sum_{i=1}^{k} \sqrt{p_i q_i} \langle w_i, v_i\rangle \\
&= \sum_{i=1}^{k} \sqrt{p_i q_i}\, \mathrm{Tr}(w_i^\dagger v_i) \\
&= \langle p_\tau, q_\tau\rangle_\tau,
\end{aligned} \quad (40)
$$

where the second equality is because w_i and w_j are orthogonal for $i \neq j$. Thus, the distance $d_\tau(p_\tau, q_\tau)$ is nothing but the standard Hilbert-Schmidt distance between the generalised purifications $|p_\tau\rangle$ and $|q_\tau\rangle$.

As in Eq. (32), if we take the w_i's as (row) vectors $|w_i\rangle = \Big[|e_{i,1}\rangle\ |e_{i,2}\rangle\ \dots\ |e_{i,r_i}\rangle\Big]$ whose entries are (column) vectors $|e_{i,j}\rangle$, one can by analogy generalise the quantum part of the metric for the non-degenerate case, the so-called *"interferometric metric"*, which has $r_i = 1$, $i = 1, \dots, k$,

$$
\begin{aligned}
g_I^{\mathrm{Q}} &= \sum_{i=1}^{k} p_i \langle dw_i|(I_n - w_i w_i^\dagger)|dw_i\rangle \\
&= \sum_{i=1}^{k} p_i \langle de_{i,1}|(I_n - |e_{i,1}\rangle\langle e_{i,1}|)|de_{i,1}\rangle,
\end{aligned} \quad (41)
$$

to the degenerate case, in which $\mathrm{U}(1)$ degree of freedom of each $w_i = |e_i\rangle$ is replaced by the $\mathrm{U}(r_i)$ degree of freedom of each $w_i = \Big[|e_{i,1}\rangle\ |e_{i,2}\rangle\ \dots\ |e_{i1,r_i}\rangle\Big]$,

$$
\begin{aligned}
g_I^{\mathrm{Q}} &= \sum_{i=1}^{k} p_i \langle dw_i|\big(I_n - w_i w_i^\dagger\big)|dw_i\rangle \\
&= \sum_{i=1}^{k} p_i \langle dw_i|\Big[I_n - \big(\sum_{j=1}^{r_i} |e_{i,j}\rangle\langle e_{i,j}|\big)\Big]|de_i\rangle \\
&= \sum_{i=1}^{k} p_i \langle dw_i|\big(I_n - P_i\big)|dw_i\rangle,
\end{aligned} \quad (42)
$$

with $|dw_i\rangle = \Big[|de_{i,1}\rangle\ |de_{i,2}\rangle\ \dots\ |de_{i,r_i}\rangle\Big]$, $i = 1, \dots, k$.

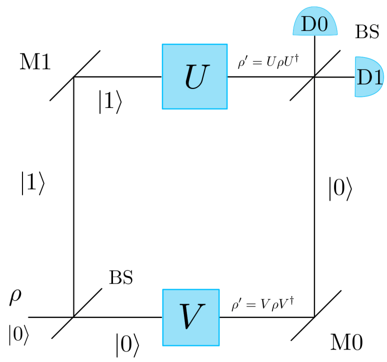


Figure 2: Interferometric measurement to probe the generalised metric g_I.

3.3. Interferometric measurement interpretation

Consider the following experiment depicted in FIG 2. A particle is entering the Mach-Zehnder interferometer from the input arm 0, given by the state $|0\rangle$, with its internal degree of freedom in a mixed state ρ. Both the input and the output beam-splitters are balanced, described by the same unitary matrix, say, the one given by $|0\rangle \to (|0\rangle + i|1\rangle)/\sqrt{2}$. In arm 0 a unitary $V = \sum_{i=0}^{k} P_i V P_i$ is applied to the internal degree of freedom, i.e., V is the most general unitary that commutes with ρ. In arm 1 a unitary $U = U(\delta t) \in \mathrm{U}(n)$ is applied for a time period δt, changing the state of the internal degree of freedom to $\rho' = U\rho U^\dagger$. The particle is detected at detectors D0 and D1, with the corresponding probabilities pr_0 and pr_1. In our case, we have that $\mathrm{pr}_1 \leq \mathrm{pr}_0$, and for $U = V$ we have full constructive interference at the output arm 0, giving $\mathrm{pr}_0 = 1$. In general, we have that

