Quantum information geometry and applications

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Resumo

Na primeira parte desta tese, apresentamos uma breve introdução à geometria quântica da informação. Começamos com uma discussão sobre a geometria clássica da informação e derivamos a métrica de Fischer-Rao. Em seguida, procedemos à generalização da teoria ao contexto quântico e derivamos a métrica de Fubini-Study. Mostramos como os estados quânticos normalizados ganham um significado geométrico mais profundo através da sua ambiguidade de gauge e como esta propriedade conduz a uma fase conhecida como a fase de Berry, induzida pela conexão de Berry. Finalmente, generalizamos estes resultados para o caso do estado misto, derivando a métrica do estado misto, conhecida como métrica de Bures. Na segunda parte desta tese, apresentamos uma generalização natural de uma estrutura Riemanniana, ou seja, uma métrica, recentemente introduzida por Sjoqvist para o espaço de matrizes de densidade não degenerada, para o caso degenerado, ou seja, em que os espaços próprios têm dimensão maior ou igual a um. Apresentamos uma interpretação física da métrica em termos de um resultado de uma experiência de interferometria. Aplicamos esta métrica, fisicamente interpretada como uma susceptibilidade interferométrica, ao estudo de transições de fase topológica a temperaturas finitas para isoladores de banda. Comparamos os comportamentos desta susceptibilidade e os que provêm da conhecida métrica de Bures, mostrando que são dramaticamente diferentes. Enquanto ambas inferem transições de fase a temperatura zero, apenas a primeira prevê transições de fase a temperaturas finitas também.

Palavras-chave: geometria da informação; fases geométricas; transições de fase; susceptibilidade; métrica interferométrica.

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 Sjoqvist 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 apply 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.

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

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BZ	Brillouin zone
FS	Fubini-Study
TKNN	Thouless-Komoto-Nightingale-den Nihjs

List of Symbols

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Chapter 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 of the temperature, characterize topological features at zero temperature. Therefore, it is crucial to understand the effect of temperature on topological phase transitions, specially with regard 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 regard 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.

We start this work with an overview of quantum geometry: we first present the classical statistical theory of information geometry and derive the Fisher-Rao metric, as well as the information geometric tensor. Next, we transport these results to the quantum realm and discuss how geometric phases arise in quantum mechanics. We derive the Fisher-Rao metric quantum counterpart, the Fubini-Study distance and we also derive the quantum geometric tensor. We show how the quantum geometric tensor captures both the metric and the Berry curvature together. We present a simple application of these concepts by considering a two level system. Finally, we turn to mixed systems and derive the respective metric in this space and show that it reduces to the Fubini-Study metric for a pure quantum state when considering one state only.

In the second part of this thesis, we provide, through what is called the Ehresmann connection, a natural generalization of a Riemannian structure over the space of non degenerate density matrices, introduced by Sjöqvist in Ref. [29], to the degenerate case. Our natural construction reveals a symmetry breaking mechanism by reducing the gauge group of the Uhlmann principal bundle [30], to a smaller subgroup preserving the *type*, i.e., the ranks of the spectral projectors of the density matrix (see Sec. 3.1 for details). This symmetry breaking mechanism explains the natural enhanced distinguishability provided by the interferometric Riemannian metric. Introducing the notion of a generalized purification, we naturally generalize Sjöqvist's result to the case of degenerate density matrices, see Sec. 3.3. In Sec. 3.5, we discuss an interferometric measurement probing the Riemannian metric derived. In Sec. 3.6, we apply the derived metric to study finite temperature phase transitions in the context of band insulators. We present results for this metric in the case of the massive Dirac model, a Chern insulator, in two spatial dimensions, and compare them with those obtained using the Bures metric. Our analysis of equilibrium phase transitions showed to be consistent with the previous study of dynamical phase transitions – the interferometric metric is more sensitive to the change of the parameters than the Bures one. Finally, we present the conclusions in Sec. 4.

The results presented in this thesis are submitted for publication in the Journal of American Society Physical Review B. They are also available in preprint format in Ref. [31] .

Chapter 2

Introduction to Quantum Information Geometry

2.1 Distinguishability in classical and quantum systems

Understanding quantum physics means having a deep understanding of statistical systems. A statistical ensemble is a collection of identical physical systems, with each system being fully characterized by its intrinsic properties (such as position, velocity, charge, (rest) mass etc.), allowing us to differentiate one system from another. Given that we can distinguish a given system A from another system B, we can then try to estimate the number of systems that are in a particular configuration (of a system)[1] and, in this way, define the proportion of systems that are in a given configuration, to which we associate a probability distribution

$$p_i = \frac{\text{\# of systems that are in a particular configuration}}{\text{Total \# of systems}}. \tag{2.1}$$

We can perform this association for every configuration possible in the ensemble and create a probability distribution. In this way, we can fully describe the ensemble through its probability distribution.

We can mix different ensembles by adding the individual systems in a larger, all encompassing ensemble. By doing this we lose (forget) the correspondence of the systems to the sub-ensembles. At this point, one can define two types of ensembles: homogeneous that correspond to ensembles that are not a mixture of different ensembles and mixed that are. In classical physics, physical states[2] are assigned to individual systems. In quantum mechanics, however, we attribute pure physical states to homogeneous ensembles, as it is intrinsically a statistical theory. In this sense, pure states are physical states of homogeneous ensembles and mixed states are physical states of mixed ensembles.

[1] The configuration of a system is the set of properties that characterize a system.
[2] Note that, as it is used in quantum mechanics, the word “state” is used as a synonym for ensemble.

2.2 Classical information geometry

Now that we have made the connection between physical states and statistical ensembles, we can begin to figure out how we can distinguish different states.

Pure states are assigned to homogeneous ensembles. The probability distributions of pure classical states are always trivial (1 for one value, 0 for all others), as a consequence of the fact that classical systems in pure states have all their properties well-defined. This makes it possible to completely distinguish any pure state from other pure states. This, however, is not true for mixed classical states, and more importantly for our study, both pure and mixed quantum states.

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.,

$$F(p,q) = \sqrt{\boldsymbol{p}} \cdot \sqrt{\boldsymbol{q}} = \sum_i \sqrt{p_i q_i}\,. \tag{2.2}$$

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, the scalar product gives us, by definition, 0 fidelity. More explicitly, when taking the scalar product of two orthogonal probability vectors we have

$$F(p,q) = 0 \Leftrightarrow \sqrt{\boldsymbol{p}} \cdot \sqrt{\boldsymbol{q}} = \sum_i \sqrt{p_i q_i} \; = 0, \tag{2.3}$$

when $\sqrt{\boldsymbol{p}} \perp \sqrt{\boldsymbol{q}}$. This means that for each i either p_i and/or q_i must be zero, hence for each system i one can completely distinguish from where it originated. In this sense, orthogonality means that the ensembles are fully distinguishable.

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 $(n-1)-\text{sphere}\,, \{(p_1, p_2, ..., p_n) \in \mathbb{R}^n \mid \sum_i (\sqrt{p_i})^2 = 1 \;\text{ and}\, p_i \geq 0\}$. This means that we can use the induced Fisher-Rao distance, which reads:

$$d_{\text{Fisher-Rao}} = \|\sqrt{p} - \sqrt{q}\| = \sqrt{2(1 - F(p,q))}. \tag{2.4}$$

The respective infinitesimal version is

$$ds^2_{\text{Fisher-Rao}} = \sum_{i=1}^n dx_i\, dx_i = \sum_{i=1}^n d(\sqrt{p_i})\; d(\sqrt{p_i}) = \frac{1}{4}\sum_{i=1}^n \frac{dp_i}{\sqrt{p_i}} \frac{dp_i}{\sqrt{p_i}} = \frac{1}{4}\sum_{i=1}^n \frac{dp_i^2}{p_i}. \tag{2.5}$$

We can already begin to see from this definition the geometric nature of statistics, which will be much of the ground-work of our thesis. Let us suppose our probability distribution depends on some vector of parameters $\boldsymbol{\theta} = (\theta_1, \theta_2, ..., \theta_d) \in U \subset \mathbb{R}^d$, such that our probability distribution is a function of these parameters, i.e., $p_i = p_i(\boldsymbol{\theta})$. Then, the above metric can be expressed as

$$ds^2_{\text{Fisher-Rao}} = \frac{1}{4}\sum_{i=1}^{n}\frac{dp_i^2}{p_i} = \frac{1}{4}\sum_{i=1}^{n} p_i(\boldsymbol{\theta})(d(\log p_i(\boldsymbol{\theta})))^2 = \frac{1}{4}\sum_{i=1}^{n} p_i(\boldsymbol{\theta})\frac{\partial(\log p_i(\boldsymbol{\theta}))}{\partial\theta^\mu}\frac{\partial(\log p_i(\boldsymbol{\theta}))}{\partial\theta^\nu} d\theta^\mu d\theta^\nu, \tag{2.6}$$

where we have used the Einstein summation convention.

Hence, we have found the metric tensor over parameter space

$$g_{\mu\nu}(\boldsymbol{\theta}) = \frac{1}{4}\sum_{i=1}^{n} p_i(\boldsymbol{\theta})\frac{\partial(\log p_i(\boldsymbol{\theta}))}{\partial\theta^\mu}\frac{\partial(\log p_i(\boldsymbol{\theta}))}{\partial\theta^\nu}. \tag{2.7}$$

The information or *surprise* of a certain event is given by the logarithm of the probability associated to that event

$$i_{p_i} = -\log p_i\,. \tag{2.8}$$

We can then rewrite equation (2.7) as

$$g_{\mu\nu}(\boldsymbol{\theta}) = \frac{1}{4}\sum_{i=1}^{n} p_i(\boldsymbol{\theta})\frac{\partial i_{p_i}}{\partial\theta^\mu}\frac{\partial i_{p_i}}{\partial\theta^\nu} = \frac{1}{4}\,\mathrm{E}_{p(\boldsymbol{\theta})}\left[\frac{\partial i_p}{\partial\theta^\mu}\frac{\partial i_p}{\partial\theta^\nu}\right], \tag{2.9}$$

where $\mathrm{E}_{p(\boldsymbol{\theta})}\left[\,\cdot\,\right]$ is the operation that takes the average value of some quantity, with respect to a given probability distribution $p(\boldsymbol{\theta})$. If we consider a single parameter θ, Fisher information is a way of measuring how much information about an unknown parameter θ we can get from a probability distribution and it is formally defined by

$$I(\theta) = \mathrm{Var}\left[\frac{\partial i(\theta)}{\partial\theta}\right] = \mathrm{E}\left[\left(\frac{\partial i(\theta)}{\partial\theta}\right)^2\right] - \mathrm{E}\left[\left(\frac{\partial i(\theta)}{\partial\theta}\right)\right]^2. \tag{2.10}$$

The latter term can be shown to be zero and we are left with

$$I(\theta) = \mathrm{E}\left[\left(\frac{\partial i(\theta)}{\partial\theta}\right)^2\right]. \tag{2.11}$$

This result can be generalized for the collection of parameters $\boldsymbol{\theta}$ we defined above, so that we can relate the statistical metric tensor with the Fisher information matrix, defined by

$$I = [I_{\mu\nu}] = E\left[(\nabla i)(\nabla i)^\dagger\right], \tag{2.12}$$

hence,

$$I_{\mu\nu}(\boldsymbol{\theta}) = 4g_{\mu\nu}(\boldsymbol{\theta}). \tag{2.13}$$

By now it is quite clear that there can be established a connection between statistics and differential geometry [32, 33]. The aim of our thesis is to make use of the tools of differential geometry to study quantum physical systems.

2.3 Pure state geometry

Next, we would like to generalize the notions and results from the past section to the quantum setting. The probability vectors introduced in the previous section are replaced, in the context of quantum mechanics, 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

$$F\left(|\psi\rangle, |\phi\rangle\right) = |\langle\psi|\phi\rangle|, \tag{2.14}$$

where $|\psi\rangle$ and $|\phi\rangle$ are normalized vectors in $\mathcal{H} = \mathbb{C}^n$. It is easy to check that if two states are the same, fidelity is equal to one (if the states are normalized) and if they are orthogonal, fidelity is zero. Physically, this means that if the fidelity between states is one, then it is impossible to dinstinguish between them, while if their fidelity is zero one can tell them apart with no uncertainty. Suppose we are given a machine that shoots out electrons that have up or down spin along the z axis. Indeed, if we are given an electron in state $|\psi\rangle$ belonging to the set $\{|\uparrow\rangle, |\downarrow\rangle\}$, one can perform a measurement in this same basis (e.g. using a Stern–Gerlach apparatus) which is able to identify the two states with no uncertainty. Hence, fidelity quantifies how much a given measurement can distinguish two quantum states. Generally speaking,

$$F\big(|\psi\rangle, |\phi\rangle\big) = |P_\psi|\phi\rangle|. \tag{2.15}$$

The notion of a distance can be defined as

$$d^2(|\psi\rangle, |\phi\rangle) = \; 2\left(1 - |\langle\psi|\phi\rangle|\right). \tag{2.16}$$

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 $\mathcal{H}$

$$\mathbb{P}(\mathcal{H}) = \{[|\psi\rangle] : |\psi\rangle \in \mathcal{H}\} \tag{2.17}$$

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

$$\pi : |\psi\rangle \longmapsto P_\psi = |\psi\rangle\langle\psi| = e^{i\phi}|\psi\rangle\langle\psi|\, e^{-i\phi}. \tag{2.18}$$

Note that, unlike the vector representatives of quantum states, the orthogonal projector is gauge invariant,

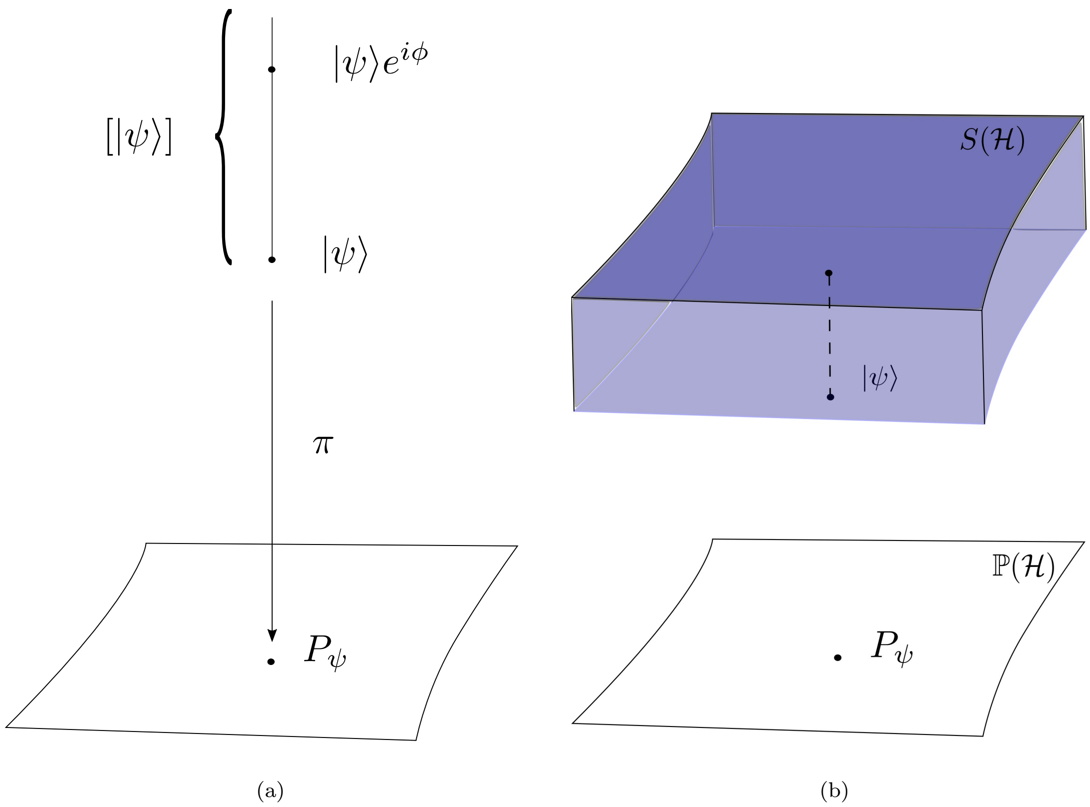


Figure 2.1: (a) Representation of a fiber: There is an equivalence class of states separated by a phase $e^{i\phi}$ that all project onto the same projector P_ψ. (b) Representation of a fiber bundle: there is a fiber for each point in the space of projectors $\mathbb{P}(\mathcal{H})$. This construction, along with the projection π defines a fiber bundle over the base space $\mathbb{P}(\mathcal{H})$

