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Geodesic paths and topological charges in quantum systems

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Dissertation

GEODESIC PATHS AND TOPOLOGICAL CHARGES
IN QUANTUM SYSTEMS

by

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“It is not the critic who counts;
not the man who points out how the strong man stumbles,
or where the doer of deeds could have done them better.
The credit belongs to the man who is actually in the arena,
whose face is marred by dust and sweat and blood;
who strives valiantly; who errs, who comes short again and again,
because there is no effort without error and shortcoming;
but who does actually strive to do the deeds;
who knows great enthusiasms, the great devotions;
who spends himself in a worthy cause;
who at the best knows in the end the triumph of high achievement,
and who at the worst, if he fails, at least fails while daring greatly,
so that his place shall never be with those cold and timid souls
who neither know victory nor defeat.”
—Theodore Roosevelt, The Man in the Arena
To my two mothers, Mariza and Yeda Souza, and my soulmate, Scarlett Sousa, with all my love and gratitude.
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Firstmost, I must thank my advisor, Professor Anatoli Polkovnikov, for without him this work would have never been possible. Apart from providing me with projects to work on and to learn from, I highly appreciate the freedom I have had to pursue my own ideas.

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To Michael Kolodrubetz, my first collaborator, I will forever be in debt for his ability
to make the right judgment call when the crucial moment arrived. I also learned a lot from him on how to network within the community, how scientific research is made, and most importantly in his keen ability to bridge theoretical ideas to experimentalist collaborators.

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To all the great friends I had the pleasure to make, thank you for changing me on the quest to become a better human being. Tadeusz Pudlik, I should thank you in every piece of scientific work I might ever write in this lifetime, and all the time we shared together was always naturally very special; Hila Hashemi, the sister life was hiding from me in Boston, if today I have faster reaction reflexes, it is only because I had the privilege to watch you
glide through much harder challenges time and time again; Hayk Yegoryan, the brother life was hiding from me in Boston, there are so many things I learned from you (e.g., writing a thesis...) and yet many others that will take a long time to hone and practice - you and Hila are deep sources of inspiration in my life, and I thank you both for always being here, wherever I am. Artur Domingues, the brother life gave me in Brazil, science is ever present in my life as consequence of the shared passion which initially was our bond as kids, moving forward to the longest brother-ship I have ever had. To my real, greatest brother, Fernando Jose, you are the sweetest brother one could ever wish to have, always so lovingly kind and considerate. Tamiro Villazon, you are the doppelgänger life was waiting to introduce me - we share so many passions, and I am honored to have met you in my life just...in...time. Erik Lascaris, I was so fortunate to have you by my side through all these years, sharing with you my “Boston home” for the longest time. You have always been an extremely kind and resourceful friend, and I thank you for always extending your helping hand when I needed without even blinking before saying yes. To my previous advisor, Ernesto Raposo, you will always be a great reference to me of what is the definition of a complete physicist - a person able to skillfully balance personal and professional life, while simultaneously keeping the beautiful mystery of what doing research in physics entails. Thank you for letting me live that perspective while I was under your guidance years ago, which directly and profoundly influenced my beliefs of what success is in the academic world.

My deepest gratitude to Paolinda Fiorella, for profoundly changing my life in its most crucial and decisive moment. My life would be radically different today if it were not for the lucky moment when I met her.

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Most especially, I would like to extend the biggest thank you ever to Jimin Guo, an outstanding human being who my guardian angel put on my path at the right moment and at the right place (...eh?). He took care of me for the past three months, opening his house and giving me shelter where I could comfortably stay, cheering me up at the right times, and giving me all the infrastructure I needed to write this thesis. I really could not have done without him, and he deserves a special place in this section. He taught me the main lesson of the year 2016: “if a problem can be solved with money, it is not a problem.”. I will be always in debt to him. But as he taught me, this is not a problem. Thank you, Jimin.

I dedicate this work to my two mothers, mother and grandmother, Mariza Souza and Yeda Souza (in memoriam) and to my soulmate, Scarlett Sousa. To my mother and grandmother, for raising me as a man of value: the fruits I am savoring today came from the seeds you both sowed throughout my lifetime, with love and dedication, and there are simply no words to express all my gratitude. You both are and will always be with me, as a simple consequence of all the values you taught me.

And to my bubble of joy, Scarlett Sousa, this achievement is ours. You helped me to get up and carry out the work that needed to be done, guided me to the right path whenever needed, gave me wisdom and courage in the moments of weakness, and on top of all that, you held yourself together during all this time. I realize how hard it was to endure my absence, all the highs and lows, and still give me the smile and happiness I needed to carry through. I could not have done it without you, and for that, I will always thank you with all my love.
GEODESIC PATHS AND TOPOLOGICAL CHARGES IN QUANTUM SYSTEMS

TIAGO AECIO GRANGEIRO SOUZA BARBOSA LIMA
Boston University Graduate School of Arts and Sciences, 2016
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ABSTRACT

This dissertation focuses on one question: how should one drive an experimentally prepared state of a generic quantum system into a different target-state, simultaneously minimizing energy dissipation and maximizing the fidelity between the target and evolved-states? We develop optimal adiabatic driving protocols for general quantum systems, and show that these are geodesic paths.

Geometric ideas have always played a fundamental role in the understanding and unification of physical phenomena, and the recent discovery of topological insulators has drawn great interest to topology from the field of condensed matter physics. Here, we discuss the quantum geometric tensor, a mathematical object that encodes geometrical and topological properties of a quantum system. It is related to the fidelity susceptibility (an important quantity regarding quantum phase transitions) and to the Berry curvature, which enables topological characterization through Berry phases.

A refined understanding of the interplay between geometry and topology in quantum mechanics is of direct relevance to several emergent technologies, such as quantum computers, quantum cryptography, and quantum sensors. As a demonstration of how powerful geometric and topological ideas can become when combined, we present the results of an experiment that we recently proposed. This experimental work was done at the Google Quantum Lab, where researchers were able to visualize the topological nature of a two-qubit system in sharp detail, a startling contrast with earlier methods. To achieve this feat, the optimal protocols described in this dissertation were used, allowing for a great...
improvement on the experimental apparatus, without the need for technical engineering
advances.

Expanding the existing literature on the quantum geometric tensor using notions from
differential geometry and topology, we build on the subject nowadays known as quantum
gometry. We discuss how slowly changing a parameter of a quantum system produces
a measurable output of its response, merely due to its geometric nature. Next, we topo-
logically characterize different classes of Hamiltonians using the Berry monopole charges,
and establish their topological protection. Finally, we explore how such knowledge allows
one to access topologically forbidden regions by adiabatically breaking and reestablishing
symmetries.
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<td>$A$</td>
<td>Berry connection</td>
</tr>
<tr>
<td>$\text{ch}_1$</td>
<td>First Chern number</td>
</tr>
<tr>
<td>$\mathbb{CP}$</td>
<td>Complex projective space</td>
</tr>
<tr>
<td>$d$</td>
<td>Exterior derivative operator</td>
</tr>
<tr>
<td>E&amp;M</td>
<td>Electromagnetism</td>
</tr>
<tr>
<td>$f$</td>
<td>Overlap (inner product) between quantum states</td>
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<tr>
<td>$F$</td>
<td>Fidelity</td>
</tr>
<tr>
<td>FS</td>
<td>Fubini-Study</td>
</tr>
<tr>
<td>g.s.</td>
<td>Ground-state</td>
</tr>
<tr>
<td>$\text{LZ}$</td>
<td>Landau-Zener</td>
</tr>
<tr>
<td>$\text{LZ-}\phi$</td>
<td>Landau-Zener with additional angular parameter $\phi$</td>
</tr>
<tr>
<td>$\mathcal{M}$</td>
<td>Parameter space manifold</td>
</tr>
<tr>
<td>$\mathcal{PH}$</td>
<td>Projective Hilbert Space</td>
</tr>
<tr>
<td>QGT</td>
<td>Quantum Geometric Tensor</td>
</tr>
<tr>
<td>QMT</td>
<td>Quantum Metric Tensor</td>
</tr>
<tr>
<td>$S^2$</td>
<td>2-Sphere</td>
</tr>
<tr>
<td>$\bigwedge$</td>
<td>Wedge Operator</td>
</tr>
<tr>
<td>$\Delta E$</td>
<td>Energy fluctuation</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Quantum Geometric Tensor</td>
</tr>
<tr>
<td>$\bar{x}$</td>
<td>Fubini-Study metric</td>
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Chapter 1

Introduction

Some people say, “How can you live without knowing?” I do not know what they mean. I always live without knowing. That is easy. How you get to know is what I want to know.

– Richard. P. Feynman, in The Meaning of It All

1.1 The Quest for Quantum Optimal Control

Consider the situation where one wants to make measurements involving the time evolved ground-state\(^1\) of a quantum system, the target state, with the goal of studying its properties. Due to experimental constraints, however, the experimentalist is only able to accurately prepare the ground-state for particular initial values of the system parameters. Examples are initial conditions involving a high-degree of symmetry, as zero external magnetic fields, or zero couplings between the parts of the system.

After initializing under these settings, the experimentalist next switches and/or changes a certain number of the system’s couplings, parameter of which it depends. Such procedure evolves the readily available prepared state into the desired target state. The final evolved state is then used to perform the necessary quantum manipulations.

\(^1\)The choice for the ground-state here is merely illustrative – the arguments put forth in what follows applies for any other eigenstate as well. We mainly refer to the ground-state in the remainder of this thesis, but the previous observation should be kept in mind throughout.
This thesis addresses the question of how to perform the above described procedure adiabatically in order to achieve a high degree of similarity (referred as \textit{fidelity}) between the evolved and target states, thus reducing the effects of external noise and circumventing decoherence. We develop optimal adiabatic driving protocols for quantum systems which minimize and keep the energy fluctuation of the system constant along the entire evolution path, simultaneously maximizing the fidelity locally between its evolved and target states. These protocols are shown to be \textit{geodesic paths}.

\subsection*{1.1.1 Examples of Applicability}

Knowledge of optimal ways to accurately prepare quantum states is a fundamental requirement for the realization of many emergent technologies, with immediate repercussions:

\textbf{Quantum Computation:} The most prominent one is for \textit{adiabatic quantum computation} (Nielsen and Chuang, 2000). It often is viable to experimentally prepare the ground-state of a simpler Hamiltonian $\hat{H}_0$, but instead it is the ground-state of a convoluted Hamiltonian $\hat{H}_f$ that encodes the solution of a hard computational problem. One can experimentally interpolate between these two Hamiltonians by defining $\lambda(t) = \frac{t}{t_f}$ and writing

$$\hat{H} = (1 - \lambda) \hat{H}_0 + \lambda \hat{H}_f,$$

effectively yielding a generic scheme for a working quantum computer (Farhi et al., 2001).

The $\lambda(t)$ protocol defined above is a simple but not necessarily optimal way to interpolate the two Hamiltonians. Finding an optimal protocol for such interpolations can have broad consequences on the future engineering of quantum computation.

\textbf{Quantum Phase Transitions:} It also is important on the study of quantum phase transitions. The experimental protocol commonly used nowadays is the same as delineated in the previous section. A famous recent example is the observation of the paradigmatic superfluid-Mott insulator transition in cold atoms (Greiner et al., 2002).
**Geometrical and Topological Properties of Quantum Systems:** Finally, it is of fundamental importance for the study of geometrical and topological properties of quantum eigenstates manifolds. A refined understanding will enable advances in quantum metrology, and in measurements of Chern numbers and complex phase diagrams (Schroer et al., 2014; Roushan et al., 2014). Other examples of impact are in quantum sensors (Schirhagl et al., 2014; Ivanov et al., 2015), quantum cryptography (Ekert, 1991), and quantum simulators (Feynman, 1982; Baumann et al., 2010; Blatt and Roos, 2012; Islam et al., 2013).

The field of quantum optimal control (Walmsley and Rabitz, 2003; D’Alessandro, 2007) provides powerful methods, which have been implemented in cold atomic systems (Chu, 2002), atom chips (Lovecchio et al., 2016), superconducting quantum circuits (Huang and Goan, 2014) and in adiabatic quantum computation (Farhi et al., 2001).

One of the major constraints in quantum experiments is time: each apparatus is only able to keep coherence for a set period. For small quantum systems, it is possible to develop arbitrarily fast protocols with a perfect fidelity between the evolved and target states. The important question still remains on how to extend these protocols for many-body quantum systems. Optimal control algorithms for quantum many-body systems have recently been developed (Doria et al., 2011; Rahmani and Chamon, 2011), but the ideas are model specific. So far, attempts have relied on brute-force techniques, or have been based on *ansatzes*, thus tied to specific systems where they work well. Those can broadly be characterized as unstructured methods. A general, well-prescribed and robust approach to optimal control for many-body quantum systems has so far been lacking.

Recently, basic research on quantum mechanics has seen a burst of ideas coming from differential geometry and topology (Zanardi et al., 2007; Gritsev and Polkovnikov, 2012; Kolodrubetz et al., 2013). The necessary tool to address the aforementioned quest is the quantum geometric tensor (QGT), a mathematical object that encodes geometrical and topological properties of a quantum system. It is related to the fidelity susceptibility (an important quantity regarding quantum phase transitions) and to the Berry curvature, which enables topological characterization through Berry phases.
Figure 1.1: Left: Parameter space manifold, \( \mathcal{M} \): the \( xy \)-axes represent two tunable parameters in the system, \( \lambda^1 \) and \( \lambda^2 \). The \( z \)-axis corresponds to the squared energy fluctuation, \( \Delta E^2 \). The optimal adiabatic path from \( i \) to \( f \) is a minimal level curve on \( \mathcal{M} \) (red). A linear path (green) increases the squared energy fluctuation, thereby increasing the probability of excitations and decreasing the fidelity along the path (consequently with the target state). Right: The linear and geodesic paths projected on a two dimensional plane. For a constrained amount of time, the projected curves erroneously suggest that a linear path is preferable for adiabatic evolution.

The goal in this thesis is to systematically explore the properties, applicability, limits of validity, and experimental constraints of such approach. We thus show how it addresses the following question: “After preparing the initial state of an experimentally accessible Hamiltonian, how should one drive it to a different final Hamiltonian in order to simultaneously maximize the fidelity and minimize the energy fluctuation along the entire driven path?”

1.2 Geodesic Paths in Quantum Systems

Let us consider the scenario where no knowledge is available on the location of degeneracies in a certain region of the parameter space \( \mathcal{M} \). An experimentalist wants to go from the accessible initial state \( i \) to a generic final one \( f \), both represented as points on \( \mathcal{M} \), with very
limited knowledge of the system’s Hamiltonian.

What is be the best strategy to drive the system connecting these two points? With limited knowledge of the Hamiltonian, a good strategy is to find a path that minimizes and keeps constant the energy fluctuations of the quantum system along its entire adiabatic evolution. The motivation for such strategy lies on the fact that energy fluctuations increase the likelihood of excitations. The idea is illustrated in Figure 1.1: in the landscape defined by the squared energy fluctuations of a quantum system, \[ \Delta E^2 = \langle \Psi_0 | \hat{H}^2 | \Psi_0 \rangle - \langle \Psi_0 | \hat{H} | \Psi_0 \rangle^2, \]
given a starting point i, remaining on the same level while evolving to the final target point f maintains \( \Delta E^2 \) minimal and stationary (constant) along the evolution. The path taken (shown in red) might mislead one’s intuition when projected down on a two dimensional plot, as it does not seem to correspond to the shortest path between the initial and final points (shown in green). But in reality, a straight path when seen in the parameter space manifold \( M \) might highly increase the energy fluctuations along the evolution, thereby introducing excitations and compromising the evolved state to remain adiabatically connected throughout the path (Figure 1.1). In sum, by remaining always adiabatically close to the

![Figure 1.2: Evolution of a quantum system (hyperbloch spheres) along the geodesic path in the parameter space \( M \). The curvature of \( M \) is given by the square of energy fluctuations \( \Delta E^2 \). The geodesic path is the leveled trajectory connecting \( A \) and \( C \), corresponding to a stationary value for \( \Delta E^2 \).](image-url)
path of constant $\Delta E^2$ for given initial and final conditions, a good overlap between the instantaneous eigenstate and the evolved state is attained at every point along the way. Schematically, as the system travels along the path, its instantaneous ground-state at every point can be represented by a hyperbloch sphere (Figure 1.2), and the above procedure evolves the system maintaining the overlap of the evolved and target states maximized at all times.

Minimizing the energy fluctuation allows one to define a cost function, specified by the metric defining the landscape, and minimizing this cost function gives the geodesic paths, essentially the shortest path in terms of energy fluctuation and local fidelity.

1.3 Topological Applications

Of particular interest are novel ways to obtain topological information of a quantum system. We also discuss how geodesic ramping allows for a better adiabatic exploration of quantum systems, and consequently the gathering of their topological properties.

Interestingly, the mathematical tools needed to explore geometry and topology topics are interlinked. For the former, we develop notions of quantum geometry, derived from the fact that the Hilbert space is a metric system, as it has a well-defined inner product. The fact that the Hilbert space is a complex vector space ties its geometrical and topological properties. The inner product defines a complex tensor, known as the Quantum Geometric Tensor (QGT) (Provost and Vallee, 1980). This tensor has both a real part, a Riemannian metric structuring the Hilbert Space, and also an imaginary part, the Berry curvature field describing the topology of the system.

In what follows, we develop the necessary mathematical tools to explore both the geometric and topological properties of quantum systems. Those allow for the development of optimal adiabatic protocols and a better exploration of topological ideas. Finally, we present experimental realizations of the approach hereby developed, showing a considerably more refined experimental resolution achieved merely by using the fostered knowledge on the fundamentals of geometry and topology applied to basic quantum mechanics.
Chapter 2

Quantum Metric Tensor: defining distance in quantum systems

Philosophy is written in this grand book – I mean the universe – which stands continually open to our gaze, but it cannot be understood unless one first learns to comprehend the language in which it is written. It is written in the language of mathematics, and its characters are triangles, circles, and other geometric figures, without which it is humanly impossible to understand a single word of it; without these, one is wandering about in a dark labyrinth.

– Galileo Galilei, in The Assayer

In this chapter, we aim to address the following question: after preparing an initial eigenstate of an experimentally accessible Hamiltonian $\hat{H}_i$, how should one drive it to a final target eigenstate of the Hamiltonian $\hat{H}_f$ simultaneously extremizing the fidelity $F$ and energy fluctuation $\Delta E$ of the driven-state at all times? We develop an optimal adiabatic driving protocol for quantum systems where the optimal paths are given by geodesic curves.

2.1 Introduction

The manifestation of geometry in quantum systems evolving adiabatically was first described by M. V. Berry (Berry, 1984). In this reference, he showed that an eigenstate
accumulates a phase factor when the parameters of the quantum system are varied adiabatically along a closed path in parameter space. The phase factor is given by the sum of a dynamical phase (the time integral of the energy) and an additional phase with one remarkable geometric property: its value depends only on the path taken in parameter space, but not on the (adiabatic) rate of evolution. Nowadays, this additional phase is known in the literature as the Berry or geometric phase. Soon after its discovery, many surprising applications of the geometric phase were carried over into various branches of physics: the Aharonov-Bohm effect (Berry, 1984; Aharonov and Anandan, 1987), quantized transport (Thouless, 1983; Niu, 1990), the quantum Hall effect (Thouless et al., 1982; Xiao et al., 2010), anomalies in quantum field theories (Fujikawa, 2006), the advent of high-precision quantum measurements (Roos et al., 2006; Filipp et al., 2009; Martin-Martinez et al., 2013) and adiabatic quantum computation (Jones et al., 2000).

In the past two decades, the use of geometrical and topological ideas to better understand fundamental aspects of quantum mechanics has culminated with the definition of the quantum geometric tensor (QGT) (Provost and Vallee, 1980). Many subsequent works have analyzed old and predicted new phenomena based on the behavior of the QGT (Zanardi et al., 2007; Gritsev and Polkovnikov, 2012; Avron et al., 2011; Schroer et al., 2014; Roushan et al., 2014).

### 2.2 Quantum Metric Space – Preliminaries

Consider a quantum system given by a Hamiltonian $\hat{H}$ with $N$ variable parameters $\lambda^\mu$ ($\mu = 1, \ldots, N$), i.e., $\hat{H} \equiv \hat{H}(\lambda^1, \ldots, \lambda^N) = \hat{H}(\vec{\lambda})$. The set $\{\lambda^\mu\}$ defines the parameter space $\mathcal{M}$, a $N$-dimensional manifold. Let $\mathcal{H}$ denote the Hilbert space of the quantum system and $|\Psi_n⟩ \in \mathcal{H}$ its $n$–th eigenstate$^1$. A natural map $s$ exists from the parameter space $\mathcal{M}$ to the Hilbert space $\mathcal{H}$, namely $s : \mathcal{M} \to \mathcal{H}$, $\vec{\lambda} \to |\Psi_n(\vec{\lambda})⟩$. The formalism and results here developed are general for all eigenstates, but for the sake of notational simplicity, from now on we restrict our focus to the ground-state $|\Psi_0⟩$.

$^1$We assume there are no degeneracies, for simplicity.
For an infinitesimal parameter variation $\bar{\lambda} \rightarrow \bar{\lambda} + \delta \bar{\lambda}$, we calculate the overlap $f$ between the eigenstates $|\Psi_0(\bar{\lambda})\rangle \equiv |\psi\rangle$ and $|\Psi_0(\bar{\lambda} + \delta \bar{\lambda})\rangle \equiv |\psi + \delta \psi\rangle$,

$$f(\psi, \psi + \delta \psi) \equiv |\langle \psi | \psi + \delta \psi \rangle| \ ,$$

(2.1)

with $||\psi|| = ||\psi + \delta \psi|| = 1$. The functional $f$ defines the Fubini-Study distance, $d_{FS} \equiv \arccos[f(\psi, \psi + \delta \psi)]$ (Zanardi et al., 2007). Since $\delta \psi$ is infinitesimally small, $f$ is very close to unit, and we write $d_{FS}^2 = 2 (1 - f)$. Expanding $f(\psi, \psi + \delta \psi) \simeq |\langle \psi | \psi \rangle + \langle \psi | \delta \psi \rangle + (1/2)\langle \psi | \delta \psi^2 \rangle|$, $d_{FS}^2(\psi, \psi + \delta \psi) = \langle \delta \psi | \delta \psi \rangle - |\langle \psi | \delta \psi \rangle|^2$.

(2.2)

Writing $\delta |\Psi_0(\bar{\lambda})\rangle = \sum_\mu |\partial_\mu \Psi_0\rangle d\lambda^\mu$ with $\partial_\mu \equiv \partial/\partial \lambda^\mu$ ($\mu = 1, \ldots, \text{dim } \mathcal{M}$) and substituting in Eq. (2.2), one gets the formal expression for a Riemannian metric $g_{\mu\nu}$ on the parameter manifold $\mathcal{M}$,

$$ds^2 = \sum_{\mu\nu} \text{Re} \left[ \langle \partial_\mu \Psi_0 | \partial_\nu \Psi_0 \rangle - \langle \partial_\mu \Psi_0 | \Psi_0 \rangle \langle \Psi_0 | \partial_\nu \Psi_0 \rangle \right] d\lambda^\mu d\lambda^\nu$$

(2.3)

where,

$$g_{\mu\nu} \equiv \text{Re} \left[ \langle \partial_\mu \Psi_0 | \partial_\nu \Psi_0 \rangle - \langle \partial_\mu \Psi_0 | \Psi_0 \rangle \langle \Psi_0 | \partial_\nu \Psi_0 \rangle \right] .$$

(2.4)

The Riemannian metric tensor $g_{\mu\nu}$ is the quantum metric tensor (QMT), symmetric under exchange of indexes $\mu$ and $\nu$. The QMT is the real (symmetric) part of the complex quantum geometric tensor $\chi_{\mu\nu}$.

### 2.3 Quantum Geometric Tensor

The quantum geometric tensor was introduced by Provost and Vallee (Provost and Vallee, 1980), but the term itself first appeared in a work from M. Berry (Berry, 1989). For the ground-state $|\Psi_0\rangle$ of a generic quantum system, it is given by

$$\chi_{\mu\nu} \equiv \langle \Psi_0 | \partial_\mu \hat{H} | \partial_\nu \Psi_0 \rangle - \langle \Psi_0 | \partial_\mu | \Psi_0 \rangle \langle \Psi_0 | \partial_\nu | \Psi_0 \rangle$$

(2.5)

Alternatively, it can also be expressed as

$$\chi_{\mu\nu} = \sum_{m \neq 0} \frac{\langle \Psi_0 | \partial_\mu \hat{H} | \Psi_m \rangle \langle \Psi_m | \partial_\nu \hat{H} | \Psi_0 \rangle}{(E_0 - E_m)^2} ,$$

(2.6)
by using the resolution of identity $\sum_m |\Psi_m\rangle\langle \Psi_m| = \hat{1}$ in the first term of Eq. (2.5), followed by the relation $\langle \Psi_m | \partial_\mu \hat{H} | \Psi_n \rangle = (E_n - E_m) / (E_n - E_m)$, valid for $m \neq n$ (see Appendix D for details).

We note that for two-level systems $\{ |\Psi_0\rangle, |\Psi_1\rangle \}$, the quantum geometric tensor is given by

$$\chi_{\mu\nu} = \langle \Psi_0 | \partial_\mu | \Psi_1 \rangle \langle \Psi_1 | \partial_\nu | \Psi_0 \rangle .$$  \hspace{1cm} (2.7)

### 2.3.1 Quantum Metric Tensor

The symmetric part of the quantum geometric tensor

$$g_{\mu\nu} \equiv \chi_{\mu\nu} + \chi_{\nu\mu} \frac{2}{2} = \text{Re}(\chi_{\mu\nu}) ,$$  \hspace{1cm} (2.8)

corresponds to the previously introduced quantum metric tensor (Equation (2.4)). It defines a Riemannian metric in the parameter space $\mathcal{M}$ with local coordinates $\{ \lambda^\mu \}$, and consequently a measure of distances between different ground-states, identified as points in $\mathcal{M}$. The distance $ds$ between two ground-states differing by an infinitesimal variation of parameters $\vec{\lambda} \in \mathcal{M}$ is given by

$$ds^2 = g_{\mu\nu} d\lambda^\mu d\lambda^\nu ,$$  \hspace{1cm} (2.9)

where Einstein summation convention over repeated indices is implied.

### 2.3.2 Berry curvature

The anti-symmetric part of the QGT defines the Berry curvature

$$F_{\mu\nu} \equiv i(\chi_{\mu\nu} - \chi_{\nu\mu}) = -2 \text{Im}(\chi_{\mu\nu}) ,$$  \hspace{1cm} (2.10)

a symplectic two-form which gives rise to the Berry phase and the topological invariant Chern number. We discuss the Berry curvature in depth in Chapter 4.
Figure 2.1: *Left:* Parameter space $\mathcal{M}$ in local coordinates $\{\lambda^\mu\}$. *Right:* Hilbert space $\mathbb{C}P^m$ with an illustrative line representing the ground state $|\Psi_0\rangle$ image as function of $\vec{\lambda}$ on a given path. The map $s : \mathcal{M} \to \mathbb{C}P^m$, $s(\lambda) = |\Psi_0(\lambda)\rangle$ connects both spaces. As $\mathbb{C}P^m$ possesses the complex Fubini-Study metric $\bar{\chi}$, the pullback $s^*$ endows $\mathcal{M}$ with the structure of a complex manifold, with the *quantum geometric tensor* $\chi$ as its Kähler metric.

### 2.3.3 Quantum Geometric Tensor as Sum of the Quantum Metric Tensor and the Berry Curvature

The QGT is thus written as

$$\chi_{\mu\nu} = g_{\mu\nu} - i \frac{1}{2} F_{\mu\nu}. \quad (2.11)$$

It is the pullback $s^*\bar{\chi} \equiv \chi$ of the Fubini-Study metric\(^2\) $\bar{\chi}$ on $\mathbb{C}P^m$ by the map $s : \mathcal{M} \to \mathbb{C}P^m$, $s(\lambda) = |\Psi_0(\lambda)\rangle$, and seen as a Kähler metric\(^3\) on the parameter manifold $\mathcal{M}$, thus endowed with a natural Riemannian metric $g_{\mu\nu}$ and a sympletic two-form $F_{\mu\nu}$ (see Figure 2.1).

### 2.4 Quantum Optimal Control: Local Fidelity

The measure of optimality we have chosen is the fidelity $\mathcal{F}$, a quantifier of the similarity between the evolved state and the exact ground-state at a value for the parameters $\lambda = \lambda(t)$,

$$\mathcal{F}(\lambda(t)) = |\langle \Psi(\lambda(t)) | \Psi_0(\lambda) \rangle|^2 = |\langle \Psi(\lambda) | \Psi_0(\lambda) \rangle|^2. \quad (2.12)$$

\(^2\) $\bar{\chi} \equiv f$, Eq. (2.1).

\(^3\) The metric of a complex manifold (e.g., the Hilbert space) is called a Kähler metric.
It is equal to the absolute value squared of the overlap \( f \) between the exact ground-state at \( \lambda, |\Psi_0(\lambda)\rangle \), and the time-evolved state from \( \lambda(0) = \lambda_i \) to \( \lambda(t), |\Psi(\lambda(t))\rangle \),

\[ f = \langle \Psi(\lambda(t)) | \Psi_0(\lambda) \rangle . \]  

(2.13)

Observe this is a different goal than considering as a measure of optimality the fidelity measured solely at the target-state (i.e., at the final evolution time \( t_f \)). Here, instead, we consider adiabatic protocols maximizing the fidelity at every infinitesimal time step along the evolution. As we present in the next few sections, these are obtained by making use of Variational Calculus techniques, where solving the corresponding Euler-Lagrange equations yields geodesic paths maximizing the local fidelity defined by Equation 2.12 (see Section 2.5 and Chapter 3 for more details).