$$\mathrm{pr}_1^{\max} = \max_{\{V_i\}}(\mathrm{pr}_1) = 1 - \frac{1}{4} d_I^2(\rho, \rho + \delta\rho), \tag{43}$$

where $d_I^2(\rho, \rho+\delta\rho) \approx g_I(\dot\rho, \dot\rho)\delta t^2$ is the "infinitesimal" distance between ρ and $\rho' = \rho + \delta\rho$, where $\delta\rho = \dot\rho\delta t$. Note that in the case of the Hadamard matrix, given by $|\ell\rangle \to (|0\rangle + (-1)^\ell |1\rangle)/\sqrt{2}$, with $\ell \in \{0, 1\}$, the roles of arms 0 and 1 are exchanged.

3.4. Interferometric metric in the context of band insulators

Suppose we have a family of band insulators with two bands described by the Hamiltonian

$$\mathcal{H}(M) = \int_{\mathrm{BZ}^d} \frac{d^d k}{(2\pi)^d}\, \psi_{\mathbf{k}}^\dagger d^\mu(\mathbf{k}; M)\sigma_\mu \psi_{\mathbf{k}}, \tag{44}$$

parametrized by M (M can be some intrinsic parameter, such as the hopping), where σ_μ, $\mu = 1, 2, 3$, are the Pauli matrices, $\mathbf{k}$ is the crystalline momentum in a d-dimensional Brillouin zone BZ^d, with $d = 1, 2, 3$, and $\Psi_{\mathbf{k}}^\dagger$ is an array of 2 creation operators for fermions at momentum $\mathbf{k}$. We assume that the system is gapped for generic values of M, meaning that the vector $d = (d^1, d^2, d^3)$ is non-vanishing as a function of $\mathbf{k}$. For a certain value of M_c, we assume that the vector has isolated zeroes. This assumption is generically correct for the $d = 1, 2$ momenta coordinates plus the mass M, as one needs to tune three parameters for an Hermitian matrix to have two eigenvalues cross.

The pullback of the interferometric metric that we have desribed in Sec. 3.2,

$$g = \frac{1}{4}\sum_i r_i \frac{dp_i^2}{p_i} + \sum_i p_i \operatorname{Tr}(P_i dP_i dP_i), \tag{45}$$

with $\rho = \sum_i p_i P_i$ and $\operatorname{Tr} P_i = r_i$, by the map induced by the Gibbs state

$$M \mapsto \rho(M) = Z^{-1}\exp(-\beta\mathcal{H}(M)), \tag{46}$$

where Z is the partition function, is given by

$$ds^2 = \frac{1}{4}\int_{\mathrm{BZ}^d} \frac{d^d k}{(2\pi)^d}\Big[\frac{1}{\cosh(\beta E) + 1} \tag{47}$$
$$\times \left(\beta^2 \left(\frac{\partial E}{\partial M}\right)^2 + \cosh(\beta E)\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\right)\Big] dM^2,$$

where we omitted the obvious dependence on $\mathbf{k}$ and M of the quantities E and n^μ. This result should be compared to the pullback of the Bures metric for $d = 2$, which yields (see Ref. [24])

$$g_{\mathrm{Bures}} = \frac{1}{4}\int_{\mathrm{BZ}^d}\frac{d^d k}{(2\pi)^d}\Big[\frac{1}{\cosh(\beta E)+1}\beta^2\left(\frac{\partial E}{\partial M}\right)^2 \tag{48}$$
$$+ \frac{\cosh(\beta E) - 1}{\cosh(\beta E)}\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\Big] dM^2.$$

The two expressions have dramatically different behaviours, when it comes to taking the zero temperature limit.