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 principal 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. Now, let us define a smooth curve $t \mapsto |\psi(t)\rangle$, such that $|\psi(0)\rangle = |\psi\rangle$, so that we can take derivatives of states. We know that our states live in the sphere in $\mathcal{H}$, hence the tangent space to this sphere is defined by

$$T_{|\psi\rangle}\mathcal{S}(\mathcal{H}) = T_{|\psi\rangle}S^{2n+1} = \{|v\rangle \in \mathcal{H} : \langle v|\psi\rangle + \langle\psi|v\rangle = 0\}, \tag{2.19}$$

which can be derived from the normalization condition for the states, i.e., $\frac{d}{dt}\left(\langle\psi|\psi\rangle\right) = 0$. Due to the unitary gauge ambiguity of states $|\psi\rangle$, when taking variation of a given state, two contributions will arise: a component proportional to the unitary phase and a component proportional to the differential of the physical state. These two components define the vertical and horizontal components, respectively. We will see below that pure gauge transformations completely specify a subbundle of the tangent bundle, i.e. a subspace of each tangent space, which we call the vertical subbundle. Pure gauge transformations induce no change in the quantum states. Therefore, one would like to have a complement of the vertical bundle, which we would then associate to variations of the states. For the case at hand, one natural choice is provided by the inner product structure of the Hilbert space, namely, we can consider the orthogonal complement so that:

$$T_{|\psi\rangle}S^{2n+1} = V_{|\psi\rangle} \oplus H_{|\psi\rangle}. \tag{2.20}$$

Quite intuitively so, the vertical space is defined as the collection of vectors that are tangent to the fiber. This can be easily seen if we consider a smooth curve that only has time dependence in the phase (it only moves within the fiber), i.e., $t \mapsto |\psi(t)\rangle = |\psi\rangle e^{i\phi t}$. Taking the derivative of this curve we have $\frac{d|\psi(t)\rangle}{dt} = i\phi\,|\psi(t)\rangle$, hence

$$V_{|\psi\rangle} = \{|\psi\rangle \cdot i\phi : \phi \in \mathbb{R}\} \subset T_{|\psi\rangle}\mathcal{H}. \tag{2.21}$$

Meanwhile, the horizontal space is defined as the orthogonal of the vertical space

$$H_{|\psi\rangle} = \{|v\rangle \in T_{|\psi\rangle}S^{2n+1} : \langle v|\psi\rangle = 0\}. \tag{2.22}$$

Generally, when a state evolves, it moves both vertically and horizontally within the principal bundle. In other words, its evolution will depend on both its phase and state itself. Hence, we will consider a curve on a state that has time dependence on both of these terms

$$|\psi'(t)\rangle = |\psi(t)\rangle \cdot e^{i\phi(t)}. \tag{2.23}$$

Now, we want to parallel transport this state, so it must follow the horizontality condition, that is

$$\langle \frac{d\psi'}{dt}|\psi'\rangle = 0 \Leftrightarrow i\frac{d\phi}{dt} = -\langle\psi|\frac{d\psi}{dt}\rangle \Leftrightarrow \phi = i\int \langle\psi|\frac{d}{dt}|\psi\rangle dt \tag{2.24}$$

This is the so-called *Berry phase*: as the state evolves it can move in two directions (vertically and horizontally), by adding a geometrical phase, the state is forced to stay within the horizontal subspace. This is the notion of *parallel transport* in the space of quantum states. The state then reads

$$|\psi'(t)\rangle = |\psi(t)\rangle \cdot \exp\left(-\int \langle\psi|\frac{d}{dt}|\psi\rangle dt\right). \tag{2.25}$$

Note that this is the same phase that appears in the quantum adiabatic theorem [34]. The term inside the integral

$$A = \langle\psi|\, d\,|\psi\rangle, \tag{2.26}$$

is the $U(1)$ *Berry connection*. Using this result, one can derive another representation of tangent horizontal vectors, by deriving the expression in Eq. (2.25) at $t = 0$, i.e.,

$$\frac{d|\psi'(t)\rangle}{dt}\Big|_{t=0} = \frac{d|\psi(t)\rangle}{dt}\Big|_{t=0} - \langle\psi(t)|\frac{d\psi}{dt}\rangle\Big|_{t=0}|\psi(t)\rangle. \tag{2.27}$$

In this sense, tangent horizontal vectors can also be described by

$$|\widetilde{v}^H\rangle = |\widetilde{v}\rangle - \langle\psi|\widetilde{v}\rangle|\psi\rangle, \tag{2.28}$$

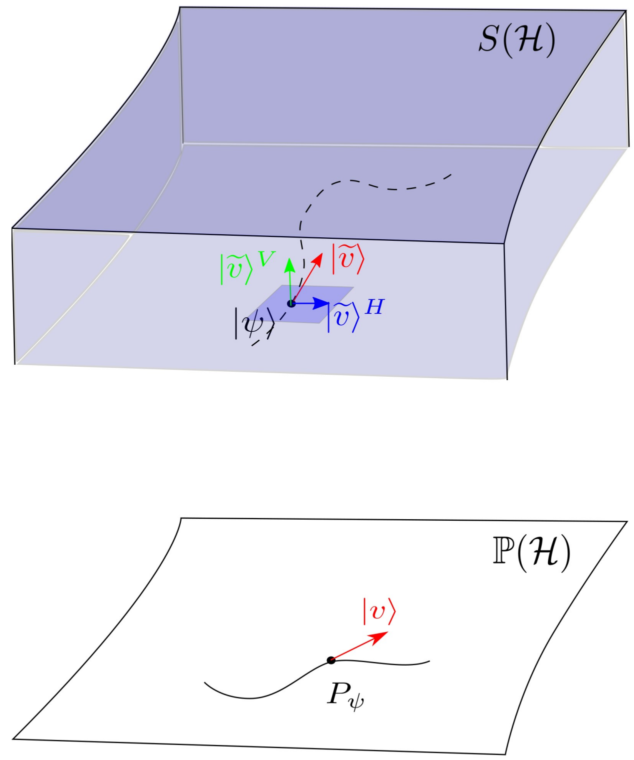


Figure 2.2: A curve in $\mathcal{S}(\mathcal{H})$ and its respective projection onto the base space, with their respective tangent vectors. The tangent vector in $\mathcal{S}(\mathcal{H})$ can be split into $|\widetilde{v}\rangle = |\widetilde{v}\rangle^H + |\widetilde{v}\rangle^V$. With this splitting one can identify isomorphisms such that $\pi(|\widetilde{v}\rangle) = |v\rangle^H$.

where $|\widetilde{v}\rangle^H$ is the horizontal component of a tangent vector $|\widetilde{v}\rangle = \frac{d|\psi(t)\rangle}{dt}\Big|_{t=0} \in T_\psi S^{2n+1}$. We now have a complete notion of horizontal subspaces of the tangent spaces to $\mathcal{H}$ and we can identifify isomorphisms $H_\psi \cong T_{P_\psi}\mathbb{P}(\mathcal{H})$ provided by the projection π, where $T_{P_\psi}\mathbb{P}(\mathcal{H})$ is the tangent space to the base space.

So far, we have seen how geometrical aspects naturally appear as a result of the gauge invariance of quantum states. Now, we must find out the metric on the space of quantum pure states. To proceed further, let us once again consider a curve in the space of quantum states and compute the distance between two infinitesimally close points

$$d^2(P_{\psi(t)}, P_{\psi(t+\delta t)}) = \; 2\Big(1 - |\langle\psi(t)|\psi(t+\delta t)\rangle|\Big). \tag{2.29}$$

Then, Taylor expand $|\psi(t+\delta t)\rangle$ up to second order as

$$|\psi(t+\delta t)\rangle = |\psi(t)\rangle + \frac{d|\psi(t)\rangle}{dt}\delta t + \frac{1}{2}\frac{d^2|\psi(t)\rangle}{dt^2}\delta t^2 + \mathcal{O}(\delta t^3). \tag{2.30}$$

The term $|\langle\psi(t)|\psi(t+\delta)\rangle|^2$ becomes

$$\begin{aligned} |\langle\psi(t)|\psi(t+\delta)\rangle|^2 &= \left(1 + \langle\psi|\dot{\psi}\rangle\delta t + \frac{1}{2}\langle\psi|\ddot{\psi}\rangle\delta t^2\right)\left(1 + \langle\dot{\psi}|\psi\rangle\delta t + \frac{1}{2}\langle\ddot{\psi}|\psi\rangle\delta t^2\right) \\ &= 1 + \left(\langle\psi|\dot{\psi}\rangle + \langle\dot{\psi}|\psi\rangle\right)\delta t + \left[\langle\dot{\psi}|\psi\rangle\langle\psi|\dot{\psi}\rangle + \frac{1}{2}\left(\langle\psi|\ddot{\psi}\rangle + \langle\ddot{\psi}|\psi\rangle\right)\right]\delta t^2, \end{aligned} \tag{2.31}$$

where $|\dot{\psi}\rangle$ and $|\ddot{\psi}\rangle$ are the first and second order time derivatives of $|\psi\rangle$, respectively. By taking derivatives of states, we are dealing with tangent vectors that follow condition (2.19), hence the second term in the equation above is zero. Meanwhile, the third term can be simplified through the tangent vector condition

$$\tfrac{d}{dt}\left[\langle\psi|\dot{\psi}\rangle + \langle\dot{\psi}|\psi\rangle\right] = 0 \iff \tfrac{1}{2}\left(\langle\ddot{\psi}|\psi\rangle + \langle\psi|\ddot{\psi}\rangle\right) = -\langle\dot{\psi}|\dot{\psi}\rangle. \tag{2.32}$$

We then have

$$\begin{aligned}|\langle\psi(t)|\psi(t+\delta)\rangle|^2 &= 1 + \left(\langle\dot{\psi}|\psi\rangle\langle\psi|\dot{\psi}\rangle - \langle\dot{\psi}|\dot{\psi}\rangle\right)\delta t^2 \\ &= 1 - \langle\dot{\psi}|\big(1 - |\psi\rangle\langle\psi|\big)|\dot{\psi}\rangle\delta t^2\end{aligned} \tag{2.33}$$

We need to square root this equation giving

$$\begin{aligned}|\langle\psi(t)|\psi(t+\delta)\rangle| &= \sqrt{1 - \langle\dot{\psi}|\big(1 - |\psi\rangle\langle\psi|\big)|\dot{\psi}\rangle\delta t^2} \\ &= 1 - \frac{1}{2}\langle\dot{\psi}|\big(1 - |\psi\rangle\langle\psi|\big)|\dot{\psi}\rangle\delta t^2,\end{aligned} \tag{2.34}$$

where we have used the binomial approximation to first order, i.e., $(1-x)^\alpha \sim 1-\alpha x$ for small x. Plugging this onto Eq. (2.29) we have

$$d^2(P_{\psi(t)}, P_{\psi(t+\delta t)}) = ds^2_{\text{FS}} = \langle\dot{\psi}|\big(1 - |\psi\rangle\langle\psi|\big)|\dot{\psi}\rangle\delta t^2. \tag{2.35}$$

which is the *Fubini-Study metric*. In terms of more general parameters $\theta^\mu(t)$ we can write

$$ds^2_{\text{FS}} = \langle\partial_\mu\psi|\left(I - |\psi\rangle\langle\psi|\right)|\partial_\nu\psi\rangle d\theta^\mu d\theta^\nu, \tag{2.36}$$

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

There is more to this tensor than meets the eye: it actually contains the information of all geometrical objects that we have been deriving so far. To see this let us first take the symmetric product $d\theta^\mu d\theta^\nu = \frac{1}{2}\left(d\theta^\mu d\theta^\nu + d\theta^\nu d\theta^\mu\right)$, such that we have

$$Q_{\mu\nu}d\theta^\mu d\theta^\nu = \frac{1}{2}\left(Q_{\mu\nu}d\theta^\mu d\theta^\nu + Q_{\mu\nu}d\theta^\nu d\theta^\mu\right). \tag{2.37}$$

We can exchange the indices in the second term since they are dummy indices

$$\frac{1}{2}\left(Q_{\mu\nu}d\theta^\mu d\theta^\nu + Q_{\mu\nu}d\theta^\nu d\theta^\mu\right) = \frac{1}{2}\left(Q_{\mu\nu}d\theta^\mu d\theta^\nu + Q_{\nu\mu}d\theta^\mu d\theta^\nu\right). \tag{2.38}$$

Now, simply note that

$$Q_{\nu\mu} = \langle\partial_\nu\psi|\left(I - |\psi\rangle\langle\psi|\right)|\partial_\mu\psi\rangle = \overline{\langle\partial_\mu\psi|\left(I - |\psi\rangle\langle\psi|\right)|\partial_\nu\psi\rangle} = \overline{Q}_{\mu\nu}, \tag{2.39}$$

such that, in the end, we have

$$\begin{aligned}Q_{\mu\nu}d\theta^\mu d\theta^\nu =& \frac{1}{2}\left(Q_{\mu\nu}+\overline{Q}_{\mu\nu}\right)d\theta^\nu d\theta^\mu \\ =& \operatorname{Re}Q_{\mu\nu}.\end{aligned}\tag{2.40}$$

We can now rewrite Eq. (2.36) as

$$ds^2_{\text{FS}} = \operatorname{Re}(Q_{\mu\nu})d\theta^\mu d\theta^\nu = g_{\mu\nu}d\theta^\mu d\theta^\nu,\tag{2.41}$$

where we have defined the metric as $g_{\mu\nu} = \operatorname{Re}Q_{\mu\nu}$.