**Log–Fidelity**

A useful way to express the fidelity is by making use of the logarithm function. Comparing Eqs. (2.9) and (2.2), one can write

\[ g_{\mu \nu} d\lambda^\mu d\lambda^\nu = 1 - |\langle \delta \Psi | \Psi \rangle|^2 \equiv 1 - \mathcal{F} , \]  

(2.14)

from which we derive

\[ \log(\mathcal{F}) = \log(1 - g_{\mu \nu} d\lambda^\mu d\lambda^\nu) = -g_{\mu \nu} d\lambda^\mu d\lambda^\nu , \]  

(2.15)

where the Taylor expansion of the logarithmic function was used in the last equality. Thus,

\[ -\log(\mathcal{F}) = g_{\mu \nu} d\lambda^\mu d\lambda^\nu = ds^2 . \]  

(2.16)

For infinitesimal displacements, \(-\log(\mathcal{F})\) gives a distance measure between infinitesimally close ground-states.

The main advantage of expressing the line-element in this way lies on the fact that fidelity is bounded, \( 0 \leq \mathcal{F} \leq 1 \), and \(-\log(x)\) behaves as a monotonically increasing function when plotted versus the reciprocal of the final time, lying in the interval \( 1 \leq -\log(x) < \infty \). This allows for a more refined graphical reading of fidelity plots, as presented in the next section.
2.5 Geodesic Paths in Parameter Space

With a Riemannian metric $g_{\mu\nu}$ defined in the parameter space $\mathcal{M}$, one can calculate critical curves between initial and final distinct points. These are geodesic paths, satisfying the well-known geodesic equations,

$$\ddot{\lambda}^\mu + \Gamma^\mu_{\nu\rho} \dot{\lambda}^\nu \dot{\lambda}^\rho = 0, \quad (2.17)$$

where $\Gamma^\mu_{\nu\rho}$ are the Christoffel symbols of the second kind, defined by

$$\Gamma^\mu_{\nu\rho} = \frac{1}{2} g^{\mu \xi} \left( \partial_\rho g_{\xi \nu} + \partial_\nu g_{\xi \rho} - \partial_\xi g_{\nu \rho} \right), \quad \text{with } \partial_\mu \equiv \partial / \partial \lambda^\mu, \quad g_{\mu\nu} = (g^{\mu\nu})^{-1}, \quad (2.18)$$

and the following quantity must be stationary along the path (Kolodrubetz et al., 2013; Tomka et al., 2016),

$$g_{\mu\nu} \dot{\lambda}^\mu \dot{\lambda}^\nu = \text{const.} \equiv \Delta E^2, \quad (2.19)$$

where $\Delta E^2$ is the energy fluctuation squared, given by

$$\Delta E^2 = \langle \Psi_0(\lambda) | (\hat{H}(\lambda))^2 | \Psi_0(\lambda) \rangle - \langle \Psi_0(\lambda) | \hat{H}(\lambda) | \Psi_0(\lambda) \rangle^2. \quad (2.20)$$

We detailedy discuss these results in Chapter 3. For now, let us exemplify the usage of the mathematical machinery above by applying it to different quantum systems and analyzing the interesting physical consequences.

2.5.1 Example I – Geodesics for One $1/2$–Spin Particle in an External Magnetic Field

Consider the quantum system defined by a $1/2$–spin particle (a quantum bit, or "qubit") in the presence of an external time-dependent magnetic field $\vec{B}(t)$ with magnitude $B \equiv |\vec{B}|$,

$$\vec{B}(t) = (B_x(t), B_y(t), B_z(t))^T \equiv B (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T. \quad (2.21)$$

The external field $\vec{B}$ couples with the spin, such that the Hamiltonian of the system reads

$$\hat{H}_{qb}(t) \equiv \vec{B}(t) \cdot \vec{\sigma} = B_x \hat{\sigma}_x + B_y \hat{\sigma}_y + B_z \hat{\sigma}_z$$

$$= B (\sin \theta \cos \phi \hat{\sigma}_x + \sin \theta \sin \phi \hat{\sigma}_y + \cos \theta \hat{\sigma}_z), \quad (2.22)$$
where \( \vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)^T \) are the usual Pauli matrices,

\[
\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

The Hamiltonian written in matrix form is

\[
\hat{H}_{qb}(B_x, B_y, B_z) = \begin{pmatrix} B_z & B_z - iB_y \\ B_z + iB_y & -B_z \end{pmatrix},
\]

\[
\hat{H}_{qb}(B, \theta, \phi) = \begin{pmatrix} B \cos \theta & e^{-i\phi} B \sin \theta \\ B \sin \theta e^{i\phi} & -B \cos \theta \end{pmatrix}, \quad \hat{H}_{qb}(B_\perp, B_\parallel, \phi) = \begin{pmatrix} B_\parallel & B_\perp e^{-i\phi} \\ B_\perp e^{i\phi} & -B_\parallel \end{pmatrix},
\]

where we used the following equalities relating cartesian \((B_x, B_y, B_z)\), cylindrical \((B_\perp, B_\parallel, \phi)\) and spherical \((B, \theta, \phi)\) coordinates,

\[
B_z = B \cos \theta \equiv B_\parallel,
\]

\[
B_x \pm i B_y = B \sin \theta \left( \cos \phi \pm i \sin \phi \right) = B \sin \theta e^{\pm i\phi} \equiv B_\perp e^{\pm i\phi}.
\]

**Eigenenergies and Eigenstates**

The eigenstates of \( \hat{H}_{qb} \), written on the eigenstate basis of \( \hat{\sigma}_z \), \(|\uparrow\rangle = (1, 0)^T\) and \(|\downarrow\rangle = (0, 1)^T\), are

\[
|\Psi_{0,1}\rangle = \mp \frac{B \mp B_z}{\sqrt{2B(B \pm B_z)}} |\uparrow\rangle + \frac{B_x \mp i B_y}{\sqrt{2B(B \pm B_z)}} |\downarrow\rangle,
\]

or, equivalently,

\[
|\Psi_{0,1}\rangle = \mp \frac{B \mp B_\parallel}{\sqrt{2B(B \mp B_\parallel)}} |\uparrow\rangle + \frac{B_\perp}{\sqrt{2B(B \mp B_\parallel)}} e^{i\phi} |\downarrow\rangle.
\]

In spherical coordinates, the eigenstates of (2.22) take a simpler form,

\[
|\Psi_0\rangle = -\sin \frac{\theta}{2} |\uparrow\rangle + \cos \frac{\theta}{2} e^{i\phi} |\downarrow\rangle, \quad |\Psi_1\rangle = \cos \frac{\theta}{2} |\uparrow\rangle + \sin \frac{\theta}{2} e^{i\phi} |\downarrow\rangle.
\]

The corresponding eigenenergies are \( E_{0,1} = \mp B = \mp \sqrt{B_x^2 + B_y^2 + B_z^2} = \mp \sqrt{B_\perp^2 + B_\parallel^2} \).
Quantum Geometric Tensor for One 1/2–Spin Particle in an External Magnetic Field

Equation (2.7) gives the QGT for a two-level quantum system. We use the eigenstates written in spherical coordinates (Eq. (2.28)) to calculate the matrix elements \( \langle \Psi_0 | \partial_\mu | \Psi_1 \rangle \) and \( \langle \Psi_1 | \partial_\nu | \Psi_0 \rangle \), with \{\mu, \nu\} \in \{B, \theta, \phi\}. The derivatives with respect to \( B \) vanish as the eigenstates do not depend on it. The QGT for the system in consideration is equal to

\[
\chi_{\mu\nu} = \frac{1}{4} \begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & i \sin \theta \\
0 & -i \sin \theta & \sin^2 \theta
\end{pmatrix},
\]

and the metric tensor reads

\[
g_{\mu\nu} \equiv \text{Re}(\chi_{\mu\nu}) = \frac{1}{4} \begin{pmatrix}
0 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & \sin^2 \theta
\end{pmatrix}.
\]

The matrix element \( g_{BB} \) vanishes, which means that the distance between two states lying on the same line passing through \( \vec{B} = 0 \) is zero.

Let us restrict ourselves to the case of a magnetic field with constant magnitude \( B = c \), such that \( \mu, \nu = (\theta, \phi) \) (with the index correspondence \( 1 = \theta, 2 = \phi \)); the metric and its inverse are given by

\[
g_{\mu\nu} = \frac{1}{4} \begin{pmatrix}
1 & 0 \\
0 & \sin^2 \theta
\end{pmatrix} \quad \Rightarrow \quad g^{\mu\nu} = (g_{\mu\nu})^{-1} = 4 \begin{pmatrix}
1 & 0 \\
0 & \frac{1}{\sin^2 \theta}
\end{pmatrix}.
\]

The non-vanishing Christoffel symbols of the second kind \( \Gamma^\mu_{\nu\rho} \) for the present example are equal to

\[
\Gamma^1_{22} = -\cos \theta \sin \theta, \quad \Gamma^2_{12} = \Gamma^2_{21} = \cot \theta.
\]

The geodesic equations, generically given by Eq. (2.17), are written in the problem original notation, \( \lambda^1 = \theta, \lambda^2 = \phi \), as

\[
\ddot{\theta} - \cos \theta \sin \theta \dot{\phi}^2 = 0,
\]

\[
\ddot{\phi} + 2 \cot \theta \dot{\theta} \dot{\phi} = 0,
\]
where the dot refers to derivatives taken with respect to the proper time $\tau$, with $0 \leq \tau \leq 1$. These differential equations are not straightforward to solve with general initial conditions for $\theta$ and $\phi$.

A conserved quantity, $k$, exists, obtainable from Eq. (2.34). It is associated to a “conservation of angular momentum” over the spherical surface,

$$\sin^2 \theta \dot{\phi} = k .$$

To verify that it is an integral of motion for Eq. (2.34), one only has to take its derivative, and the geodesic equation for $\phi$ is obtained.

If one uses the equation for $k$ and chooses the initial condition $\theta(0) = \pi/2$, corresponding to starting at the north pole, the geodesic equations (2.33) and (2.34) are easily solved, with solutions

$$\theta(t) = \arccos \left( \pm \sqrt{1 - k^2 \sin(t)} \right), \quad \phi(t) = \arctan \left( k \tan(t) \right) + \phi(0) .$$

For a constant value of $B$, these are the defining equations of an arc along the sphere’s great circle connecting the north pole to the final point, which is the smallest distance between two points along the surface of a sphere (see Figure 2.2). Moreover, rotations are isometries of the sphere and hence the initial condition assumed above can be changed arbitrarily. One then concludes that sphere geodesics are arc segments of great circles.

**General Solution of the Geodesic Equations (2.33) and (2.34)**

The geodesic solution for curves constrained on a sphere of constant radius are used in many situations, and we derive their general solution in Appendix A (see Eqs. (A.53)–(A.57)). The reason of their importance is that for two-level systems, the Hilbert space of the quantum system in consideration is $\mathbb{CP}^1$, which is diffeomorphic to the 2–sphere $S^2$ (known in the literature as the Bloch sphere).
Figure 2.2: Geodesic path for a 1/2-spin particle in a magnetic field, evolving from an initial point i to a final point f. The geodesics for this system are arcs of a half-great-circle (half-orthodrome).

2.5.2 Example II – The Landau-Zener Model: A Simple Two-Level System

The Landau-Zener problem, referred by M. Berry as “the simplest non-simple quantum problem” (Berry, 1995), is commonly defined by the following time-dependent Hamiltonian (Damski, 2005),

\[
\hat{H}_{LZ}(h(t)) = (h(t)\hat{\sigma}_x + \epsilon \hat{\sigma}_z) = \begin{pmatrix}
\epsilon & h(t) \\
h(t) & -\epsilon
\end{pmatrix}.
\]  

(2.37)

The parameter \( h \equiv h(t) \) changes as a function of time, usually defined as \( h(t) = \nu t \), with \(-\tau < t < \tau \) and \( \nu \) constant. The parameter \( \epsilon \) in the Landau-Zener Hamiltonian is fixed and sets the minimum gap value attained by the driven system at \( h = 0 \) (see Fig. 2.3).
Eigenenergies and Eigenstates

The eigenenergies of $\hat{H}_{LZ}$ are given by $E_{0,1} = \mp \sqrt{\epsilon^2 + h^2(t)} \equiv \mp \Omega$, and the corresponding eigenstates, written in the basis defined by the eigenstates of $\hat{\sigma}_z$ are

$$|\Psi_{0,1}\rangle = \mp \frac{\Omega \mp \epsilon}{\sqrt{2 \Omega (\Omega \mp \epsilon)}} |\uparrow\rangle + \frac{h(t)}{\sqrt{2 \Omega (\Omega \mp \epsilon)}} |\downarrow\rangle , \quad (2.38)$$

The energy gap $(E_1 - E_0) \equiv \delta E$ is minimal for $h = 0$, when $E_1(h = 0) - E_0(h = 0) = 2 \epsilon$.

Linear Paths – Landau-Zener

First, consider the simplest standard protocol, where $\epsilon$ is time-independent and $h(t)$ linearly depends on time$^4$: $h_{lin}(t) = h_i + (h_f - h_i) t / t_f$. This protocol corresponds to the paradigmatic Landau-Zener problem (Vitanov and Garraway, 1996), and the initial adiabatic ground-state tunnels to the excited-state during the evolution with a finite probability, which yields a final fidelity given by

$$F(t_f) \approx 1 - \exp \left[ -\pi \frac{\epsilon^2 t_f}{(h_f - h_i)} \right] . \quad (2.39)$$

Geodesic Paths – Landau-Zener

An intuitive way to improve this protocol would be to simply adjust the speed $\dot{h}(t)$ during the evolution, slowing down near the avoided level-crossing, thereby reducing transitions to the excited-state. The geodesic protocol slows down close to the avoided level-crossing (Fig. 2.3, right panel), and hence minimizes the tunneling probability to the excited-state during the evolution (Fig. 2.4, right panel).

Equation (2.7) expresses the QGT for any two-level system. The parameter space here is $\mathcal{M}_{LZ} = \mathbb{R}^1$, defined by the coordinate $h$ parametrized by the time $t$. For the Landau-Zener system, we calculate the matrix elements $\langle \Psi_0 | \partial_{\mu} | \Psi_1 \rangle$ and $\langle \Psi_1 | \partial_{\nu} | \Psi_0 \rangle$, with $\{ \mu, \nu \} \in \{ h \}$. The quantum metric tensor is

$$g_{hh} = \frac{\epsilon^2}{4 (\epsilon^2 + h^2)^2} . \quad (2.40)$$

$^4$To avoid strong non-adiabatic effects related to initial and final transients, we always deal with protocols sufficiently smoothened around the initial and final times. We checked that all our results are insensitive to the details of the smoothing procedure. For more details, refer to Appendix C.
The single non-vanishing Christoffel symbols of the second kind is \( \Gamma_{hh}^{h} = -\frac{2h}{(\epsilon^2 + h^2)^2} \), and the geodesic equation \( \ddot{\lambda}^1 + \Gamma_{11}^{1}(\dot{\lambda}^1)^2 = 0 \), with \( \lambda^1 = h \), becomes

\[
\ddot{h} - \frac{2h}{(\epsilon^2 + h^2)^2} h^2 = 0 \implies h(t) = \epsilon \tan \left[ \epsilon c_1 (t + c_2) \right], \quad (2.41)
\]

where \( c_1 \) and \( c_2 \) are constants determined by the boundary conditions.

**Boundary Conditions: Expressions for \( c_1 \) and \( c_2 \)**

For \( t = 0 \), writing \( h(0) \equiv h_i \),

\[
h_i = \epsilon \tan \left[ \epsilon c_1 c_2 \right] \implies \epsilon c_1 c_2 = \arctan \left( \frac{h_i}{\epsilon} \right) \quad . \quad (2.42)
\]

For \( t = t_f \), writing \( h(t_f) \equiv h_f \),

\[
h_f = \epsilon \tan \left[ \epsilon c_1 (t_f + c_2) \right] \implies \epsilon c_1 t_f + \arctan \left( \frac{h_i}{\epsilon} \right) = \arctan \left( \frac{h_f}{\epsilon} \right) \quad . \quad (2.43)
\]

Solving these two equations for \( \epsilon c_1 \) yields \( \epsilon c_1 = (1/t_f) (\arctan (h_f/\epsilon) - \arctan (h_i/\epsilon)) \). Applying the above solutions in Eq. (2.41), one obtains the geodesic curve for the Landau-Zener system with boundary conditions \( h(0) = h_i \) and \( h(t_f) = h_f \),

\[
h_{\text{geo}}(t) = \epsilon \tan \left[ \arctan \left( \frac{h_f}{\epsilon} \right) \left( \frac{t}{t_f} \right) + \arctan \left( \frac{h_i}{\epsilon} \right) \left( 1 - \frac{t}{t_f} \right) \right]. \quad (2.44)
\]

Equivalently, writing \( \tau = t/t_f \) \((0 \leq \tau \leq 1)\) and defining \( \alpha_{i,f} = \arctan (h_{i,f}/\epsilon) \), the geodesic solution is written as

\[
h_{\text{geo}}(t) = \epsilon \tan \left( \alpha_i + \tau (\alpha_f - \alpha_i) \right). \quad (2.45)
\]

**The Squared Energy Fluctuation as a Stationary Quantity along the Path**

We could have obtained the geodesic path (2.45) from Equation (2.19), the differential equation for the stationary value of the squared energy fluctuation \( \Delta E^2 \) along the geodesic path,

\[
\sum_{\mu,\nu} g_{\mu\nu} \dot{\lambda}^\mu \dot{\lambda}^\nu = g_{hh} \dot{h}^2 = \frac{\epsilon^2}{4(\epsilon^2 + h^2)^2} \dot{h}^2 = \Delta E^2 \implies \dot{h}^2 = \left( \frac{2 \Delta E}{\epsilon} \right)^2 (\epsilon^2 + h^2)^2 \quad \dot{h}(\tau) = \epsilon \tan \left( 2 \Delta E \tau + \epsilon c_0 \right) \quad . \quad (2.46)
\]
Writing \( h(0) = h_i, \epsilon c_0 = \arctan \left( \frac{h_x}{\epsilon} \right) \equiv \alpha_i \) and the resulting equation for \( h(\tau) \) is

\[
h_{\text{geo}}(t) = \epsilon \tan \left( 2 \Delta E \tau + \alpha_i \right) ,
\]

the same as Equation (2.45), with \( 2\Delta E \equiv (\alpha_f - \alpha_i) / 2 \).

One important feature of the solution as written above becomes clear by defining \( \beta(\tau) \equiv h(\tau)/\epsilon \) and \( \beta_i \equiv \alpha_i \),

\[
\beta_{\text{geo}}(\tau) = \tan \left( 2 \Delta E \tau + \beta_i \right) .
\]

Since \( \epsilon \) only defines the system energy scale, \( 2\Delta E \) is thus seen as the system “proper speed” while traveling along the geodesic path, which we refer to as the geodesic speed, \( v_{\text{geo}} \). As \( \Delta E \) is stationary, \( v_{\text{geo}} \) is a constant speed along the path. An analogous feature is observed for the magnitude of the 4-velocity in special and general relativity: it is stationary along the traveled geodesic path, and corresponds to the integrand of the action \( S \) which gives rise to the geodesic equations\(^5\), Eq. (2.17).

In what follows, we show that merely introducing an additional tunable parameter is enough to boost the fidelity of the quantum system defined by exactly the same Hamiltonian.

### 2.5.3 Example III – The Landau-Zener Model with an Additional Tunable Parameter

We here extend the original Landau-Zener system in Eq. (2.37), introducing a second angular variable \( \phi \),

\[
\hat{H}_{LZ-\phi}(\epsilon, h, \phi) = h (\cos \phi \hat{\sigma}_x + \sin \phi \hat{\sigma}_y) + \epsilon \hat{\sigma}_z = h_x \hat{\sigma}_x + h_y \hat{\sigma}_y + \epsilon \hat{\sigma}_z = \hat{H}_{LZ-\phi}(h_x, h_y, \epsilon) ,
\]

where \( h_x^2 + h_y^2 = h^2 \) and \( \tan \phi = h_y/h_x \); equivalently,

\[
\hat{H}_{LZ-\phi}(\epsilon, h, \phi) = \begin{pmatrix} \epsilon & h e^{-i\phi} \\ h e^{i\phi} & -\epsilon \end{pmatrix} .
\]

\(^5\)q.v. Chapter 3.
Figure 2.3: **Left:** Landau-Zener eigenenergies $E_{\pm}$ as a function of $h$ for $\epsilon = 2$. **Right:** Landau-Zener geodesic paths as a function of time for different values of $\epsilon$, from $h_i = -10$ to $h_f = 10$. The linear path is shown in dotted red.

### Eigenenergies and Eigenstates

The eigenenergies of $\hat{H}_{LZ-\phi}$ are given by $\tilde{E}_{0,1}(\epsilon,h) = \mp \sqrt{\epsilon^2 + h^2} \equiv \mp \Omega$, while the eigenstates, written in the basis of $\hat{\sigma}_z$, are

$$|\Psi_{0,1}\rangle_{\phi} = \mp \frac{\Omega \mp \epsilon}{\sqrt{2 \Omega (\Omega \mp \epsilon)}} e^{-i \frac{\phi}{2}} |\uparrow\rangle + \frac{h}{\sqrt{2 \Omega (\Omega \mp \epsilon)}} e^{i \frac{\phi}{2}} |\downarrow\rangle.$$  

(2.51)

The motivation to extended the LZ–system by adding another parameter is to enable paths defined in a two-dimensional space. The parameters now are $(h, \phi)$. Such modification allows one to go around the minimum energy gap of the original LZ system by also tuning $\phi$.

### Quantum Metric Tensor and Geodesic Equations for $h$ and $\phi$:

For $\mu, \nu = \{h, \phi\}$, the terms in $\chi_{\mu\nu}$ are equal to

$$\langle \Psi_1 | \partial_h | \Psi_0 \rangle = -\frac{\epsilon \text{sign}(h)}{2 (\epsilon^2 + h^2)}, \quad \langle \Psi_1 | \partial_\phi | \Psi_0 \rangle = \frac{i \sqrt{h^2}}{2 (\epsilon^2 + h^2)^{1/2}}.$$  

(2.52)

and thus

$$\chi_{\mu\nu} = \frac{1}{4} \begin{pmatrix} \frac{\epsilon^2}{(\epsilon^2 + h^2)^{3/2}} & \frac{i \epsilon h}{(\epsilon^2 + h^2)^{1/2}} \\ \frac{i \epsilon h}{(\epsilon^2 + h^2)^{3/2}} & \frac{h^2}{(\epsilon^2 + h^2)} \end{pmatrix},$$  

(2.53)
from which the quantum metric tensor can be read,

\[ g_{\mu\nu} = \begin{pmatrix} gh & g_{h\phi} \\ g_{\phi h} & g_{\phi\phi} \end{pmatrix} = \frac{1}{4} \begin{pmatrix} \epsilon^2 + h^2 & 0 \\ 0 & \frac{h^2}{\epsilon^2 + h^2} \end{pmatrix}. \] (2.54)

**Case I:** For \( \epsilon = 0 \), the above metric becomes degenerate, since the metric element \( g_{hh} \) vanishes due to the vanishing gap at \( h = 0 \),

\[ g_{\mu\nu} = \begin{pmatrix} gh & g_{h\phi} \\ g_{\phi h} & g_{\phi\phi} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{4} \end{pmatrix}. \] (2.55)

This is the metric of the sphere with initial conditions \( \theta = 0 \) and \( \dot{\theta} = 0 \), corresponding to solutions on the equator. The metric element for \( \phi \) is constant, and thus, the solution for the corresponding polar angle, here represented by \( h \), satisfy the equation \( \ddot{h} = 0 \) (this is a consequence of applying the initial conditions for \( \theta \) on the sphere geodesic equations, Eqs (2.33) and (2.34)). Since the ground-state \( |\Psi_0\rangle \) becomes independent of \( h \), there is no notion of distance along the \( h \) direction. We are free to choose \( h(t) \), with \( h > 0 \) since our goal is to avoid the \( E_0 = E_1 \) degeneracy. Let us take the simplest choice of \( h(t) \) as a constant function. All Christoffel symbols vanish, and the geodesic equation for \( \phi(t) \) simply becomes

\[ \ddot{\phi} = 0 \quad \implies \quad \phi(t) = (\phi_f - \phi_i) \delta t + \phi_i, \] (2.56)

assuming the boundary conditions given by \( \phi(0) = \phi_i \) and \( \phi(t_f) = \phi_f \).

**Case II:** For \( \epsilon \neq 0 \), we can recast the metric tensor (2.54) by performing the rescaling given by \( h = \epsilon \tilde{h} \). Observe that the infinitesimal line element \( ds^2 \) has its \( g_{hh} \) metric tensor component rescaled accordingly,

\[ ds^2 = g_{hh} dh^2 + g_{\phi\phi} d\phi^2 = \left( g_{hh}/\epsilon^2 \right) d\tilde{h}^2 + g_{\phi\phi} d\phi^2. \] (2.57)

The metric can be thus be simplified to

\[ g_{\mu\nu} = \begin{pmatrix} gh & g_{h\phi} \\ g_{\phi h} & g_{\phi\phi} \end{pmatrix} = \frac{1}{4} \begin{pmatrix} \frac{1}{(\epsilon^2 + h^2)} & 0 \\ 0 & \frac{h^2}{(\epsilon^2 + h^2)} \end{pmatrix}. \] (2.58)
Changing variables allows us to simplify the metric even further,

$$\tilde{h}(t) = \tan \alpha(t), \quad (2.59)$$

where now

$$ds^2 = g_{\tilde{h}\tilde{h}} d\tilde{h}^2 + g_{\phi\phi} d\phi^2 = \left( g_{\tilde{h}\tilde{h}} \sec^4 \alpha \right) d\alpha^2 + g_{\phi\phi} d\phi^2. \quad (2.60)$$

Hence, we obtain the metric of a sphere in the new coordinates,

$$(g_{\mu
u}) = \begin{vmatrix} g_{\alpha\alpha} & g_{\alpha\phi} \\ g_{\phi\alpha} & g_{\phi\phi} \end{vmatrix} = \frac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & \sin^2 \alpha \end{pmatrix}. \quad (2.61)$$

The non-vanishing Christoffel symbols are

$$\Gamma^\alpha_{\phi\phi} = -\cos \alpha \sin \alpha, \quad \Gamma^\phi_{\phi\alpha} = \cot \alpha = \Gamma^\phi_{\alpha\phi}, \quad (2.62)$$

such that the geodesic equations for $\alpha$ and $\phi$ are

$$\ddot{\alpha} - \sin \alpha \cos \alpha \dot{\phi}^2 = 0, \quad \ddot{\phi} + 2 \cot \alpha \dot{\alpha} \dot{\phi} = 0. \quad (2.63)$$

For two points along the same meridian (an arc of the great circle that connects the two poles), the shortest distance should also be along the meridian. That, in fact, is our desired solution. Let us show that such a curve satisfies the geodesic equations above.

Substituting

$$\phi(t) = \phi_i = 0, \quad \dot{\phi} = 0, \quad \ddot{\phi} = 0,$$

$$\alpha(t) = c_1 t + c_2, \quad \dot{\alpha} = c_1, \quad \ddot{\alpha} = 0, \quad (2.64)$$

in the geodesic equation (2.61), we get

$$\ddot{\alpha} - \sin \alpha \cos \alpha \dot{\phi}^2 = 0 - \sin (c_1 t + c_2) \cos (c_1 t + c_2) 0^2 = 0,$$

$$\ddot{\phi} + 2 \cot \alpha \dot{\alpha} \dot{\phi} = 0 + 2 \cot (c_1 t + c_2) c_1 0 = 0. \quad (2.65)$$

So they do indeed satisfy the geodesic equation, and thereby are valid solutions, corresponding on part of a great circle on the $xz$–plane (constant azimuth angle $\phi(t) = 0$) with the polar angle $\alpha(t)$ changing linearly from $\alpha_i$ to its supplement, $\alpha_f = \pi - \alpha_i$. 

Boundary Conditions for $\alpha(t)$

At $t = 0$, labelling $\alpha(0) = \alpha_i$, we get $c_2 = \alpha_i$. At $t = t_f$, labelling $\alpha(t_f) = \alpha_f$, we get $c_1 t_f + \alpha_i = \alpha_f \rightarrow c_1 = \delta (\alpha_f - \alpha_i)$, where, as usual, we defined $\delta = 1/t_f$. Thus, $\phi(t) = 0$ and $\alpha(t) = (\alpha_f - \alpha_i) \delta t + \alpha_i$ are the geodesic solutions, with $\alpha_{i,f} = \arctan (h_{i,f}/\epsilon)$ from Eq. (2.59).

In terms of the coordinates $(h(t), \phi(t))$, the solutions are

$$h(t) = \epsilon \tan \left[ (\alpha_f - \alpha_i) \delta t + \alpha_i \right], \quad \phi(t) = 0,$$

with $\alpha_{i,f} = \arctan (h_{i,f}/\epsilon)$.