Naively, one would say that both yield the pullback of the Fubini-Study metric, which is the pure-state metric,

$$g_0 = \frac{1}{4}\int_{\mathrm{BZ}^d}\frac{d^d k}{(2\pi)^d}\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M} dM^2. \tag{49}$$

Note that for gapless points the vector n is not defined and the expression for g_0 becomes (potentially) singular. However, due to the gapless points, the integrands must be carefully analysed in the neighbourhoods of these points, as the singularities can be avoided in some cases. In fact, it was shown that if the gapless points are isolated in momentum space, then an expansion near these points of the integrand function yields a regular result [24]. Namely, because of the inequality

$$\frac{1}{2}\frac{1}{\cosh(x)} < \frac{1}{\cosh(x)+1}\frac{1}{\cosh(x)}, \quad \text{for all } x \in \mathbb{R}, \tag{50}$$

we can write,

$$\frac{1}{\cosh(\beta E)+1}\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + \frac{\cosh(\beta E)-1}{\cosh(\beta E)}\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M} \tag{51}$$
$$< \frac{1}{\cosh(\beta E)}\left[\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + (\cosh(\beta E) - 1))\,\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\right].$$

Expansion for small βE yields that up to $\mathrm{O}\left((\beta E)^4\right)$ the integrand is upper bounded by

$$\frac{\beta^2}{\cosh(\beta E)}\delta_{\mu\nu}\frac{\partial d^\mu}{\partial M}\frac{\partial d^\nu}{\partial M}, \tag{52}$$

which is regular in the limit $\beta \to \infty$. Hence, the potential singularities arising from the gapless region are regularized by the Bures prescription. However, in the case of the interferometric metric, considering the integrand

$$\frac{1}{\cosh(\beta E)+1}\left(\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + \cosh(\beta E)\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\right), \tag{53}$$

near $E = 0$ gives us

$$\frac{1}{\cosh(\beta E)+1}\Big[\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + (1 + \frac{1}{2}\beta^2 E^2)\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}$$
$$+ \mathrm{O}\left((\beta E)^4\right)\Big]. \tag{54}$$

In this case, we cannot get rid of the singular factor

$$\delta_{\mu\nu}\frac{\partial n^{\mu}}{\partial M}\frac{\partial n^{\nu}}{\partial M}, \tag{55}$$

which appears once in the second term without the regularizing coefficient $\beta^2 E^2$ which above allowed for the identification of the regular quantity

$$\beta^2\left(\frac{\partial E}{\partial M}\right)^2+\beta^2E^2\delta_{\mu\nu}\frac{\partial n^{\mu}}{\partial M}\frac{\partial n^{\nu}}{\partial M}=\beta^2\delta_{\mu\nu}\frac{\partial d^{\mu}}{\partial M}\frac{\partial d^{\nu}}{\partial M}. \tag{56}$$

This implies that the limit $\beta\to\infty$ yields singular behaviour for g, provided the same happens with g_0. But not the other way around, i.e., singular behaviour on the finite temperature metric does not imply zero temperature singular behaviour. In other words, while in the case of the Bures metric the thermodynamic and the zero temperature limits did not commute, in the interferometric case they do, because the singular behaviour of the gapless points is recovered, as one considers a small neighbourhood of these points and takes the zero temperature limit. In the following, we will consider the massive Dirac model to illustrate the different behaviours of the two metrics.

4. Results

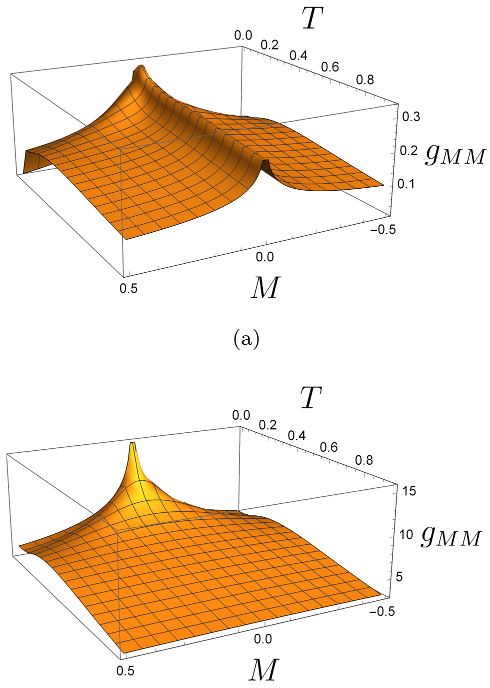
4.1. Massive Dirac model

We consider the massive Dirac model, a band insulator in two spatial dimensions, described by Eq. (44), with