Taking into account the gauge invariance of $Q_{\mu\nu}$, one might ask, rightly so, what the imaginary part of this part would give us. To see this, we will follow a similar reasoning as the preceeding one. Consider now the 2-form

$$Q_{\mu\nu}d\theta^\mu \wedge d\theta^\nu.\tag{2.42}$$

We can write the differential as $d\theta^\mu \wedge d\theta^\nu = \frac{1}{2}\left(d\theta^\mu \wedge d\theta^\nu - d\theta^\nu \wedge d\theta^\mu\right)$, which gives us

$$Q_{\mu\nu}d\theta^\mu \wedge d\theta^\nu = \frac{1}{2}\left(Q_{\mu\nu}d\theta^\mu \wedge d\theta^\nu - Q_{\mu\nu}d\theta^\nu \wedge d\theta^\mu\right).\tag{2.43}$$

Once again the indices can be interchanged giving

$$\frac{1}{2}\left(Q_{\mu\nu}d\theta^\mu \wedge d\theta^\nu - Q_{\mu\nu}d\theta^\nu \wedge d\theta^\mu\right) = \frac{1}{2}\left(Q_{\mu\nu} - Q_{\nu\mu}\right)d\theta^\mu \wedge d\theta^\nu.\tag{2.44}$$

Let us now compute explicitly the anti-symmetric quantity $Q_{\mu\nu} - Q_{\nu\mu}$,

$$\begin{aligned}Q_{\mu\nu} - Q_{\nu\mu} &= \langle\partial_\mu\psi|\left(I - |\psi\rangle\langle\psi|\right)|\partial_\nu\psi\rangle - \langle\partial_\nu\psi|\left(I - |\psi\rangle\langle\psi|\right)|\partial_\mu\psi\rangle \\ &= \langle\partial_\mu\psi|\partial_\nu\psi\rangle - \langle\partial_\nu\psi|\partial_\mu\psi\rangle - \langle\partial_\mu\psi|\psi\rangle\langle\psi|\partial_\nu\psi\rangle + \langle\partial_\nu\psi|\psi\rangle\langle\psi|\partial_\mu\psi\rangle.\end{aligned}\tag{2.45}$$

The last two terms cancel each other through the identity $\langle\psi|\partial_\mu\psi\rangle = -\langle\partial_\mu\psi|\psi\rangle$, so that

$$Q_{\mu\nu} - Q_{\nu\mu} = \langle\partial_\mu\psi|\partial_\nu\psi\rangle - \langle\partial_\nu\psi|\partial_\mu\psi\rangle.\tag{2.46}$$

Substituting this on Eq. (2.44) gives

$$\begin{aligned}Q_{\mu\nu}d\theta^\mu \wedge d\theta^\nu &= \frac{1}{2}\left(\langle\partial_\mu\psi|\partial_\nu\psi\rangle - \langle\partial_\nu\psi|\partial_\mu\psi\rangle\right)d\theta^\mu \wedge d\theta^\nu \\ &= d\mathcal{A} \\ &= F,\end{aligned}\tag{2.47}$$

where $F = \left(\langle\partial_\mu\psi|\partial_\nu\psi\rangle - \langle\partial_\nu\psi|\partial_\mu\psi\rangle\right)d\theta^\mu \wedge d\theta^\nu$ is a differential form known as the *Berry curvature* and

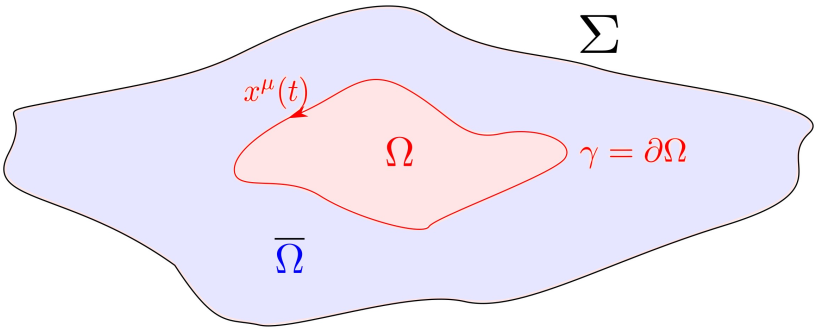


Figure 2.3: Visualization of Stokes' theorem and partition of $\mathbb{P}(\mathcal{H})$

$\mathcal{A} = \mathcal{A}_\mu dx^\mu$ is the Berry connection 1-form. On the other hand,

$$\begin{aligned} Q_{\mu\nu} d\theta^\mu \wedge d\theta^\nu &= \frac{1}{2}\left(Q_{\mu\nu} - Q_{\nu\mu}\right) d\theta^\mu \wedge d\theta^\nu \\ &= \frac{1}{2}\left(Q_{\mu\nu} - \overline{Q}_{\mu\nu}\right) d\theta^\mu \wedge d\theta^\nu \\ &= i \operatorname{Im} Q_{\mu\nu} d\theta^\mu \wedge d\theta^\nu \\ &= \frac{1}{2} F_{\mu\nu} d\theta^\mu \wedge d\theta^\nu, \end{aligned} \tag{2.48}$$

so that $F_{\mu\nu} = 2i \operatorname{Im} Q_{\mu\nu}$. The quantum geometric tensor can then be separated into its real and imaginary parts

$$\begin{aligned} Q_{\mu\nu} &= \operatorname{Re} Q_{\mu\nu} + i \operatorname{Im} Q_{\mu\nu} \\ &= g_{\mu\nu} + \frac{1}{2} F_{\mu\nu}, \end{aligned} \tag{2.49}$$

so that the real part corresponds to the metric tensor and the imaginary part corresponds to the Berry curvature.

Now, let us look again at Eq. (2.25): one can compute the phase that a given state acquires in a closed curve γ, given by $x^\mu(t)$ when parametrized by a set of coordinates $x^\mu \in U$, where U is an open neighborhood within our manifold $\mathbb{P}(\mathcal{H})$. Hence, a given state can be written as $|\psi(t)\rangle = |\psi\left(x^\mu(t)\right)\rangle$ and we can compute the explicit formula for the Berry phase

$$\exp\left(-\int_\gamma \langle\psi|\frac{d}{dt}|\psi\rangle dt\right) = \exp\left(-\int_\gamma \langle\psi|\partial_\mu|\psi\rangle \frac{dx^\mu}{dt} dt\right) = \exp\left(-\int_\gamma A\right), \tag{2.50}$$

If we consider that $\Sigma \subset \mathbb{P}(\mathcal{H})$ is a 2D compact connected surface, Stokes' theorem tells us that the integral of the Berry connection differential form A over the boundary of some orientable manifold $\partial\omega = \gamma$ is equal to the integral of its exterior derivative $dA = F$ over the whole of Ω (see Fig. 2.3), i.e.,

$$\int_\gamma A = \int_\Omega F. \tag{2.51}$$

There is another equality that can be found by identifying the complement of Ω - $\overline{\Omega}$ - such that $\Omega \cup \overline{\Omega} = \Sigma$.

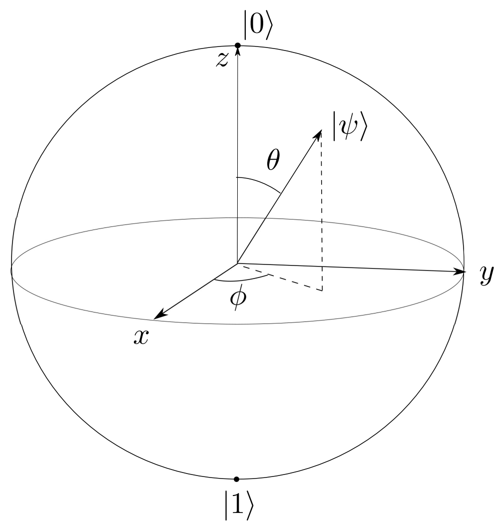


Figure 2.4: Parametrization of Bloch sphere using polar coordinates

We then have

$$\int_\gamma A = \int_\Omega F = -\int_{\overline{\Omega}} F. \tag{2.52}$$

Then, the Berry phase that is acquired in a closed loop can also be written as

$$\exp\left(\int_\gamma A\right) = \exp\left(\int_\Omega F\right) = \exp\left(-\int_{\overline{\Omega}} F\right), \tag{2.53}$$

from where one can conclude that

$$\exp\left(\int_{\Omega\cup\overline{\Omega}} F\right) = 1 \quad \therefore \quad \int_\Sigma F = 2\pi i n_1, n \in \mathbb{N}. \tag{2.54}$$

From this relation, one can define the *Chern number* of a compact manifold as

$$C_1 = i\int_\Sigma \frac{F}{2\pi}. \tag{2.55}$$

This quantity is a topological invariant, since one can deform these manifolds and their Chern number will still remain invariant. These invariants form the basis for the theory of topological phases of matter.

This concludes our discussion of pure quantum state geometry. We have gone over concepts that will not be used in our work direcly, but which are in any case important for the comprehension of the theory overall. In the next section, we will apply these notions to a simple two level system - a qubit, as they are known in quantum information.

Example: Single qubit state

Let us apply these notions to the single qubit state. Its respective Hilbert space is $\mathcal{H} = \mathbb{C}^2$ and the corresponding complex projective space is $\mathbb{C}P^1 \cong S^2$ - a spherical shell in $\mathbb{R}^3$ (see Fig. 2.4). In this space, qubits are given by the superpostion of two orthogonal states $|0\rangle$ and $|1\rangle$, i.e.

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle, \tag{2.56}$$

where (θ, ϕ) are the standard spherical angles that parametrize the spherical shell. Let us compute the quantum geometric tensor for this system. For this purpose we will need to compute the derivatives of $|\psi\rangle$ in spherical coordinates, i.e.,

$$|\partial_\theta\psi\rangle = \frac{1}{2}\left(-\sin\frac{\theta}{2}|0\rangle + e^{i\phi}\cos\frac{\theta}{2}|1\rangle\right) \tag{2.57}$$

$$|\partial_\phi\psi\rangle = ie^{i\phi}\sin\frac{\theta}{2}|1\rangle. \tag{2.58}$$

Using these results, in the first term of the tensor $\langle\partial_\mu\psi|\partial_\nu\psi\rangle$ we have

$$\langle\partial_\theta\psi|\partial_\theta\psi\rangle = \frac{1}{4}\left(\sin^2\frac{\theta}{2} + \cos^2\frac{\theta}{2}\right) = \frac{1}{4}, \tag{2.59}$$

$$\langle\partial_\theta\psi|\partial_\phi\psi\rangle = \frac{i}{2}\cos\frac{\theta}{2}\sin\frac{\theta}{2} = \frac{i}{4}\sin\theta, \tag{2.60}$$

$$\langle\partial_\phi\psi|\partial_\phi\psi\rangle = \sin^2\frac{\theta}{2}, \tag{2.61}$$

where we have used the identity $\frac{1}{2}\sin\theta = \cos\frac{\theta}{2}\sin\frac{\theta}{2}$. As for the second term $\langle\partial_\mu\psi|\psi\rangle\langle\psi|\partial_\nu\psi\rangle$ we have

$$\langle\psi|\partial_\theta\psi\rangle = \frac{1}{2}\left(-\sin\frac{\theta}{2}\cos\frac{\theta}{2} + \sin\frac{\theta}{2}\cos\frac{\theta}{2}\right) = 0 \tag{2.62}$$

$$\langle\psi|\partial_\phi\psi\rangle = i\sin^2\frac{\theta}{2}. \tag{2.63}$$

We are now ready to compute all the components of the tensor

$$Q_{\theta\theta} = \langle\partial_\theta\psi|\partial_\theta\psi\rangle - \langle\partial_\theta\psi|\psi\rangle\langle\psi|\partial_\theta\psi\rangle = \frac{1}{4} \tag{2.64}$$

$$Q_{\theta\phi} = \langle\partial_\theta\psi|\partial_\phi\psi\rangle - \langle\partial_\theta\psi|\psi\rangle\langle\psi|\partial_\phi\psi\rangle = \frac{i}{4}\sin\theta \tag{2.65}$$

$$Q_{\phi\theta} = Q^\dagger_{\theta\phi} = -\frac{i}{4}\sin\theta \tag{2.66}$$

$$Q_{\phi\phi} = \langle\partial_\phi\psi|\partial_\phi\psi\rangle - \langle\partial_\phi\psi|\psi\rangle\langle\psi|\partial_\phi\psi\rangle = \sin^2\frac{\theta}{2}\left(1 - \sin^2\frac{\theta}{2}\right) = \frac{1}{4}\sin^2\theta. \tag{2.67}$$

As we have seen in the previous section, $g_{\mu\nu} = \mathrm{Re}\, Q_{\mu\nu}$, hence our metric tensor reads

$$g_{\theta\theta} = \frac{1}{4} \tag{2.68}$$

$$g_{\theta\phi} = g_{\phi\theta} = 0 \tag{2.69}$$

$$g_{\phi\phi} = \frac{1}{4}\sin^2\theta. \tag{2.70}$$

This gives us the following infinitesimal line element

$$ds^2_{\mathrm{FS}} = \frac{1}{4}\left(d\theta^2 + \sin^2\theta d\phi^2\right), \tag{2.71}$$

which is the standard metric of a sphere of radius $\frac{1}{2}$. Meanwhile, the Berry curvature, given by $F_{\mu\nu} = 2i\,\mathrm{Im}\,Q_{\mu\nu}$, is

$$F_{\theta\theta} = F_{\phi\phi} = 0 \tag{2.72}$$
$$F_{\theta\phi} = \frac{i}{2}\sin\theta \tag{2.73}$$
$$F_{\phi\theta} = -\frac{i}{2}\sin\theta, \tag{2.74}$$

which defines the following 2-form

$$\begin{aligned} F &= \frac{1}{2}F_{\mu\nu}dx^\mu dx^\nu = \frac{1}{2}\left(F_{\theta\phi}d\theta\wedge d\phi + F_{\theta\phi}d\phi\wedge d\theta\right) = F_{\theta\phi}d\theta\wedge d\phi \\ &= \frac{i}{4}\sin\theta d\theta\wedge d\phi - \frac{i}{4}\sin\theta d\phi\wedge d\theta = \frac{i}{2}\sin\theta d\theta\wedge d\phi, \end{aligned} \tag{2.75}$$

Differential forms provide us a way of integrating over manifolds. More specifically, we know that the integral of this 2-form will give us the Chern number for the Bloch sphere. Let us perform this calculation. In this case, $\Sigma = \mathbb{P}(\mathcal{H}) = S^2$, therefore we have

$$\begin{aligned} C_1 &= i\int_{S^2}\frac{F}{2\pi} \\ &= -\frac{1}{4\pi}\int_0^\pi\int_0^{2\pi}\sin\theta d\theta d\phi \\ &= -\frac{1}{2}\int_0^\pi \sin\theta d\theta \\ &= \frac{1}{2}\int_0^\pi \frac{d\cos\theta}{d\theta}d\theta \\ &= -1. \end{aligned} \tag{2.76}$$

2.4 Mixed state geometry

Let us now turn our attention to mixed states. These 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 $|\varphi_j\rangle$. Within the context of the discussion in section 2.1, these pure states are homogeneous ensembles with a degree of "*mixing*" specified 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

$$\rho = \sum_{j=1}^{\ell} q_j|\varphi_j\rangle\langle\varphi_j|. \tag{2.77}$$

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

$$S = -\operatorname{Tr}\left(\rho \ln \rho\right). \tag{2.78}$$

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

$$\rho = \sum_{i=1}^{k} p_i P_i, \tag{2.79}$$

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 introduce matrices w called *amplitudes* of ρ, with $w \in \mathbb{C}^{n\times r}$, such that we can restate the density matrix as

$$\rho = ww^\dagger. \tag{2.80}$$

Essentially, w is a matrix whose columns are eigenvectors of ρ, that is, $w = (|e_1\rangle\, |e_2\rangle \ldots |e_r\rangle)$, with appropriate weights concerning the eigenvalues, i.e.,

$$\rho = ww^\dagger = \begin{pmatrix} |e_1\rangle & |e_2\rangle & \ldots & |e_k\rangle \end{pmatrix} \begin{pmatrix} \langle e_1| \\ \langle e_2| \\ \ldots \\ \langle e_k| \end{pmatrix} = \sum_{\alpha=1}^{r} |e_\alpha\rangle\langle e_\alpha| = \sum_{\alpha=1}^{r} p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|, \tag{2.81}$$

where $|e_\alpha\rangle = \sqrt{p_\alpha}|\psi_\alpha\rangle$ and, for each orthogonal projector P_i, the corresponding eigenvalue p_i appears r_i times. Much like the standard quantum pure states, these amplitudes can be defined up to an unitary matrix $U \in U(r)$, since when replacing $w \to w \cdot U$ expression (2.80) remains invariant

$$ww^\dagger \to (w \cdot U)\left(U^\dagger \cdot w^\dagger\right) = ww^\dagger = \rho. \tag{2.82}$$

Our objective is to find a metric for such a mixed quantum system and, for this purpose, we will follow a similar reasoning to what was done in the previous secion for the pure case.