Transforming back to the original variables $(x(t), y(t))$, the solutions are

$$x(t) = h(t) \cos \phi(t) = \epsilon \tan \left[ (\alpha_f - \alpha_i) \delta t + \alpha_i \right], \quad y(t) = h(t) \sin \phi(t) = 0,$$

which is the geodesic path\textsuperscript{6} as a function of time $t$ for variations in $x$ and $y$ on the Hamiltonian (2.49). In Figure 2.4, we show a comparison of three ways of driving the LZ system for different final times: linearly (blue); on a one-parameter geodesic $h(t)$ (green); and with a two-parameters geodesic protocol, $h(t)$ and $\phi(t)$. One can clearly see that the addition of parameters gives an improvement of orders of magnitude for the final fidelity, even beyond the adiabatic regime.

\textsuperscript{6}In order to numerically simulate the time evolution of a quantum state along any path, one has to make use of mollifying functions. These smoothening protocols inhibit the oscillatory behavior known as the \textit{Gibbs phenomenon} caused by the time domain derivative discontinuity at $t = 0$. A piecewise function in the time domain introduces oscillatory behavior in the frequency domain. Refer to Appendix C for more details about mollifying functions and their use in the numerical simulations here presented.
Figure 2.4: Left: Landau-Zener geodesic and linear protocols (green and blue, respectively) with $h(t)$ as the single tuning parameter, and with both tuning parameters $(h(t), \phi(t))$ (orange). The addition of an extra parameter further enables the avoidance of regions with a small gap. Right: $-\log_{10}(F)$ ($F \equiv$ final fidelity) as a function of the driving “speed” $1/t_f$ for linear driving (blue), one and two parameters geodesic driving (green and orange, respectively) shown on a logarithmic scale. An improvement in orders of magnitude is observed for shorter times with the addition of a parameter (green vs. orange).

Map Between the LZ/LZ--$\phi$ System and a 1/2--Spin Particle in a Magnetic Field System

Mapping LZ

There is a mapping between the two previous two-level systems studied. To highlight it, consider Eq. (2.5.1) with $B_y = 0$, $B_z = \epsilon$ and $B_x(t) \equiv h(t)$, the last variable considered as the only tunable parameter. The Hamiltonian becomes

$$\hat{H}_{q\bar{b}}(h(t), 0, \epsilon) = \begin{pmatrix} \epsilon & h(t) \\ h(t) & -\epsilon \end{pmatrix} \equiv \hat{H}_{LZ}(h(t)),$$

which is exactly the Landau-Zener Hamiltonian introduced in the previous section, with $\epsilon$ assumed to be constant.
26

Mapping LZ−ϕ

Let us now consider Eq. (2.5.1) with $B_y = h(t) \sin \phi$, $B_z = \epsilon$ and $B_x(t) \equiv h(t) \cos \phi$, with $h$ and $\phi$ considered as tunable parameters. The Hamiltonian reads

$$\hat{H}_{qb}(h(t) \cos \phi, h(t) \sin \phi, \epsilon) = \begin{pmatrix} \epsilon & h e^{-i\phi} \\ h e^{i\phi} & -\epsilon \end{pmatrix} \equiv \hat{H}_{LZ}(h(t), \phi),$$

which is the extended Landau-Zener Hamiltonian with $h$ and $\phi$ as tunable parameters, and $\epsilon$ assumed to be constant.

2.5.4 Example IV – The XY Spin Chain: a quintessential many-body system

The XY spin chain system is defined by (Kolodrubetz et al., 2013)

$$\hat{H}_{XY} = -\sum_{j=1}^{N} \left( J_x \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + J_y \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + h \hat{\sigma}_j^z \right),$$

where $\hat{\sigma}_j^\alpha$, with $\alpha = x, y, z$, are the Pauli matrices acting on the spin at the $j$-th site of the chain. We assume periodic boundary conditions, $\hat{\sigma}_N^\alpha = \hat{\sigma}_1^\alpha$. A common practice is to parametrize the couplings $J_{x,y}$ in terms of an energy scale and an anisotropy parameter $\gamma$ as follows,

$$J_x = J \left( \frac{1+\gamma}{2} \right), \quad J_y = J \left( \frac{1-\gamma}{2} \right).$$

One can then rescale the energy of $\hat{H}_{XY}$ setting $J = 1$. The parameters of the model are the anisotropy $\gamma$ of the nearest neighbor spin-spin exchange interaction along the $x, y$ directions, and the transverse magnetic field $h$.

We introduce an additional parameter $\phi$, describing a simultaneous rotation of all spins around the $z$-axis by an angle $\phi/2$ (Kolodrubetz et al., 2013; Tomka et al., 2016). The corresponding Hamiltonian is given by

$$\hat{H}_{XY}(h, \gamma, \phi) = R_z(\phi) \hat{H}_{XY} R_z^\dagger(\phi),$$

where $R_z(\phi) = \prod_{j=1}^{N} \exp \left( -i \frac{\phi}{2} \sigma_j^z \right)$. As shown below, a rotation of the system by $\phi$ does not affect its the spectrum, but it modifies the eigenstates.
Transforming the XY Hamiltonian to a Free Fermionic System

The XY spin chain Hamiltonian (2.72) can be mapped to non-interacting spin−1/2 model through a Jordan-Wigner transformation (Sachdev, 1999) followed by a Fourier transform,

$$\hat{H}_{XY} = \sum_k c_k^\dagger \hat{H}_k c_k, \quad \text{where} \quad \hat{H}_k = \begin{pmatrix} h - \cos k & \gamma e^{i\phi} \sin k \\ \gamma e^{-i\phi} \sin k & -(h - \cos k) \end{pmatrix},$$

with $k = \pm \frac{2\pi n}{N}$, $n \in [1, N/2]$, and $c_k^\dagger = (c_{-k}, c_k^\dagger)$ the Fourier transform of the Jordan-Wigner fermions (Dutta et al., 2015). A Bogoliubov transform on Eq. (2.73) maps $\hat{H}_{XY}$ to a free fermionic Hamiltonian with excitation spectrum $\epsilon_k = \sqrt{(h - \cos k)^2 + \gamma^2 \sin^2 k}$. Once the fermion parity is fixed, the map yields a unique ground-state for $\hat{H}_{XY}$ throughout the entire phase diagram (Lieb et al., 1961), factorable as $|\Psi_0\rangle = \prod_k |\psi_0\rangle_k$. The ground-state of $\hat{H}_k$, $|\psi_0\rangle_k$, is given by a Bloch-sphere vector with azimuthal angle $\phi$ and polar angle

$$\theta_k = \arctan\left(\frac{\gamma \sin k}{h - \cos k}\right).$$

Written explicitly,

$$|\psi_0\rangle_k = \cos \frac{\theta_k}{2} e^{i\phi} |0\rangle_k |0\rangle_{-k} + \sin \frac{\theta_k}{2} e^{-i\phi} |1\rangle_k |1\rangle_{-k},$$

$$|\psi_1\rangle_k = \sin \frac{\theta_k}{2} e^{i\phi} |0\rangle_k |0\rangle_{-k} - \cos \frac{\theta_k}{2} e^{-i\phi} |1\rangle_k |1\rangle_{-k},$$

where $|1\rangle_k = c_k^\dagger |0\rangle_k$. The phase diagram of the model is illustrated in Fig. 2.5.

We focus on the $|h| \leq 1$ region of the parameter space and study the fidelity $F(t_f) = |\langle \Psi(t_f) | \Psi_0(t_f) \rangle|^2$ for the preparation of a target ground-state $|\Psi_0(t_f)\rangle$ from an initial ground-state $|\Psi_0(0)\rangle$, lying in a different phase region than the target state. Let us analyze the passage through the anisotropic transition line with fixed $h = 0.5$, for the initial $\gamma_i = 1$ and final $\gamma_f = -1$ points. As in the previously studied case, we compare the three different protocols: a linear $\gamma_{\text{lin}}(t)$, a geodesic $\gamma_{\text{geo}}(t)$ and a geodesic one which avoids the quantum phase transition $\lambda_{\text{geo}}(t) = |\gamma(t)|(\cos \phi(t), \sin \phi(t))^T$. 
XY Spin Chain: $\gamma - \phi$ Geodesics

The quantum metric tensor for the XY spin chain was calculated in (Zanardi et al., 2007; Kolodrubetz et al., 2013) and reads

$$
g_{\gamma\gamma} = \frac{1}{16} \frac{1}{|\gamma|(|\gamma| + 1)^2}, \quad g_{\phi\phi} = \frac{1}{8} \frac{|\gamma|}{(|\gamma| + 1)}, \quad g_{\gamma\phi} = 0.
$$

(2.76)

Performing the change of coordinates

$$
\gamma = \tan^2 \eta \implies d\gamma = 2 \tan \eta \sec^2 \eta \, d\eta, \quad \phi = \sqrt{2} \varphi \implies d\phi = \sqrt{2} \, d\varphi.
$$

(2.77)

The infinitesimal line element $ds^2$ is rewritten as

$$
ds^2 = g_{\gamma\gamma} d\gamma^2 + g_{\phi\phi} d\phi^2 = \frac{4 \tan^2 \eta \sec^4 \eta}{g_{\eta\eta}} \, d\eta^2 + \frac{2 \tan^2 \eta}{g_{\varphi\varphi}} \, d\varphi^2.
$$

(2.78)

The metric in the new coordinates reads

$$
g_{\eta\eta} = g_{\gamma\gamma} \left(4 \tan^2 \eta \sec^4 \eta\right) = \frac{4 \tan^2 \eta \sec^4 \eta}{16 \tan^2 \eta \sec^4 \eta} = \frac{1}{4},
$$

$$
g_{\varphi\varphi} = 2 g_{\phi\phi} = \frac{2 \tan^2 \eta}{8 (\tan^2 \eta + 1)} = \frac{1}{4 \sec^2 \eta} = \frac{1}{4} \, \sin^2 \eta.
$$

(2.79)

Hence, we obtain the metric of a sphere in the new coordinates,

$$
(g_{\mu\nu}) = \begin{pmatrix} g_{\eta\eta} & g_{\eta\varphi} \\ g_{\varphi\eta} & g_{\varphi\varphi} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \sin^2 \eta \end{pmatrix}.
$$

(2.80)

The non-vanishing Christoffel symbols are

$$
\Gamma^\eta_{\varphi\varphi} = -\cos \eta \sin \eta, \quad \Gamma^\varphi_{\eta\eta} = \cot \eta = \Gamma^\varphi_{\varphi\eta},
$$

(2.81)

such that the geodesic equations for $\eta$ and $\varphi$ are

$$
\ddot{\eta} - \sin \eta \cos \eta \dot{\varphi}^2 = 0,
$$

(2.82)

$$
\ddot{\varphi} + 2 \cot \eta \dot{\eta} \dot{\varphi} = 0.
$$

(2.83)

The variable $\eta$ plays the role of the polar angle and $\varphi$ the azimuth angle in a spherical coordinate system.
Figure 2.5: Geodesic passage through a quantum phase transition – Left: The phase diagram of the rotated XY spin chain in cylindrical coordinates ($|\gamma| \cos \phi, |\gamma| \sin \phi, h$) is depicted. The two red planes ($|h| = 1$) indicate the Ising criticality, where the system undergoes a continuous transition between a paramagnetic and a ferromagnetic phase. The line $\gamma = 0$ marks the anisotropic transition, separating the two different aligned ferromagnetic phases. The blue/green and orange lines illustrate the driving protocols for crossing and avoiding the quantum criticality, respectively. Right: $-\log_{10}(\mathcal{F})/N$ ($\mathcal{F}$ ≡ final fidelity and $N = 1024$ the number of spins) as a function of the driving “speed” $1/t_f$ for linear driving (blue), one and two parameters geodesic driving (green and orange, respectively) is shown on a logarithmic scale, with $\gamma_i = 1$, $\gamma_f = -1$, $h = 0.5$. As in the Landau-Zener case before, an improvement in orders of magnitude is observed for shorter times with the addition of a parameter (green vs. orange).

The geodesic path we want is one that avoids the critical line at $\gamma = 0$. In polar coordinates, our geodesic path is written as $|\gamma(t)| (\sin \phi(t), \cos \phi(t))$, with boundary conditions given by $\gamma(0) = \gamma(t_f) = 1$, and $\phi(0) = 0$, $\phi(t_f) = \pi$. In terms of the new coordinates, this translates to $\eta(0) = \pi/4$, $\eta(t_f) = 3\pi/4$, and $\varphi(0) = 0$, $\varphi(t_f) = \sqrt{2} \pi$. The analytical expression for the geodesic path is calculated in detail in Appendix B.

In Figure 2.5, we show a comparison of three ways of driving the XY system for different final times: linearly (blue); on a one-parameter geodesic $\gamma(t)$ (green); and with a two-
parameters geodesic protocol, $\gamma(t)$ and $\phi(t)$. One clearly sees the addition of parameters giving an improvement in orders of magnitude to the final fidelity, for shorter times beyond the adiabatic regime.

2.6 Conclusion

In this chapter, a geometric approach was used to obtain optimal protocols for the adiabatic preparation of ground-states in quantum many-body systems close to the adiabatic limit. Those ares shown to be geodesics in the space of control parameters, maximizing the overlap between the evolved-state and the target state, while simultaneously keeping the quantity $g_{\mu\nu}\dot{\lambda}^\mu\dot{\lambda}^\nu$, equal to the energy fluctuation squared $\Delta E^2$ (Section 2.5), stationary along the path. Further, it was shown that increasing the number of control parameters while tuning them along geodesic paths on the extended parameter space provides a further increase in the final fidelity. Such method can be applied to various optimization problems like finding best quantum annealing protocols, optimum adiabatic path for quantum simulation or minimization of heating in experiments with ultra-cold atoms.
Chapter 3

The Hilbert Space – a Complex Metric Space

*Everything should be made as simple as possible, but not simpler.*

– Albert Einstein, in *On the Method of Theoretical Physics*

3.1 The Quantum Metric Tensor and Geodesics in Parameter Space

The QMT provides a natural way of obtaining distances along the evolution path in the parameter space $\mathcal{M}$. The distance between two eigenstates can be expressed in a differential-geometric form as shown in Eq. (2.9).

In addition, if the eigenstate of the system evolves adiabatically from $\vec{\lambda}_i$ to $\vec{\lambda}_f$ on a generic path $\gamma \equiv \gamma(\vec{\lambda})$ with boundary values $\gamma(\vec{\lambda}_i) \equiv \gamma_i$ and $\gamma(\vec{\lambda}_f) \equiv \gamma_f$, the quantum distance $L(\gamma(\vec{\lambda})) \equiv L(\gamma)$ in parameter space can be written as

$$L(\gamma) = \int_{\gamma_i}^{\gamma_f} ds = \int_{\vec{\lambda}_i}^{\vec{\lambda}_f} (g_{\mu\nu} d\lambda^\mu d\lambda^\nu)^{1/2}.$$  (3.1)

One can further parametrize the curve $\gamma = \gamma(\vec{\lambda})$ by parametrizing the variable parameters $\vec{\lambda} \equiv \vec{x}(t)$ such that $\vec{x}(t_i) = \vec{x}_i$ and $\vec{x}(t_f) = \vec{x}_f$, and consequently $\gamma \equiv \gamma(\vec{\lambda}) = \gamma(\vec{x}(t))$. After such parametrization, the previous equation can be rewritten as

$$L(\gamma) = \int_{t_i}^{t_f} \left( g_{\mu\nu} \frac{d\lambda^\mu}{dt} \frac{d\lambda^\nu}{dt} \right)^{1/2} dt = \int_{t_i}^{t_f} \left( g_{\mu\nu} \dot{\lambda}^\mu \dot{\lambda}^\nu \right)^{1/2} dt.$$  (3.2)
A fundamental property of the functional \( L \) is its invariance under any smooth monotonic reparameterization of \( t \), such as \( t = \alpha t' + \beta \), with \( \alpha \neq 0 \) and \( \beta \) constants. Paths have the same length regardless of how you travel (and for how long) along the path, as long as you keep moving in the same direction on the path. The stationary curve for the functional \( L \), \( \bar{\gamma}(t) \) will naturally inherit this property. This is an important result — we refer to the stationary curve as the geodesic connecting the boundary points.

A convenient parametrization is given by \( t = t_f \tau, \; dt = t_f d\tau \), in which case Eq. (3.2) becomes

\[
\tilde{L}(\gamma) = \int_0^1 \left( g_{\mu\nu} \frac{d\lambda^\mu}{d\tau} \frac{d\lambda^\nu}{d\tau} \right)^{1/2} d\tau.
\]  

(3.3)

Such choice is often referred as the proper parametrization.

3.1.1 Principle of Stationary Action: Euler-Lagrange Equations

The functional \( L(\gamma) \) defined above can be used to find the distance for any path \( \gamma \) with fixed boundary points, namely \( \vec{\lambda}_0 \) and \( \vec{\lambda}_f \). A natural question thus arises about which path \( \bar{\gamma} \) minimizes the distance between the fixed endpoints. To obtain this curve, we enforce the variation of the above action with respect to \( \gamma \) to be stationary,

\[
\frac{\delta \tilde{L}[\gamma(\vec{\lambda})]}{\delta \vec{\lambda}} = 0.
\]  

(3.4)

One then resorts to Variational Calculus techniques, applying Euler-Lagrange’s equations on the variation above, thereby obtaining differential equations for the stationary path connecting the two eigenstates at \( \vec{\lambda}_0 \) and \( \vec{\lambda}_f \).

3.1.2 The Energy Action

As it turns out, the action \( \tilde{L}(\gamma) \) is hard to attack analytically due to the square root in the integrand of Eq. (3.3). To circumvent this analytical hurdle, let us find instead the critical path for what is referred in the literature as the Energy functional \( \tilde{E} \) (Milnor, 1963; Petersen, 1998; Spivak, 1999), defined by

\[
\tilde{E} = \frac{1}{2} \int_0^1 \left( g_{\mu\nu} \frac{d\lambda^\mu}{d\tau} \frac{d\lambda^\nu}{d\tau} \right) d\tau,
\]  

(3.5)
which has a much nicer integrand.

From Cauchy-Schwarz’s inequality,

\[
\left( \int_a^b f h \, dt \right)^2 \leq \left( \int_a^b f^2 \, dt \right) \left( \int_a^b h^2 \, dt \right),
\]

if one sets \( f(t) = 1 \) and \( h(t) = (g_{\mu\nu} (d\lambda^\mu/d\tau) (d\lambda^\nu/d\tau))^{1/2}, a = 0 \) and \( b = 1 \), we conclude that

\[
(\tilde{L})^2 \leq 2 \tilde{E},
\]

where equality holds if and only if the integrand of \( \tilde{E} \) is constant. Hence, if we apply the principle of stationary action to the functional \( \tilde{E} \), we consequently obtain the stationary solutions for \( \tilde{L} \), with one very important caveat: the functional \( \tilde{E} \) is not invariant under change of parametrization, as one can easily verify in Eq. (3.5). Consequently, the stationary curve of \( \tilde{E} \) is only stationary for \( \tilde{L} \) under affine reparametrizations on \( \tau \), i.e., provided that the solution curve \( \tilde{\gamma}(\tau) \) is only reparametrized by linear functions\(^1\), \( \tau(t) = \alpha t + \beta, \alpha \neq 0 \) (Spivak, 1999; Milnor, 1963).

The Euler-Lagrange equations of motion for the functional \( \tilde{E} \) in local coordinates \( \{\lambda^\mu\} \) are given by (Spivak, 1999)

\[
\frac{d^2 \lambda^\mu}{d\tau^2} + \Gamma_{\nu\rho}^{\mu} \frac{d\lambda^\nu}{d\tau} \frac{d\lambda^\rho}{d\tau} = 0,
\]

where \( \Gamma_{\mu}^{\nu\rho} \) are the Christoffel symbols of the second kind, defined by

\[
\Gamma_{\nu\rho}^{\mu} = \frac{1}{2} g^{\mu\xi} \left( \partial_\rho g_{\xi\nu} + \partial_\nu g_{\xi\rho} - \partial_\xi g_{\nu\rho} \right), \text{ with } \partial_\mu \equiv \partial/\partial \lambda^\mu \text{ and } g^{\mu\xi} = (g_{\mu\xi})^{-1}.
\]

In summary, to obtain the geodesic paths in parameter space, one first calculates the quantum metric tensor, its derivatives and Christoffel symbols to solve the differential equations (3.8). The solution is a path which makes both functionals \( \tilde{L} \) and \( \tilde{E} \) stationary, i.e., one that has the shortest length connecting the fixed points in the parameter manifold \( \mathcal{M} \) while also minimizing the energy. In the adiabatic limit, traveling along this path yields the opti-

\(^1\)This condition is also referred in the literature as the requirement for the curve \( \gamma(\tau) \) to be parametrized by its arc-length.
mal control we initially set as our goal, i.e., one that maximizes fidelity while simultaneously minimizing the energy fluctuation.\(^2\)

It should be noted that different quantum metrics have been defined in the literature, but the one outlined above stands out since it is directly related to the concept of susceptibility, that is, of the system’s response after a given parameter change is made\(^3\). This makes this theoretical tool very suitable and naturally connected to experiments that can measure its predictions and properties.

### 3.2 Energy Fluctuation and the Quantum Geometric Tensor

In this section, we derive in detail the relationship between energy fluctuations \(\Delta E\) and the quantum metric tensor \(g_{\mu\nu}\).

The energy fluctuation is given by

\[
\Delta E^2 \equiv \langle \Psi | \hat{H}^2 | \Psi \rangle - \langle \Psi | \hat{H} | \Psi \rangle^2.
\]  

(3.10)

Within adiabatic perturbation theory (De Grandi and Polkovnikov, 2010; Gritsev and Polkovnikov, 2012; Kolodrubetz et al., 2013), we calculate \(|\Psi\rangle\) on its instantaneous eigenbasis in powers of the driving velocities \(\dot{\lambda}^\mu\), assuming that the parameter driving speed rate is small for all \(\mu\),

\[
|\Psi\rangle = \left(1 + \beta^\mu (\dot{\lambda}^\mu)^2 \right)|\Psi_0\rangle - i \dot{\lambda}^\mu \sum_{m \neq 0} \alpha_m^\mu |\Psi_m\rangle + \ldots,
\]  

(3.11)

where

\[
\alpha_m^\mu = \frac{\langle \Psi_m | \partial_\mu \hat{H} | \Psi_0 \rangle}{(E_m - E_0)^2}, \quad \beta^\mu = -\frac{1}{2} \sum_{n \neq 0} |\alpha_n^\mu|^2.
\]  

(3.12)

The constant \(\beta^\mu\) normalizes the state up to second-order in terms of \(\dot{\lambda}^\mu\).

Since variances are invariant by shifts of a real number, let us subtract the ground-state

\(^2\)These are functional paths of shortest length in the projective Hilbert space, adiabatically connecting two ground-states.

\(^3\)This is shown to be extremely important in subsequent chapters, particularly Chapter 6.
energy \( E_0 \) from the Hamiltonian\(^4\),

\[
\Delta E^2 = \langle \Psi | (\hat{H} - E_0)^2 | \Psi \rangle - \langle \Psi | (\hat{H} - E_0) | \Psi \rangle^2 .
\] (3.13)

The first term gives

\[
\langle \Psi | (\hat{H} - E_0)^2 | \Psi \rangle = \left( 1 + \beta^\mu (\dot{\lambda}^\mu)^2 \right) \langle \Psi_0 | + i \dot{\lambda}^\mu \sum_{n \neq 0} (\alpha_n^\mu)^* \langle \Psi_n | \right) \left( \hat{H}^2 - 2 \hat{H} E_0 + E_0^2 \right) \times \\
\times \left( 1 + \beta^\nu (\dot{\lambda}^\nu)^2 \right) \langle \Psi_0 | - i \dot{\lambda}^\nu \sum_{m \neq 0} \alpha_m^\nu \langle \Psi_m | \right).
\] (3.14)

The crossed terms all vanish since they connect \( \langle 0 | \) with \( \hat{H}^p | m \rangle \equiv E_m^p | m \rangle \) \((p = \{0, 1, 2\} \) and \( m \neq 0 \)). Also vanishing is the direct product of \( | \Psi_0 \rangle \),

\[
\left( 1 + \beta^\mu (\dot{\lambda}^\mu)^2 \right) \left( 1 + \beta^\nu (\dot{\lambda}^\nu)^2 \right) \langle \Psi_0 | \left( \hat{H}^2 - 2 \hat{H} E_0 + E_0^2 \right) | \Psi_0 \rangle = 0 .
\] (3.15)

The non-vanishing terms are

\[
\dot{\lambda}^\mu \dot{\lambda}^\nu \sum_{m, n \neq 0} (\alpha_n^\mu)^* \alpha_m^\nu \langle \Psi_n | \left( \hat{H}^2 - 2 \hat{H} E_0 + E_0^2 \right) | \Psi_m \rangle = \dot{\lambda}^\mu \dot{\lambda}^\nu \sum_{m \neq 0} (\alpha_m^\mu)^* \alpha_m^\nu (E_m - E_0)^2 .
\] (3.16)

The second term gives

\[
\langle \Psi | (\hat{H} - E_0) | \Psi \rangle^2 = \left[ \left( 1 + \beta^\mu (\dot{\lambda}^\mu)^2 \right) \langle \Psi_0 | + i \dot{\lambda}^\mu \sum_{n \neq 0} (\alpha_n^\mu)^* \langle \Psi_n | \right) \left( \hat{H} - E_0 \right) \times \\
\times \left( 1 + \beta^\nu (\dot{\lambda}^\nu)^2 \right) \langle \Psi_0 | - i \dot{\lambda}^\nu \sum_{m \neq 0} \alpha_m^\nu \langle \Psi_m | \right) \right]^2 \sim \mathcal{O} \left[ (\dot{\lambda}^\mu \dot{\lambda}^\nu)^2 \right].
\] (3.17)

Keeping only the lowest order correction, Equation 3.13 reduces to

\[
\Delta E^2 = \lambda^\mu \lambda^\nu \sum_{m \neq 0} \frac{\langle \Psi_0 | \partial_\mu \hat{H} | \Psi_m \rangle \langle \Psi_m | \partial_\nu \hat{H} | \Psi_0 \rangle}{(E_m - E_0)^2} \frac{(E_m - E_0)^2}{(E_m - E_0)^2} (E_m - E_0)^2 \\
= \left( \sum_{m \neq 0} \frac{\langle \Psi_0 | \partial_\mu \hat{H} | \Psi_m \rangle \langle \Psi_m | \partial_\nu \hat{H} | \Psi_0 \rangle}{(E_m - E_0)^2} \right) \dot{\lambda}^\mu \dot{\lambda}^\nu \\
= \lambda_{\mu \nu} \dot{\lambda}^\mu \dot{\lambda}^\nu = \left( g_{\mu \nu} - \frac{i}{2} F_{\mu \nu} \right) \dot{\lambda}^\mu \dot{\lambda}^\nu = g_{\mu \nu} \dot{\lambda}^\mu \dot{\lambda}^\nu ,
\] (3.18)

\(^4\)More accurately, \( \hat{H}_0 = \hat{H} - \hat{I} E_0 \), where \( \hat{I} \) is the identity operator and \( \dim \hat{I} \equiv \dim \hat{H} \). For simplicity, we write \( \hat{H}_0 = \hat{H} - E_0 \) and relabel \( \hat{H}_0 \equiv \hat{H} \).
where in the last equality, the contribution from $F_{\mu\nu}$ vanishes in the implicit sum due to its anti-symmetric nature.

The metric tensor thus defines the leading (up to fourth-order in $\dot{\lambda}^\mu$) non-adiabatic correction to the energy fluctuation,

$$\Delta E^2 = g_{\mu\nu} \dot{\lambda}^\mu \dot{\lambda}^\nu. \quad (3.19)$$

Finally, we note that due to energy conservation, the energy fluctuations in a closed system equals the fluctuations of the work done on the system, $\Delta W^2$. Therefore, the quantum metric tensor can as well be obtained through the measurement of the work fluctuations. We emphasize that this result is not tied to the ground-state, as it applies to any other initial eigenstate.

### 3.2.1 Geodesics as Critical Paths for the Squared Energy Fluctuation

The action

$$\mathcal{E}_0^T(\gamma) = \frac{1}{2} \int_0^{t_f} \left( g_{\mu\nu} \frac{d\lambda^\mu}{dt} \frac{d\lambda^\nu}{dt} \right) dt = \frac{1}{2 t_f} \int_0^1 \left( g_{\mu\nu} \frac{d\lambda^\mu}{d\tau} \frac{d\lambda^\nu}{d\tau} \right) d\tau \equiv \tilde{\mathcal{E}}(\gamma), \quad (3.20)$$

from which one derives the geodesic equation by performing $\delta \tilde{\mathcal{E}} = 0$ implies that, along the stationary curve, the above integrand is a constant of motion. As shown in the previous section (Equation (3.19)), the constant of motion is equal to the squared energy fluctuation $\Delta E^2 \equiv \langle \Psi|\hat{H}^2|\Psi \rangle - (\langle \Psi|\hat{H}|\Psi \rangle)^2$. The integrand of $\mathcal{E}_0^T$ along $\dot{\gamma}$ is therefore constant and equal to $(1/2 t_f) \Delta E^2$.

### 3.2.2 Measuring the Quantum Metric Tensor from Energy Fluctuations

Equation (3.19) establishes a way to directly measure the quantum metric experimentally as the leading-order non-adiabatic response of a quantum system (Kolodrubetz et al., 2013).