$$d(\mathbf{k};M)=(\sin(k_x),\sin(k_y),M-\cos(k_x)-\cos(k_y)), \tag{57}$$

where $\mathbf{k}=(k_x,k_y)$ is the quasi-momentum in the two-dimensional Brillouin zone BZ^2 and M is a real parameter. The model exhibits topological phase transitions [31]. We will focus at the one occurring at $M=0$, where the Chern number goes from $+1$, for $M\to0^-$, to -1, for $M\to0^+$. The following two figures describe the inteferometric metric (Fig. 3(a)) and the Bures metric (Fig. 3(b)) in the thermodynamic limit.

As argued above, the Bures metric is regular if one considers the thermodynamic limit and then the zero temperature limit. The same does not hold for the interferometric metric. In fact, we can see that the interferometric metric knows about the quantum phase transition taking place at $T=0$ even at finite temperatures. The reason is that in passing from one metric to the other the symmetry was broken, namely $\mathrm{U}(r)\to\prod_{i=1}^{k}\mathrm{U}(r_i)$, and, therefore, there is enhanced distinguishability. Indeed, in the interferometric case, whenever the gap closes, we expect a phase transition, even at finite temperatures, because then there are states which according to a Boltzmann-Gibbs distribution become degenerate in probability, hence the gap closing changes the type of the density matrix involved. Whether such singular begavior of the interferometric



(a)

(b)

Figure 3: (a) Interferometric metric for the massive Dirac model — the topological phase transition is captured for all temperatures. (b) Bures metric for the massive Dirac model — the topological phase transition is captured only at zero temperature. The figures illustrate the different behaviour of the metrics with temperature T and the parameter M driving the topological phase transition.

metric is indeed observable for macroscopic many-body systems is an open question. While the straightforward implementation of the interferometric experiment described in Sec. 3.3 seems to be, at least technologically, infeasible, as it would require maintaining Schrödinger cat-like macroscopic states, possible variations are argued to be able to reveal the singular behaviour of the interferometric metric at finite temperatures (see Sec. V of Ref. [32]).

5. Conclusions

5.1. Conluding remarks

In this work, we have generalized Sjöqvist's interferometric metric introduced in [29], to the degenerate case. For this purpose, we have introduced generalized amplitudes and purifications. We have analysed an interpretation of the metric in terms of a suitably generalized interferometric measurement, accommodating for the non-Abelian character of our gauge group, as opposed to the Abelian gauge group used in the non degenerate case. We have applied the induced Riemannian structure, physically interpreted as a susceptibility, to the study of topological phase transitions at finite temperatures for band insulators. To the best of our knowledge, this is the first study of finite-temperature equilibrium phase transitions using interferometric geometry. The inferred critical behaviour is very different from that of the Bures metric. The interferometric metric is more sensitive to the change of parameters than the Bures one, and unlike the latter, in addition to zero temperature phase transitions, infers finite temperature phase transitions as well. This sensitivity can be traced back to a symmetry breaking mechanism, much in the same spirit of Landau-Ginzburg theory. In our case, by fixing the type of the density matrix considered, a gauge group is broken down to a subgroup.

5.2. Future work

It would be very interesting to analyse the inteferometric curvature, an analogue of the usual Berry curvature, generalized to this mixed setting, associated with the Ehresmann connection presented in this manuscript. Since the curvature is intrinsically related to topological phenomena, this analysis might very well unravel new symmetry protected topological phases in the mixed state case and potentially help refining the classification of topological matter. It would be also interesting to compare the critical behaviour of different many-body systems in terms of interferometric metrics corresponding to different types of density matrices. Recent study of the fidelity susceptibility indicated that its singular behaviour around regions of criticality has preferred directions on the parameter space [33]. Performing a similar analysis for the interferometric critical geometry is another possible line of future research. Finally, probing experimentally the introduced interferometric metrics is a relevant topic of future investigation.

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