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

$$\langle w, v\rangle := \operatorname{Re}\operatorname{Tr}\left(w^\dagger v\right), \tag{2.83}$$

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

$$\begin{aligned} d_B^2\left(\rho, \sigma\right) &= \inf_{\{w,v\}} ||w - v||^2 \\ &= \inf_{\{w,v\}} \operatorname{Tr}\left[(w - v)^\dagger (w - v)\right] \end{aligned}$$

$$= 2 - \sup_{\{w,v\}} \mathrm{Tr}\left[w^\dagger v + v^\dagger w\right], \tag{2.84}$$

where $||\cdot||$ is the Hilbert Schmidt scalar product on the space $\mathbb{C}^{n\times r}$. Let us go a little further and see that $\mathrm{Tr}\left[w^\dagger v + (w^\dagger v)^\dagger\right]$ is maximized if $w^\dagger v$ is positive and Hermitian, i.e,

$$w^\dagger v = v^\dagger w > 0. \tag{2.85}$$

This is the *Uhlmann parallelity condition* [30]: two amplitudes are said to be parallel if the above condition holds. Choosing $w = \sqrt{\rho}\,U$ and $v = \sqrt{\sigma}\,V$, we have

$$\begin{aligned} d_B^2(\rho,\sigma) &= 2\left(1 - \mathrm{Re}\,\mathrm{Tr}\, w^\dagger v\right) \\ &= 2\left(1 - \mathrm{Re}\,\mathrm{Tr}\sqrt{\rho}\sqrt{\sigma}VU^\dagger\right) \\ &= 2\left(1 - \mathrm{Re}\,\mathrm{Tr}\,|\sqrt{\rho}\sqrt{\sigma}|^{1/2}\cdot|\sqrt{\rho}\sqrt{\sigma}|^{1/2}\mathcal{U}VU^\dagger\right) \\ &\overset{\text{C-S}}{\geq} 2\left(1 - \mathrm{Tr}\sqrt{\sqrt{\rho}\,\sigma\sqrt{\rho}}\right) \\ &= 2\left(1 - F(\rho,\sigma)\right). \end{aligned} \tag{2.86}$$

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

$$F(\rho,\sigma) = \mathrm{Tr}\sqrt{\sqrt{\rho}\,\sigma\sqrt{\rho}}. \tag{2.87}$$

and $F(\rho,\sigma) = \mathrm{Tr}\,\mathcal{F}(\rho,\sigma)$. Eq.(2.86) is the mixed state counterpart of the Fubini-Study distance in Eq. (2.16). The definition of fidelity in Eq. (2.87) is the generalization of the fidelity that encompasses both the classical and the pure quantum state fidelity, since, as we have discussed previously, mixed states are simply the conjuction of a classical contribution, the statistical weights p_i, and a quantum contribution represented by pure states $|\psi_i\rangle$. Therefore, Eq. (2.87) should reduce to the classical and to the pure quantum state fidelity, when considering specific states.

Let us check the first case: consider another state $\sigma = \sum_{\alpha=1}^{r} q_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|$ that commutes with ρ. In this case, the fidelity between states ρ and σ is

$$\begin{aligned} F(\rho,\sigma) &= \mathrm{Tr}\sqrt{\sqrt{\rho}\,\sigma\sqrt{\rho}} \\ &= \mathrm{Tr}\sqrt{\sqrt{\sum_{\alpha=1}^{r} p_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|}\sum_{\beta=1}^{4} q_\beta|\psi_\beta\rangle\langle\psi_\beta|\sqrt{\sum_{\gamma=1}^{r} p_\gamma|\psi_\gamma\rangle\langle\psi_\gamma|}} \\ &= \mathrm{Tr}\sqrt{\sum_{\alpha,\beta,\gamma=1}\sqrt{p_\alpha}|\psi_\alpha\rangle\langle\psi_\alpha|q_\beta|\psi_\beta\rangle\langle\psi_\beta|\sqrt{p_\gamma}|\psi_\gamma\rangle\langle\psi_\gamma|} \\ &= \mathrm{Tr}\sqrt{\sum_{\alpha=1}^{r} p_\alpha q_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|} \\ &= \mathrm{Tr}\left(\sum_{\alpha=1}^{r}\sqrt{p_\alpha q_\alpha}|\psi_\alpha\rangle\langle\psi_\alpha|\right) \end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=\alpha}^{n} \sqrt{p_\alpha q_\alpha} \\
&= F_{cl}(p,q),
\end{aligned}
$$

where we have used the fact that the square root of a diagonal matrix with positive entries is just the square root of each entry, i.e., $\sqrt{\sum_i a_i |i\rangle\langle i|} = \sum_i \sqrt{a_i}|i\rangle\langle i|$. Physically, this result tells us that the fidelity between two quantum systems comprised of the same pure states is really just the classical fidelity between their relative distributions.

Next, we consider the fidelity between a pure state $\rho = |\psi\rangle\langle\psi|$ and a general mixed state σ. With this in mind, the fidelity reads

$$
\begin{aligned}
F(|\psi\rangle, \sigma) &= \mathrm{Tr}\sqrt{\sqrt{|\psi\rangle\langle\psi|}\sigma\sqrt{|\psi\rangle\langle\psi|}} \\
&= \mathrm{Tr}\sqrt{|\psi\rangle\langle\psi|\sigma|\psi\rangle\langle\psi|} \\
&= \sqrt{\langle\psi|\sigma|\psi\rangle}.
\end{aligned}
\tag{2.88}
$$

This case is quite useful since it comes up frequently in laboratory experiments: oftentimes in experiments one sends pure states (electrons or photons) which interact with the environment, resulting in a mixed state. The formula above reduces to the pure state fidelity when $\sigma = |\phi\rangle\langle\phi|$, i.e., when σ is also a pure state,

$$
F\Big(|\psi\rangle, \sigma = |\phi\rangle\langle\phi|\Big) = \sqrt{\langle\psi|\sigma|\psi\rangle} = \sqrt{\langle\psi|\phi\rangle\langle\phi|\psi\rangle} = F(|\psi\rangle, |\phi\rangle). \tag{2.89}
$$

Consider now the space 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_{Uhl}, by

$$
\begin{aligned}
\pi : P_{\mathrm{Uhl}} &\to B \\
w &\mapsto \rho = ww^\dagger.
\end{aligned}
\tag{2.90}
$$

We must remind ourselves that each amplitude has an $U(r)$ gauge freedom, so that $(\pi, P_{\mathrm{Uhl}}, B, U(r))$ define a principal $U(r)$-bundle. Once again, we will define horizontal tangent directions orthogonal to the vertical, i.e., gauge transformation geometry directions and hence find a geometry for mixed states.

Consider now a curve of rank r amplitudes

$$
\gamma_w : [0,1] \ni t \mapsto \gamma_w(t) \in P_{\mathrm{Uhl}} \tag{2.91}
$$

subject to the initial conditions $\gamma_w(0) = w$ and $\frac{d\gamma_w}{dt}|_{t=0} = \dot{w}$. The vertical subspace is then the collection of tangent vectors such that when they are projected onto the base space they give zero, that is

$$
\frac{d}{dt}\left(\pi\left(\gamma_w(t)\right)\right)|_{t=0} = 0 \leftrightarrow \frac{d}{dt}\left(\gamma_w(t)\gamma_w(t)^\dagger\right)|_{t=0} = \dot{w}w^\dagger + w\dot{w}^\dagger = 0, \tag{2.92}
$$

hence the vertical space at w is defined as

$$V_w = \{\dot{w} \in T_w P_{\text{Uhl}} : \dot{w}w^\dagger + w\dot{w}^\dagger = 0\}. \tag{2.93}$$

We can think of this space similarly to what we did in the last section, by saying that the vertical curve along the fiber can be written as $t \mapsto w(t) = w \cdot e^{tX}$, where $X \in \mathfrak{u}(r)$ is an anti-Hermitian matrix. Clearly, the projection onto the base state is invariant under this transformation

$$\begin{aligned} w(t)w^\dagger(t) =& we^{tX} \left(we^{tX}\right)^\dagger \\ &= we^{tX}e^{-tX}w^\dagger = ww^\dagger. \end{aligned} \tag{2.94}$$

The vector tangent to the fiber can now be written as $\frac{dw}{dt}|_{t=0} = \dot{w} = w \cdot X$, which satisfies the condition for vertical matrices

$$\dot{w}w^\dagger + w\dot{w}^\dagger = wXw^\dagger + wX^\dagger w^\dagger = wXw^\dagger - wXw^\dagger = 0 \tag{2.95}$$

Hence, our vertical space can also be seen as

$$V_w = \{\dot{w} \in T_w P_{\text{Uhl}} : \dot{w} = w \cdot X,\, X^\dagger = -X\}. \tag{2.96}$$

We are now in condition to define the horizontal subspaces, which will simply be the collection of tangent vectors $\dot{w}$ that are orthogonal to V_w, that is

$$H_w = \{\dot{w} \in T_w P_{\text{Uhl}} : \langle \dot{w}, \dot{w}' \rangle = 0, \text{ where } \dot{w}' \in V_w\}. \tag{2.97}$$

In this case, the connection is defined again by the horizontality condition, given by

$$\langle \dot{w}, \dot{w}' \rangle = 0, \tag{2.98}$$

where $\dot{w}$ is a tangent vector under consideration and $\dot{w}'$ is an arbitrary vertical tangent vector. Using the definition for the Hermitian form, the condition is then given by

$$\begin{aligned} &\operatorname{Re}\operatorname{Tr}\left(\dot{w}^\dagger w \cdot X\right) = 0, \text{ for every } X \in \mathfrak{u}(r) \\ &\qquad \Longrightarrow \dot{w}^\dagger w - w^\dagger \dot{w} = 0, \end{aligned} \tag{2.99}$$

where the implication stems from the fact that X is anti-Hermitian, so that $\dot{w}^\dagger w$ can only be Hermitian. [3]

[3] To see this, observe that a complex matrix can be split into its Hermitian and anti-Hermitian components: $Z = Z^H + Z^{AH}$, where $Z^H = \frac{1}{2}(Z + Z^\dagger)$ and $Z^{AH} = \frac{1}{2}(Z - Z^\dagger)$. This real-linear decomposition divides the full matrix into two orthogonal components. Indeed, $\operatorname{Re}\operatorname{Tr}\left[(Z_1^{AH})^\dagger Z_2^H\right] = \frac{1}{2}\left\{\operatorname{Tr}\left[\left(Z_1^{AH}\right)^\dagger Z_2^H\right] + \operatorname{Tr}\left[\left(Z_2^H\right)^\dagger Z_1^{AH}\right]\right\} = \frac{1}{2}\left\{-\operatorname{Tr}\left[\left(Z_1^{AH}\right) Z_2^H\right] + \operatorname{Tr}\left[\left(Z_2^H\right) Z_1^{AH}\right]\right\} = 0$. Moreover, since the real vector space of Hermitian matrices and anti-Hermitian matrices both have dimension $k \times k$, we conclude that if a complex matrix is (real-)orthogonal to an anti-Hermitian matrix, then it must be Hermitian.

We can then restate the horizontal space as

$$H_w = \{\dot{w} \in T_w P_{\mathrm{Uhl}} : w^\dagger \dot{w} = \dot{w}^\dagger w\}. \tag{2.100}$$

Finally, now that we have a notion of horizontal subspaces of the tangent spaces to P_{Uhl}, we have unique isomorphisms of $H_w \cong T_\rho \mathcal{B}$ provided by the projection π. This means that for each $v \in T_\rho \mathcal{B}$ there exists a unique $\widetilde{v}^H \in H_w \subset T_w P_{\mathrm{Uhl}}$, such that its projection is v, i.e., $\pi(\widetilde{v}^H) = \widetilde{v}^H w^\dagger + w \widetilde{v}^{H\dagger} = v$, and the converse is also true. This lift is called the "horizontal lift" for obvious reasons. Any other lift of v to $T_w P_{\mathrm{Uhl}}$, i.e., any tangent vector projecting to v, would differ from the horizontal by an element of the kernel of the derivative of the projection, i.e., a vertical vector. As a consequence of this isomorphism, the Riemannian metric in the base space is $g(v_1, v_2) := \langle \widetilde{v}_1^H, \widetilde{v}_2^H \rangle = \mathrm{Re}\,\mathrm{Tr}\left[\left(\widetilde{v}_1^H\right)^\dagger \widetilde{v}_2^H\right]$, where $\widetilde{v}^H$, are horizontal lifts of tangent vectors $v_1, v_2 \in T_P \mathrm{Gr}_r(\mathbb{C}^n)$. Moreover, the expression $g(v_1, v_2)$ does not depend on the point of the fiber over P, because the horizontal subspaces are $\mathrm{U}(r)$-equivariant and the metric is $\mathrm{U}(r)$-invariant. Indeed, if $\widetilde{v}^H \in H_w$ is an horizontal lift of $v \in T_\rho \mathcal{B}$, then $\widetilde{v}^H \cdot U$ is a horizontal lift belonging to $H_{w \cdot U}$, for every $U \in \mathrm{U}(r)$: $w^\dagger \widetilde{v}^H = 0 \Rightarrow (w \cdot U)^\dagger (\widetilde{v}^H \cdot U) = U^\dagger w^\dagger \widetilde{v}^H U = 0$. Note that, in $\widetilde{v}^H \cdot U$, right multiplication should be understood as the tangent map of right multiplication at w_i. Finally, $\mathrm{Re}\,\mathrm{Tr}\left[\left(\widetilde{v}_1^H\right)^\dagger \widetilde{v}_2^H\right] = \mathrm{Re}\,\mathrm{Tr}\left[\left(\widetilde{v}_1^H \cdot U\right)^\dagger \widetilde{v}_2^H \cdot U\right]$, by the cyclic property of the trace, which shows that this expression defines a metric in the base space.