As an illustrative example, consider a quantum system depending on two externally tunable parameters, $\lambda_x$ and $\lambda_z$. We prepare the system at $t = 0$ in its ground-state $|\Psi_0(t = 0)\rangle$ for an initial set of values $(\lambda_{x_i}, \lambda_{z_i})$. The goal is to measure the quantum metric tensor of
the ground-state at a given point \((\lambda_{xf}, \lambda_{zf})\),
\[
g(\lambda_{xf}, \lambda_{zf}) = \begin{pmatrix}
g_{xx}(\lambda_{xf}, \lambda_{zf}) & g_{xz}(\lambda_{xf}, \lambda_{zf}) \\
g_{zx}(\lambda_{xf}, \lambda_{zf}) & g_{zz}(\lambda_{xf}, \lambda_{zf})
\end{pmatrix}.
\]
(3.21)

We assume no prior knowledge of the system’s Hamiltonian. Therefore, we propose a method to measure the quantum metric tensor \(g_{\mu\nu}\) through the energy fluctuation at the point \((\lambda_{xf}, \lambda_{zf})\) by performing linear ramps arriving from three mutually independent directions (Anandan and Aharonov, 1990; Kolodrubetz et al., 2013). These three measurements are sufficient to determine the quantum metric tensor since \(g_{\mu\nu}\) is a symmetric tensor.

Initially, assume \(\lambda_z\) fixed, i.e., \(\lambda_z = \lambda_{zf}\) and adiabatically change \(\lambda_x\) according to \(\lambda_x(t) = v_x t + \lambda_{x0}, 0 \leq t \leq t_f\), such that \(\lambda_x(t_f) = \lambda_{xf}\). The energy fluctuation of the ground-state after the ramp is given by
\[
\Delta E^2 = \langle \Psi(t_f)|\hat{H}^2|\Psi(t_f)\rangle - \langle \Psi(t_f)|\hat{H}|\Psi(t_f)\rangle^2.
\]
(3.22)

Equation (3.19) allows to write the quantum metric element \(g_{xx}\) as
\[
g_{xx} = \frac{\Delta E_x^2}{v_x^2}.
\]
(3.23)
The same reasoning is used to obtain \(g_{zz}\), by fixing \(\lambda_x\) and varying \(\lambda_z\) \((x \leftrightarrow z)\),
\[
g_{zz} = \frac{\Delta E_z^2}{v_z^2}.
\]
(3.24)
Finally, for the non-diagonal term \(g_{xz}\), define \(\lambda_w = (\lambda_x + \lambda_z)/2\) and ramp along the line \(\lambda_x = \lambda_w\) (Anandan and Aharonov, 1990). This yields \(d\lambda_x = d\lambda_z = d\lambda_w\), which implies
\[
ds^2 = g_{xx}d\lambda_x^2 + 2g_{xx}d\lambda_x d\lambda_z + g_{zz}d\lambda_z^2 = g_{ww}d\lambda_w^2 = (g_{xx} + 2g_{xz} + g_{zz})d\lambda_w^2.
\]
(3.25)
From the last equality, we extract the off-diagonal element as
\[
g_{xz} = \frac{1}{2}(g_{ww} - g_{xx} - g_{zz}),
\]
(3.26)
where \(g_{xx}\) and \(g_{xx}\) have been measured at first.
3.3 Geodesics for Non-Exactly Solvable Systems

For systems that are not exactly solvable, the expression for the quantum geometric tensor can be obtained numerically. More importantly, geodesic paths for such systems are also obtainable with proper numerical techniques. The main difficulty to solve the geodesic equations numerically lies in the computation of the Christoffel symbols,

$$\Gamma^\mu_{\nu\rho} = \frac{1}{2} g^{\mu\xi} \left( \frac{\partial g_{\xi\nu}}{\partial \lambda^\rho} + \frac{\partial g_{\xi\rho}}{\partial \lambda^\nu} - \frac{\partial g_{\nu\rho}}{\partial \lambda^\xi} \right),$$

since they depend on derivatives of the quantum metric tensor. In this section, we show the analytical expression for derivatives of the QGT.

3.3.1 Analytic Expressions for Numerical Simulations

The Quantum Geometric tensor is defined by

$$\chi_{\beta\gamma} = \sum_{m \neq n} \langle \Psi_n | \tilde{\partial}_\beta | \Psi_m \rangle \langle \Psi_m | \partial_\gamma | \Psi_n \rangle . \quad (3.27)$$

Using the expressions for bra/ket derivatives in terms of Hamiltonian derivatives\(^5\),

$$\chi_{\beta\gamma} = \sum_{m \neq n} \langle \Psi_n | \tilde{\partial}_\beta | \Psi_m \rangle \langle \Psi_m | \partial_\gamma | \Psi_n \rangle = \sum_{m \neq n} \frac{\langle \Psi_n | \partial_\beta \hat{H} | \Psi_m \rangle \langle \Psi_m | \partial_\gamma \hat{H} | \Psi_n \rangle}{(E_n - E_m)^2} \quad (3.28)$$

Let us define the notations,

$$\tilde{M}_\mu = \partial_\mu \hat{H}, \quad M_{\mu}^{nm} \equiv \langle \Psi_n | \partial_\mu \hat{H} | \Psi_m \rangle = \langle \Psi_n | \tilde{M}_\mu | \Psi_m \rangle ,$$

$$M_{ \mu}^{nm} = \langle \Psi_n | \partial_\mu \hat{H} | \Psi_n \rangle = \partial_\mu E_n , \quad \Delta_{nm} \equiv E_n - E_m . \quad (3.29)$$

We thus rewrite the QGT as

$$\chi_{\beta\gamma} = \sum_{m \neq n} \frac{\langle \Psi_n | \tilde{M}_{\beta} | \Psi_m \rangle \langle \Psi_m | \tilde{M}_{\gamma} | \Psi_n \rangle}{(E_n - E_m)^2} . \quad (3.30)$$

This expression can be used to calculate \(\chi_{\beta\gamma}\) by numerically diagonalizing for the eigenenergies and eigenstates, and performing the derivative operation directly on the known Hamiltonian \(\hat{H}\).

\(^5\)These expressions are detailedly derived in Appendix D.
Derivative of the Quantum Geometric Tensor

From Equation (3.30), we calculate the derivative of the geometric tensor $\partial_\alpha \chi_{\beta\gamma}$, given by

$$\partial_\alpha \chi_{\beta\gamma} = \partial_\alpha \left[ \sum_{m \neq n} \frac{\langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle}{(E_n - E_m)^2} \right]$$

$$= \sum_{m \neq n} \Delta_{nm}^{-2} \left[ \partial^2 \hat{H} - \frac{\partial_\beta \Delta_{nm} M_{\alpha m} M_{\gamma n}^{\alpha}}{\Delta_{nm}} + \frac{\partial_\gamma \Delta_{nm} M_{\beta n} M_{\alpha m}^{\gamma}}{\Delta_{nm}} + 2 \partial_\alpha \Delta_{nm} M_{\beta m} M_{\gamma n}^{\alpha} \right] +$$

$$+ \sum_{\ell \neq n, m} \frac{M_{\alpha \ell} M_{\beta m} M_{\gamma n}^{\alpha} + M_{\beta \ell} M_{\gamma n}^{\gamma} + M_{\alpha \ell} M_{\beta m} M_{\gamma n}^{\alpha} + M_{\beta \ell} M_{\gamma n}^{\gamma} + M_{\alpha \ell} M_{\beta m} M_{\gamma n}^{\alpha} + M_{\gamma n}^{\alpha}}{\Delta_{n\ell}} \right], \quad (3.31)$$

where $\partial^2 \hat{H} = \langle \Psi_n | \partial_\alpha \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \partial_\alpha \hat{M}_\gamma | \Psi_n \rangle$.

Since $\text{Re} (\partial_\alpha \chi_{\beta\gamma}) = \partial_\alpha g_{\beta\gamma}$, by taking the real part of the above expression, the Christoffel symbols can be numerically calculated, and the geodesic equations are thus solvable numerically.

---

A careful derivation of this expression can be found in Appendix E.
Chapter 4

Berry Connection and Curvature

If there is a God, He is a great mathematician.

– Paul Dirac, quoted by Margit Wigner.

4.1 Berry connection

We start differentiating by \( \partial_\mu \) both sides of the normalization condition for quantum states, \( \langle \Psi \mid \Psi \rangle = \text{const.} \),

\[
\partial_\mu (\langle \Psi \mid \Psi \rangle) = 0 \implies \langle \partial_\mu \Psi \mid \Psi \rangle + \langle \Psi \mid \partial_\mu \Psi \rangle = 0 \implies \langle \Psi \mid \partial_\mu \Psi \rangle = -\langle \partial_\mu \Psi \mid \Psi \rangle .
\] (4.1)

Since \( \langle \Psi \mid \partial_\mu \Psi \rangle = (\langle \partial_\mu \Psi \mid \Psi \rangle)^* \equiv \alpha \), we can rewrite Eq. (4.1) as \( \alpha = -\alpha^* \), which lead us to the mutually excluding conclusion:

- \( \alpha = 0 \) if \( \langle \Psi \mid \partial_\mu \Psi \rangle \in \mathbb{R} \);
- \( \alpha \) is purely imaginary and can be written as \( i \text{Im}\{\alpha}\).

We thus define the Berry connection \( A_\mu \) by

\[
A_\mu \equiv i \langle \Psi \mid \partial_\mu \Psi \rangle .
\] (4.2)

The above expression can be rewritten as

\[
A_\mu = i \langle \Psi \mid \partial_\mu \Psi \rangle = \langle \Psi \mid i \partial_\mu \mid \Psi \rangle \equiv \langle \Psi \mid \hat{A}_\mu \mid \Psi \rangle ,
\] (4.3)
where we defined the Berry connection gauge operator $\hat{A}_\mu \equiv i \partial_\mu$. The Berry connection is the expectation value of $\hat{A}_\mu$ over a given quantum state.

**Conclusion:** The Berry connection is the product of two purely imaginary numbers, $i$ and $\alpha$, so it is a real number, unless $\alpha$ is a real number, in which case the Berry connection vanishes. The Berry connection gauge operator $\hat{A}_\mu$ is an Hermitian operator since its expectation value is always a real number\(^1\).

### 4.2 Berry curvature

Let us now obtain an expression for the Berry curvature. Differentiating the Berry connection $A_\nu$ by $\partial_\mu$,

$$
\partial_\mu A_\nu = \partial_\mu (\langle \Phi | \hat{A}_\nu | \Phi \rangle) = (\partial_\mu \langle \Phi | \hat{A}_\nu | \Phi \rangle) + \langle \Phi | \partial_\mu (\hat{A}_\nu | \Phi \rangle) .
$$

(4.4)

Recap Eq. (4.1),

$$
\langle \Phi | \Phi \rangle = \text{const.} \implies (\partial_\mu \langle \Phi | | \Phi \rangle + \langle \Phi | (\partial_\mu | \Phi \rangle) = 0 \implies (\partial_\mu \langle \Phi | | \Phi \rangle = -\langle \Phi | (\partial_\mu | \Phi \rangle .
$$

(4.5)

Introduce the notation $\partial_\mu \langle \Phi \equiv \langle \Phi | \tilde{\partial}_\mu \equiv \langle \Phi | \partial_\mu | \Phi \rangle$, and one can rewrite Eq. (4.5) as

$$
\langle \Phi | \tilde{\partial}_\mu | \Phi \rangle = -\langle \Phi | \partial_\mu | \Phi \rangle \iff \langle \partial_\mu | \Phi \rangle = -\langle \Phi | \partial_\mu | \Phi \rangle ,
$$

(4.6)

which is sensible, since in the previous section we showed the Berry connection to be a purely imaginary number. Thus, from the definition for $\hat{A}_\nu \equiv i \partial_\nu$, Eq. (4.4) is equivalent to

$$
\partial_\mu A_\nu = i (\langle \partial_\mu \Phi | \partial_\nu \Phi \rangle + \langle \Phi | \partial_\mu \partial_\nu | \Phi \rangle) = i \left( \langle \Phi | \tilde{\partial}_\mu \partial_\nu | \Phi \rangle + \langle \Phi | \partial_\mu \partial_\nu | \Phi \rangle \right) = \langle \Phi | \tilde{\partial}_\mu \hat{A}_\nu | \Phi \rangle + \langle \Phi | \partial_\mu \hat{A}_\nu | \Phi \rangle .
$$

(4.7)

At this point, one needs to be careful about the notation, since $\langle \Phi | \tilde{\partial}_\mu \partial_\nu | \Phi \rangle \neq -\langle \Phi | \partial_\mu \partial_\nu | \Phi \rangle$.

The reason lies on the fact that in Eq. (4.1), we started from the equality $\langle \Phi | \Phi \rangle = \text{const.}$, from which we concluded $\tilde{\partial}_\mu = -\partial_\mu$. It was crucial, however, that the right-hand side of

\(^1\)This is a consequence of the *Spectral Theorem* (Reed and Simon, 1980).
the equality was a constant, independently of \(\mu\), so taking the partial derivative gave a vanishing result.

As a general illustrative example, let us carry out the same derivation for two distinct orthonormal vectors, labeled by \(n, m\),

\[
\langle \Psi_n | \Psi_m \rangle = \delta_{nm} \implies \langle \Psi_n | \partial_\mu | \Psi_m \rangle = -\langle \Psi_n | \partial_\mu | \Psi_m \rangle,
\]

\[
\partial_\mu = -\partial_\mu, \text{ if } \{m, n\} \text{ satisfy } \langle \Psi_n | \Psi_m \rangle = \delta_{nm}.
\]

Back to Equation (4.4), for notational simplicity, we write \(\hat{A}_\mu | \varphi \rangle \equiv | \varphi \rangle, \)

\[
\partial_\mu A_\nu = \langle \Psi | \partial_\mu | \varphi \rangle + \langle \Psi | \partial_\mu | \varphi \rangle.
\]

Since |\(\Psi\rangle\) and |\(\varphi \rangle\) are not required to be orthonormal, the relation \(\partial_\mu = -\partial_\mu\) does not necessarily hold.

The correct relationship is given by

\[
\langle \Psi | \partial_\mu \partial_\nu | \Psi \rangle = \text{const.} \implies \langle \Psi | \partial_\nu \partial_\mu | \Psi \rangle + \langle \Psi | \partial_\mu \partial_\nu | \Psi \rangle = 0,
\]

\[
\partial_\mu \left( \langle \Psi | \partial_\nu | \Psi \rangle + \langle \Psi | \partial_\nu | \Psi \rangle \right) = \langle \Psi | \partial_\nu \partial_\mu | \Psi \rangle + \langle \Psi | \partial_\nu \partial_\mu | \Psi \rangle + \langle \Psi | \partial_\nu \partial_\mu | \Psi \rangle + \langle \Psi | \partial_\mu \partial_\nu | \Psi \rangle = 0,
\]

so the correct expression for \(\langle \Psi | \partial_\mu \partial_\nu | \Psi \rangle\) is given by

\[
\langle \Psi | \partial_\mu \partial_\nu | \Psi \rangle = -\left( \langle \Psi | \partial_\nu \partial_\mu | \Psi \rangle + \langle \Psi | \partial_\nu \partial_\mu | \Psi \rangle + \langle \Psi | \partial_\mu \partial_\nu | \Psi \rangle \right).
\]

Back to Eq. (4.7), we now write the full expression for \(F_{\mu \nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu, \)

\[
F_{\mu \nu} = \partial_\mu A_\nu - \partial_\nu A_\mu = \left( \langle \Psi | \partial_\mu \hat{A}_\nu | \Psi \rangle + \langle \Psi | \partial_\mu \hat{A}_\nu | \Psi \rangle \right) - \left( \langle \Psi | \partial_\nu \hat{A}_\mu | \Psi \rangle + \langle \Psi | \partial_\nu \hat{A}_\mu | \Psi \rangle \right)
\]

\[
= \left( \langle \Psi | \partial_\mu \hat{A}_\nu | \Psi \rangle - \langle \Psi | \partial_\nu \hat{A}_\mu | \Psi \rangle \right) - \left( \langle \Psi | \partial_\nu \hat{A}_\mu | \Psi \rangle - \langle \Psi | \partial_\mu \hat{A}_\nu | \Psi \rangle \right)
\]

\[
= \langle \Psi | \left( \partial_\mu \hat{A}_\nu - \partial_\nu \hat{A}_\mu \right) | \Psi \rangle - \langle i | \partial_\mu \hat{A}_\nu - \partial_\nu \hat{A}_\mu | \Psi \rangle = -i \langle \Psi | \left( i \partial_\mu \hat{A}_\nu - i \partial_\nu \hat{A}_\mu \right) | \Psi \rangle,
\]

where we have restrained the focus to abelian gauge fields, so the second term vanishes, and multiplied the remaining equation by \(1 = -i^2\). Writing \(i \partial_\mu \equiv \hat{A}_\mu^\dagger = \hat{A}_\mu, \) one gets a final formal expression for \(F_{\mu \nu}\) in terms of the Berry connection gauge operator,

\[
F_{\mu \nu} = i \langle \Psi | [\hat{A}_\mu, \hat{A}_\nu] | \Psi \rangle.
\]
4.3 Covariant definition of the Berry connection

In the previous section, a coordinate system defined by the set of $\{\mu\}$ has been chosen. One can write the Berry connection in a covariant form\(^2\) by making use of the exterior derivative operator $d$,

$$A \equiv \langle \Psi | i d | \Psi \rangle . \quad (4.14)$$

The Berry connection is a one-form in the parameter space manifold $\mathcal{M}$. A one-form is associated with a vector in any given manifold, and can be written in a coordinate set by choosing a coordinate system. The manifold $\mathcal{M}$ is defined by the variable parameters in the Hamiltonian $\hat{H} \equiv \hat{H}(\vec{\lambda})$, the operator defining $|\Psi\rangle \equiv |\Psi(\vec{\lambda})\rangle$ through Schrödinger equation. As an illustrative example, consider the ground-state $|\Psi\rangle = |\Psi_0\rangle$ of a quantum system. The system’s Hamiltonian is a function of the parameters $\vec{\lambda} \equiv (\lambda_1, \lambda_2, \ldots)$, and the ground-state changes as a function of $\vec{\lambda}$, defining a fiber bundle $\eta$ on the projective Hilbert space $\mathcal{PH}$ by the following equation

$$\hat{H}(\vec{\lambda}) |\Psi_0(\vec{\lambda})\rangle = E_0(\vec{\lambda}) |\Psi_0(\vec{\lambda})\rangle . \quad (4.15)$$

The projective Hilbert space is defined by the equivalence class of vectors $[|\Psi_0\rangle]$, as one can multiply the state by an arbitrary phase $\exp(i \theta)$ and it will not affect observables measured from the state. We define the equivalence class $[|\Psi(\lambda)\rangle] \equiv \{e^{i\theta} \sim |\Psi(\lambda)\rangle\}$, and the set of all elements in this equivalence class defines the manifold $\mathcal{PH}$.

The definition of the projective Hilbert space $\mathcal{PH}$ above highlights the fact that $A$ is a gauge field. One can choose any element belonging to the equivalence class $[|\Psi(\lambda)\rangle]$ to calculate $A$, which corresponds to what is referred as making a gauge choice.

---

\(^2\)i.e., independent of choice for a coordinate system.
4.4 Covariant definition of the Berry curvature

The Berry curvature is a two-form (i.e., a tensor) obtained from the Berry connection by taking its exterior derivative,

$$ F \equiv dA. \quad (4.16) $$

This definition implies that $F$ is a exact form (it is writeable as the exterior derivative of a one form) and a closed form (its exterior derivative vanishes, since $ddf \equiv 0$ by definition)\(^3\).

A couple of interesting consequences arise from the definition,

- $dF = ddA = 0$ if $A$ is smooth, since $d(d)f = 0$ for any smooth function $f$.

This last statement implies that $F$ is also a closed form, i.e. $dF = 0$. Of course it is, since every exact form is closed, as can be inferred from the general statement I made for $d^2f = 0$ above. The converse is not always true, and the Poincaré Lemma states the conditions for which the converse is valid.

---

\(^3\)Formally, a $k$-form is said to be closed if $d\omega = 0$, and $\omega$ is said to be exact if $\omega = d\alpha$ for some $(k-1)$-form $\alpha$. Since by the exterior derivative definition $d^2 = 0$, every exact form is also closed.
The exterior derivative $d$ allows us to write $A$ in a given basis as

$$A = A_\nu dx^\nu,$$

(4.17)

where $A_\mu$ are the components of the one-form Berry connection. Using Eq. (4.16), we can write an expression for $F$ in a given basis as

$$F_{\mu\nu} dx^\mu dx^\nu = \partial_\mu A_\nu dx^\mu \wedge dx^\nu,$$

(4.18)

where $\wedge$ is the wedge product operator. A notable property of the wedge product is that it is anti-symmetric, i.e., $dx^\mu \wedge dx^\nu = -dx^\nu \wedge dx^\mu$, which obviously implies that $dx^\mu \wedge dx^\mu = 0$. Thus, elements in the sum on Eq. (4.16) can be rewritten in the more familiar fashion,

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu.$$

(4.19)

Finally, notice that the Berry curvature $F$ is a gauge invariant quantity, for if we rewrite $A \to A + d\phi$, the Berry curvature remains unchanged since $dF = dA + d^2\phi = dA$.

### 4.5 Berry connection and curvature expressed in local coordinates

As discussed in the previous section, the Berry connection is a connection one-form on the parameter space $\mathcal{M}$, defined in general by $A \equiv i\langle \Psi | d | \Psi \rangle$, with $d$ the exterior derivative operator. The Berry curvature is an exact two-form, defined by $F = dA$.

The Berry connection can be written in local coordinates $(x^1, x^2, \ldots)$ as

$$A = A_\mu dx^\mu, \quad A_\mu = i\langle \Psi | \partial_\mu | \Psi \rangle,$$

(4.20)

and where $\partial_\mu = \partial/\partial x^\mu$, $\mu = 1, 2, \ldots$.

Similarly, the Berry curvature in local coordinates reads

$$F = \frac{1}{2} F_{\mu\nu} dx^\mu \wedge dx^\nu, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu,$$

(4.21)

\[ \text{This is the definition of how an exterior derivative is applied on a } k\text{-form.} \]
where $dx^\mu \wedge dx^{\nu}$ is the wedge product of two one-forms.

For a three-dimensional parameter space $\mathcal{M}$, the components of the Berry connection one-form $A_\mu$ can be collected in a vector as $\vec{A} = i \langle \Psi | \nabla | \Psi \rangle$. Similarly, the Berry curvature two-form can be mapped to a vector through the Levi-Civita connection, $F_k = \epsilon^{ijk}F_{ij}$, also written as $\vec{F} = \nabla \times \vec{A}$.

Such mapping is seen explicitly from the Berry curvature definition in local coordinates, $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, an antisymmetric tensor. In three dimensions, it reduces to

$$
(F_{\mu\nu}) = \begin{pmatrix}
F_{11} & F_{12} & F_{13} \\
F_{21} & F_{22} & F_{23} \\
F_{31} & F_{32} & F_{33}
\end{pmatrix}
= \begin{pmatrix}
0 & F_3 & -F_2 \\
-F_3 & 0 & F_1 \\
F_2 & -F_1 & 0
\end{pmatrix},
$$

(4.22)

and thus we can write $\vec{F} = (F_1, F_2, F_3)^T = (F_{23}, F_{31}, F_{12})^T$.

In view of the discussion in the previous paragraph, the Berry connection in Cartesian coordinates, $(x, y, z)$, reads

$$
\vec{A}^{(C)}(x, y, z) = A_x \hat{x} + A_y \hat{y} + A_z \hat{z},
$$

(4.23)

where $A_\mu = i \langle \Psi | \partial_\mu | \Psi \rangle$, with $\mu = \{x, y, z\}$, $\partial_\mu = \partial/\partial \mu$, and $\hat{x}$, $\hat{y}$ and $\hat{z}$ are the unit vectors in Cartesian coordinates.

One should be wary, since there is a potential for ambiguity in this notation if a different choice of coordinate system is considered. For example, with respect to spherical coordinates $(r, \theta, \phi)$, the Berry connection becomes

$$
\vec{A}^{(S)}(r, \theta, \phi) = A_r \hat{r} + A_\theta \hat{\theta} + A_\phi \hat{\phi},
$$

(4.24)

where now we must define

$$
A_r = i \langle \Psi | \partial_r | \Psi \rangle,
$$

$$
A_\theta = i \frac{1}{r} \langle \Psi | \partial_\theta | \Psi \rangle,
$$

$$
A_\phi = i \frac{1}{r \sin \theta} \langle \Psi | \partial_\phi | \Psi \rangle,
$$

(4.25)
since in spherical coordinates the operator $\nabla$ is given by

$$\nabla f = \frac{\partial f}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial f}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} \hat{\phi}, \quad (4.26)$$

where

$$\hat{r} = \sin \theta \cos \phi \hat{x} + \sin \theta \sin \phi \hat{y} + \cos \theta \hat{z},$$

$$\hat{\theta} = \cos \theta \cos \phi \hat{x} + \cos \theta \sin \phi \hat{y} - \sin \theta \hat{z},$$

$$\hat{\phi} = -\sin \phi \hat{x} + \cos \phi \hat{y}, \quad (4.27)$$

are the local orthogonal unit vectors in the directions of increasing $r$, $\theta$ and $\phi$, respectively.

Note that the Cartesian unit vectors can be expressed as

$$\hat{x} = \sin \theta \cos \phi \hat{r} + \cos \theta \cos \phi \hat{\theta} - \sin \phi \hat{\phi},$$

$$\hat{y} = \sin \theta \sin \phi \hat{r} + \cos \theta \sin \phi \hat{\theta} + \cos \phi \hat{\phi},$$

$$\hat{z} = \cos \theta \hat{r} - \sin \theta \hat{\theta}, \quad (4.28)$$

or the spherical unit vectors as

$$\hat{r} = \frac{x \hat{x} + y \hat{y} + z \hat{z}}{\sqrt{x^2 + y^2 + z^2}},$$

$$\hat{\theta} = \frac{zx \hat{x} + yz \hat{y} - (x^2 + y^2) \hat{z}}{\sqrt{x^2 + y^2} \sqrt{x^2 + y^2 + z^2}},$$

$$\hat{\phi} = \frac{-y \hat{x} + x \hat{y}}{\sqrt{x^2 + y^2}}. \quad (4.29)$$

The Berry phase, given by the integral of the Berry connection along a closed loop $C$ in parameter space, can be written as

$$\gamma = \int_C \bar{A}^{(C)} \cdot d\vec{r} = \int_C \bar{A}^{(S)} \cdot d\vec{r}, \quad (4.30)$$

where $d\vec{r} = dx \hat{x} + dy \hat{y} + dz \hat{z}$ in Cartesian coordinates and $d\vec{r} = dr \hat{r} + r d\theta \hat{\theta} + r \sin \theta d\phi \hat{\phi}$ in spherical coordinates.
Chapter 5

Topological Transitions in Parameter Space

*The miracle of the appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve.*

– Eugene Wigner, in *The Unreasonable Effectiveness of Mathematics in the Natural Sciences.*

In this chapter, we study a system of two coupled qubits interacting with external magnetic fields. The analogy between the Berry curvature and magnetic fields in parameter space is outlined, with degeneracies in the spectrum associated to magnetic charges.

Sharp topological transitions on the charge distributions occur when symmetries are broken. This effect is used here to bypass crossing degeneracies – it enables adiabatic passages between regions adiabatically disconnected within a given parameter manifold. We also investigate the curl of the Berry curvature, which together with its divergence uniquely defines this field. Finally, we suggest a simple method for measuring the Berry curvature, with experimental results shown in chapter 6.

This chapter is based on Souza et al. (2015).
5.1 Introduction

We consider the case where the Hamiltonian of a system $H(\vec{\lambda})$ depends on three real-valued parameters $\vec{\lambda} = (\lambda^1, \lambda^2, \lambda^3)^T \in \mathbb{R}^3$, thereby describing a three-dimensional parameter space. Focusing on the ground-state manifold, the Berry phase $\gamma$ acquired by $|\Psi_0(\vec{\lambda})\rangle$ after the parameters evolve adiabatically along a closed path $C$ reads

$$\gamma(C) = \oint_C \vec{A} \cdot d\vec{\lambda} = \iint_S \vec{F} \cdot d\vec{S},$$

(5.1)

where $\vec{A} = i \langle \Psi_0 | \vec{\nabla} | \Psi_0 \rangle$ is the Berry connection. The last equality defines the Berry curvature $\vec{F} = \vec{\nabla} \times \vec{A}$, where the surface $S$ is bounded by the path $C$. The Berry connection behaves like a $U(1)$ gauge potential and therefore cannot directly be observed, whereas the Berry curvature is a local and gauge-invariant object manifesting the geometric properties of its associated eigenstate.

An analogy with electromagnetism (E&M), also presented by M. V. Berry (Berry, 1984), shows that the Berry connection plays the role of a magnetic vector potential and yields through its curl the Berry curvature, which can be interpreted as an effective magnetic field. For each degeneracy in the spectrum, one can choose a closed Gaussian surface $\Sigma_i$ that encloses it in parameter space. The flux of the Berry curvature through $\Sigma_i$ defines a topological quantized invariant

$$\text{ch}_1 = \frac{1}{2\pi} \iint_{\Sigma_i} \vec{F} \cdot d\Sigma_i,$$

(5.2)

known as the first Chern number. By noting that $\vec{\nabla} \cdot \vec{F} = \vec{\nabla} \cdot (\vec{\nabla} \times \vec{A})$, one can see that the Berry curvature has zero divergence except at singularities. These singularities correspond to the degeneracies in the spectrum of the Hamiltonian, which play the role of effective magnetic charges in parameter space. The first Chern number quantization simply reflects the quantization of these magnetic charges. Various systems illustrating this analogy have been studied, each exhibiting different monopole charge configurations in parameter space (Oh, 2009; Li et al., 2014; Wu et al., 2011; Wiener and Zhou, 2004; Sjöqvist et al., 2010; Viennot, 2006; Nesterov and Aceves de la Cruz, 2008; Bruno, 2006).
5.2 Two-qubit System

We consider a system of two interacting qubits (represented here by quantum spins−1/2), coupled to tunable external magnetic fields. This choice was inspired by a recent experiment which measured the Berry curvature (Roushan et al., 2014). The Hamiltonian of the system is given by

$$\hat{H} = \vec{B} \cdot (\gamma_1 \vec{\sigma}_1 + \gamma_2 \vec{\sigma}_2) + \frac{g}{2}(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + g_z \sigma_1^z \sigma_2^z + B_0 \sigma_1^z,$$

where $\vec{\sigma}_i \equiv (\sigma_i^x, \sigma_i^y, \sigma_i^z)^T$ are Pauli matrices for the $i$–th spin, $\vec{B}$ is the external magnetic field acting simultaneously on both spins, anisotropically (isotropically) if $\gamma_1 \neq \gamma_2$ ($\gamma_1 = \gamma_2$), $g$ describes the $xy$ coupling, $B_0$ is an offset magnetic field applied only to the first spin, breaking the exchange symmetry if non-zero, and $g_z$ indicates the interaction in the $z$ direction, which can turn the system into the $SU(2)$ Heisenberg Hamiltonian for the choice of constants $g_z = 1$, $g = 2$, $\gamma_1 = \gamma_2 = 1$ and $B_0 = 0$.

In the present analysis, we will fix $\gamma_1$, $\gamma_2$, $g$, $B_0$ and $g_z$ and restrict ourselves to consider the Berry curvature with respect to the external applied magnetic field $\vec{B} \in \mathbb{R}^3$, defining our parameter space. The vector $\vec{B}$ will interchangeably be written in spherical $(B, \theta, \phi)$ or Cartesian $(B_x, B_y, B_z) \equiv (x, y, z)$ coordinates, whichever is more convenient. The term $g$ merely sets the energy scale, and so we will consider units in which $g = 2$ from here onward.

The eigenenergies of (5.3) possess azimuthal symmetry, since the Hamiltonian and
ground-state at arbitrary $\phi$ are trivially connected to their expressions at $\phi = 0$. In other words,

$$\hat{H}(B, \theta, \phi) = R^1(\phi)H(B, \theta, 0)R(\phi), \quad (5.4)$$

where $R(\phi) = \exp(i \phi \sigma_z^{\text{tot}}/2)$, and similarly for the ground-state,

$$|\Psi_0(B, \theta, \phi)\rangle = R^\dagger(\phi)|\Psi_0(B, \theta, 0)\rangle. \quad (5.5)$$

The Hamiltonian is real at $\phi = 0$, and therefore a gauge choice is made requiring the eigenfunctions to be real-valued. As a consequence of this gauge, the components $A_B$ and $A_{\theta}$ of the Berry connection vanish, and the only non-zero component $A_\phi$ can be calculated explicitly.

$$\vec{A} = \frac{1}{B \sin \theta} \frac{\langle \sigma_z^{\text{tot}} \rangle}{2} \hat{\phi}. \quad (5.6)$$

One can thus use this result to experimentally measure the Berry connection by measuring the ground-state expectation value of the total magnetization, with the Berry curvature obtained by taking the curl of Eq. (5.6).

In analogy with E&M, one of Maxwell’s equations in $\mathbb{R}^3$ for the vector field $\vec{F}$ is

$$\vec{\nabla} \cdot \vec{F} = 2\pi \rho_m, \quad (5.7)$$

with $\rho_m$ denoting the effective magnetic charge density. The expression above is nothing but the differential form of Eq. (5.2), showing that the divergence of $\vec{F}$ is equal to the effective magnetic charge (first Chern number). The role of Chern numbers as topological quantifiers in quantum systems has been widely investigated, and it is still a very active field (Wen, 2004; Bernevig and Hughes, 2013). A direct measurement of the Berry curvature was proposed in (Gritsev and Polkovnikov, 2012; Avron et al., 2011), where it was shown to be given by the non-adiabatic response of certain physical observables. This was experimentally confirmed with systems of superconducting qubits (Schroer et al., 2014; Roushan et al., 2014), where the first Chern number quantization was readily confirmed.

However, the role of $\vec{\nabla} \times \vec{F}$ has not been explored so far. In three-dimensional space, any vector field is uniquely represented by its divergence and curl. The divergence of $\vec{F}$,
as seen from Eq. (5.7), is given by effective magnetic charges, while the curl is analogous to “electric” currents. In what follows, we then study in detail the divergence and curl of $\mathbf{F}$ for different fixed set of values of the parameters $\gamma_1, \gamma_2, g_z$ and $B_0$. We start with the choice that makes the Hamiltonian (5.3) $SU(2)$ symmetric, and break symmetries in each subsequent case.

### 5.3 Heisenberg interaction

The simplest system extending the aforementioned E&M analogy to continuous magnetic charge densities has the Hamiltonian

$$\hat{H}_{\text{Heis}} = \mathbf{B} \cdot (\mathbf{\hat{\sigma}}_1 + \mathbf{\hat{\sigma}}_2) + \mathbf{\hat{\sigma}}_1 \cdot \mathbf{\hat{\sigma}}_2.$$  \hspace{1cm} (5.8)

A similar system and its charge configuration was studied in (Oh, 2009). The Hamiltonian $\hat{H}_{\text{Heis}}$ corresponds to the two-spin Heisenberg model in an external $\mathbf{B}$ field. It is obtained from the Hamiltonian (5.3) by setting the parameters to $\gamma_1 = \gamma_2 = g_z = 1$, $B_0 = 0$. The parameter space is $\mathcal{M} \equiv \mathbb{R}^3$, defined in local spherical coordinates by $(B, \theta, \phi)$. This Hamiltonian has $SU(2)$ symmetry, which can be seen immediately using spherical coordinates $(B, \theta, \phi)$

$$\hat{H}_{\text{Heis}}(B, \theta, \phi) = B \mathbf{\hat{B}}(\theta, \phi) \cdot (\mathbf{\hat{\sigma}}_1 + \mathbf{\hat{\sigma}}_2) + \mathbf{\hat{\sigma}}_1 \cdot \mathbf{\hat{\sigma}}_2.$$  \hspace{1cm} (5.9)

Namely, one observes that

$$D(\mathbf{\hat{B}}, \alpha) \hat{H}_{\text{Heis}} D^\dagger(\mathbf{\hat{B}}, \alpha) = H_{\text{Heis}},$$  \hspace{1cm} (5.10)

where $D(\mathbf{\hat{B}}, \alpha) = \exp[i \alpha \mathbf{\hat{B}} \cdot (\mathbf{\hat{\sigma}}_1 + \mathbf{\hat{\sigma}}_2)]$ is a generic element of $SU(2)$ and can be interpreted as a rotation around the axis $\mathbf{\hat{B}}(\theta, \phi)$ by an angle $\alpha$. The system also has exchange symmetry between $\mathbf{\hat{\sigma}}_1 \leftrightarrow \mathbf{\hat{\sigma}}_2$.

Using the property $\hat{H}_{\text{Heis}}(B, \theta, \phi) = R^\dagger(\phi) \hat{H}_{\text{Heis}}(B, \theta, 0) R(\phi)$, we calculate the eigenenergies, eigenstates, and thus the Berry connection.
Figure 5.2: **Left:** The Berry curvature in Cartesian coordinates (5.16) is plotted in parameter space ($B_x, B_y, B_z$). The sphere of radius $B = 2$ carries a magnetic charge $q_m = 2$, which is uniformly distributed over the surface of this sphere. **Right:** The Energy spectrum of the Heisenberg Hamiltonian $H_{\text{Heis}}$ as a function of $B$ is depicted. The ground-state energy $E_0(B)$ is shown by the thick red line.

### Eigenenergies and Eigenstates

The ground-state energy is given by

$$E_0(B) = \begin{cases} -3, & B < 2, \\ 1 - 2B, & B > 2, \end{cases} \quad (5.11)$$

and the corresponding ground-state reads

$$|\tilde{\Psi}_0(\phi)\rangle = \begin{cases} \frac{1}{\sqrt{2}}(0, 1, -1, 0)^T, \\ \left(e^{-i\phi} \sin^2 \frac{\theta}{2}, -\sin \frac{\theta}{2}, -\sin \frac{\theta}{2}, e^{i\phi} \cos^2 \frac{\theta}{2}\right)^T, \end{cases} \quad (5.12)$$

for $B < 2$ and $B > 2$, respectively, where we used the basis $\{|\uparrow\uparrow\rangle = (1, 0, 0, 0)^T, |\uparrow\downarrow\rangle = (0, 1, 0, 0)^T, |\downarrow\uparrow\rangle = (0, 0, 1, 0)^T, |\downarrow\downarrow\rangle = (0, 0, 0, 1)^T\}$, since $\{|\uparrow\rangle = (1, 0)^T, |\downarrow\rangle = (0, 1)^T\}$ are the eigenstates of $\sigma_i^z$.

As illustrated in what follows, this degeneracy surface can be interpreted as a magnetically charged sphere in parameter space which creates an effective magnetic field, the Berry curvature $\vec{F}$. 
Berry connection and curvature

The Berry connection in spherical coordinates can be calculated explicitly, and we find

\[ \vec{A}^{(S)}(B, \theta, \phi) = A_\phi \hat{\phi} = \begin{cases} 0, & B < 2, \\ -\frac{1}{B} \cot \theta \hat{\phi}, & B > 2, \end{cases} \]  

(5.13)

The Berry curvature, obtained by taking the curl of \( \vec{A}^{(S)}(B, \theta, \phi) \) in spherical coordinates, reads

\[ \vec{F}^{(S)}(B, \theta, \phi) = \frac{1}{B \sin \theta} \partial_\theta (A_\phi \sin \theta) \hat{B} = \begin{cases} 0, & B < 2, \\ \frac{1}{2} q_m \frac{1}{B^2} \hat{B}, & B > 2, \end{cases} \]  

(5.14)

where \( q_m = 2 \) can be interpreted as an effective magnetic charge. The Berry curvature allows us to read the first Chern number, which indeed corresponds to the effective magnetic charge \( q_m \),

\[ \text{ch}_1 = \frac{1}{2\pi} \int \int \vec{F}^{(S)} \cdot d\vec{S} = \frac{1}{2\pi} \int_0^\pi \int_0^{2\pi} \frac{1}{B^2} B^2 \sin \theta d\theta d\phi = 2 = q_m. \]  

(5.15)

We used the fact that the surface element \( d\vec{S} \) is strictly radial \( d\vec{S} = B^2 \sin \theta d\theta d\phi \hat{B} \), and choose a spherical Gaussian surface \( \Sigma \) centered at the origin with radius \( B > 2 \) to calculate the above integral. In Fig. 5.2 we show the spectrum of \( H_{\text{Heis}} \) and the effective magnetic field given by the Berry curvature

\[ \vec{F}^{(C)}(B_x, B_y, B_z) = \begin{cases} 0, & \sqrt{B_x^2 + B_y^2} < 2, \\ \frac{1}{2} q_m \frac{B}{(B_x^2 + B_y^2 + B_z^2)^{3/2}}, & \sqrt{B_x^2 + B_y^2 + B_z^2} > 2, \end{cases} \]  

(5.16)

for \( \sqrt{B_x^2 + B_y^2 + B_z^2} < 2 \) and \( \sqrt{B_x^2 + B_y^2 + B_z^2} > 2 \), respectively.

The ground-state degenerates on the sphere of radius \( B = 2 \), dividing the parameter space into two disjoint regions. The Berry curvature in this case is

\[ \vec{F} = \begin{cases} 0, & B < 2, \\ \frac{1}{2} q_m \frac{B}{B^2}, & B > 2, \end{cases} \]  

(5.17)

where \( q_m = 2 \) gives the effective magnetic charge.
5.3 \textit{XXZ-interaction} ($g_z = 0$): \textit{Left:} Berry curvature $\vec{F}$ (light arrows) and magnetic surface charge density $\sigma_m$ (colorbar). \textit{Right:} $\vec{\nabla} \times \vec{F}$, with magnitude shown in the $xz$-plane. The curl has only a $\phi$ component, and the colors on the ellipsoid illustrate the magnitude of the electric surface current density $\vec{K}_e = K_e \hat{\phi}$, with direction indicated by the darker arrows.

The effective magnetic field defined by the Berry curvature above is akin to the electric field of a hollow conducting sphere of radius two. The total magnetic charge is equal to the Chern number, $\text{ch}_1 = 2$, and can be obtained from Eq. (5.2). The magnetic charge density distribution $\rho_m$ is uniform since the sphere is a surface of constant curvature. The curl of $\vec{F}$ is equal to zero since the field falls of radially as $1/B^2$. This will not be the case in the following examples.

5.4 \textbf{XXZ interaction}

Consider now the case where $g_z \neq 1$, and as before, $\gamma_1 = \gamma_2 = 1$, $B_0 = 0$. The two-qubit Hamiltonian with XXZ interaction reads

$$\hat{H}_{\text{XXZ}} = \vec{B} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2) + (\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + g_z \sigma_1^z \sigma_2^z$$

$$= \vec{B} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2) + \vec{\sigma}_1 \cdot \vec{\sigma}_2 - (1 - g_z) \sigma_1^z \sigma_2^z. \quad (5.18)$$
Figure 5.4: Left: Locus of ground-state degeneracies (ellipsoid) of Eq. (5.20) in parameter space. Right: The lowest two eigenenergies of $H_{\text{XXZ}}$ as function of $B_x$, $B_z$ for $g_z = 0.01$ and $B_y = 0$. The singlet-state has constant energy ($E_{\text{singlet}} = -(2 + g_z)$), shown by the (orange) plane. It cuts the (blue) surface corresponding to the next lowest eigenenergy. The crossing curve (yellow), intersection of the two lowest eigenenergies, is given by an ellipse.

If $|g_z| < 1$ ($|g_z| > 1$), the $SU(2)$ symmetry is broken, and the charged sphere of the Heisenberg interaction case gets squeezed (stretched) along the $z$-axis, becoming an oblate (prolate) ellipsoid of revolution. In analogy to the charge distribution on conductors in electrostatics, the magnetic charge density is no longer uniformly distributed. Instead, it accumulates in regions of higher curvature (see Fig. 5.3, left panel). In spite of the non-uniform surface charge density, the total charge on the entire surface remains the same as for the Heisenberg interaction case ($ch_1 = 2$). This can be concluded from the fact that the ground-state remains fully polarized at large $B$, yielding the total effective charge enclosed as a topologically protected integer equal to $ch_1 = 2$.

Figure 5.3 (right panel) shows the existence of a surface current $\vec{K} \neq 0$ defined by the discontinuity of the parallel component of $\vec{F}$ across the surface, which implies that $\hat{\nabla} \times \vec{F} \neq 0$. The Berry curvature has only $\hat{B}$ and $\hat{\theta}$ components, and therefore its curl is parallel to $\hat{\phi}$. The non-uniform magnetic charge distribution produces a quadrupole in the curl of $\vec{F}$. 
Eigenergies and Eigenstates

Although the XXZ interaction Hamiltonian is no longer $SU(2)$ symmetric, it still has the exchange symmetry between the two-qubits. Further, due to the property $\hat{H}_{XXZ}(B, \theta, \phi) = R^\dagger(\phi) \hat{H}_{XXZ}(B, \theta, 0) R(\phi)$, we can set $B_y = 0$ and using a more appropriate basis given by $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}, (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}\}$, the Hamiltonian is written as a $4 \times 4$ matrix,

$$H_{XXZ} = \begin{pmatrix} 2B_z + g_z & 0 & \sqrt{2}B_x & 0 \\ 0 & -2B_z + g_z & \sqrt{2}B_x & 0 \\ \sqrt{2}B_x & \sqrt{2}B_x & 2 - g_z & 0 \\ 0 & 0 & 0 & -2 - g_z \end{pmatrix}. \quad (5.19)$$

One can immediately see that the singlet-state $\langle |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \rangle/\sqrt{2}$ is an eigenstate with eigenenergy $E_{\text{singlet}} = -(2 + g_z)$. More precisely, the singlet-state is the ground-state inside the locus of crossing points given by

$$\frac{B_z^2}{2(1 + g_z)} + \frac{B_y^2}{2(1 + g_z)} + \frac{B_z^2}{(1 + g_z)^2} = 1. \quad (5.20)$$

The above expression defines the surface of an ellipsoid in the parameter space $(B_x, B_y, B_z)$, and can be obtained by solving the equation for the energy crossing between the singlet-state and the only other state with negative energy for $B_y = 0$, applying next the rotation $R(\phi) = \exp(i \phi \sigma_{tot.}^z / 2)$ to obtain the result (5.20) for $B_y \neq 0$ (see Fig. 5.4). The ground-state inside the ellipsoid is thus the Bell entangled singlet-state

$$|\Psi_0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}} (0, 1, -1, 0)^T, \quad (5.21)$$

and hence the Berry connection vanishes inside the ellipsoid, since $\hat{A}^{(S)} = \frac{1}{B \sin \theta} \langle \sigma_{tot.}^z \rangle \hat{\phi}$. The Berry connection acquires only a non-zero value outside the ellipsoid, which was calculated numerically using the standard numerical diagonalization techniques. The corresponding Berry curvature and its curl are depicted in Fig. 5.6.
5.4.1 Surface and Charge Density on the Ellipsoidal Surface of Degen-
eracies

The magnetic surface charge density $\sigma_m$ and effective electric surface current $\vec{K}_e$ associated with the curl of $\vec{F}$ are calculated in the following by considering the discontinuity in the normal and parallel components of the magnetic field $\vec{F}$ across the degeneracy surface (the ellipsoid) (Griffiths, 1999). The magnetic surface charge density can be calculated from the identity

$$\left( F_{\perp}^{\text{out}} - F_{\perp}^{\text{in}} \right) = 2\pi \sigma_m, \quad (5.22)$$

where $F_{\perp}^{\text{out}}$ ($F_{\perp}^{\text{in}}$) refers to the perpendicular component of $\vec{F}$ just outside (inside) the charged boundary surface. The total charge $q_m$ in this example is obtained by $q_m = \frac{1}{2\pi} \iint_S \sigma_m(\vec{r}) \, dS$, where $dS$ is the differential area element of the ellipsoid surface. Further, the electric surface current can be calculated through

$$\hat{n} \times \left( \vec{F}_{\text{out}} - \vec{F}_{\text{in}} \right) = 2\pi \vec{K}_e, \quad (5.23)$$
Figure 5.6: a) Surface charge density $\sigma_m$ on the ellipsoid with $\vec{F}$ for $g_z = 0$. b) The corresponding $|\vec{F}|$ in the $xz$-plane. c) Surface electric current density $K_e$ with $\vec{\nabla} \times \vec{F}$ for $g_z = 0$. d) $(\vec{\nabla} \times \vec{F})_y$ in the $xz$-plane.

where $\vec{F}_{\text{out}}$ ($\vec{F}_{\text{in}}$) refers to $\vec{F}$ just outside (inside) the ellipsoid and $\hat{n}$ is a unit vector perpendicular to the surface. Both the surface charge density and surface current density are plotted in Fig. 5.5 versus the polar angle $\theta$ for different values of $g_z$. We note that the property $\hat{H}_{XXZ}(B, \theta, \phi) = R^\dagger(\phi)\hat{H}_{XXZ}(B, \theta, 0)R(\phi)$ implies that $\sigma_m$ and $K_e$ are independent of the azimuthal angle $\phi$. In Fig. 5.6 we plot $\sigma_m$ and $K_e$ on the surface of the ellipsoid. The total charge was also computed numerically and found to be $q_m = +2$ for any value of $g_z$, as required from topological considerations ($ch_1 = 2$).

In the previous two cases we have explored situations of high symmetry, where the magnetic charges occur as surface densities spread on closed degeneracy surfaces, instead of the more commonly studied discrete monopole charges (Berry, 1984). Similar cases of continuous surfaces with magnetic charge densities have been explored elsewhere (Oh, 2009). The new aspect of the aforementioned results is shown by the curl of the Berry curvature, which displays a characteristic quadrupole pattern.

### 5.5 Bypassing degeneracy crossings

The points belonging to the closed surfaces in the two previous cases indicate the locus in parameter space where there are degeneracies in the ground-state. Interestingly, inside all the previous surfaces, the ground-state is a singlet $|\Psi_0\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, i.e., a Bell
entangled state of the two qubits. Equation (5.6) then implies a vanishing Berry connection and curvature; in the region outside the closed surfaces, $|\Psi_0\rangle$ has contributions of the other vectors in the spin-product basis. At first sight, it might seem impossible to experimentally start with a high polarizing field $B_z \gg B_x \approx 0$ where $|\Psi_0\rangle \approx |\uparrow\uparrow\rangle$ to subsequently prepare adiabatically a pure singlet-state without crossing the continuous degeneracy surface, which would introduce excitations and break the adiabaticity. The procedure is illustrated in figure 5.7, and it goes as follows: We start from a point in parameter space corresponding to a state outside the sphere defined by the Heisenberg Hamiltonian (first panel). Next, as depicted in the second and third panel, we adiabatically break the symmetry by introducing a pinning field in one of the spins. This creates a different topological magnetic charge distribution (with the total magnetic charge conserved). One can now evolve the system to a previously adiabatically inaccessible region. Finally, we reintroducing the symmetry by removing the symmetry-breaking term, allowing one to bypass the continuous crossing surface and enter a previously adiabatically disconnected region in parameter space (fourth panel).

In order to bypass this topological constraint, we now consider situations with significantly reduced symmetry, and we observe a sharp collapse of the surface charge density to the more familiar case of magnetic monopoles. This singular change in the topology of the monopole charge density is unlike anything in classical E&M, and we explore this
phase transition to open a passage and access the interior regions of the previous cases by adiabatically breaking and reestablishing symmetries (see Fig. 5.7). We also show how the effective electromagnetic fields respond to this transition.

5.6 Anisotropic fields

Anisotropy is introduced by setting $\gamma_1 = 1 + \alpha$, $\gamma_2 = 1 - \alpha$ with $\alpha \neq 0$ and $g_z = B_0 = 0$. The two-qubit anisotropic Hamiltonian has the magnetic field $\vec{B}$ acting anisotropically on each spin,

$$\hat{H}_{\text{ani}} = \vec{B} \cdot [(1 + \alpha) \vec{\sigma}_1 + (1 - \alpha) \vec{\sigma}_2] + \frac{g}{2} (\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y).$$  \hspace{1cm} (5.24)

Writing this Hamiltonian in spherical coordinates, it can be seen that $\hat{H}_{\text{ani}}(B, \theta, \phi) = R^\dagger(\phi)\hat{H}_{\text{ani}}(B, \theta, 0)R(\phi)$, still holds and therefore it is sufficient to study the spectrum for $B_y = 0$. The parameter $\alpha$ breaks the symmetry which permits the existence of two-dimensional surface manifolds as the locus where ground-state degeneracies occur. The

Figure 5.8: Anisotropic fields ($g_z = 0$, $\alpha = 0.3$): Left: Curl of Berry curvature, shown only in the $xz$–plane due to azimuthal symmetry. Right: Berry curvature $\vec{F}$ (light arrows), showing two charges (yellow dots) on the $z$–axis, plus an uncharged ring (green) in the $xy$–plane.
previous surfaces now collapse to two points, located on the z-axis at $\pm g/(2\sqrt{(1-\alpha^2)})$ due to azimuthal symmetry of the eigenenergies. These two points correspond to energy level crossings in the ground-state manifold and act like sources of $\vec{F}$. The total Chern number in the entire parameter space is topologically protected and equal to +2, therefore each source carries an effective magnetic charge equal to +1.

These magnetic monopoles are visible as singularities in the divergence of the Berry curvature, which is unsurprisingly zero away from these two singularities. For the curl of the Berry curvature, we find a quadrupolar field pattern very similar to what we saw in the previous section for the charged surface. However, surprisingly we also find the appearance of two other points on the x-axis. Respecting the model’s symmetry by revolving the plotted planes around the z-axis, one can see that these points in fact correspond to a ring of degeneracies, centered at the origin in the xy-plane, with radius $\varrho = \sqrt{2(1+\alpha^2)/(1-\alpha^2)}$ (see Fig. 5.8). Most interestingly, this ring is uncharged as can be inferred from a topological argument: the total Chern number for the entire parameter manifold must remain equal to +2, and the monopoles on the z-axis each carries a unit charge, as can be verified using Gauss law. The Berry curvature in its vicinity exhibits a saddle-point behavior, rather than acting like a sink or source for the $\vec{F}$ vector field. The analogous configuration in E&M are two electric charges with a conducting ring placed halfway in between, which introduces boundary conditions for the fields. As can be seen in Fig. 5.8, the curl of Berry curvature shows a hexapole pattern for the intersections on the xy-plane. Thus, the presence of the uncharged ring, although not obvious from the Berry curvature field, can clearly be observed in the $\vec{\nabla} \times \vec{F}$ graph, as they exhibit a distinct pattern compared to degeneracies having an effective charge. The curl then apparently contains additional geometric information about the ground-state manifold of the system, which has not been explored so far.

It is readily confirmed that the gap vanishes at this ring of singularities despite the absence of effective magnetic charge. Interestingly, crossing this degeneracy by fixing $B_x = \varrho$ and varying $B_z$, we find that the energies exhibit a quadratic touching, which in the chemistry literature is known as Renner-Teller intersection points (Zwanziger and Grant, 1987;
Figure 5.9: **Left:** plot of the energy spectrum of $H_{\text{ani}}(0,0,B_z)$. **Center:** Eigenenergies of $H_{\text{ani}}(B_x,0,0)$. **Right:** Ground-state degeneracies in the parameter space $(B_x,B_y,B_z)$.

Yarkony, 1996, 1998; Oh, 2009), fundamentally different from conical intersections since they do not give rise to a geometric phase, and consequently have a Chern number equal to 0. This quadratic touching comes from a symmetry of the Hamiltonian, namely $B_z \rightarrow -B_z$, and therefore is not present for curves that do not cross the degeneracy vertically, e.g., the energy levels for fixed $B_z = 0$ when varying $B_x$.

### 5.6.1 Crossings in the $z$-axis: $B_x = B_y = 0$

Let us rewrite $H_{\text{ani}}$ for $B_y = 0$ in the basis \{\ket{\uparrow\uparrow}, \ket{\uparrow\downarrow}, \ket{\downarrow\uparrow}, \ket{\downarrow\downarrow}\}, defining $\alpha_{\pm} \equiv (1 \pm \alpha)$ for notational brevity,

$$H_{\text{ani}}(B_x,B_z) = \begin{pmatrix} 2B_z & \alpha_- B_x & \alpha_+ B_x & 0 \\ \alpha_- B_x & 2\alpha B_z & 2 & \alpha_+ B_x \\ \alpha_+ B_x & 2 & -2\alpha B_z & \alpha_- B_x \\ 0 & \alpha_+ B_x & \alpha_- B_x & -2B_z \end{pmatrix}.$$  \hspace{1cm} (5.25)

For $B_x = 0$, the matrix becomes block-diagonal, and the ground-state energy crossings are located at

$$\beta_z^{(+)} = \pm \frac{1}{\sqrt{(1 - \alpha^2)}}.$$  \hspace{1cm} (5.26)

The Fig. 5.3 above shows the plots of the choice $\alpha = 0.3$ for the Berry curvature on the first panel on the $xz$-plane and the second panel in 3D, obtained by revolving the first
Figure 5.10: Renner-Teller level touching for \( B_x = \varrho \) and changing \( B_z \) (vertically crossing the ring).

Panel around the \( z \)-axis. The two leftmost panels show two monopole sources in the \( z \)-axis colored in yellow, and the uncharged ring colored in green on the \( xy \)-plane (the ring shows up in the \( xz \)-plane as two symmetrical points on the \( x \)-axis). Observe the behavior of the vector field in the vicinity of the green points — it shows a saddle-point behavior, and thus the flux of \( \vec{F} \) vanishes. However, these points can clearly be located on the third panel, where \( \vec{\nabla} \times \vec{F} \) is shown.

5.6.2 Crossings in the \( x \)-axis: \( B_z = B_y = 0 \)

In the case of \( B_z = 0 \), the Hamiltonian \( \hat{H}_\text{ani}(B_x, 0, 0) \) commutes with \( \sigma_1^x \sigma_2^x \) and therefore they have a common basis of eigenvectors given by \( \{(-|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}, (-|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}, (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}, (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}\} \). With respect to this basis, \( \hat{H}_\text{ani}(B_x, 0, 0) \) is block-diagonal,

\[
\hat{H}_\text{ani}(B_x, 0, 0) = \begin{pmatrix}
0 & -2\alpha B_x & 0 & 0 \\
-2\alpha B_x & -2 & 0 & 0 \\
0 & 0 & 0 & 2B_x \\
0 & 0 & 2B_x & 2 \\
\end{pmatrix}, \quad (5.27)
\]
where the corresponding eigenenergies can easily be calculated,

\[ E_1 = 1 - \sqrt{1 + 4 B_x^2}, \quad E_2 = -1 - \sqrt{1 + 4 \alpha^2 B_x^2}, \]
\[ E_3 = -1 + \sqrt{1 + 4 \alpha^2 B_x^2}, \quad E_4 = 1 + \sqrt{1 + 4 B_x^2}, \quad (5.28) \]

and it can be seen that the ground-state energy degenerates \( E_1 = E_2 \) at

\[ B_x^{(\pm)} = \pm \sqrt{\frac{2(1 + \alpha^2)}{(1 - \alpha^2)}}. \quad (5.29) \]

The azimuthal invariance of the eigenenergies as expressed in Eq. (5.4), implies that these two points in the \( xz \)-plane actually correspond to a ring centered at the origin in the \( xy \)-plane, with radius

\[ \varrho = \sqrt{\frac{2(1 + \alpha^2)}{(1 - \alpha^2)}}. \quad (5.30) \]

In Fig. 5.9 we plot the spectrum of the two-qubit Hamiltonian with an anisotropic magnetic field and the ground-state degeneracies in parameter space \( (B_x, B_y, B_z) \), given by a ring in the \( xy \)-plane and two points on the \( z \)-axis.