Now every tangent vector $\widetilde{v} \in T_w P_{\mathrm{Uhl}}$ is uniquely projected to a horizontal vector $\tilde{v}^H \in H_w$, which is mapped to a base space tangent vector $v \in T_\rho \mathcal{B}$. Given the decomposition $T_w P_{\mathrm{Uhl}} = V_w \oplus H_w$, we can always find unique projection operators onto the vertical and horizontal subspaces, that perform the splitting

$$\widetilde{v} = \widetilde{v}^V + \widetilde{v}^H, \text{ where } \widetilde{v}^V \in V_w, \widetilde{v}^H \in H_w. \tag{2.101}$$

We claim that horizontal vectors can be written as transformation of the amplitudes w, i.e.,

$$\widetilde{v}^H = Gw, \text{where } G = G^\dagger \tag{2.102}$$

and we can check that this is true, replacing it in Eq. (2.100), i.e.

$$(\widetilde{v}w)^\dagger = w^\dagger \widetilde{v} \implies (Gw)^\dagger w = w^\dagger (Gw) \implies w^\dagger G w = w^\dagger G w. \tag{2.103}$$

Now, we have the identity

$$g(v_1, v_2) = \langle \widetilde{v}_1^H, \widetilde{v}_2^H \rangle. \tag{2.104}$$

which through the claim above, yields

$$\begin{aligned} g(v, v) &= \langle \widetilde{v}^H, \widetilde{v}^H \rangle \\ &= \mathrm{Re}\,\mathrm{Tr}\left(w^\dagger G G w\right) \end{aligned}$$

$$
\begin{aligned}
&= \mathrm{Tr}\left(ww^\dagger GG\right) \\
&= \mathrm{Tr}\,\rho G^2. \qquad (2.105)
\end{aligned}
$$

We can rewrite this equation in a different way, noting that

$$
v = \frac{d\rho}{dt}\Big|_{t=0} = \frac{d}{dt}(ww^\dagger) = \widetilde{v}w^\dagger + w\widetilde{v}^\dagger = G\rho + \rho G. \qquad (2.106)
$$

If we multiply $d\rho$ by G and take its trace, we have

$$
\mathrm{Tr}\,d\rho G = \mathrm{Tr}\left(G\rho G + \rho G^2\right) = 2\,\mathrm{Tr}\,\rho G^2, \qquad (2.107)
$$

which is just two times the Bures metric in Eq. (2.105), hence

$$
ds^2_{\text{Bures}} = \frac{1}{2}\,\mathrm{Tr}\,d\rho G. \qquad (2.108)
$$

Next, we would like to find out the matrix G, for this purpose, consider a given diagonalization of $\rho = \sum_i p_i|i\rangle\langle i|$, such that using the formula above

$$
\begin{aligned}
d\rho &= \sum_{ij} \langle i|d\rho|j\rangle |i\rangle\langle j| \qquad (2.109) \\
&= \sum_{ij} \langle i|(G\rho + \rho G)|j\rangle |i\rangle\langle j| \\
&= \sum_{ij} \langle i|(p_i + p_j)G|j\rangle |i\rangle\langle j|.
\end{aligned}
$$

This equation can be inverted for $p_i, p_j \neq 0$ yielding

$$
G = \sum_{ij} \frac{\langle i|d\rho|j\rangle}{p_i + p_j} |i\rangle\langle j|. \qquad (2.110)
$$

Plugging this into Eq. (2.105)

$$
\begin{aligned}
g_\rho &= \mathrm{Tr}\,\rho G^2 \\
&= \sum_{ij} p_i \langle j|G|i\rangle\langle i|G|j\rangle \\
&= \sum_{ij} \frac{p_i}{(p_i + p_j)^2} |\langle i|d\rho|j\rangle|^2. \qquad (2.111)
\end{aligned}
$$

Using $d\langle i|j\rangle = 0$, it can be shown that the differential of ρ is

$$
d\rho = \langle i|d\rho|j\rangle + \langle i|dj\rangle(p_j - p_i), \qquad (2.112)
$$

such that the explicit form of the Bures metric is

$$g_\rho = \frac{1}{4}\sum_i \frac{dp_i^2}{p_i} + \sum_{i\neq j} p_i \frac{(p_i - p_j)^2}{(p_i + p_j)^2} |\langle i|dj\rangle|^2, \tag{2.113}$$

since the cross terms of the square of Eq. (2.112) give zero. The first term on this equation is the classical Fischer-Rao metric derived in Eq. (2.5), while the second term corresponds to variations of the state and is the quantum contribution to the metric.

Now, it can be shown that this equation reduces to the Fubini-Study metric (2.36) when considering a single pure state. Consider a collection of eigenstates $\{|i\rangle\}$ such that there is one state $|\psi\rangle = |i = 1\rangle$ that is populated, i.e., $p_1 = 1, p_i = 0$ for $i \neq 1$. The first term is zero since we have only one state with constant probability, while in the second sum, the only term that survives is the one where $i = 1$ and $j \neq 1$ for which $p_j = 0$. We then have

$$g_\rho = \sum_{j\neq 1} |\langle \psi|dj\rangle|^2 = \sum_{j\neq 1} \langle \psi|dj\rangle\langle dj|\psi\rangle, \tag{2.114}$$

which through the identity $\langle \psi|dj\rangle = -\langle d\psi|j\rangle$ gives

$$g_\rho = \sum_{j\neq 1} \langle d\psi|j\rangle\langle j|d\psi\rangle. \tag{2.115}$$

Finally notice that $\sum_i |i\rangle\langle i| = I$ which implies that $\sum_{j\neq 1} |j\rangle\langle j| = I - |\psi\rangle\langle\psi|$. Replacing this in the equation above

$$g_\rho = \langle d\psi|\left(I - |\psi\rangle\langle\psi|\right)|\psi\rangle \tag{2.116}$$

we arrive at the Fubini-Study metric.

Now that we have gone through a comprehensive introduction of the main concepts, we are ready to explore the new ideas we produced during this thesis.

Chapter 3

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

3.1 The geometry of the Sjöqvist metric

We begin by briefly recapitulating the work of Erik Sjöqvist in Ref. [29]. In this paper, 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

$$\{\sqrt{p_j(t)}e^{if_j(t)}|n_j(t)\rangle\}_{j=1}^N, \tag{3.1}$$

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

$$\pi\left(\sqrt{p_j(t)}e^{if_j(t)}|n_j(t)\rangle\right) = \sum_{j=1}^N \sqrt{p_j(t)}\sqrt{p_j(t)}e^{if_j(t)}|n_j(t)\rangle\langle n_j(t)|e^{-if_j(t)} = \sum_{j=1}^N p_j|n_j(t)\rangle\langle n_j(t)|. \tag{3.2}$$

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

$$ds^2 = \frac{1}{4}\sum_k \frac{dp_k^2}{p_k} + \sum_k p_k\langle dn_k|\left(1 - |n_k\rangle\langle n_k|\right)|dn_k\rangle. \tag{3.3}$$

This metric has a special property, not featured in the Bures case. From Eq. (3.3) we see that the Sjöqvist metric can be separated into the classical Fisher-Rao metric of Eq. (2.5) 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 respective probabilities p_k.

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

3.2 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

$$\rho = \sum_{i=0}^{k} p_i P_i, \tag{3.4}$$

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 $r \in \{1, \dots, n\}$ 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 $\tau \equiv (r_1, r_2, \dots r_k) \in \mathcal{T}$, with $k \in \{1, \dots, n\}$ 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

$$\sum_{i=1}^{k} r_i p_i = 1. \tag{3.5}$$

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,

$$B = \bigcup_{\tau \in \mathcal{T}} B_\tau = \{\rho \in \mathcal{H} \otimes \mathcal{H}^* : \rho^\dagger = \rho \text{ and } \rho \geq 0 \text{ and } \operatorname{Tr} \rho = 1\}. \tag{3.6}$$

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 (3.5), 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 that is given by

$$\pi_\tau(p_\tau) \equiv \sum_{i=1}^{k} p_i P_i = \rho, \tag{3.7}$$

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

$$G_\tau \equiv \prod_{i=1}^{k} \mathrm{U}(r_i). \tag{3.8}$$

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

$$|e_{i,j}\rangle \mapsto \sum_{j'=1}^{r_i} |e_{i,j'}\rangle (U_i)^{j'}_{j}, \; j = 1, ..., r_i. \tag{3.9}$$

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., $w_i \equiv \big(|e_{i,1}\rangle \; |e_{i,2}\rangle \ldots |e_{i,r_i}\rangle\big)$, $i = 1, ..., k$, we can see P_τ as

$$P_\tau = \{\big((p_i, w_i)\big)_{i=1}^{k} : \sum_{i=1}^{k} p_i \; w_i w_i^\dagger \in B_\tau \text{ and } w_i^\dagger w_i = I_{r_i}, \text{ for all } i = 1, ..., k, \text{ and } p_i \neq p_j, \text{ for all } i \neq j\}, \tag{3.10}$$

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

$$\begin{aligned}\langle p_\tau, p'_\tau\rangle_\tau &\equiv \sum_{i=1}^{k} \sqrt{p_i p'_i}\, \mathrm{Tr}(w_i^\dagger w'_i) \\ &= \sum_{i=1}^{k} \mathrm{Tr}[(\sqrt{p_i} w_i^\dagger)(\sqrt{p'_i} w'_i)].\end{aligned} \tag{3.11}$$

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

$$P_{\text{Uhl}} = \{w \in \mathbb{C}^{n\times r} : \pi(w) \equiv w w^\dagger = \rho \in B, \text{ with } \operatorname{rank}(\rho) = r\}, \tag{3.12}$$

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

$$\langle w, w'\rangle = \mathrm{Tr}(w^\dagger w'). \tag{3.13}$$

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_{Uhl}. This follows from the map

$$P_\tau \ni ((p_i, w_i))_{i=1}^k \mapsto (\sqrt{p_1}w_1, ..., \sqrt{p_k}w_k) \in \bigoplus_{i=1}^k \mathbb{C}^{n\times r_i}, \tag{3.14}$$

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 [35] 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.

3.3 Distance measures and Riemannian metrics

Consider now two points, $p_\tau = ((p_i, w_i))_{i=1}^k$ and $q_\tau = ((q_i, v_i))_{i=1}^k \in P_\tau$. By making use of Eq. (3.11) one can define a distance between elements p_τ and q_τ in the total space of the principal bundle given by

$$\begin{aligned} d_\tau^2(p_\tau, q_\tau) &= 2\Big(1 - \mathrm{Re}\left(\langle p_\tau, q_\tau\rangle_\tau\right)\Big) \\ &= 2\left(1 - \sum_{i=1}^k \sqrt{p_i q_i}\ \mathrm{Re}\left(\mathrm{Tr}(w_i^\dagger v_i)\right)\right). \end{aligned} \tag{3.15}$$

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. (3.14). One can use this distance to define a distance on B_τ, through the formula:

$$d_I^2(\rho,\sigma) = \inf\{d_\tau^2(p_\tau, q_\tau) : \pi(p_\tau) = \rho \text{ and } \pi(q_\tau) = \sigma,\ \text{for } p_\tau, q_\tau \in P_\tau\}. \tag{3.16}$$

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 $i = 1, 2, \ldots k$, 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

$$|p_\tau\rangle = \sum_{i=1}^k \sqrt{p_i} w_i \otimes \mathrm{w}_i. \tag{3.17}$$

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

$$\begin{aligned} \langle p_\tau, q_\tau\rangle &= \sum_{i,j=1}^k \sqrt{p_i q_j}\langle w_i, v_j\rangle\langle \mathrm{w}_i, \mathrm{w}_j\rangle \\ &= \sum_{i=1}^k \sqrt{p_i q_i}\langle w_i, v_i\rangle \\ &= \sum_{i=1}^k \sqrt{p_i q_i}\,\mathrm{Tr}(w_i^\dagger v_i) \\ &= \langle p_\tau, q_\tau\rangle_\tau, \end{aligned} \tag{3.18}$$

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. (3.10), if we take the w_i's as (row) vectors $|w_i\rangle = \Big[|e_{i,1}\rangle\ |e_{i,2}\rangle\ \ldots\ |e_{i,r_i}\rangle\Big]$ 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 $r_i = 1$, $i = 1, ..., k$,

$$\begin{aligned} g_I^{\mathrm{Q}} &= \sum_{i=1}^k p_i\langle dw_i|(I_n - w_i w_i^\dagger)|dw_i\rangle \\ &= \sum_{i=1}^k p_i\langle de_{i,1}|(I_n - |e_{i,1}\rangle\langle e_{i,1}|)|de_{i,1}\rangle, \end{aligned} \tag{3.19}$$

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

$$\begin{aligned} g_I^{\mathrm{Q}} &= \sum_{i=1}^k p_i\langle dw_i|\big(I_n - w_i w_i^\dagger\big)|dw_i\rangle \\ &= \sum_{i=1}^k p_i\langle dw_i|\Big[I_n - \big(\sum_{j=1}^{r_i}|e_{i,j}\rangle\langle e_{i,j}|\big)\Big]|de_i\rangle \\ &= \sum_{i=1}^k p_i\langle dw_i|\big(I_n - P_i\big)|dw_i\rangle, \end{aligned} \tag{3.20}$$

with $|dw_i\rangle = \Big[|de_{i,1}\rangle\ |de_{i,2}\rangle\ \ldots\ |de_{i,r_i}\rangle\Big]$, $i = 1, ..., k$. Indeed, in the next chapter we prove that this intuitive generalization is the correct result describing the infinitesimal counterpart of the distance in Eq. (3.16).

3.4 Induced Riemannian metrics

Let us look again at the principal bundle P_τ, for a fixed type $\tau = (r_1, ..., r_k)$. In this case, a point in P_τ is given by $p_\tau = \big((p_i, w_i)\big)_{i=1}^k$ and can be equivalently represented as $p_\tau = \big((p_i)_{i=1}^k, (w_i)_{i=1}^k\big)$. With this identification, we can separate p_τ into its "*classical*" and "*quantum*" parts:

(i) A classical probability amplitude vector $\sqrt{\mathbf{p}} = (\sqrt{p_1}, ..., \sqrt{p_k})$, with $\sum_{i=1}^k p_i = 1$ and, for each $i \in \{1, ..., k\}$, $p_i > 0$. Note that the set of all classical probability amplitudes is in fact contained in the $k-1$-dimensional sphere and the associated classical Fisher metric is, up to a factor of $1/4$, the usual round metric in the sphere S^{k-1}.

(ii) A quantum part which is a k-tuple, i.e., a sequence of matrices $(w_1, ..., w_k)$, each of them identifying a r_i-unitary frame in $\mathbb{C}^n$, i.e., $w_i \in \mathrm{V}_{r_i}(\mathbb{C}^n)$, where

$$V_{r_i}(\mathbb{C}^n) = \{w_i \in \mathbb{C}^{n\times r_i} : w_i^\dagger w_i = I_k\} \subset \mathbb{C}^{n\times r_i},$$
$$i = 1, ..., k, \tag{3.21}$$

commonly known as the *Stiefel* manifold of r_i-unitary frames in $\mathbb{C}^n$.

Our aim is to compute the Riemannian metric in the base space B_τ for a given type $\tau = (r_1, ..., r_k)$. For this purpose, we will first look at the tangent space at a point p_τ, which is isomorphic to the direct sum

$$T_{p_\tau} P_\tau \cong T_{\sqrt{\mathbf{p}}} S^{k-1} \oplus \left(\bigoplus_{i=1}^k T_{w_i} V_{r_i}(\mathbb{C}^n) \right). \tag{3.22}$$

This isomorphism follows from the factorization into classical and quantum parts: for every curve in the total space P_τ, there will be a tangent vector for each of the curves induced by projection in the different factors of P_τ.

The classical components have no gauge ambiguity. The quantum components, however, have a $\mathrm{U}(r_i)$ gauge degree of freedom for each matrix w_i, $i = 1, ..., k$. This gauge ambiguity corresponds to variations along the fibres, as we will mention later on. From a physical standpoint, the exact point in the fibre has no significance, since the matrices w_i will be projected onto the base space, where the projectors P_i are gauge invariant: namely, w_i and $w_i \cdot U$, for $U \in \mathrm{U}(r_i)$, give rise to the same projector $P_i = w_i w_i^\dagger = w_i U U^\dagger w_i^\dagger$, for all $i = 1, ..., k$. Hence, we need to define the horizontal subspaces of the tangent spaces to P_τ, in order to uniquely represent the tangent spaces to the base space upstairs, i.e., in the tangent spaces to P_τ. Mathematically, this notion is referred to as an *Ehresmann connection*, see, for example, Sec. 6.3 of Ref. [36].