Finally, we note that the ring has no charge, which can be seen by calculating the first Chern number numerically, \( \text{ch}_1(\text{ring}) = 0 \). On the contrary, the two point charges on the \( z \)-axis carry each a charge of +1. This was also confirmed by a numerical evaluation of the first Chern number. Energy-level crossings that yield a trivial Berry phase when encircled, and therefore have an associated zero Chern number, are know as Renner-Teller level touchings (Yarkony, 1996). The energy level touching can be observed by fixing \( B_x = \varrho \) and varying \( B_z \) (see Fig. 5.10).

\section{5.7 Broken exchange symmetry}

For the final case, consider \( \gamma_1 = \gamma_2 = 1, g_z = 0 \) and \( B_0 = 1 \). Due to the pinning field \( B_0 \) on the first spin the exchange symmetry between the two spins is broken, and only the azimuthal symmetry in the eigenenergies is left. The crossing points now lie solely on the \( z \)-axis, with the two monopoles located at \( B_z^{(\pm)} \equiv (-B_0 \pm \delta)/2 \), where \( \delta \equiv \sqrt{B_0^2 + g_z^2} \) is the degenerate ground-state energy for the case in consideration. The curl of \( \vec{\Phi} \) for this case
Figure 5.11: Broken exchange symmetry ($g_z = 0 = \alpha = 0$, $B_0 = 1$): Left: $\nabla \times \vec{F}$ shown in the $xz$-plane. Right: Berry curvature $\vec{F}$ (light arrows) showing the only two magnetic charges on the $z$-axis.

shows a persistent quadrupole pattern around the crossing points in the $z$-axis, although one observes a bending of the lobes toward each other, which increases with $B_0$ (see Fig. 5.11). The point charges along the $z$-axis are no longer symmetric with respect to the $xy$-plane, and their location varies as a function of $B_0$, given by $B_z^{(\pm)}$.

We now calculate the Berry connection $\vec{A}$ (vector potential), Berry curvature $\vec{F}$ (magnetic field) and the curl of the Berry curvature $\nabla \times \vec{F}$ (current) using a degenerate perturbation theory for the interacting two-qubit system with broken exchange symmetry. First, we derive the location of the ground-state degeneracies (level crossings) in the parameter space. Next, we compute the ground-state of the system up to second-order using a degenerate perturbation theory. The resulting ground-state allows us then to calculate the Berry connection, Berry curvature and the curl of the Berry curvature in the vicinity of the effective magnetic monopole charges (ground-state degeneracies).
5.7.1 Location of the magnetic monopoles (level crossings)

The Hamiltonian for two interacting qubits with a broken exchange symmetry is given by

\[ \hat{H}_{\text{BES}} = \vec{B} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2) + \frac{g}{2}(\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y) + B_0 \sigma_1^z, \]  

(5.31)

which can be obtained by setting \( \gamma_1 = \gamma_2 = 1 \) and \( g_z = 0 \) in the Hamiltonian (5.3).

The ground-state degeneracies are restricted to the \( B_z \) axis, since the eigenenergies of the Hamiltonian (5.31) have an azimuthal symmetry, and since the Hamiltonian (5.31) itself has no more symmetries. The positions of the ground-state degeneracies in parameter space can therefore be determined by diagonalizing the Hamiltonian (5.31) for \( B_x = B_y = 0 \). In the basis \{\text{\{\uparrow\uparrow\}, \text{\{\uparrow\downarrow\}, \text{\{\downarrow\uparrow\}, \text{\{\downarrow\downarrow\}\}}\} the Hamiltonian becomes block-diagonal

\[ \hat{H}_{\text{BES}}(0, 0, B_z) = \begin{pmatrix} B_0 + 2B_z & 0 & 0 & 0 \\ 0 & B_0 & g & 0 \\ 0 & g & -B_0 & 0 \\ 0 & 0 & 0 & -B_0 - 2B_z \end{pmatrix}, \]  

(5.32)

and thus the corresponding eigenenergies \( E_n \) and eigenstates \( |\psi_n\rangle \), with \( n = 1, 2, 3, 4 \), are given by

\[ E_1 = -B_0 - 2B_z, \quad |\psi_1\rangle = (0, 0, 0, 1)^T, \]
\[ E_2 = -\delta, \quad |\psi_2\rangle = \frac{1}{\sqrt{(B_z^+)^2 + \left(\frac{g}{2}\right)^2}}(0, -B_z^+, \frac{g}{2}, 0)^T, \]
\[ E_3 = B_0 + 2B_z, \quad |\psi_3\rangle = (1, 0, 0, 0)^T, \]
\[ E_4 = \delta, \quad |\psi_4\rangle = \frac{1}{\sqrt{(B_z^-)^2 + \left(\frac{g}{2}\right)^2}}(0, -B_z^-, \frac{g}{2}, 0)^T, \]  

(5.33)

where we defined

\[ \delta \equiv \sqrt{B_0^2 + g^2}, \]
\[ B_z^+ \equiv \frac{1}{2}(-B_0 + \delta), \quad B_z^- \equiv \frac{1}{2}(-B_0 - \delta). \]  

(5.34)

In Fig. 5.12, we plot the eigenenergies \( E_n \) as a function of \( B_z \) for \( B_x = B_y = 0 \) with fixed \( B_0 \) and \( g \). It shows that the ground-state energy-level crosses with the excited energy-levels
Figure 5.12: Eigenenergies as a function of $B_z$ for $B_x = B_y = 0$ and fixed $B_0$ and $g$. The degeneracies of the ground-state occur at $B_z = B_z^-$ and $B_z = B_z^+$.

at $B_z = B_z^-$ and $B_z = B_z^+$. These degeneracies act as magnetic monopoles in parameter space. The ground-state energy of the system as a function of $B_z$ for $B_x = B_y = 0$ can be written as

$$E_0(B_z) = \begin{cases} 
-B_0 - 2B_z, & B_z \geq B_z^+, \\
-\delta, & B_z^- \leq B_z \leq B_z^+, \\
B_0 + 2B_z, & B_z \leq B_z^-
\end{cases}$$

and the corresponding ground-state reads

$$|\Psi_0(B_z)\rangle = \begin{cases} 
(0,0,1)^T, & B_z \geq B_z^+, \\
(0, -B_z^+, g/2)^T / \sqrt{(B_z^+)^2 + (g/2)^2}, & B_z^- \leq B_z \leq B_z^+, \\
(1,0,0)^T, & B_z \leq B_z^-
\end{cases}$$

5.7.2 Degenerate perturbation theory

Coordinate system centered at monopoles

In what follows we use a degenerate perturbation theory to calculate the ground-state of our two-qubit system close to the degeneracies at $B_z^+$ and $B_z^-$. We will present only the results for small deviations around the degeneracy $B_z^+$; the results around $B_z^-$ are obtained in a similar way. Let us consider the location of the degeneracy, given vectorially by $\vec{B}' = (0,0,B_z^+)^T$, as the origin of a new coordinate system. With respect to this new
coordinate system, a point in parameter space \((B_x, B_y, B_z)\) is indicated by the vector \(d\vec{B} = (dB_x, dB_y, dB_z)^T\) and it is related to the original coordinate system by \(d\vec{B} = \vec{B} - \vec{B}'\), which yields the following relations between the two coordinate systems

\[
\vec{B} = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} = \vec{B}' + d\vec{B} = \begin{pmatrix} dB_x \\ dB_y \\ dB_z + B_z^+ \end{pmatrix}, \tag{5.37}
\]

The Hamiltonian (5.31) in the new coordinates reads

\[
\hat{H}_{\text{BES}} = dB_x (\sigma_1^x + \sigma_2^x) + dB_y (\sigma_1^y + \sigma_2^y) + dB_z (\sigma_1^z + \sigma_2^z) + B_z^+ (\sigma_1^z + \sigma_2^z) + \frac{g}{2} (\sigma_1^x \sigma_2^y + \sigma_1^y \sigma_2^x + B_0 \sigma_1^z). \tag{5.38}
\]

We treat the deviation from the monopole (degeneracy) as a small perturbation, i.e., \(|d\vec{B}| \ll 1\). It is therefore useful to express (5.37) in spherical coordinates

\[
d\vec{B} = \begin{pmatrix} dB \sin \vartheta \cos \phi \\ dB \sin \vartheta \sin \phi \\ dB \cos \vartheta \end{pmatrix} = \vec{B} - \vec{B}' = \begin{pmatrix} B \sin \vartheta \cos \phi \\ B \sin \vartheta \sin \phi \\ B \cos \vartheta - B_z^+ \end{pmatrix}, \tag{5.39}
\]

which yields the relations

\[
dB \sin \vartheta = B \sin \vartheta, \quad dB \cos \vartheta = B \cos \vartheta - B_z^+. \tag{5.40}
\]
Let us focus on the \(xz\)-plane defined by \(B_y = 0\), or in spherical coordinates, by \(\phi = 0\). Such choice implies \(dB_y = 0\), and thus we have

\[
\hat{H}_{\text{BES}} = dB_x (\sigma^x_1 + \sigma^x_2) + dB_z (\sigma^y_1 + \sigma^y_2) + B^+_z (\sigma^x_1 + \sigma^x_2) + \frac{g}{2} (\sigma^x_1 \sigma^x_2 + \sigma^y_1 \sigma^y_2) + B_0 \sigma^z_1
\]

\[
= \hat{H}_0 + dB \hat{H}', \tag{5.41}
\]

where

\[
\hat{H}_0 = B^+_z (\sigma^x_1 + \sigma^x_2) + \frac{g}{2} (\sigma^x_1 \sigma^x_2 + \sigma^y_1 \sigma^y_2) + B_0 \sigma^z_1,
\]

\[
\hat{H}' = \sin \vartheta (\sigma^x_1 + \sigma^x_2) + \cos \vartheta (\sigma^y_1 + \sigma^y_2). \tag{5.42}
\]

### 5.7.3 Berry connection and curvature: effective magnetic vector potential and field

The leading order term for \(A_{\phi,+}\) we have

\[
A_{\phi,+} \approx -\frac{1}{2} \frac{1}{dB \sin \vartheta} \left(1 + \frac{\cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right). \tag{5.43}
\]

The Berry curvature \(\vec{F}^{(S)}(dB, \vartheta, \phi)\) is obtained by taking the curl of (5.43). As detailed in Appendix F, in the leading order of \(dB\) we find

\[
\vec{F}^{(S)}_+(dB, \vartheta, \phi) = \nabla \times \vec{A}^{(S)}_+(dB, \vartheta, \phi) \approx \frac{1}{2} \frac{1}{\gamma^2 (1 - \beta^2 \sin^2 \vartheta)^{3/2}} \frac{1}{dB^2} dB, \tag{5.44}
\]

where we introduced \(\gamma \equiv 1/\sqrt{1 - \beta^2}\).

### 5.7.4 Curl analysis

To understand the curl behavior of \(\vec{F}\) analytically, we calculate the Berry connection for the broken exchange symmetry case at the degeneracy points \(B^\pm_z\) using perturbation theory and obtain \(\nabla \times \vec{F}\) around \(B^\pm_z\) (see Appendix F). The leading order expression for the curl is given by

\[
\nabla \times \vec{F}^{(\pm)} = -\frac{3}{4} \frac{\beta^2 \sin 2 \vartheta}{\gamma^2 (1 - \beta^2 \sin^2 \vartheta)^{5/2}} \frac{1}{dB^3} dB \hat{\phi} + \cdots, \tag{5.45}
\]

where \(\beta^2 \equiv g/\delta\), \(\gamma \equiv 1/\sqrt{(1 - \beta^2)}\), and with respect to the coordinate system centered at the monopole \(B^\pm_z\) respectively, given in spherical coordinates \((dB, \vartheta, \phi)\). This expression
reproduces qualitatively the quadrupole seen numerically (see Fig. 5.14 and Appendix F) and suggests the possibility that this pattern may be robust in the vicinity of Berry curvature sources.

## 5.8 Conclusion

The analogy between E&M and degeneracies in quantum systems has been outlined many years ago, and it is still a field of active research, mainly due to its applications to adiabatic quantum computing and the recent burst of interest in topological transitions. For highly symmetric systems, we have shown how symmetry-breaking perturbations allows one to open adiabatic passages in previously topologically disjoint regions, thereby allowing the full parameter space to be explored. The procedure outlined in this paper is general and robust, and not necessarily restricted to qubits. We note that by identifying angles of the magnetic field with quasi-momenta, the two-spin system here analyzed can be mapped
to a four-band model of a topological insulator with a rich phase diagram, similar to the construction in (Roushan et al., 2014). Therefore results presented in this paper can find direct analogues in other systems. The system in analysis was chosen as a good illustrative example due to experimental feasibility of measuring the Berry connection $\vec{A}$ by relating it to the ground-state expectation value of the total magnetization. The Berry curvature and its curl can then be experimentally obtained, and the results here presented can be verified.

We also highlighted the existence of degeneracy points with vanishing Chern number, and exemplified how they fit within the E&M analogy as boundary conditions for the $\vec{F}$ field. Finally, the curl of the Berry curvature was explored, with different behavior near charged and uncharged points, indicating the possibility that this quantity might carry geometrical information about the ground-state manifold previously unexplored.
Chapter 6

Visualizing Singularities of a Ground-State Landscape Using Superconducting Circuits

Nature isn’t classical, dammit, and if you want to make a simulation of nature, you’d better make it quantum mechanical, and by golly it’s a wonderful problem, because it doesn’t look so easy.


In this Chapter, we present the measurements of an experimental proposal realized at the Google Quantum Lab (Dunsworth et al., 2016). Researchers were able to visualize the topological nature of a two-qubit system with sharper detail, in startling contrast with earlier methods. To achieve this feat, geodesic paths as optimal adiabatic driving protocols were used. This enabled a great improvement on the measurements made by the experimental apparatus, without the need for technical engineering advances. The results are a demonstration of how powerful geometric and topological ideas can become when combined, allowing for a refined understanding of the connection between the topology of the parameter space (with degeneracies associated with magnetic charge densities) and adiabaticity in quantum systems\(^1\).

\(^1\)The author would like to thank A. Dunsworth, P. Roushan, C. Neill, J. Martinis and all his group for their kindness in providing their unpublished experimental data here presented.
6.1 Singularities Curve the Space

The ground-state of a quantum system distinguishes itself from the other excited-states for carrying many features of interest in condensed matter physics. Frequently, one wants to investigate the ground-state properties in various points of the parameter space. Knowledge about the location of degeneracies in the parameter space is crucial for the problems exemplified in Section 1.1.1. If one wants to study ground-state manifolds, having a well-prescribed way of moving in parameter space is a desired goal to find the degeneracy locations.

Interestingly, singularities leave a fingerprint on the parameter manifold by curving it in a manner similar to how the fabric of space-time is warped by the presence of energy, as described by the general theory of relativity. Such curvature, resulting from the presence of the singularity, can be measured. In this chapter, we describe how and present the experimental outcome.

6.2 Berry Curvature as an Effective Magnetic Field

Let us recap the main results discussed in previous chapters.

The geometric phase is defined by

\[ \gamma = i \oint_C \langle \Psi_0(\vec{\lambda}) | \nabla \vec{\lambda} | \Psi_0(\vec{\lambda}) \rangle \cdot d\vec{\lambda} \equiv \oint_C \vec{A} \cdot d\vec{\lambda}, \quad (6.1) \]

where \( |\Psi_0(\vec{\lambda})\rangle \) is the ground-state, \( \vec{\lambda} \) is a set of parameters being varied in the Hamiltonian, and \( \vec{A} \) is the gauge dependent Berry connection. The phase \( \gamma \) is calculated along a path \( C \) in the three-dimensional parameter space \( \mathcal{M} \) defined in local coordinates by \( \{\lambda^\mu\}, \mu = \{1, 2, 3\} \).

Using Stoke’s theorem, the line integral above is written as an integral over a closed (gaussian) surface,

\[ \gamma = \oint_C \vec{A} \cdot d\vec{\lambda} = \int_S (\nabla \times \vec{A}) \cdot d\vec{S} \equiv \int_S \vec{F} \cdot d\vec{S}, \quad (6.2) \]

where \( \vec{F} = \nabla \times \vec{A} \) is the gauge independent Berry curvature, and \( S \) represents the surface boundary.

2The words degeneracy and singularity are used interchangeably here.

3We here consider \( \hbar = 1/2\pi \). Energy is measured in units of 1 MHz, and time in units of \( 1\mu s = 1000\text{ns} \).
In analogy with E&M, the equations above map the Berry connection $\vec{A}$ to the magnetic vector potential and the Berry curvature $\vec{F}$ to an effective magnetic field. The geometric phase $\gamma$ equals the effective magnetic field flux. When computed on a closed surface, it is proportional to the effective charge enclosed (Gauss’s law).

As phases are well-defined only up to mod($2\pi$), the integer-valued integral

$$ch_1 = \frac{1}{2\pi} \oint_S \vec{F} \cdot d\vec{S}$$

(6.3)

along the closed surface $S$ defines a topological invariant, the (first) Chern number $ch_1$, seen as effective magnetic charges giving rise to the field $\vec{F}$ and its flux.

### 6.3 Experimental Adiabatic State Preparation

Figure 6.1 is a picture of the chip where the measurements were performed. It consists of a 3-gmon device incorporating a fast tunable coupling for each qubit in the $xy$-control line.
and an inductively coupled $z$-control line (Chen et al., 2014; Martinis and Osborne, 2003). Two qubits\footnote{Qubits are two-state quantum mechanical systems, and can be represented by 1/2-spin particles q.v. Chapter 5.} and their couplers have been isolated (Figure 6.1, right panel).

We thus consider a system of two coupled qubits with a constant offset $B_0$ in a tunable external magnetic field $\vec{B}$. The Hamiltonian is given by\footnote{q.v. Section 5.2.} Eq. (5.3),

$$\hat{H}(B_x, B_y, B_z) = \vec{B} \cdot (\vec{\sigma}_1 + \vec{\sigma}_2) + B_0 \sigma^z_1 + g (\sigma^x_1 \sigma^x_2 + \sigma^y_1 \sigma^y_2),$$

(6.4)

where $\vec{B} = B \hat{n}(\theta, \phi) = B (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ is the external magnetic field coupled to both qubits, $g$ is the $xy$-coupling and $B_0$ is a constant offset on the $z$-control line.

Due to azimuthal symmetry, the Hamiltonian at arbitrary $\phi$ can be mapped to $\phi = 0$ by a rotation of the spins around the $z$-axis, with the same being valid for the eigenstates\footnote{Note: in the previous chapter, the $xy$-coupling term in the Hamiltonian is written as $g/2$, whereas here $g$ is used instead - these choices were kept to maintain consistency with (Souza et al., 2015) (previous chapter), and (Dunsworth et al., 2016) (current chapter).}

For the gauge choice $\phi = 0$ ($B_y = 0$), we write $|\Psi_0(B_x, 0, B_z)\rangle \equiv |\Psi_0(B_x, B_z)\rangle$, and the Berry connection equals to $\vec{A} = (1/B \sin \theta) (\langle \sigma^z_{\text{tot.}} \rangle / 2) \hat{\phi}$, where $\langle \sigma^z_{\text{tot.}} \rangle = \langle \sigma^z_1 \rangle + \langle \sigma^z_2 \rangle$ is the expectation value of the total magnetization for the spins taken with respect to the ground-state $|\Psi_0(B_x, B_z)\rangle$ at $(B_x, B_z)$.

Figure 6.2 shows the Hamiltonian phase diagram and the effects of the parameters $g$ and $B_0$ on the system. The applied pulses for $B_x$ and $B_z$ are mirrored on both qubits for $g = B_0 = 0$ and the system is equivalent to two single qubits. Coupling them in the $xy$-direction ($g$ parameter) generates a surface of degeneracies, where the singlet-state is the ground-state inside ($\langle \sigma^z_{\text{tot.}} \rangle = 0$). Finally, detuning the qubits ($B_0$ parameter) breaks the exchange symmetry, coalescing the degeneracies to two points in the $z$-axis.

### 6.4 Experimental Description

The experiment consists of measuring the expectation value of the total magnetization

$$\langle \sigma^z_{\text{tot.}} \rangle = \langle \sigma^z_1 \rangle + \langle \sigma^z_2 \rangle$$

at the end of the ramps. Since $\langle \sigma^z_{\text{tot.}} \rangle \sim \vec{A}$ (Eq. (5.6)), the Berry
connection is thus experimentally measurable. The curl of the Berry connection is equal to the Berry curvature, numerically obtained \textit{a posteriori}.

The analogy with E&M exhibits the motivation for the experiment: singularities are conceptually similar to magnetic monopoles, and the integral of the effective magnetic field over Gaussian surfaces is equal to the number of singularities enclosed. We are then able to find the location of the singularities.

6.4.1 Initialization Procedure

We consider the Hamiltonian for two qubits with four parameters: $B_x, B_z, B_0$ and $g$ (Equation (6.4) with $B_y = 0$). The initialization procedure is achieved by applying $\pi/2$ pulses to bring the qubits to the equator ($x$-axis). The system is thus prepared at the point with
Figure 6.3: Pulse sequence schematics. Q1,2 represent the qubits, and cp12 their coupling. Initially, a $\pi/2$ pulse is applied to align the spins along the $x$-axis, preparing them at the parameter values of point A. Next, RF pulses are ramped according to linear or geodesic protocols to adiabatically transfer the system from A to parameter values at the point C.

parameter values $A$: $(B_z = 10 \text{ MHz}, B_x = 0 \text{ MHz}, B_0 = 0 \text{ MHz}, g = 0 \text{ MHz})$. The starting point A is easy to produce experimentally, and the ground-state is given by two non-entangled qubits.

Next, the task is to move the system from the starting point A to a family of arbitrary end points $C$: $(B_{xf}, B_{zf}, B_{0f}, g_f)$, lying on an $80 \times 80$ rectangular grid within the interval $-10 \text{ MHz} < B_x/2\pi, B_z/2\pi < 10 \text{ MHz}$. Finally, the fields are turned off and the magnetization of each qubit $\langle \sigma_1^z \rangle$ and $\langle \sigma_2^z \rangle$ is measured (see Figure 6.3).

The procedure delineated above is realized for two different ramps: a linear one connecting the initial and final points, and across geodesic pulses obtained by using the real part of the QGT\textsuperscript{8}. The quantum metric tensor acts as a cost function, yielding the geodesic pulse sequences. Those prescribe how to go between the initial and final points minimizing the energy fluctuation and maximizing the local fidelity along the path.

\textsuperscript{8}q.v. Chapters 2 and 3
## 6.5 Paths in the Parameter Space

### 6.5.1 Linear Ramps

Figure 6.4 shows the total magnetization $\langle \sigma^z_{\text{tot.}} \rangle$ for linear ramps: *Left*: Exact diagonalization numerical simulation. *Center*: Numerical evolution simulation. *Right*: Experimental data.

The panels from left to right show: numerical simulation results from exact diagonalization; numerical evolution simulation for linear ramps; the experimental measurements of $\langle \sigma^z_{\text{tot.}} \rangle$ for linear ramps, with $t_f = 600$ ns, $\delta E_{\text{min}} \sim 1.7$ MHz (top panel), and $t_f = 800$ ns, $\delta E_{\text{min}} \sim 1.25$ MHz (bottom panel).
\[ \delta E \equiv (E_1 - E_0)/2\pi \text{ [MHz]} , \ g/2\pi = 4.0 \text{ MHz} , \ B_0/2\pi = 5.0 \text{ MHz} \]

Figure 6.5: Gap map vs. simulated linear ramp results. Regions where the gap is small decrease the resolution due to the higher likelihood of excitations.

A small gap region is observed for the no coupling case (top panel) for the numerical simulation and the experimental data, the latter showing a considerable amount of noise. This is not observed in the exact diagonalization numerical simulation. The case with a finite coupling and detuning (bottom panel) also show this lack of resolution near singularities.

Energy Gap Limits Resolution

The spots in Figure 6.4 where the linear ramp results are not exactly mimicking the exact numerical simulations are regions where the energy gap gets small. Figure 6.5 shows energy gap \( \delta E = E_1 - E_0 \) for the \( B_0 = 5 \text{ MHz} , g = 4 \text{ MHz} \) case. Observe that the black regions in the left panel plot – corresponding to a small energy gap – coincide precisely with the regions where the resolution is lost on the measurements of the total magnetization, shown in the right panel.
6.5.2 Geodesic Ramps

The top panel of Figure 6.6 shows the total magnetization for the two qubits driven by geodesic ramps with $B_0 = 5\, \text{MHz}$, $g = 4\, \text{MHz}$. The panels from left to right show, as in Figure 6.4, the numerical simulation results from exact diagonalization, numerical evolution simulation for geodesic ramps and the experimental measurements of $\langle \sigma_z^{\text{tot.}} \rangle$ for geodesic ramps, with $t_f = 800\, \text{ns}$, $\delta E_{\text{min}} \sim 1.25\, \text{MHz}$. The bottom panel shows the experimental
measure for the same values, but obtained with linear ramps. Regions of small gap are better resolved with geodesic ramps (top panel) in comparison with linear ramps (bottom panel). This better resolution has immediate repercussions in the next step of taking numerical derivatives of the Berry connection in order to obtain the Berry curvature ($\vec{F} = \nabla \times \vec{A}$).

### 6.6 Curvature: Fingerprint of Singularities

Figure 6.7 shows the total magnetization $\langle \sigma^z_{\text{tot.}} \rangle \sim \vec{A}$ experimentally measured with geodesic ramps. The Berry connection is given by $\vec{A} = (1/B \sin \theta)(\langle \sigma^z_{\text{tot.}} \rangle/2) \hat{\phi}$, and taking the curl of $\vec{A}$, one gets the Berry curvature, shown as vectors overlaid in both graphs.

In the left panel ($B_0 = g = 0 \text{ MHz}$), the vectors are seen to emanate from the origin, where two effective magnetic monopole charges are located; in the right panel ($B_0/2\pi = 5 \text{ MHz}, g/2\pi = 4 \text{ MHz}$), two separate sources of effective magnetic field are observed lying on the $z$-axis.

![Figure 6.7: Total magnetization $\langle \sigma^z_{\text{tot.}} \rangle \sim \vec{A}$ experimentally measured with geodesic ramps. The Berry curvature $\vec{F}$ field is overlaid (white arrows). Left: $B_0 = g = 0 \text{ MHz}$; charges at the origin. Right: $B_0 = 5 \text{ MHz}, g = 4 \text{ MHz}$; charges on the $z$-axis. The black circle is a Gaussian surface where the flux is obtained numerically.](image-url)
6.7 Visualizing the Ground-state Singularities

We finally locate the singularities by calculating the Berry curvature field flux on Gaussian surfaces from the experimental data. The origin of the surface is iteratively changed to span the plane and the integral in Equation (6.3) is computed, yielding the (first) Chern number \( \text{ch}_1 \) measurement map.

6.7.1 First set of measurements

Figure 6.8 exhibits the first results obtained. On the left panel, exact diagonalization numerical simulation is shown, while the center/right panel is the experimental measurements of the (first) Chern number for linear and geodesic ramps, respectively. As seen in plots, the monopole charges are smeared out in the linear ramp protocol due to a low final fidelity after evolution, whereas a higher contrast is observed for geodesic protocols, where one is thus able to visualize the location of the singularities. The \( B_z^{(\pm)} \) values where the singularities lie is given by Equation (5.7.1), here equal to \( B_z^+ \approx 2.22 \) MHz and \( B_z^- \approx -7.22 \) MHz.

Figure 6.8: Two-qubit ground-state degeneracies for \( B_0/2\pi = 5 \) MHz, \( g/2\pi = 4 \) MHz. \( \text{Left:} \) Exact diagonalization simulations. \( \text{Center:} \) Linear ramping protocol experimental result. \( \text{Right:} \) Geodesic ramping protocol experimental result. Charges location are given by Eq (5.7.1), here equal to \( B_z^+ \approx 2.22 \) MHz and \( B_z^- \approx -7.22 \) MHz.
A second set of measurements performed a couple of months later is shown in Figure 6.9. In the $B_0 = g = 0$ MHz case, one singularity at the origin is captured by the measurements, corresponding to the overlapping degeneracies for two uncoupled qubits. In the more interesting case of $B_0/2\pi = 5$ MHz, $g/2\pi = 4$ MHz, the two degeneracies are split and the monopole charges spread apart along the $z$-axis away from each other. The location of the singularities is given by Eq (5.7.1), and equal to $B_z^+ \approx 2.22$ MHz and $B_z^- \approx -7.22$ MHz, in perfect agreement with what is shown in both Figures 6.8 and 6.9.

### 6.8 Conclusion

In this final chapter, we exhibit an experimental realization of the ideas developed in previous chapters. Geodesic ramps are obtainable by minimizing and keeping constant the energy fluctuations along the path. This procedure works even in the absence of an $a$
priori knowledge on the location of degeneracies, how to ramp the system, or any potentially useful information about the parameter space itself. Geodesics paths are the shortest distance between any two points in parameter space in the sense that they keep the local fidelity maximized along a quantum adiabatic evolution while simultaneously minimizing and keeping the energy fluctuation stationary at each point along the path.

By making use of this technique, experimentalists have obtained the necessary geodesic pulses, comparing their application to linear pulses for a two-qubit system. They also reported the ability to better measure the energy landscape, as well as all different quantum correlations.

Finally, for the two-qubit system in consideration, due to its azimuthal symmetry, they measured the total magnetization and obtained the Berry curvature, which by topological considerations, can be thought as fingerprint of singularities. Using Gauss’s law, the visualization of the location of singularities in the probed region of the parameter space was achieved with a higher resolution comparatively to naive singular ramps. Most importantly, the ideas developed in this thesis allowed for a great improvement on the measurements made by the same experimental apparatus, without the need for costly technical engineering advances.
Appendices
Appendix A

General Solution for the Sphere Geodesic

A.1 Metric Tensor for the 2–Sphere ($S^2$) and Geodesic Solutions

The 2–sphere ($S^2$) is defined by the two-dimensional surface of a three-dimensional ball in $\mathbb{R}^3$. It is topologically equivalent to the complex projective line $\mathbb{C}P^1$, a two-dimensional Hilbert space known as the Bloch sphere.

As most of the quantum metric tensors analyzed in this dissertation are isometric to the

Figure A.1: Depiction of the isometry between $S^2$ and $\mathbb{C}P^1$. The blue points are one and the same, shown in two different manifolds. This map is known in the literature as the stereographic projection.
2-sphere, in this appendix we derive its geodesic solution for arbitrary boundary conditions.

The infinitesimal distance $ds$ between two points on the two-dimensional surface of a sphere is given by

$$ds^2 = R^2 d\theta^2 + R^2 \sin^2 \theta d\phi^2,$$

(A.1)

where $R$ is a constant, representing the sphere radius when viewed in three dimensions. On the sphere surface, however, $R$ is a parameter which rescales distances accordingly.

From (A.1), one can read the associated metric tensor (see Eq. (2.9)),

$$g_{\mu\nu} = \begin{pmatrix} g_{\theta\theta} & g_{\theta\phi} \\ g_{\phi\theta} & g_{\phi\phi} \end{pmatrix} = \begin{pmatrix} R^2 & 0 \\ 0 & R^2 \sin^2 \theta \end{pmatrix}$$

(A.2)

The systems diffeomorphic to $\mathbb{CP}^1$ considered in previous chapters had the quantum metric written as (2.31),

$$g_{\mu\nu} = \frac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & \sin^2 \theta \end{pmatrix} \quad \implies \quad g^{\mu\nu} = (g_{\mu\nu})^{-1} = 4 \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\sin^2 \theta} \end{pmatrix}.$$ 

(A.3)

and hence one reads the radius $R = 1/2$, for the systems here treated. The Christoffel symbols of the second kind $\Gamma^\mu_{\nu\rho}$ are defined by Eq. (2.18), and for the metric above, the only non-vanishing components are

$$\Gamma^1_{22} = -\cos \theta \sin \theta, \quad \Gamma^2_{12} = \cot \theta = \Gamma^2_{21}.$$ 

(A.4)

The geodesic equations are

$$\ddot{\lambda}^1 + \left( \Gamma^1_{11} \dot{\lambda}^1 \dot{\lambda}^1 + \Gamma^1_{12} \dot{\lambda}^1 \dot{\lambda}^2 + \Gamma^1_{21} \dot{\lambda}^2 \dot{\lambda}^1 + \Gamma^1_{22} \dot{\lambda}^2 \dot{\lambda}^2 \right) = 0,$$

(A.5)

$$\ddot{\lambda}^2 + \left( \Gamma^2_{11} \dot{\lambda}^1 \dot{\lambda}^1 + \Gamma^2_{12} \dot{\lambda}^1 \dot{\lambda}^2 + \Gamma^2_{21} \dot{\lambda}^2 \dot{\lambda}^1 + \Gamma^2_{22} \dot{\lambda}^2 \dot{\lambda}^2 \right) = 0.$$ 

(A.6)

and referring to the notation, $\lambda^1 = \theta$, $\lambda^2 = \phi$,

$$\ddot{\theta} - \cos \theta \sin \theta \dot{\phi}^2 = 0,$$

(A.7)

$$\ddot{\phi} + 2 \cot \theta \dot{\theta} \dot{\phi} = 0.$$ 

(A.8)

where, for simplicity, the dot refers to derivatives taken with respect to the proper time $\tau$, $0 \leq \tau \leq 1$. As the solution is invariant to affine transformations, one is free to later change
variables, $\tau = \alpha t + \beta$, $\alpha \neq 0$. Let us solve Equations (A.7) and (A.8) for generic boundary conditions, $\phi(0) = \phi_i$, $\phi(1) = \phi_f$ and $\theta(0) = \theta_i$, $\theta(1) = \theta_f$.

### A.2 Integrals of Motion

#### A.2.1 Sphere Isometries – Angular Momentum Conservation

An integral of motion, $k$, is obtained by integration of Eq. (A.8). It is associated to rotation isometries of a sphere, equivalent to a “conservation of angular momentum”,

$$\sin^2 \theta \dot{\phi} = k \tag{A.9}$$

It is straightforward to verify the integral of motion above – by taking its derivative, Eq. (A.8) is readily obtained.

Rearranging Eq. (A.9) for an explicit expression of $\dot{\phi}^2$,

$$\dot{\phi}^2 = \frac{k^2}{\sin^4 \theta}. \tag{A.10}$$

#### A.2.2 Path Length – Energy Variance Conservation

Another integral of motion is given by $\Delta E^2$, the integrand of the energy functional (Equation (3.5)). The principle of stationary action enforces the integrand to be constant along the solution path, as illustrated in Eq.3.20,

$$\frac{1}{4} \dot{\theta}^2 + \frac{1}{4} \sin^2 \theta \dot{\phi}^2 = \Delta E^2$$

$$\dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2 = 4 \Delta E^2 \equiv \sigma^2, \tag{A.11}$$

where we defined $\sigma^2 \equiv 4 \Delta E^2$ (or more generically, $\sigma^2 \equiv \Delta E^2/R^2$).

### A.3 Integrals of Motion and Sphere Geodesic Solution

The two integrals of motion allows one to solve the sphere geodesic equations. Making use of Eq (A.10) on Eq. (A.11),

$$\dot{\theta}^2 + \sin^2 \theta \dot{\phi}^2 = \sigma^2 \implies \dot{\theta}^2 + \sin^2 \theta \left(\frac{k^2}{\sin^4 \theta}\right) = \sigma^2 \implies \dot{\theta}^2 = \sigma^2 - \left(\frac{k^2}{\sin^2 \theta}\right), \tag{A.12}$$
and defining \( \kappa \equiv k/\sigma \),
\[
\dot{\theta}^2 = \frac{\sigma^2}{\sin^2 \theta} \left( \sin^2 \theta - \frac{k^2}{\sigma^2} \right) = \frac{\sigma^2}{\sin^2 \theta} \left( \sin^2 \theta - \kappa^2 \right). \quad (A.13)
\]
Define \( \alpha^2 = 1 - \kappa^2 \),
\[
\dot{\theta}^2 = \frac{\sigma^2}{\sin^2 \theta} \left( 1 - \cos^2 \theta - \kappa^2 \right) = \frac{\sigma^2}{\sin^2 \theta} \left( \alpha^2 - \cos^2 \theta \right) \implies \dot{\theta} = \pm \sigma \frac{\sqrt{(\alpha^2 - \cos^2 \theta)}}{\sin \theta} \quad (A.14)
\]
The differential equation above is solved by integration,
\[
\sigma \int_0^{\tau} d\tau' = \pm \int_{\theta_i}^{\theta} \frac{\sin \theta'}{\sqrt{(\alpha^2 - \cos^2 \theta')}} d\theta' \quad (A.15)
\]
and we obtain an implicit analytic solution for \( \theta \),
\[
\mp \sigma \tau = \arctan \left[ \frac{\cos \theta}{\sqrt{\alpha^2 - \cos^2 \theta}} \right] - \arctan \left[ \frac{\cos \theta_i}{\sqrt{\alpha^2 - \cos^2 \theta_i}} \right] \quad (A.16)
\]
\[A.3.1 \text{ Boundary Values and Solution for } \sigma\]
Equation (A.16) transforms in one algebraic equation for the parameters when the boundary conditions are applied – at \( \tau = 1, \theta = \theta_f \),
\[
\mp \sigma = \arctan \left[ \frac{\cos \theta_f}{\sqrt{\alpha^2 - \cos^2 \theta_f}} \right] - \arctan \left[ \frac{\cos \theta_i}{\sqrt{\alpha^2 - \cos^2 \theta_i}} \right] \equiv (\chi_f - \chi_i) \quad (A.17)
\]
where we defined
\[
\chi_{i,f} = \arctan \left[ \frac{\cos \theta_{i,f}}{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}} \right]. \quad (A.18)
\]
Since \( \sigma \geq 0 \), Eq. (A.17) is also writable as
\[
\sigma = \text{sgn} \left( \chi_f - \chi_i \right) \left( \chi_f - \chi_i \right) = \text{sgn} \left( \chi_f - \chi_i \right) \left( \arctan \left[ \frac{\cos \theta_f}{\sqrt{\alpha^2 - \cos^2 \theta_f}} \right] - \arctan \left[ \frac{\cos \theta_i}{\sqrt{\alpha^2 - \cos^2 \theta_i}} \right] \right). \quad (A.19)
\]
\[A.4 \text{ Geodesic Solution for } \theta(\tau)\]
From \( \mp \sigma = (\chi_f - \chi_i) \) in Eq. (A.17), we rewrite Eq. (A.16),
\[
\underbrace{(\chi_f - \chi_i) \tau + \chi_i}_{\equiv X(\tau)} = \arctan \left[ \frac{\cos \theta}{\sqrt{\alpha^2 - \cos^2 \theta}} \right] \implies \cos \theta = \tan \left[ X(\tau) \right] \sqrt{\alpha^2 - \cos^2 \theta}. \quad (A.20)
\]
Squaring both sides,

\[
\cos^2 \theta = \tan^2 [X(\tau)] (\alpha^2 - \cos^2 \theta) \implies (1 + \tan^2 [X(\tau)]) \cos^2 \theta = \alpha^2 \tan^2 [X(\tau)].
\] (A.21)

The identity \(1 + \tan^2 x = \sec^2 x\) simplifies the equation above to

\[
\cos^2 \theta = \alpha^2 \sin^2 [X(\tau)],
\] (A.22)

or, in terms of \(\theta(\tau)\),

\[
\theta(\tau) = \arccos \left[ \sqrt{1 - \kappa^2 \sin ((\chi_f - \chi_i) \tau + \chi_i)} \right].
\] (A.23)

The last equation is the geodesic solution for \(\theta(\tau)\).

### A.5 Geodesic Solution for \(\phi(\tau)\)

We now integrate Eq. (A.9) to obtain the solution for \(\phi(\tau)\). By making use of the identity \(\sin^2 \theta = 1 - \cos^2 \theta = 1 - \alpha^2 \sin^2 \theta\) (last equality is from Eq. (A.22)),

\[
k = \sin^2 \theta \dot{\phi} = (1 - \alpha^2 \sin^2 [X(\tau)]) \dot{\phi} \implies \int_{\phi_i}^{\phi} d\phi = k \int_0^\tau \frac{1}{1 - \alpha^2 \sin^2 [X(\tau)]} d\tau.
\] (A.24)

and we obtain an analytic solution for \(\phi(\tau)\),

\[
\phi(\tau) - \phi_i = \mp \left( \arctan \left[ \kappa \tan [X(\tau)] \right] - \arctan \left[ \kappa \tan [X(0)] \right] \right)
\] (A.25)

also writeable as

\[
\phi(\tau) = \phi_i + \text{sgn} (\chi_f - \chi_i) \left( \arctan \left[ \kappa \tan ((\chi_f - \chi_i) \tau + \chi_i) \right] - \arctan \left[ \kappa \tan (\chi_i) \right] \right)
\] (A.26)

#### A.5.1 Expressions for \(\phi(\tau)\) in terms of \text{ArcSec}(x) :

The angle \(\phi(\tau)\) is an azimuthal angle measured from the \(x\)-axis counterclockwise, and due to the domain definition of the inverse trigonometric functions, we write the solutions for \(\phi\) in terms of \text{arcsec}.
By taking the tangent of both sides on equation (A.26),
\[
\tan \left[ \text{sgn} \left( \chi_f - \chi_i \right) \left( \phi(\tau) - \phi_i \right) + \arctan \left( \kappa \tan (\chi_i) \right) \right] = \kappa \tan \left( (\chi_f - \chi_i) \tau + \chi_i \right) \quad (A.27)
\]

Squaring both sides and using the trigonometric identity \(1 + \tan^2 x = \sec^2 x\),
\[
\tan^2 \phi(\tau) = \kappa^2 \tan^2 \left( (\chi_f - \chi_i) \tau + \chi_i \right) \implies \sec^2 \phi(\tau) = \kappa^2 \tan^2 \left( (\chi_f - \chi_i) \tau + \chi_i \right) + 1
\]

\[
\varphi(\tau) = \arcsin \left[ \text{sgn} \left( \chi_f - \chi_i \right) \kappa \tan (\chi_i) \right] - \arcsin \left[ \text{sgn} \left( \chi_f - \chi_i \right) \kappa \tan (\chi_i) \right] = \vartheta_i \rho_f \cos (\vartheta_i) + \sin (\vartheta_f) \sin (\vartheta_i) \quad (A.30)
\]

where we defined
\[
\vartheta_i,\rho_f = \arctan \left( \text{sgn} \left( \chi_f - \chi_i \right) \kappa \tan (\chi_i) \right) \quad (A.31)
\]

The trigonometric identities
\[
\cos (\arctan (x)) = \frac{1}{\sqrt{1 + x^2}}, \quad \sin (\arctan (x)) = \frac{x}{\sqrt{1 + x^2}} = x \cos (\arctan (x)) \quad (A.32)
\]

simplify the terms in Eq. (A.30) to
\[
\cos \left[ \arctan \left( \text{sgn} \left( \chi_f - \chi_i \right) \kappa \tan (\chi_i) \right) \right] = \frac{1}{\sqrt{1 + \kappa^2 \tan (\chi_i, \rho_f)^2}} \quad (A.33)
\]
Recalling the definition for $\chi_{i,f}$ (Eq. (A.18)),

$$\tan(\chi_{i,f}) = \tan\left(\arctan\left[\frac{\cos \theta_{i,f}}{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}\right]\right) = \frac{\cos \theta_{i,f}}{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}.$$  \hspace{1cm} (A.34)

Thus, Eq. (A.33) simplifies to

$$\cos\left[\arctan\left(\text{sgn}(\chi_f - \chi) \kappa \tan(\chi_{i,f})\right)\right] = \cos\left[\frac{\alpha^2 \tan(\theta_{i,f})^2 - \cot^2(\theta_{i,f})}{1 - \cos^2(\theta_{i,f})/\alpha^2}\right]^{-1/2}.$$ \hspace{1cm} (A.35)

The previous equation is rewritten as

$$\cos \phi_{i,f} = \frac{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}} = \frac{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}{\sqrt{\alpha^2 (1 - \cos^2 \theta_{i,f})}} = \frac{\sqrt{1 - \cos^2(\theta_{i,f})/\alpha^2}}{|\sin(\theta_{i,f})|} = \frac{\sqrt{\alpha^2 \csc^2(\theta_{i,f}) - \cot^2(\theta_{i,f})}}{\alpha}.$$ \hspace{1cm} (A.36)

For $\sin \phi_{i,f}$, note that $\sin(\arctan(x)) = x \cos(\arctan(x))$,

$$\sin(\arctan(\theta_{i,f})) = \text{sgn}(\chi_f - \chi_i) \left(\frac{\kappa \cos \theta_{i,f}}{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}\right) \frac{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}{\alpha |\sin(\theta_{i,f})|} = \text{sgn}(\chi_f - \chi_i) \frac{\kappa \cos \theta_{i,f}}{\alpha |\sin(\theta_{i,f})|} = \frac{\text{sgn}(\chi_f - \chi_i) \kappa}{\text{sgn}(\cos \theta_{i,f})} |\cot(\theta_{i,f})|.$$ \hspace{1cm} (A.37)

Inserting Eqs. (A.36) and (A.37) in (A.30),

$$\alpha^2 \cos (\phi_f - \phi_i) = \sqrt{(\alpha^2 \csc^2 \theta_i - \cot^2 \theta_i) (\alpha^2 \csc^2 \theta_f - \cot^2 \theta_f) + \kappa^2 |\cot \theta_i| |\cot \theta_f|}$$

$$= |\cot \theta_i| |\cot \theta_f| \left(\sqrt{\alpha^2 \tan^2 \theta_i - \kappa^2} (\alpha^2 \tan^2 \theta_f - \kappa^2) + \kappa^2\right)$$

Rearranging the terms,

$$\alpha^2 \cos (\phi_f - \phi_i) |\tan \theta_i| |\tan \theta_f| - \kappa^2 = \sqrt{(\alpha^2 \tan^2 \theta_i - \kappa^2) (\alpha^2 \tan^2 \theta_f - \kappa^2)},$$ \hspace{1cm} (A.39)

we square the right-hand side,

$$\alpha^4 \tan^2 \theta_i \tan^2 \theta_f - \kappa^2 \alpha^2 (\tan^2 \theta_i + \tan^2 \theta_f) + \kappa^4$$ \hspace{1cm} (A.40)

and the left-hand side,

$$\alpha^4 \tan^2 \theta_i \tan^2 \theta_f \cos^2 (\phi_f - \phi_i) - 2 \kappa^2 \alpha^2 \cos (\phi_f - \phi_i) |\tan \theta_i| |\tan \theta_f| + \kappa^4.$$ \hspace{1cm} (A.41)
Simplifying the equality between Eqs. (A.40) and (A.41),

\[ \alpha^2 \tan^2 \theta_i \tan^2 \theta_f \sin^2 (\phi_f - \phi_i) = \kappa^2 (\tan^2 \theta_i + \tan^2 \theta_f - 2 \cos (\phi_f - \phi_i)|\tan \theta_i| |\tan \theta_f|) \]
\[ \alpha^2 \sin^2 (\phi_f - \phi_i) = \kappa^2 (\cot^2 \theta_i + \cot^2 \theta_f - 2 \cos (\phi_f - \phi_i)|\cot \theta_i| |\cot \theta_f|) \] (A.42)

For further simplification, define \( z_{i,f} \equiv |\cot \theta_{i,f}| e^{i \phi_{i,f}} \),

\[ |z_f - z_i|^2 = \cot^2 \theta_i + \cot^2 \theta_f - 2 \cos (\phi_f - \phi_i)|\cot \theta_i| |\cot \theta_f| \] (A.43)

so Eq. (A.42) simplifies to

\[ \kappa = \frac{|\sin (\phi_f - \phi_i)|}{\sqrt{|z_f - z_i|^2 + \sin^2 (\phi_f - \phi_i)}}, \quad z_{i,f} \equiv |\cot \theta_{i,f}| e^{i \phi_{i,f}}, \] (A.44)

or equivalently,

\[ \kappa = \frac{1}{\sqrt{|z_f - z_i|^2 \csc^2 (\phi_f - \phi_i) + 1}}. \] (A.45)

The equation above is the solution for the parameter \( \kappa \) in terms of the boundary values.

### A.7 Boundary Values and Solution for \( \sigma \)

To obtain an expression for \( \sigma \) in terms of the boundary values, take the cosine of Eq. (A.19) and use the identity \( \pm \arctan (x) = \arctan (\pm x) \),

\[ \cos \sigma = \cos \left[ \text{sgn} (\chi_f - \chi_i) \left( \arctan \left[ \tan (\chi_f) \right] - \arctan \left[ \tan (\chi_i) \right] \right) \right] \]
\[ = \cos \left[ \arctan \left( \text{sgn} (\chi_f - \chi_i) \tan (\chi_f) \right) - \arctan \left( \text{sgn} (\chi_f - \chi_i) \tan (\chi_i) \right) \right] \]
\[ = \cos \eta_f \cos \eta_i + \sin \eta_f \sin \eta_i \] (A.46)

where we defined

\[ \eta_{i,f} = \arctan \left[ \text{sgn} (\chi_{i,f} - \chi_{i,i}) \tan (\chi_{i,f}) \right]. \] (A.47)

Using the trigonometric identities (A.32),

\[ \cos \left[ \arctan \left( \text{sgn} (\chi_{i,f} - \chi_{i,i}) \tan (\chi_{i,f}) \right) \right] = \frac{1}{\sqrt{1 + \tan^2 (\chi_{i,f})}} \] (A.48)
Recalling the result from Eq. (A.34),

\[
\cos (\eta_{i,f}) = \left[ 1 + \left( \frac{\cos \theta_{i,f}}{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}} \right)^2 \right]^{-1/2} = \frac{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}{\alpha} = \frac{\sqrt{\sin^2 \theta_{i,f} - \kappa^2}}{\sqrt{1 - \kappa^2}}. \tag{A.49}
\]

For \(\sin \theta_{i,f}\), as before,

\[
\sin \left[ \arctan \left( \frac{\text{sgn} (\chi_f - \chi_i) \tan (\chi_{i,f})}{\sqrt{1 + \tan^2 (\chi_{i,f})}} \right) \right] = \frac{\text{sgn} (\chi_f - \chi_i) \tan (\chi_{i,f})}{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}} \frac{\sqrt{\alpha^2 - \cos^2 \theta_{i,f}}}{\alpha} = \frac{\text{sgn} (\chi_f - \chi_i) \cos \theta_{i,f}}{\sqrt{1 - \kappa^2}}. \tag{A.50}
\]

Substituting the above expressions in Eq. (A.46),

\[
\cos \sigma = \frac{\sqrt{\left( \sin^2 \theta_i - \kappa^2 \right)(\sin^2 \theta_f - \kappa^2)} + \cos \theta_i \cos \theta_f}{1 - \kappa^2}. \tag{A.51}
\]

As \(\sigma \geq 0\) and the inverse cosine function is defined by \(\text{arccos} : [0, \pi] \rightarrow [-1, 1]\), the solution for sigma is correctly written as

\[
\sigma = \arccos \left( \frac{\sqrt{(\sin^2 \theta_i - \kappa^2)(\sin^2 \theta_f - \kappa^2)} + \cos \theta_i \cos \theta_f}{1 - \kappa^2} \right) \tag{A.52}
\]

with \(\kappa\) given by Eq. (A.44).

### A.8 Conclusion

We have thus solved for the geodesic paths in \(S^2 - \mathbb{CP}^1\) given arbitrary boundary values:

- The solution for \(\theta(\tau)\) is given by Eq. (A.23),

\[
\theta(\tau) = \arccos \left[ \sqrt{1 - \kappa^2} \sin ((\chi_f - \chi_i) \tau + \chi_i) \right] \tag{A.53}
\]

where

\[
\chi_{i,f} = \arccos \left( \frac{\sqrt{(1 - \kappa^2) - \cos^2 \theta_{i,f}}}{\sqrt{1 - \kappa^2}} \right). \tag{A.54}
\]
• The solution for $\phi(\tau)$ is given by Eq. (A.29),

$$
\phi(\tau) = \phi_i + \text{arcsec}\left[ \text{sgn}(\Upsilon^2(\tau) + 1) \sqrt{\Upsilon^2(\tau) + 1} \right] - \text{arcsec}\left[ \text{sgn}(\Upsilon^2(0) + 1) \sqrt{\Upsilon^2(0) + 1} \right]
$$

(A.55)

where $\Upsilon(\tau) = \kappa \tan((\chi_f - \chi_i) \tau + \chi_i)$.

• The parameter $\kappa$ is given by Eq. (A.44),

$$
\kappa = \frac{|\sin(\phi_f - \phi_i)|}{\sqrt{|z_f - z_i|^2 + \sin^2(\phi_f - \phi_i)}}, \quad z_{i,f} \equiv |\cot \theta_{i,f}| e^{i \phi_{i,f}}.
$$

(A.56)

• Finally, the parameter $\sigma = \Delta E / R$ is given by

$$
\sigma = \arccos\left( \frac{\sqrt{(\sin^2 \theta_i - \kappa^2)(\sin^2 \theta_f - \kappa^2) + \cos \theta_i \cos \theta_f}}{1 - \kappa^2} \right)
$$

(A.57)

For a different time interval, $[0, t_f]$, $t_f \neq 1$, the affine parametrization $\tau \equiv t / t_f$ gives the solution for the geodesic equations (A.7) and (A.8) with boundary conditions $\phi(0) = \phi_i$, $\phi(t_f) = \phi_f$ and $\theta(0) = \theta_i$, $\theta(t_f) = \theta_f$. 
Appendix B

General Solution for the Sphere Geodesics – II

B.1 Geodesic Path for the XY spin chain

The boundary conditions for the XY spin chain geodesic in Chapter 2 are \( \eta(0) = \pi/4, \eta(t_f) = 3\pi/4 \) and \( \varphi(0) = 0, \varphi(t_f) = \pi/\sqrt{2} \).

The parameter \( \kappa \) is given by Eq. (A.56). We have

\[
|z_f - z_i|^2 = \cot^2 \eta_i + \cot^2 \eta_f - 2 \cos (\varphi_f - \varphi_i) |\cot \eta_i| |\cot \eta_f|
= 2 \left( 1 - \cos \left( \frac{\pi}{\sqrt{2}} \right) \right) = 4 \sin^2 \left( \frac{\pi}{2\sqrt{2}} \right).
\]

(B.1)

Thus,

\[
\kappa = \frac{|\sin (\varphi_f)|}{\sqrt{|z_f - z_i|^2 + \sin^2 (\varphi_f)}} = \frac{|\sin \left( \frac{\pi}{\sqrt{2}} \right)|}{\sqrt{4 \sin^2 \left( \frac{\pi}{2\sqrt{2}} \right) + \sin^2 \left( \frac{\pi}{2\sqrt{2}} \right)}},
\]

(B.2)

so that

\[
\kappa^2 = \frac{1}{1 + \sec^2 \left( \frac{\pi}{2\sqrt{2}} \right)}.
\]

(B.3)

Consequently,

\[
\alpha^2 = 1 - \kappa^2 = \frac{1 + \sec^2 \left( \frac{\pi}{2\sqrt{2}} \right)}{1 + \sec^2 \left( \frac{\pi}{2\sqrt{2}} \right)} - 1 = \frac{\sec^2 \left( \frac{\pi}{2\sqrt{2}} \right)}{1 + \sec^2 \left( \frac{\pi}{2\sqrt{2}} \right)} = \frac{1}{1 + \cos^2 \left( \frac{\pi}{2\sqrt{2}} \right)}.
\]

(B.4)
The parameter \( \sigma = \Delta E / R \) is given by Eq. (A.57),

\[
\sigma = \arccos \left( \frac{\sqrt{(\sin^2 \left( \frac{\pi}{4} \right) - \kappa^2)(\sin^2 \left( \frac{3\pi}{4} \right) - \kappa^2) + \cos \left( \frac{\pi}{4} \right) \cos \left( \frac{3\pi}{4} \right)}}{1 - \kappa^2} \right)
\]

\[
= \arccos \left( \cos \left( \frac{\pi}{2 \sqrt{2}} \right) \right)
\]

(B.5)

The solution for \( \theta(\tau) \) is given by Eq. (A.53),

\[
\theta(\tau) = \arccos \left[ \sqrt{1 - \kappa^2} \sin \left( (\chi_f - \chi_i) \tau + \chi_i \right) \right]
\]

(B.6)

where

\[
\chi_{i,f} = \arctan \left[ \frac{\cos \eta_{i,f}}{\sqrt{\alpha^2 - \cos^2 \eta_{i,f}}} \right],
\]

(B.7)

i.e.,

\[
\chi_i = \arctan \left[ \frac{\cos \eta_i}{\sqrt{\alpha^2 - \cos^2 \eta_i}} \right] = \arctan \left[ \frac{\cos \left( \frac{\pi}{4} \right)}{\sqrt{\alpha^2 - \cos^2 \left( \frac{\pi}{4} \right)}} \right] = \arctan \left[ -\frac{1}{\sqrt{2\alpha^2 - 1}} \right]
\]

(B.8)

Similarly,

\[
\chi_f = \arctan \left[ \frac{\cos \eta_f}{\sqrt{\alpha^2 - \cos^2 \eta_f}} \right] = \arctan \left[ \frac{\cos \left( \frac{3\pi}{4} \right)}{\sqrt{\alpha^2 - \cos^2 \left( \frac{3\pi}{4} \right)}} \right] = \arctan \left[ -\frac{1}{\sqrt{2\alpha^2 - 1}} \right]
\]

(B.9)

which implies

\[
\chi_f = -\arctan \left[ \sqrt{\csc^2 \left( \frac{\pi}{2 \sqrt{2}} \right) + \cot^2 \left( \frac{\pi}{2 \sqrt{2}} \right)} \right] = -\chi_i.
\]

(B.10)

Since \( \chi_i > 0 \), \( \chi_f - \chi_i = -2\chi_i < 0 \). Moreover, from Eq. (A.19), \( \sigma = 2\chi_i \). Thus, \( \chi_f - \chi_i = -\sigma / 2 \),

\[
(\chi_f - \chi_i) \tau + \chi_i = -\frac{\sigma}{2} \tau + \frac{\sigma}{2}
\]

(B.11)

The solution for \( \varphi(\tau) \) is given by Eq. (A.55),

\[
\varphi(\tau) = \varphi_i + \arccos \left[ \text{sgn} \left( \Upsilon^2(\tau) + 1 \right) \sqrt{\Upsilon^2(\tau) + 1} \right] - \arccos \left[ \text{sgn} \left( \Upsilon^2(0) + 1 \right) \sqrt{\Upsilon^2(0) + 1} \right]
\]

(B.12)

where \( \Upsilon(\tau) = \kappa \tan \left( (\chi_f - \chi_i) \tau + \chi_i \right) = \frac{\tan(\chi_f - \chi_i) \tau + \chi_i)}{1 + \sec^2 \left( \frac{\pi}{2 \sqrt{2}} \right)} \).
Appendix C

Simulating Evolution of Quantum Observables Numerically

C.1 On The Use of Mollifiers

When numerically simulating the evolution of a quantum state using the quantum evolution operator $U(t; t_0)$,

$$U(t; t_0) = \int_{t_0}^{t} \exp \left( -\frac{i \hat{H}(\tau)(\tau - t_0)}{\hbar} \right) d\tau,$$

one undesired phenomenon shows up consistently.