Before we proceed, let us focus on one of the Stiefel manifolds, say for a fixed $i \in \{1, ..., k\}$, $V_{r_i}(\mathbb{C}^n)$. For convenience, we define the projection onto the space of projectors of rank r_i, identified with the Grassmannian of r_i-planes in $\mathbb{C}^n$, i.e., the manifold of linear subspaces of dimension r_i in $\mathbb{C}^n$,

$$\begin{aligned} \pi_i : V_{r_i}(\mathbb{C}^n) &\to \mathrm{Gr}_{r_i}(\mathbb{C}^n) \\ w_i &\mapsto P_i = w_i w_i^\dagger. \end{aligned} \tag{3.23}$$

Consider a curve in the Stiefel manifold

$$\gamma_{w_i} : [0,1] \ni t \mapsto \gamma_{w_i}(t) \in V_{r_i}(\mathbb{C}^n) \tag{3.24}$$

subject to the initial conditions $\gamma_{w_i}(0) = w_i$ and $\left.\frac{d\gamma_{w_i}}{dt}\right|_{t=0} = \dot{w}_i \equiv \widetilde{v}$. From the definition of $V_{r_i}(\mathbb{C}^n)$, the tangent spaces are

$$T_{w_i}V_{r_i}(\mathbb{C}^n) = \{\dot{w}_i \in \mathbb{C}^{n\times r_i} : \dot{w}_i^\dagger w_i + w_i^\dagger \dot{w}_i = 0\}. \tag{3.25}$$

The vertical space at $w_i \in V_{r_i}(\mathbb{C}^n)$ is the set of tangent vectors in $T_{w_i}V_{r_i}(\mathbb{C}^n)$, such that its infinitesimal projection onto the base space is zero, that is

$$\begin{aligned}&\frac{d}{dt}\left(\pi_i\left(\gamma_{w_i}(t)\right)\right)\Big|_{t=0} = 0\\ \Leftrightarrow &\frac{d}{dt}\left(\gamma_{w_i}(t)\gamma_{w_i}^\dagger(t)\right)\Big|_{t=0} = \dot{w}_i w_i^\dagger + w_i \dot{w}_i^\dagger = 0.\end{aligned} \tag{3.26}$$

The vertical space is then given by

$$V_{w_i} = \{\dot{w}_i \in T_{w_i}V_{r_i}(\mathbb{C}^n) : \dot{w}_i w_i^\dagger + w_i \dot{w}_i^\dagger = 0\}. \tag{3.27}$$

The projection π_i has derivative, $d\pi_i = w_i dw_i^\dagger + dw_i w_i^\dagger$, and the vertical tangent vectors are in the kernel of this linear map. Given a fiber of π_i and a choice of a w_i in this fibre, then we can diffeomorphically identify the fiber with $\mathrm{U}(r_i)$ by right multiplication. Suppose we take $X \in \mathfrak{u}(r_i)$, identified as an anti-Hermitian matrix in the usual way, and choose a curve $t \mapsto w_i(t) = w_i \cdot e^{tX}$. Clearly, the projection onto the base is invariant under this transformation

$$\begin{aligned}w_i(t)w_i^\dagger(t) &= w_i\, e^{tX}\left(w_i\, e^{tX}\right)^\dagger\\ &= w_i\, e^{tX} e^{-tX}\, w_i^\dagger = w_i w_i^\dagger.\end{aligned} \tag{3.28}$$

The tangent vector to the fiber can now be written as $\left.\frac{dw_i}{dt}\right|_{t=0} = \dot{w}_i = w_i \cdot X$, which satisfies the condition for vertical matrices

$$\dot{w}_i w_i^\dagger + w_i \dot{w}_i^\dagger = w_i X w_i^\dagger + w_i X^\dagger w_i = w_i X w_i^\dagger - w_i X w_i^\dagger = 0. \tag{3.29}$$

Hence, by dimensionality, our vertical space can also be seen as

$$V_{w_i} = \{\dot{w}_i \in T_{w_i}V_{r_i}(\mathbb{C}^n) : \dot{w}_i = w_i \cdot X, \text{where } X^\dagger = -X\}. \tag{3.30}$$

We are now in condition to define the horizontal subspaces, which will simply be the collection of tangent vectors $\dot{w}_i$ that are orthogonal to V_{w_i}

$$\begin{aligned}H_{w_i} &= (V_{w_i})^\perp \qquad (3.31)\\ &= \{\dot{w} \in T_{w_i}V_{r_i}(\mathbb{C}^n) :\ \langle \dot{w}_i, \dot{w}_i' \rangle = 0, \text{where } \dot{w}_i' \in V_{w_i}\}.\end{aligned}$$

Note that the operation $\langle \cdot, \cdot \rangle$ is not the Hermitian form defined in Eq. (3.11). It is instead the standard inner product in the space of complex matrices seen as a real vector space $\langle A, B\rangle \equiv \operatorname{Re}\operatorname{Tr}(A^\dagger B)$. The condition in (3.31) is then given by

$$\begin{aligned} \operatorname{Re}\operatorname{Tr}\left(\dot{w}_i^\dagger w_i \cdot X\right) &= 0, \text{ for every } X \in \mathfrak{u}(r_i) \\ &\implies \dot{w}_i^\dagger w_i - w_i^\dagger \dot{w}_i = 0, \end{aligned} \tag{3.32}$$

where the implication stems from the fact that X is anti-Hermitian, so that $\dot{w}^\dagger w$ can only be Hermitian. [1] We can go further by making use of the condition in Eq. (3.25), yielding $\dot{w}_i^\dagger w_i = -w_i^\dagger \dot{w}_i$, and substituting this in Eq. (3.32) we get

$$\dot{w}_i^\dagger w_i - w_i^\dagger \dot{w}_i = -2 w_i^\dagger \dot{w}_i = 0 \implies w_i^\dagger \dot{w}_i = 0. \tag{3.33}$$

Finally, now that we have a notion of horizontal subspaces of the tangent spaces to $V_{r_i}(\mathbb{C}^n)$, we have unique isomorphisms of $H_{w_i} \cong T_{P_i}\mathrm{Gr}_{r_i}(\mathbb{C}^n)$ provided by the projection π_i. This means that for each $v \in T_{P_i}\mathrm{Gr}_{r_i}(\mathbb{C}^n)$ there exists a unique $\widetilde{v}^H \in H_{w_i} \subset T_{w_i}\mathrm{V}_{r_i}(\mathbb{C}^n)$, such that its projection is v, i.e., $\pi_i(\widetilde{v}^H) = \widetilde{v}^H w_i^\dagger + w_i \widetilde{v}^{H\dagger} = v$, and the converse is also true. This lift is called the "horizontal lift" for obvious reasons. Any other lift of v to $T_{w_i}\mathrm{V}_{r_i}(\mathbb{C}^n)$, i.e., any tangent vector projecting to v, would differ from the horizontal by an element of the kernel of the derivative of the projection, i.e., a vertical vector. As a consequence of this isomorphism, the Riemannian metric in the base space is $g_i(v_1, v_2) := \langle \widetilde{v}_1^H, \widetilde{v}_2^H \rangle = \operatorname{Re}\operatorname{Tr}\left[\left(\widetilde{v}_1^H\right)^\dagger \widetilde{v}_2^H\right]$, where $\widetilde{v}_i^H$, are horizontal lifts of tangent vectors $v_1, v_2 \in T_{P_i}\mathrm{Gr}_{r_i}(\mathbb{C}^n)$. Moreover, the expression $g_i(v_1, v_2)$ does not depend on the point of the fiber over P_i, because the horizontal subspaces are $\mathrm{U}(r_i)$-equivariant and the metric is $\mathrm{U}(r_i)$-invariant. Indeed, if $\widetilde{v}^H \in H_{w_i}$ is a horizontal lift of $v \in T_{P_i}\mathrm{Gr}_{r_i}(\mathbb{C}^n)$, then $\widetilde{v}^H \cdot U$ is a horizontal lift belonging to $H_{w_i \cdot U}$, for every $U \in \mathrm{U}(r_i)$: $w_i^\dagger \widetilde{v}^H = 0 \Rightarrow (w_i \cdot U)^\dagger (\widetilde{v}^H \cdot U) = U^\dagger w_i^\dagger \widetilde{v}^H U = 0$. Note that, in $\widetilde{v}^H \cdot U$, right multiplication should be understood as the tangent map of right multiplication at w_i. Finally, $\operatorname{Re}\operatorname{Tr}\left[\left(\widetilde{v}_1^H\right)^\dagger \widetilde{v}_2^H\right] = \operatorname{Re}\operatorname{Tr}\left[\left(\widetilde{v}_1^H \cdot U\right)^\dagger \widetilde{v}_2^H \cdot U\right]$, by the cyclic property of the trace, which shows that this expression defines a metric in the base space.

Now every tangent vector $\widetilde{v} \in T_{w_i}\mathrm{V}_{r_i}(\mathbb{C}^n)$ is uniquely projected to a horizontal vector $\tilde{v}^H \in H_{w_i}$, which is mapped to a base space tangent vector $v \in T_{P_i}\mathrm{Gr}_{r_i}(\mathbb{C}^n)$. Given the decomposition $T_{w_i}\mathrm{V}_{r_i}(\mathbb{C}^n) = V_{w_i} \oplus H_{w_i}$, we can always find unique projection operators onto the vertical and horizontal subspaces, that perform the splitting

$$\widetilde{v} = \widetilde{v}^V + \widetilde{v}^H, \text{ where } \widetilde{v}^V \in V_{w_i}, \widetilde{v}^H \in H_{w_i}. \tag{3.34}$$

[1] To see this, observe that a complex matrix can be split into its Hermitian and anti-Hermitian components: $Z = Z^H + Z^{AH}$, where $Z^H = \frac{1}{2}(Z + Z^\dagger)$ and $Z^{AH} = \frac{1}{2}(Z - Z^\dagger)$. This real-linear decomposition divides the full matrix into two orthogonal components. Indeed, $\operatorname{Re}\operatorname{Tr}\left[\left(Z_1^{AH}\right)^\dagger Z_2^H\right] = \dfrac{1}{2}\left\{\operatorname{Tr}\left[\left(Z_1^{AH}\right)^\dagger Z_2^H\right] + \operatorname{Tr}\left[\left(Z_2^H\right)^\dagger Z_1^{AH}\right]\right\} = \dfrac{1}{2}\left\{-\operatorname{Tr}\left[\left(Z_1^{AH}\right) Z_2^H\right] + \operatorname{Tr}\left[\left(Z_2^H\right) Z_1^{AH}\right]\right\} = 0$. Moreover, since the real vector space of Hermitian matrices and anti-Hermitian matrices both have dimension $k \times k$, we conclude that if a complex matrix is (real-)orthogonal to an anti-Hermitian matrix, then it must be Hermitian.

We have the identity

$$g(v_1, v_2) = \langle \widetilde{v}_1^H, \widetilde{v}_2^H \rangle. \tag{3.35}$$

Additionally, due to the splitting of subspaces, we can write

$$\widetilde{v}^H = \widetilde{v} - \widetilde{v}^V, \tag{3.36}$$

In the following, we determine the form of the projection onto the vertical subspaces, in order to obtain a more compact form for the metric on the base space.

We claim that the vertical projection of a general tangent vector $\widetilde{v}$ is given by

$$\widetilde{v}^V = P_i \widetilde{v} = w_i w_i^\dagger \widetilde{v}. \tag{3.37}$$

Let us see why this is true. For this tangent vector to be vertical it must comply with Eq (3.27), i.e.,

$$(P_i \widetilde{v})\, w_i^\dagger + w_i\, (P_i \widetilde{v})^\dagger = w_i w_i^\dagger \widetilde{v} w_i^\dagger + w_i \widetilde{v}^\dagger w_i w_i^\dagger = 0. \tag{3.38}$$

However, we know that $\widetilde{v}$ is a tangent vector, that is, we know that $\widetilde{v}^\dagger w_i = -w_i^\dagger \widetilde{v}$. Replacing this in the expression above we have

$$w_i w_i^\dagger \widetilde{v} w_i^\dagger - w_i w_i^\dagger \widetilde{v} w_i^\dagger = 0. \tag{3.39}$$

Hence, we have verified that $P_i \widetilde{v}$ is a vertical tangent vector and the map $\widetilde{v} \mapsto w_i w_i^\dagger \widetilde{v}$ is a projection onto the vertical space. The horizontal projection is then given by

$$\widetilde{v}^H = \widetilde{v} - (w_i w_i^\dagger) \widetilde{v}. \tag{3.40}$$

Meanwhile, the metric in $\mathrm{Gr}_{r_i}(\mathbb{C}^n)$ is, using the horizontal projections, given by the following compact formula

$$\begin{aligned} g_i &= \mathrm{Re}\,\mathrm{Tr}\left[\left(dw_i^\dagger - dw_i^\dagger w_i w_i^\dagger \right) \left(dw_i - w_i w_i^\dagger dw_i \right) \right] \\ &= \mathrm{Re}\,\mathrm{Tr}\left[dw_i^\dagger dw_i - dw_i^\dagger w_i w_i^\dagger dw_i - dw_i^\dagger w_i w_i^\dagger dw_i + dw_i^\dagger (w_i w_i^\dagger)^2 dw_i \right]. \end{aligned} \tag{3.41}$$

We know that $w_i (w_i^\dagger w_i) w_i^\dagger = w_i w_i^\dagger$, since $w_i^\dagger w_i = I_k$, so the last two terms cancel each other, giving

$$\begin{aligned} g_i &= \mathrm{Re}\,\mathrm{Tr}\left[dw_i^\dagger dw_i - dw_i^\dagger w_i w_i^\dagger dw_i \right] \\ &= \mathrm{Re}\,\mathrm{Tr}\left[dw_i^\dagger (1 - w_i w_i^\dagger) dw_i \right]. \end{aligned} \tag{3.42}$$

Now, this expression is written in terms of the elements defined in the principal bundle so we want to write it in terms of the elements in the base space — the projectors P_i. For this purpose, notice that $w_i = (w_i w_i^\dagger) w_i = P_i w_i$ which, by derivation gives $dw_i = dP_i w_i + P_i dw_i$. The same can be done for the hermitian $w_i^\dagger = w_i^\dagger(w_i w_i^\dagger) = w_i^\dagger P_i$ that gives us $dw_i^\dagger = dw_i^\dagger P_i + w_i^\dagger dP_i$. Replacing these in Eq. (3.42), we get

$$\begin{aligned}
g_i &= \operatorname{Re}\operatorname{Tr}\left[dw_i^\dagger(1 - w_i w_i^\dagger)dw_i\right] \\
&= \operatorname{Re}\operatorname{Tr}\left[\left(dw_i^\dagger P_i + w_i^\dagger dP_i\right)(1 - P_i)\left(dP_i w_i + P_i dw_i\right)\right] \\
&= \operatorname{Re}\operatorname{Tr}\Big[\left(dw_i^\dagger P_i + w_i^\dagger dP_i - dw_i^\dagger P_i - w_i^\dagger dP_i P_i\right)\left(dP_i w_i + P_i dw_i\right)\Big] \\
&= \operatorname{Re}\operatorname{Tr}\Big(dw_i^\dagger P_i dP_i w_i + w_i^\dagger dP_i dP_i w_i - dw_i^\dagger P_i dP_i w_i - w_i^\dagger dP_i P_i dP_i w_i \\
&\qquad + dw_i^\dagger P_i dw_i + w_i^\dagger dP_i P_i dw_i - dw_i^\dagger P_i dw_i - w_i^\dagger dP_i P_i dw_i\Big) \\
&= \operatorname{Re}\operatorname{Tr}\Big(w_i^\dagger dP_i dP_i w_i - w_i^\dagger dP_i P_i dP_i w_i\Big) \\
&= \operatorname{Re}\operatorname{Tr}\Big(P_i dP_i dP_i\Big) - \operatorname{Re}\operatorname{Tr}\Big(P_i dP_i P_i dP_i\Big).
\end{aligned} \tag{3.43}$$

Moreover, since $P_i^2 = P_i$, we have that $dP_i = d(P_i^2) = P_i dP_i + dP_i P_i$. Multiplying this expression by P_i on both sides we get $P_i dP_i P_i = 2P_i dP_i P_i$ and we can conclude that $P_i dP_i P_i = 0$. The last term on the last expression is then zero and we see that the metric is given by

$$\begin{aligned}
g_i &= \operatorname{Re}\operatorname{Tr}\left(P_i dP_i dP_i\right) = \operatorname{Re}\operatorname{Tr}\left(P_i dP_i dP_i P_i\right) \\
&= \operatorname{Tr}\left(P_i dP_i dP_i P_i\right).
\end{aligned} \tag{3.44}$$

Now we wish to determine the metric on the total space of the principal bundle, i.e., the metric that encompasses both the classical and quantum parts. For this purpose, consider a curve in the principal bundle space given by $t \mapsto p_\tau(t) = \left(\sqrt{\mathbf{p}(t)}, \mathbf{w}(t)\right)$ and compute the distance between two infinitesimally close points t and $t + \delta t$. For the first case, we consider a static $\mathbf{w}(t) = \mathbf{w}$ and compute the distance

$$d_\tau^2\big(p_\tau(t),\, p_\tau(t+\delta t)\big) = 2\Big(1 - \sum_{i=1}^{k}\sqrt{p_i(t)p_i(t+\delta t)}\operatorname{Re}\operatorname{Tr}(w_i^\dagger w_i)\Big).$$

We have $\operatorname{Tr}(w_i^\dagger w_i) = \operatorname{Tr} P_i = r_i$, hence

$$d_\tau^2\big(p_\tau(t), p_\tau(t+\delta t)\big) = 2\left(1 - \sum_{i=1}^{k} r_i\sqrt{p_i(t)p_i(t+\delta t)}\right). \tag{3.45}$$

Let us look more closely at the expression $\sqrt{p_i(t)p_i(t+\delta t)}$. We can Taylor expand $P_i(t+\delta t)$ to second order in δt to obtain

$$\begin{aligned}
\sqrt{p_i(t)p_i(t+\delta t)} &= \sqrt{p_i(t)\left(p_i(t) + \dot{p}_i\delta t + \frac{1}{2}\ddot{p}_i\delta t^2\right)} \\
&= p_i(t)\sqrt{1 + \frac{\dot{p}_i}{p_i}\delta t + \frac{1}{2}\frac{\ddot{p}_i}{p_i}\delta t^2}
\end{aligned} \tag{3.46}$$

We can then approximate the quantity inside the square root by $\sqrt{1+x} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2$, which, ignoring higher order terms, yields

$$\begin{aligned}\sqrt{p_i(t)p_i(t+\delta t)} &\approx p_i\Big[1+\frac{1}{2}\left(\frac{\dot{p}_i}{p_i}\delta t+\frac{1}{2}\frac{\ddot{p}_i}{p_i}\delta t^2\right)-\frac{1}{8}\left(\frac{\dot{p}_i}{p_i}\delta t+\frac{1}{2}\frac{\ddot{p}_i}{p_i}\delta t^2\right)^2\Big]\\ &= p_i\left[1+\frac{1}{2}\frac{\dot{p}_i}{p_i}\delta t+\frac{1}{2}\frac{\ddot{p}_i}{p_i}\delta t^2-\frac{1}{8}\left(\frac{\dot{p}_i}{p_i}\right)^2\delta t^2\right]\\ &= p_i+\frac{1}{2}\dot{p}_i\delta t+\frac{1}{2}\ddot{p}_i\delta t^2-\frac{1}{8}\frac{\dot{p}_i^2}{p_i}\delta t^2. \end{aligned} \tag{3.47}$$

Replacing this in Eq. (3.45), we get

$$d_\tau^2\left(p_\tau(t),p_\tau(t+\delta t)\right)=2\Big[1-\sum_{i=1}^k r_i\left(p_i+\frac{1}{2}\dot{p}_i\delta t+\frac{1}{2}\ddot{p}_i\delta t^2-\frac{1}{8}\frac{\dot{p}_i^2}{p_i}\delta t^2\right)\Big]. \tag{3.48}$$

Using the condition $\sum_{i=1}^k r_i p_i=1$ we can infer that $\sum_{i=1}^k r_i\dot{p}_i=0$ and $\sum_{i=1}^k r_i\ddot{p}_i=0$. Applying these results in the expression above, we finally arrive at the Fisher-Rao metric

$$\left(ds_P^{\mathrm{Cl}}\right)^2=\frac{1}{4}\sum_{i=1}^k r_i\frac{\dot{p}_i^2}{p_i}\delta t^2=\frac{1}{4}\sum_{i=1}^k r_i\frac{dp_i^2}{p_i} \tag{3.49}$$

in terms of the probability distribution "coordinates" $\sqrt{\mathbf{p}}$.

Next, consider the case of a static classical part $\mathbf{p}(t)=\mathbf{p}$. The distance is then

$$d_\tau^2\left(p_\tau(t),p_\tau(t+\delta t)\right)=2\Big(1-\sum_{i=1}^k p_i\,\mathrm{Re}\,\mathrm{Tr}(w_i(t)^\dagger w_i(t+\delta t))\Big). \tag{3.50}$$

Expanding $w_i(t+\delta t)$ to second order $w_i(t+\delta t)\approx w_i(t)+\dot{w}_i(t)\delta t+\frac{1}{2}\ddot{w}_i(t)\delta t^2$ we have

$$\begin{aligned}\mathrm{Re}\,\mathrm{Tr}(w_i(t)^\dagger w_i(t+\delta t)) =& \mathrm{Re}\,\mathrm{Tr}(w_i^\dagger w_i)+\mathrm{Re}\,\mathrm{Tr}(w_i^\dagger\dot{w}_i)\delta t+\frac{1}{2}\mathrm{Re}\,\mathrm{Tr}(w_i^\dagger\ddot{w}_i)\delta t^2+r_i\\ &+\frac{1}{2}\mathrm{Tr}(w_i^\dagger\dot{w}_i+\dot{w}_i^\dagger w_i)\delta t+\frac{1}{4}\mathrm{Tr}(w_i^\dagger\ddot{w}_i+\ddot{w}_i^\dagger w_i)\delta t^2.\end{aligned} \tag{3.51}$$

From condition (3.25) for tangent vectors, the first order term is zero. From this same condition one can infer that $\ddot{w}_i^\dagger w_i+w_i^\dagger\ddot{w}_i=-2\dot{w}_i^\dagger\dot{w}_i$ and Eq. (3.51) becomes

$$\mathrm{Re}\,\mathrm{Tr}\left(w_i(t)^\dagger w_i(t+\delta t)\right)=r_i-\frac{1}{2}\mathrm{Tr}\left(\dot{w}_i^\dagger\dot{w}_i\right)\delta t^2. \tag{3.52}$$

Using this expression in Eq. (3.50) we get

$$d_\tau^2\big(p_\tau(t),\,p_\tau(t+\delta t)\big)=2\Big(1-\sum_{i=1}^k r_i p_i+\frac{1}{2}\sum_{i=1}^k p_i\,\mathrm{Tr}(\dot{w}_i^\dagger\dot{w}_i)\delta t^2\Big).$$

Since $\sum_{i=1}^k r_i p_i=1$, we have

$$\left(ds_{P_\tau}^{\mathrm{Q}}\right)^2=\sum_{i=1}^k p_i\,\mathrm{Tr}(\dot{w}_i^\dagger\dot{w}_i)\delta t^2=\sum_{i=1}^k p_i\,\mathrm{Tr}(dw_i^\dagger dw_i). \tag{3.53}$$

From the derivation of Eq. (3.44), it becomes clear that, restricting to the Horizontal subspaces, one obtains the induced quantum part of the metric in the Base space

$$\left(ds^{\mathrm{Q}}_{B_\tau}\right)^2 = \sum_{i=1}^{k} p_i \operatorname{Tr}\left(P_i dP_i dP_i\right). \tag{3.54}$$

So, the quantum part of the metric in the base space is the sum for $i \in \{1, ..., k\}$ of the metric on the Grassmannian given by Eq. (3.44) weighed by the relative proportions of the distribution p_i.

Finally, we are left with the task of taking a general variation, where both $\sqrt{\mathbf{p}}(t)$ and $\mathbf{w}(t)$ are non-constant, to make sure that we do not get cross terms. We have,

$$d^2_\tau\big(p_\tau(t), p_\tau(t+\delta t)\big) = 2\Big(1 - \sum_{i=1}^{k} \sqrt{p_i(t)p_i(t+\delta t)}\,\mathrm{Re}\operatorname{Tr}(w_i(t)^\dagger w_i(t+\delta t))\Big).$$

We can Taylor expand, as before, to obtain

$$d^2_\tau\big(p_\tau(t),\, p_\tau(t+\delta t)\big) = 2\Big[1 - \sum_{i=1}^{k} \Big(p_i + \frac{1}{2}\dot{p}_i\delta t + \frac{1}{2}\ddot{p}_i\delta t^2 - \frac{1}{8}\frac{\dot{p}_i^2}{p_i}\delta t^2\big(r_i - \frac{1}{2}\operatorname{Tr}(\dot{w}_i^\dagger \dot{w}_i)\delta t^2\big)\Big)\Big].$$

Collecting the terms up to second order we get

$$d^2_\tau\big(p_\tau(t), p_\tau(t+\delta t)\big) = 2\Big[1 - \sum_{i=1}^{k} \Big(p_i \operatorname{Tr}(\dot{w}_i^\dagger \dot{w}_i)\delta t^2 + \frac{1}{2}r_i\dot{p}_i\delta t + \frac{1}{2}r_i\ddot{p}_i\delta t^2 - \frac{1}{8}r_i\frac{\dot{p}_i^2}{p_i}\delta t^2\Big)\Big], \tag{3.55}$$

which, using the same arguments as before, reduces to

$$\begin{aligned} ds^2_{P_\tau} &= \sum_{i=1}^{k} \left(\frac{1}{4}r_i\frac{\dot{p}_i^2}{p_i}\delta t^2 + p_i \operatorname{Tr}(\dot{w}_i^\dagger \dot{w}_i)\delta t^2\right) \\ &= \sum_{i=1}^{k} \left(\frac{1}{4}r_i\frac{dp_i^2}{p_i} + p_i \operatorname{Tr}(dw_i^\dagger dw_i)\right). \end{aligned} \tag{3.56}$$

Hence, the metric in the principal bundle is just the sum of the respective classical and quantum metrics. We want to arrive at the metric for the base space: the classical probability distributions $\sqrt{p_i}$ have no gauge freedom so they have no vertical or horizontal components and their projection is trivial; meanwhile, the horizontal projection in the quantum part described by the amplitudes w_i proceeds as in the Stiefel manifold case, for each $i = 1, ..., k$, so that our final interferometric metric g_I is

$$\begin{aligned} g_I &= ds^2_{B_\tau} \qquad (3.57) \\ &= \left(ds^{\mathrm{Cl}}_{B_\tau}\right)^2 + \left(ds^{\mathrm{Q}}_{B_\tau}\right)^2 \\ &= \frac{1}{4}\sum_{i=1}^{k} r_i\frac{dp_i^2}{p_i} + \sum_{i=1}^{k} p_i \operatorname{Tr}\left(P_i dP_i dP_i\right). \end{aligned}$$

3.5 Interferometric measurement interpretation

Consider the following experiment depicted in FIG 3.1. 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 $\mathrm{pr}_0 = 1$.

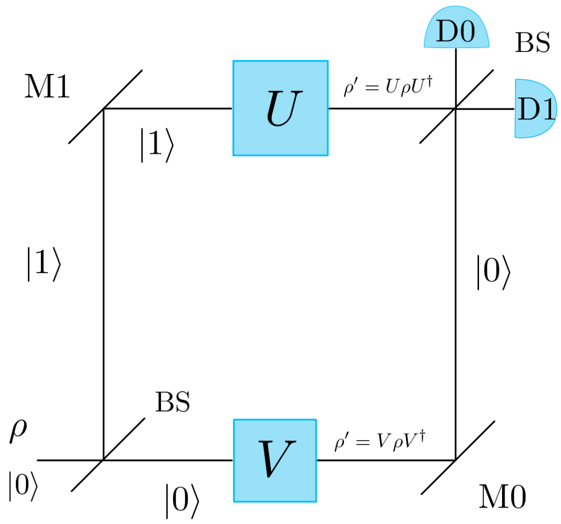


Figure 3.1: Interferometric measurement to probe the generalised metric g_I.

The input state is $|0\rangle\langle 0| \otimes \rho$. The first beam splitter $BS1 \otimes I$ acts on this state giving $\frac{1}{2}((|0\rangle + i|1\rangle)(\langle 0| - i\langle 1|) \otimes \rho$. The controlled unitary is $|0\rangle\langle 0| \otimes V + |1\rangle\langle 1| \otimes U$, which, when acting on the last state gives

$$\frac{1}{2}\Big(|0\rangle\langle 0| \otimes V\rho V^\dagger - i|0\rangle\langle 1| \otimes V\rho U^\dagger + i|1\rangle\langle 0| \otimes U\rho V^\dagger + |1\rangle\langle 1| \otimes U\rho U^\dagger\Big). \tag{3.58}$$

Upon passing through a second beam splitter and measuring the $|1\rangle$ state yields

$$\frac{1}{4}|1\rangle\langle 1| \otimes \Big[V\rho V^\dagger + V\rho U^\dagger + U\rho V^\dagger + U\rho U^\dagger\Big]. \tag{3.59}$$

Tracing out this quantity gives

$$\frac{1}{4}\left[\mathrm{Tr}\, U\rho U^\dagger + \mathrm{Tr}\, V\rho V^\dagger + 2\,\mathrm{Re}\,\mathrm{Tr}\, U\rho V^\dagger\right]. \tag{3.60}$$

We know that $\mathrm{Tr}\, U\rho U^\dagger = \mathrm{Tr}\, V\rho V^\dagger = 1$, hence

$$\frac{1}{2}\left[1 + \mathrm{Re}\,\mathrm{Tr}\, U\rho V^\dagger\right]. \tag{3.61}$$

Recall that $V = \sum_{i=0}^{k} P_i V P_i$, and that, since we can write in terms of a choice of amplitudes w_i, $i = 1, ..., k$,

$$P_i = w_i w_i^\dagger, \; i = 1, ..., k, \tag{3.62}$$

then,

$$V = P_0 V P_0 + \sum_{i=1}^{k} w_i V_i w_i^\dagger, \tag{3.63}$$

where $V_i = w_i^\dagger V w_i$ is an $r_i \times r_i$ unitary matrix, for $i = 1, ..., k$. Observe that

$$\begin{aligned} \mathrm{Tr}\left[V^\dagger U \rho\right] &= \sum_{i,j=0}^{k} p_i \,\mathrm{Tr}\left[P_j V^\dagger P_j U P_i\right] \\ &= \sum_{i=0}^{k} p_i \,\mathrm{Tr}\left[V^\dagger P_i U P_i\right], \end{aligned} \tag{3.64}$$

where in the last step we used the cyclic property of the trace and $P_i P_j = \delta_{ij} P_i$, $i, j = 0, ..., k$. Finally, introducing the expression for V of Eq. (3.63) we can write, using $w_i^\dagger w_i = I_{r_i}$, $i = 1, .., r_i$, and $p_0 = 0$,

$$\begin{aligned} \sum_{i=1}^{k} p_i \,\mathrm{Tr}\left[V^\dagger P_i U P_i\right] =& \sum_{i=1}^{k} p_i \,\mathrm{Tr}\left[(V_i^\dagger w_i^\dagger U) w_i\right] \\ &= \sum_{i=1}^{k} p_i \,\mathrm{Tr}\left[(U^\dagger w_i V_i)^\dagger w_i\right] \end{aligned} \tag{3.65}$$

observe that if we write

$$p_\tau = ((p_i, w_i))_{i=1}^{k} \text{ and } q_\tau = ((p_i, U^\dagger w_i V_i))_{i=1}^{k}, \tag{3.66}$$

then,

$$\sum_{i=1}^{k} p_i \,\mathrm{Tr}\left[V_i^\dagger w_i^\dagger U w_i\right] = \langle q_\tau, p_\tau \rangle_\tau, \tag{3.67}$$

where $\langle q_\tau, p_\tau \rangle$ is the Hermitian form defined in Eq. (3.11). Hence,

$$\begin{aligned} \mathrm{pr}_1 &= \frac{1}{2}\left(1 + \mathrm{Re}\,\mathrm{Tr}\, U \rho V^\dagger\right) \\ &= 1 - \frac{1}{2}\left(1 - \sum_{i=1}^{k} p_i \,\mathrm{Re}\,\mathrm{Tr}\left[P_i V^\dagger P_i U P_i\right]\right) \\ &= 1 - \frac{1}{2}\left(1 - \sum_{i=1}^{k} p_i \,\mathrm{Re}\langle q_\tau, p_\tau \rangle_\tau\right) \\ &= 1 - \frac{1}{4} d_\tau^2(q_\tau, p_\tau), \end{aligned} \tag{3.68}$$

where d_τ is the distance over the total space of the principal bundle $P_\tau \to B_\tau$. Maximizing over the the gauge degree of freedom given by the collection of unitary $r_i \times r_i$ matrices, V_i, $i = 1, ..., k$ (note that $P_0 V P_0$ is irrelevant), one gets the distance $d_I(\rho, U^\dagger \rho U)$. In general, we have that

$$\mathrm{pr}_1^{\max} = \max_{\{V_i\}}(\mathrm{pr}_1) = 1 - \frac{1}{4} d_I^2(\rho, \rho + \delta\rho), \tag{3.69}$$

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.

3.6 Interferometric metric in the context of band insulators

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

$$\mathcal{H}(M) = \int_{\mathrm{BZ}^d} \frac{d^d k}{(2\pi)^d}\ \psi_{\mathbf{k}}^\dagger d^\mu(\mathbf{k}; M) \sigma_\mu \psi_{\mathbf{k}}, \tag{3.70}$$

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 described in Sec. 3.3,

$$g = \frac{1}{4} \sum_i r_i \frac{dp_i^2}{p_i} + \sum_i p_i \operatorname{Tr}(P_i dP_i dP_i), \tag{3.71}$$

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

$$M \mapsto \rho(M) = Z^{-1} \exp(-\beta \mathcal{H}(M)), \tag{3.72}$$

with $\mathcal{H}(M)$ given by Eq. (3.70) and where Z is the partition function. The first thing to notice is that if $\rho = \rho_1 \otimes \rho_2$, with $\rho_\alpha = \sum_{i_\alpha} p_{i_\alpha} P_{i_\alpha}$, $\alpha = 1, 2$ we have the decomposition

$$\rho = \sum_I p_I P_I = \sum_{i_1, i_2} p_{i_1} p_{i_2} P_{i_1} \otimes P_{i_2}, \tag{3.73}$$

where $I = (i_1, i_2)$ is a multi-index describing the joint system labels. Note that,

$$\sum_{i_1, i_2} r_I \frac{dp_I^2}{p_I}$$

$$
\begin{aligned}
&= \sum_{i_1,i_2} \frac{r_{i_1} r_{i_2}}{p_{i_1} p_{i_2}} \left(p_{i_2}^2 dp_{i_1} dp_{i_1} + 2p_{i_1} p_{i_2} dp_{i_1} dp_{i_2} + p_{i_1}^2 dp_{i_2}^2\right) \\
&= \sum_{i_1} r_{i_1} \frac{dp_{i_1}^2}{p_{i_1}} + \sum_{i_2} r_{i_2} \frac{dp_{i_2}^2}{p_{i_2}},
\end{aligned} \tag{3.74}
$$

and

$$
\begin{aligned}
&\sum_I p_I \operatorname{Tr}\left(P_I dP_I dP_I\right) \\
&= \sum_{i_1,i_2} p_{i_1} \operatorname{Tr}\left[P_{i_1} \otimes P_{i_2} d\left(P_{i_1} \otimes P_{i_2}\right) d\left(P_{i_1} \otimes P_{i_2}\right)\right] \\
&= \sum_{i_1} p_{i_1} \operatorname{Tr}\left(P_{i_1} dP_{i_1} dP_{i_1}\right) + \sum_{i_2} p_{i_2} \operatorname{Tr}\left(P_{i_2} dP_{i_2} dP_{i_2}\right),
\end{aligned} \tag{3.75}
$$

where we used $PdPP = 0$ for any projector P. As a consequence, the interferometric metric, much like the Bures metric, converts tensor product states into orthogonal sum metrics.

Because the Hamiltonian is diagonal in momentum space, the density matrix factors over the momenta – it follows that the metric becomes an integral over the momentum space of individual contributions of each momentum sector. The pullback of the classical term, which also appears in the Bures metric,

$$
\frac{1}{4} \sum_i r_i \frac{dp_i^2}{p_i} \tag{3.76}
$$

was computed in the Appendix of Ref. [24] and it yields

$$
\frac{\beta^2}{4} \int_{\mathrm{BZ}^d} \frac{d^d k}{(2\pi)^d} \frac{1}{\cosh(\beta E(\mathbf{k}; M)) + 1} \left(\frac{\partial E(\mathbf{k}; M)}{\partial M}\right)^2 dM^2, \tag{3.77}
$$

where $E(\mathbf{k}; M) = |d(\mathbf{k}; M)|$ is the magnitude of $d(\mathbf{k}, M)$. With regards to the second term, one can use the mathematical fact that the embedding of the space of k-dimensional subspaces of $\mathbb{C}^N$, $\mathrm{Gr}_k(\mathbb{C}^N)$ on the space of 1-dimensional subspaces of the Fock space $\mathbb{P}\Lambda^* \mathbb{C}^N$, given by

$$
\operatorname{span}\{|1\rangle, ..., |k\rangle\} \mapsto \operatorname{span}\left\{c_1^\dagger ... c_k^\dagger |0\rangle\right\}, \tag{3.78}
$$

is isometric. In the previous equation $c_i^\dagger$ stand for creation operators for $|i\rangle$, i.e., at the single particle level, $c_i^\dagger |0\rangle = |i\rangle$, $i = 1, ..., k$. The embedding being isometric means, in this context, that if we write the rank k single-particle projector

$$
\widetilde{P} = \sum_{i=1}^{k} |i\rangle\langle i| \tag{3.79}
$$

and the rank 1 many-body projector

$$
P = c_1^\dagger ... c_k^\dagger |0\rangle\langle 0| c_k ... c_1, \tag{3.80}
$$

we have

$$\mathrm{Tr}\left(\widetilde{P}d\widetilde{P}d\widetilde{P}\right)=\mathrm{Tr}\left(PdPdP\right). \tag{3.81}$$

In particular, this means that in the gapped case for each $\mathbf{k}\in\mathrm{BZ}^d$ we will have four classes of orthogonal eigenstates,

$$|0\rangle,\ c^\dagger_{1,\mathbf{k}}|0\rangle,\ c^\dagger_{2,\mathbf{k}}|0\rangle, c^\dagger_{1,\mathbf{k}}c^\dagger_{2,\mathbf{k}}|0\rangle, \tag{3.82}$$

where $c^\dagger_{i,\mathbf{k}}$, $i=1,2$, are the Bogoliubov quasiparticle creation operators of $\mathcal{H}$ with energies $E(\mathbf{k};M)$ and $-E(\mathbf{k};M)$, respectively. The energies of the classes of eigenstates are, respectively, 0, $E(\mathbf{k};M)$, $-E(\mathbf{k};M)$ and 0. The associated single-particle 2×2 projectors are, respectively, the 0 projector, $P_1(\mathbf{k};M)=c^\dagger_{1,\mathbf{k}}|0\rangle\langle0|c_{1,\mathbf{k}}$, $P_2(\mathbf{k};M)=c^\dagger_{2,\mathbf{k}}|0\rangle\langle0|c_{2,\mathbf{k}}$ and the 2×2 identity matrix I_2. Only $P_1(\mathbf{k})$ and $P_2(\mathbf{k})$ are non-trivial and moreover, if we introduce the unit vector $n=d/|d|$, we can write,

$$\begin{aligned}
&P_1(\mathbf{k};M)=\frac{1}{2}\left(I_2+n^\mu(\mathbf{k};M)\sigma_\mu\right)\ \text{ and}\\
&P_2(\mathbf{k};M)=I_2-P_1(\mathbf{k};M).
\end{aligned} \tag{3.83}$$

As a consequence, using the identity $\mathrm{Tr}\left(PdPdP\right)=(1/2)\,\mathrm{Tr}\left(dPdP\right)$ and using the fact that the Pauli matrices are traceless, we get,

$$\begin{aligned}
\mathrm{Tr}\left(P_1dP_1dP_1\right)&=\mathrm{Tr}\left(P_2dP_2dP_2\right)\\
&=\frac{1}{4}\delta_{\mu\nu}\frac{\partial n^\mu(\mathbf{k};M)}{\partial M}\frac{\partial n^\nu(\mathbf{k};M)}{\partial M}dM^2.
\end{aligned} \tag{3.84}$$

Finally, taking into account the partition function factor $Z_{\mathbf{k}}=(2+2\cosh(\beta E(\mathbf{k};M)))$, we get that the quantum contribution is

$$\frac{1}{4}\int_{\mathrm{BZ}^d}\frac{d^dk}{(2\pi)^d}\left(\frac{\cosh(\beta E(\mathbf{k};M))}{1+\cosh(\beta E(\mathbf{k};M))}\right)\delta_{\mu\nu}\frac{\partial n^\mu(\mathbf{k};M)}{\partial M}\frac{\partial n^\nu(\mathbf{k};M)}{\partial M}dM^2. \tag{3.85}$$

Finally, we obtain,

$$g=\frac{1}{4}\int_{\mathrm{BZ}^d}\frac{d^dk}{(2\pi)^d}\Big[\frac{1}{\cosh(\beta E)+1}\left(\beta^2\left(\frac{\partial E}{\partial M}\right)^2+\cosh(\beta E)\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\right)\Big]dM^2, \tag{3.86}$$

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])

$$g_{\mathrm{Bures}}=\frac{1}{4}\int_{\mathrm{BZ}^d}\frac{d^dk}{(2\pi)^d}\Big[\frac{1}{\cosh(\beta E)+1}\beta^2\left(\frac{\partial E}{\partial M}\right)^2+\frac{\cosh(\beta E)-1}{\cosh(\beta E)}\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\Big]dM^2. \tag{3.87}$$

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,

$$g_0 = \frac{1}{4}\int_{\mathrm{BZ}^d} \frac{d^d k}{(2\pi)^d}\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}dM^2. \tag{3.88}$$

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

$$\frac{1}{2}\frac{1}{\cosh(x)} < \frac{1}{\cosh(x)+1} < \frac{1}{\cosh(x)}, \text{ for all } x \in \mathbb{R}, \tag{3.89}$$

we can write,

$$\begin{aligned}
&\frac{1}{\cosh(\beta E)+1}\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + \frac{\cosh(\beta E)-1}{\cosh(\beta E)}\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M} \\
&< \frac{1}{\cosh(\beta E)}\left[\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + \left(\cosh(\beta E)-1\right)\right)\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\right].
\end{aligned} \tag{3.90}$$

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

$$\frac{\beta^2}{\cosh(\beta E)}\delta_{\mu\nu}\frac{\partial d^\mu}{\partial M}\frac{\partial d^\nu}{\partial M}, \tag{3.91}$$

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

$$\frac{1}{\cosh(\beta E)+1}\Big(\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + \cosh(\beta E)\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}\Big), \tag{3.92}$$

near $E = 0$ gives us

$$\Big[\frac{1}{2} - \frac{1}{8}(\beta E)^2 + \mathrm{O}\left((\beta E)^4\right)\Big]\Big[\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + (1+\frac{1}{2}\beta^2 E^2)\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M} + \mathrm{O}\left((\beta E)^4\right)\Big]. \tag{3.93}$$

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

$$\frac{1}{2}\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M}, \tag{3.94}$$

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

$$\beta^2\left(\frac{\partial E}{\partial M}\right)^2 + \beta^2 E^2\delta_{\mu\nu}\frac{\partial n^\mu}{\partial M}\frac{\partial n^\nu}{\partial M} = \beta^2\delta_{\mu\nu}\frac{\partial d^\mu}{\partial M}\frac{\partial d^\nu}{\partial M}. \tag{3.95}$$

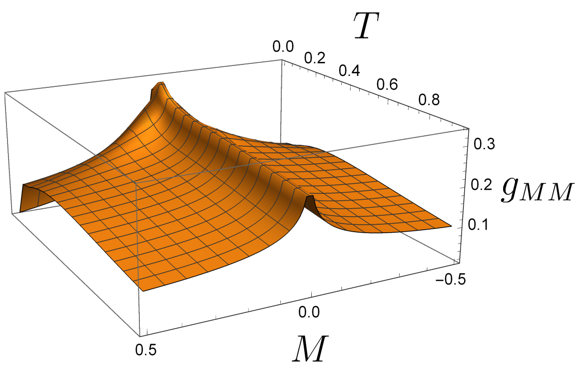
This implies that the limit $\beta \to \infty$ yields singular behaviour for g, provided the same happens with g_0. But not the other way around, i.e., singular behaviour on the finite temperature metric does not imply zero temperature singular behaviour. In other words, while in the case of the Bures 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.

3.6.1 Massive Dirac model

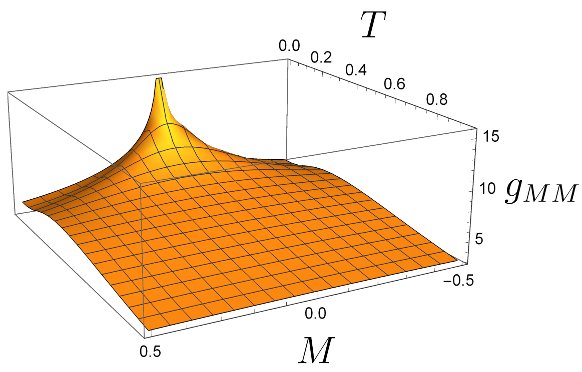
We consider the massive Dirac model, a band insulator in two spatial dimensions, described by Eq. (3.70), with

$$d(\mathbf{k}; M) = (\sin(k_x), \sin(k_y), M - \cos(k_x) - \cos(k_y)) \,, \tag{3.96}$$

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 [37]. We will focus at the one occurring at $M = 0$, where the Chern number goes from $+1$, for $M \to 0^-$, to -1, for $M \to 0^+$. The following two figures describe the inteferometric metric (Fig. 3.2(a)) and the Bures metric (Fig. 3.2(b)) in the thermodynamic limit.



(a)



(b)

Figure 3.2: (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.

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 behavior of the interferometric metric is indeed observable for macroscopic many-body systems is an open question. While the straightforward implementation of the interferometric experiment described in Sec. 3.5 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. [38]).

Chapter 4

Conclusions

4.1 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 analyzed 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 behavior 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 the Landau-Ginzburg theory. In our case, by fixing the type of the density matrix considered, a gauge group is broken down to a subgroup.

4.2 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 thesis. 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 [39]. 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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