C.1.1 Gibbs Phenomenon

Generically speaking, the Hamiltonian $\hat{H}(t)$ at different times do not necessarily commute with each other. To code Eq. (C.1) numerically, one technically discretizes the time domain in $N$ steps of small size $dt$. The state is then evolved at infinitesimal time steps according to

$$|\psi(t_n)\rangle = \Delta U(t_n, t_{n-1}) |\psi(t_{n-1})\rangle,$$

with $t_n$ and $t_{n-1} = t_n - dt$ labelling the current and previous times, respectively. The discretized unitary operator $\Delta U(t_n; t_{n-1})$ is given by

$$\Delta U(t_n; t_{n-1}) = \exp \left( -\frac{i}{\hbar} \hat{H}(t_n)(t_n - t_{n-1}) \right).$$
By using Eq. (C.2) with \( t_0 = t_{\text{initial}} = t_i \) and \( t_N = N dt = t_{\text{final}} \equiv T \), one numerically evolve any eigenstate of \( \hat{\mathcal{H}}(t) \) between \( t_0 \) and \( T \) and observes a tradeoff between accuracy and computation time as \( N = T/dt \) increases.

For an equal partition on the time domain \( [t_0, T] \), the time ramp is not differentiable at the boundaries. Thus, the time ramp derivative has jump discontinuities at those points. This discontinuity introduces what is known in the literature as the Gibbs phenomenon: an oscillatory behavior (known in signal processing as ringing artifacts) is seen in observables and in the overlap between the evolved and the instantaneous eigenstate along the ramp. This basic result follows from Benedick’s theorem, which states that it is not possible to sharply localize a function in both the time and frequency domain. Perfect specification of the protocol on the time domain boundaries implies a high temporal resolution, and the cost is a poor frequency resolution. The effect becomes more prominent\(^1\) if the energy gap at \( t_n \) is of the order of \( dt \).

There are ways to avoid the appearance of ringing artifacts, e.g., designing proper filters, making use of the Heisenberg-Gabor limit to properly balance the resolution in time and frequency domains, make use of the Weierstrass transform to smooth out the original function, among others.

### C.1.2 Mollifiers: Approximations to the Identity

We focus here on the use of functions \( g(t) \) known as mollifiers to smoothen out the boundaries of the time ramp by multiplying them by \( g(t) \). These functions have a smooth derivative at \( t = 0 \) with \( g(0) = 0 \), and after a given time \( \tau \) (the mollifier time constant) converges quickly to the identity function \( g(t) = 1 \). Multiplying the linear protocol obtained by the linear partition of the time domain by a mollifier \( g(t) \) has thus the effect of smoothening the function at the boundary for a short time period \( \tau \), with the effect becoming less prominent afterwards.

As a direct consequence of such approach, the evolution at the boundaries during the

\(^1\)In numerical simulations, \( \hbar = 1 \) and energy is measured in Hz.
interval given by the time constant $\tau$ of a given mollifier does not reflect exactly the evolution along a geodesic curve, since the later requires the velocity to be parametrized by the arclength, which computationally is the case only if the time evolution is the ramp function $f(t) = t/t_f - t_0$ linearly connecting the initial and final time. Neglecting this overshoot effect at the beginning of evolution, reliable results are obtained at the final time, where we are interested in measuring the fidelity.

C.1.3 Examples of Mollifing Functions

Several smooth functions can be used to smooth the edges of the ramp function $f(t) = t_0 + (t - t_0)$. Here are some of them.

Inductor-like Mollifier:

The mollifier function $g(t)$ is given by

$$g(t) = t_0 + (t - t_0) \left( 1 - \exp \left[ -\frac{t - t_0}{(t_f - t_0) \sigma} \right]^p \right),$$  \hspace{1cm} (C.4)

where $p$ and $\sigma$ are parameters to be chosen properly, depending on the case.

This is the mollifier function used to obtain the numerical results in Chapter 2.

Hyperbolic Tangent Mollifier:

The function $g(t)$ is given by

$$g(t) = t_0 + (t - t_0) \tanh \left( \left( \frac{t - t_0}{(t_f - t_0) \sigma} \right)^p \right)$$  \hspace{1cm} (C.5)

where $p$ and $\sigma$ are parameters to be properly chosen.

Penrose Mollifier:

The mollifier function $g(t)$ is given by

$$g(t) = t_0 + (t - t_0) \frac{\exp \left( -\frac{\alpha}{(t_f - t_0)^p} \right)}{\exp \left( -\frac{\alpha}{(t_f - t_0)^p} \right) + \exp \left( -\frac{\alpha}{(1-(t_f - t_0)^p)} \right)}$$  \hspace{1cm} (C.6)

where $\alpha$ and $p$ are parameters to be properly chosen.
Appendix D

Derivatives of Eigenvalues and Eigenkets with respect to free parameter

D.1 Eigenkets Derivatives

Let us derive the relationship between the derivatives of eigenvalues and eigenkets with respect to \( \lambda \). From Schrödinger’s equation,

\[
\hat{H}\ket{\Psi_n} = E_n\ket{\Psi_n} \implies (\partial_\lambda \hat{H})\ket{\Psi_n} + \hat{H}(\partial_\lambda \Psi_n) = (\partial_\lambda E_n)\ket{\Psi_n} + E_n(\partial_\lambda \Psi_n)
\]  

(D.1)

Taking the inner product with \( \bra{\Psi_m}, m \neq n \),

\[
\bra{\Psi_m}(\partial_\lambda \hat{H})\ket{\Psi_n} + E_m\bra{\Psi_m}(\partial_\lambda \Psi_n) = E_n\bra{\Psi_m}(\partial_\lambda \Psi_n) \implies \bra{\Psi_m}(\partial_\lambda \Psi_n) = \frac{\bra{\Psi_m}(\partial_\lambda \hat{H})\ket{\Psi_n}}{(E_n - E_m)}
\]  

(D.2)

Observe that due to the normalization of \( \ket{\Psi_n} \),

\[
\partial_\lambda \left[ \bra{\Psi_n} \right] = 0 \implies \bra{\partial_\lambda \Psi_n} = -\bra{\Psi_n}(\partial_\lambda \Psi_n) = -\bra{\partial_\lambda \Psi_n}^\dagger.
\]  

(D.3)

Thus, \( \bra{\Psi_n}(\partial_\lambda \Psi_n) \) is a purely imaginary number (as alluded in Sec. 4.1). Define

\[
\mathcal{A}_n^\lambda \equiv \bra{\Psi_n}i(\partial_\lambda \Psi_n),
\]  

(D.4)

and we can finally write

\[
\ket{\partial_\lambda \Psi_n} = \sum_{m \neq n} \frac{\bra{\Psi_m}(\partial_\lambda \hat{H})\ket{\Psi_n}}{(E_n - E_m)}\ket{\Psi_m} - i \mathcal{A}_n^\lambda \ket{\Psi_n}.
\]  

(D.5)
D.2 Eigenenergies Derivatives

Back to Equation (D.1), let us now take the inner product with $\langle \Psi_n |$,

$$
\langle \Psi_n | \partial_\lambda \hat{H} | \Psi_n \rangle + E_n \langle \Psi_n | \partial_\lambda \Psi_n \rangle = \partial_\lambda E_n \langle \Psi_n | \Psi_n \rangle + E_n \langle \Psi_n | \partial_\lambda \Psi_n \rangle .
$$

(D.6)

Hence,

$$
\partial_\lambda E_n = \langle \Psi_n | \partial_\lambda \hat{H} | \Psi_n \rangle .
$$

(D.7)

D.3 Recasting the Quantum Geometric Tensor in terms of Hamiltonian derivatives

Defining the notation $\hat{M}_\mu = \partial_\mu \hat{H}$, the two final results from the previous sections are written as

$$
\partial_\lambda E_n = \langle \Psi_n | \hat{M}_\lambda | \Psi_n \rangle ,
$$

(D.8)

and

$$
| \partial_\mu \Psi_n \rangle = \sum_{m \neq n} \frac{\langle \Psi_m | \partial_\mu \hat{H} | \Psi_n \rangle}{(E_n - E_m)} | \Psi_m \rangle + \langle \Psi_n | \partial_\mu | \Psi_n \rangle | \Psi_n \rangle

= \sum_{m \neq n} \frac{\langle \Psi_m | \hat{M}_\mu | \Psi_n \rangle}{(E_n - E_m)} | \Psi_m \rangle - i A_n^\mu | \Psi_n \rangle .
$$

(D.9)

The quantum geometric tensor $\chi_{\mu\nu}$ can thus be written as

$$
\chi_{\mu\nu} = \langle \Psi_n | \partial_\mu \partial_\nu | \Psi_n \rangle - \langle \Psi_n | \partial_\mu | \Psi_n \rangle \langle \Psi_n | \partial_\nu | \Psi_n \rangle

= \sum_m \left( \langle \Psi_n | \partial_\mu | \Psi_m \rangle \langle \Psi_m | \partial_\nu | \Psi_n \rangle \right) - \langle \Psi_n | \partial_\mu | \Psi_n \rangle \langle \Psi_n | \partial_\nu | \Psi_n \rangle

= \sum_{m \neq n} \langle \Psi_n | \partial_\mu | \Psi_m \rangle \langle \Psi_m | \partial_\nu | \Psi_n \rangle

= \sum_{m \neq n} \frac{\langle \Psi_n | \hat{M}_\mu | \Psi_m \rangle \langle \Psi_m | \hat{M}_\nu | \Psi_n \rangle}{(E_n - E_m)^2} .
$$

(D.10)
Appendix E

Derivatives of the Quantum Geometric Tensor

In this Appendix, we derive Equation (3.31) for the derivative of the quantum geometric tensor, presented in Section 3.3.

We begin by introducing the notations

$$\hat{M}^\mu = \partial^\mu \hat{H}, \quad M^{nm}_\mu = \langle \Psi^n | \partial^\mu \hat{H} | \Psi^m \rangle = \langle \Psi^n | \hat{M}^\mu | \Psi^m \rangle,$$

$$M^{nn}_\mu = \langle \Psi^n | \partial^\mu \hat{H} | \Psi^n \rangle = \partial^\mu E_n, \quad \Delta_{nm} \equiv E_n - E_m,$$

(E.1)

where the $M^{nn}_\mu$ equality is derived from Eq. (D.7).

The Quantum Geometric Tensor is given by (Eq. (2.6)),

$$\chi_{\beta\gamma} = \sum_{m \neq n} \frac{\langle \Psi^n | \partial_{\beta} \hat{H} | \Psi^m \rangle \langle \Psi^m | \partial_{\gamma} \hat{H} | \Psi^n \rangle}{(E_n - E_m)^2} = \sum_{m \neq n} \frac{\langle \Psi^n | \hat{M}_{\beta} | \Psi^m \rangle \langle \Psi^m | \hat{M}_{\gamma} | \Psi^n \rangle}{(E_n - E_m)^2},$$

(E.2)

We now proceed to calculate the derivative of the quantum geometric tensor $\chi_{\beta\gamma}$ with respect to an arbitrary parameter $\alpha$. Applying the product rule, where dots on the bra/kets refer
to derivatives with respect to $\alpha$ for the sake of notational simplicity,

$$
\partial_\alpha \chi_{\beta \gamma} = \sum_{m \neq n} \frac{1}{(E_n - E_m)^2} \left[ \langle \Psi_n | \partial_\alpha \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \partial_\alpha \hat{M}_\gamma | \Psi_n \rangle + 
\right. \\
+ \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \hat{\Psi}_n \rangle + \\
+ \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \hat{\Psi}_n \rangle \\
- 2 \frac{E_n - E_m}{(E_n - E_m)^2} \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle \right].
$$

We define $\partial^2 \hat{H} = \langle \Psi_n | \partial_\alpha \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \partial_\alpha \hat{M}_\gamma | \Psi_n \rangle$ to group the terms with double derivatives in the Hamiltonian.

Making use of the results derived in Appendix D for the derivatives on bra/kets in term of sums over other states,

$$
\partial_\alpha \chi_{\beta \gamma} = \sum_{m \neq n} \Delta^{-2}_{nm} \left[ \partial^2 \hat{H} + 
\right. \\
+ \sum_{\ell \neq n} \frac{\langle \Psi_n | \hat{M}_\alpha | \Psi_\ell \rangle \langle \Psi_\ell | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle}{\Delta_{n\ell}} + i A_{\alpha}^{m} \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle \\
+ \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \hat{\Psi}_n \rangle \\
+ \sum_{\ell \neq m} \frac{\langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_\ell \rangle \langle \Psi_\ell | \hat{M}_\alpha | \Psi_n \rangle}{\Delta_{m\ell}} + i A_{\alpha}^{m} \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle \\
+ \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \hat{\Psi}_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \hat{\Psi}_n \rangle \\
\left. - 2 \frac{\partial_\alpha \Delta_{nm}}{\Delta_{nm}} \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle \right].
$$

The above can be rewritten as

$$
\partial_\alpha \chi_{\beta \gamma} = \sum_{m \neq n} \frac{1}{\Delta_{nm}^2} \left[ \partial^2 \hat{H} - 2 \frac{\partial_\alpha \Delta_{nm}}{\Delta_{nm}} M^{mn}_\beta M^{mn}_\gamma + 
\right. \\
+ \sum_{\ell \neq n} \frac{M^{m\ell}_n M^{m\ell}_\beta M^{mn}_\gamma}{\Delta_{n\ell}} + \sum_{\ell \neq m} \frac{M^{m\ell}_n M^{m\ell}_\beta M^{mn}_\gamma}{\Delta_{m\ell}} \right].
$$

(E.5)
Extracting the $\ell = m$ term in the $\ell \neq n$ sum and the $\ell = n$ term in the $\ell \neq m$ one,

\[
\partial_{\alpha} \chi_{\beta\gamma} = \sum_{m \neq n} \Delta_{nm}^{-2} \left[ \partial^2 \hat{H} - 2 \frac{\partial_{\alpha} \Delta_{nm} M_{\gamma}^\alpha M_{\gamma}^m}{\Delta_{nm}} + \frac{M_{\alpha}^m M_{\gamma}^m \partial_\beta E_m + M_{\beta}^m M_{\alpha}^m \partial_\gamma E_m - M_{\alpha}^m M_{\gamma}^m \partial_\beta E_n - M_{\beta}^m M_{\alpha}^m \partial_\gamma E_n}{\Delta_{nm}} + \sum_{\ell \neq n, m} \frac{M_{\alpha}^m M_{\ell}^m M_{\gamma}^m + M_{\beta}^m M_{\gamma}^m M_{\ell}^m}{\Delta_{n\ell}} + \frac{M_{\beta}^m M_{\ell}^m M_{\alpha}^m}{\Delta_{m\ell}} \right], \quad (E.6)
\]

i.e.,

\[
\partial_{\alpha} \chi_{\beta\gamma} = \sum_{m \neq n} \Delta_{nm}^{-2} \left[ \partial^2 \hat{H} - \frac{\partial_\beta \Delta_{nm} M_{\alpha}^m M_{\gamma}^m}{\Delta_{nm}} + \frac{\partial_\gamma \Delta_{nm} M_{\alpha}^m M_{\gamma}^m + 2 \partial_{\alpha} \Delta_{nm} M_{\gamma}^m M_{\gamma}^m}{\Delta_{nm}} + \sum_{\ell \neq n, m} \frac{M_{\beta}^m M_{\gamma}^m M_{\ell}^m}{\Delta_{n\ell}} + \frac{M_{\alpha}^m M_{\ell}^m M_{\gamma}^m}{\Delta_{m\ell}} \right], \quad (E.7)
\]

where $\partial^2 \hat{H} = \langle \Psi_n | \partial_\alpha \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \hat{M}_\gamma | \Psi_n \rangle + \langle \Psi_n | \hat{M}_\beta | \Psi_m \rangle \langle \Psi_m | \partial_\alpha \hat{M}_\gamma | \Psi_n \rangle$.

The usefulness of the above result is two-fold:

1. To calculate geodesics for non-analytic systems, the derivative of the metric is needed for the Christoffel symbols expression. The real part of the above expression becomes necessary;

2. To obtain derivatives of the Berry curvature, the imaginary part of the above result can be used.

The geodesics used on the experiment described in Chapter 6 were obtained using the above final expression to numerically compute the necessary paths.
Appendix F

Degenerate Perturbation Theory

F.1 Degenerate perturbation theory: ground-state calculation

In this Appendix, we calculate in detail the second-order degenerate perturbation theory for the ground-state in the vicinity of the degeneracy points on the broken exchange symmetry case presented in Chapter 5. After the ground-state is obtained, we calculate the Berry connection and curvature, as well as the curl of the Berry curvature.

Perturbation Theory: Eigenenergies and Eigenstates

First, we calculate the eigenvalues and eigenstates of $\hat{H}_0$ (c.f. Eq. (5.42)). The eigenenergies are given by

$$
E^{(0)}_1 = -\sqrt{B_0^2 + g^2}, \quad E^{(0)}_2 = -\sqrt{B_0^2 + g^2}, \quad E^{(0)}_3 = \sqrt{B_0^2 + g^2}, \quad E^{(0)}_4 = \sqrt{B_0^2 + g^2},
$$

(F.1)

and the corresponding eigenstates read

$$
|\Psi^{(0)}_1\rangle = (0, 0, 0, 1)^T,

|\Psi^{(0)}_2\rangle = \left(0, -\frac{B^+_z}{\sqrt{(B^+_z)^2 + (g/2)^2}}, \frac{g/2}{\sqrt{(B^+_z)^2 + (g/2)^2}}, 0\right)^T,

|\Psi^{(0)}_3\rangle = \left(0, -\frac{B^-_z}{\sqrt{(B^-_z)^2 + (g/2)^2}}, \frac{g/2}{\sqrt{(B^-_z)^2 + (g/2)^2}}, 0\right)^T,

|\Psi^{(0)}_4\rangle = (1, 0, 0, 0)^T.
$$

(F.2)
The location of the energy level crossings of the ground-state and the first excited state on the $z$-axis appear at

$$B^+_z = \frac{-B_0 + \sqrt{B_0^2 + g^2}}{2}, \quad B^-_z = \frac{-B_0 - \sqrt{B_0^2 + g^2}}{2}. \quad (F.3)$$

We note the following useful identities

$$B^+_z + B^-_z = -B_0, \quad B^+_z - B^-_z = \sqrt{B_0^2 + g^2}. \quad (F.4)$$

Let us also introduce the following notations,

$$\delta \equiv \sqrt{B_0^2 + g^2}, \quad \beta^2 \equiv g/\delta, \quad \Delta \equiv \frac{B^+_z - g/2}{\sqrt{(B^+_z)^2 + (g/2)^2}}, \quad \eta \equiv \frac{B^-_z - g/2}{\sqrt{(B^-_z)^2 + (g/2)^2}}. \quad (F.5)$$

The unperturbed eigenstates $\{|\Psi^{(0)}_1\rangle, |\Psi^{(0)}_2\rangle\}$ and $\{|\Psi^{(0)}_3\rangle, |\Psi^{(0)}_4\rangle\}$ are degenerate, therefore one needs to use a degenerate perturbation theory to compute the first-order corrections.

To this end, we write the matrix

$$W = \begin{pmatrix}
\langle \Psi^{(0)}_1 | \hat{H}' | \Psi^{(0)}_1 \rangle & \langle \Psi^{(0)}_1 | \hat{H}' | \Psi^{(0)}_2 \rangle \\
\langle \Psi^{(0)}_2 | \hat{H}' | \Psi^{(0)}_1 \rangle & \langle \Psi^{(0)}_2 | \hat{H}' | \Psi^{(0)}_2 \rangle
\end{pmatrix} = \begin{pmatrix}
-2 \cos \vartheta & -\frac{B^+_z - g/2}{\sqrt{(B^+_z)^2 + (g/2)^2}} \sin \vartheta \\
-\frac{B^-_z - g/2}{\sqrt{(B^-_z)^2 + (g/2)^2}} \sin \vartheta & 0
\end{pmatrix}
= \begin{pmatrix}
-2 \cos \vartheta & -\Delta \sin \vartheta \\
-\Delta \sin \vartheta & 0
\end{pmatrix}. \quad (F.6)$$

The matrix $W$ has eigenvalues

$$E^{(1)}_{\pm} = -\cos \vartheta \pm \sqrt{\cos^2 \vartheta + \Delta^2 \sin^2 \vartheta} = -\cos \vartheta \pm \sqrt{1 - \beta^2 \sin^2 \vartheta}, \quad (F.7)$$

where we used the identities

$$\Delta^2 = \frac{(B^+_z - g/2)^2}{(B^+_z)^2 + (g/2)^2} = 1 - \frac{2B^+_z (g/2)}{(B^+_z)^2 + (g/2)^2} = 1 - \frac{g}{\delta} \equiv 1 - \beta^2. \quad (F.8)$$

The eigenvalues $E^{(1)}_{\pm}$ of the matrix $W$ give the first-order correction to the two lowest eigenenergies, namely $E_{1,2} = E^{(0)}_1 + dB E^{(1)}_{\pm}$. 
The eigenvectors of $W$ are written as $|w_{1,2}\rangle$ and read

$$|w_1\rangle = \left( \begin{array}{c} \frac{E_-^{(1)}}{\sqrt{(E_-^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} - \frac{\Delta \sin \vartheta}{\sqrt{(E_-^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} \end{array} \right)^T = (a_1, b_1)^T,$$

$$|w_2\rangle = \left( \begin{array}{c} \frac{E_+^{(1)}}{\sqrt{(E_+^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} - \frac{\Delta \sin \vartheta}{\sqrt{(E_+^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} \end{array} \right)^T \quad (\text{F.9})$$

The “good” linear combination for the ground-state at zeroth-order is therefore given by

$$|\Psi_0^{(0)}\rangle = a_1|\Psi_1^{(0)}\rangle + b_1|\Psi_2^{(0)}\rangle$$

$$= \frac{E_-^{(1)}}{\sqrt{(E_-^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} \left( \begin{array}{c} 0 \\ 0 \\ 1 \end{array} \right) + \frac{-\Delta \sin \vartheta}{\sqrt{(E_-^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} \left( \begin{array}{c} 0 \\ \frac{1}{\sqrt{(B_z^+)^2 + (g/2)^2}} \\ 0 \end{array} \right)$$

$$= \frac{1}{\sqrt{(E_-^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} \left( \begin{array}{c} 0, \frac{B_z^+ \Delta \sin \vartheta}{\sqrt{(B_z^+)^2 + (g/2)^2}}, -\frac{(g/2) \Delta \sin \vartheta}{\sqrt{(B_z^+)^2 + (g/2)^2}}, E_-^{(1)} \end{array} \right)^T. \quad (\text{F.10})$$

The first-order correction to the ground-state is

$$|\Psi_0^{(1)}\rangle = \sum_{n\neq \{1,2\}} \frac{\langle \Psi_n^{(0)} | \hat{H}' | \Psi_0^{(0)} \rangle}{(E_1^{(0)} - E_n^{(0)})} |\Psi_n^{(0)}\rangle = -\frac{\sin \vartheta}{2\delta \sqrt{(E_-^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} \left( \begin{array}{c} \Delta^2 \sin \vartheta \\ \frac{B_z^+ \eta^2 E_-^{(1)}}{B_z^+ - g/2} \\ -\frac{g/2 \eta^2 E_-^{(1)}}{B_z^+ - g/2} \\ 0 \end{array} \right). \quad (\text{F.11})$$

The second-order correction to the ground-state is generically given by

$$|\Psi_0^{(2)}\rangle = \sum_{k \neq \{1,2\}} \left( \sum_{l \neq \{1,2\}} \frac{\langle \Psi_k^{(0)} | \hat{H}' | \Psi_l^{(0)} \rangle}{(E_1^{(0)} - E_k^{(0)})(E_1^{(0)} - E_l^{(0)})} |\Psi_k^{(0)}\rangle + \frac{1}{2} |\Psi_0^{(0)}\rangle \frac{\langle \Psi_0^{(0)} | \hat{H}' | \Psi_k^{(0)} \rangle \langle \Psi_k^{(0)} | \hat{H}' | \Psi_0^{(0)} \rangle}{(E_1^{(0)} - E_k^{(0)})^2} - \frac{\langle \Psi_0^{(0)} | \hat{H}' | \Psi_0^{(0)} \rangle \langle \Psi_0^{(0)} | \hat{H}' | \Psi_0^{(0)} \rangle}{(E_1^{(0)} - E_k^{(0)})^2} |\Psi_k^{(0)}\rangle \right), \quad (\text{F.12})$$
and developing the previous expression,

\[
|\Psi_0^{(2)}\rangle = \frac{\Delta^2 \sin^2 \vartheta}{4 \delta^2 \sqrt{(E_+^{(1)})^2 + \Delta^2 \sin^2 \vartheta}} \left( \begin{array}{c} \frac{\eta^2 E_+^{(1)}}{B_z^+ g/2} \Delta^2 \sin \vartheta \\ \frac{B_z^+}{B_z^+ g/2} \Delta^2 \sin \vartheta \\ \frac{g/2}{B_z^+ g/2} \eta^2 \sin \vartheta \\ 0 \end{array} \right) + \frac{\Delta^2 \sin^2 \vartheta \times \left( \frac{\eta^2 (E_+^{(1)})^2 + \Delta^2 \sin^2 \vartheta}{8 \delta^2 \left( (E_+^{(1)})^2 + \Delta^2 \sin^2 \vartheta \right)^{3/2}} \right)}{\frac{\Delta^2 \sin \vartheta \times \left( E_+^{(1)} \cos \vartheta - \Delta^2 \sin^2 \vartheta \right)}{2 \delta^2 \left( (E_+^{(1)})^2 + \Delta^2 \sin^2 \vartheta \right)^{3/2}}}
\]

\[\times \left( \begin{array}{c} 0 \\ \frac{B_z^+}{B_z^+ g/2} \Delta^2 \sin \vartheta \\ \frac{g/2}{B_z^+ g/2} \eta^2 \sin \vartheta \\ E_+^{(1)} \end{array} \right) + \frac{E_+^{(1)} \sin \vartheta \times \left( \eta^2 E_+^{(1)} \right)}{2 \delta^2 \left( (E_+^{(1)})^2 + \Delta^2 \sin^2 \vartheta \right)^{3/2}} \left( \begin{array}{c} 0 \\ \frac{B_z^+}{B_z^+ g/2} \Delta^2 \sin \vartheta \\ \frac{g/2}{B_z^+ g/2} \eta^2 \sin \vartheta \\ 0 \end{array} \right) . \tag{F.13}\]

The ground-state can then be expressed up to second-order by

\[
|\Psi_0(dB, \vartheta, 0)\rangle = |\Psi_0^{(0)}\rangle + dB |\Psi_0^{(1)}\rangle + dB^2 |\Psi_0^{(2)}\rangle , \tag{F.14}\]

and the dependence on the azimuth angle \(\phi\) is obtained through the following rotation

\[
|\Psi_0(dB, \vartheta, \phi)\rangle = R(\phi) |\Psi_0(dB, \vartheta, 0)\rangle , \tag{F.15}\]

where \(R(\phi) = \exp(i \phi (\hat{\sigma}_1 + \hat{\sigma}_2)/2).\)

### F.1.1 Berry connection – Effective magnetic vector potential

We are now able to calculate the Berry connection in spherical coordinates \(\vec{A}_+^{(S)}(dB, \vartheta, \phi)\), where the + sign indicates that we are considering small radial deviations \(dB\) close to the degeneracy located at \(B_z^+\). The operator \(\vec{\nabla}\) in spherical coordinates \((dB, \vartheta, \phi)\) is given by

\[
\vec{\nabla} = \left( \frac{\partial}{\partial dB} , 1 dB \frac{\partial}{\partial \vartheta} , 1 dB \sin \vartheta \frac{\partial}{\partial \phi} \right)^T \tag{F.16}\]
therefore the only non zero component of the Berry connection is \( A_{\phi^+} \) and reads

\[
A_{\phi^+} = \frac{1}{dB \sin \vartheta} \langle \Psi_0 (dB, \vartheta, \phi) | i \partial_\phi | \Psi_0 (dB, \vartheta, \phi) \rangle \\
= \frac{1}{dB \sin \vartheta} \langle \Psi_0 (dB, \vartheta, 0) \bigg| \left( \frac{\hat{\sigma}_1 + \hat{\sigma}_2}{2} \right) \bigg| \Psi_0 (dB, \vartheta, 0) \rangle \\
= \frac{1}{dB \sin \vartheta} \left[ \langle \Psi_0^{(0)} \bigg| \left( \frac{\hat{\sigma}_1 + \hat{\sigma}_2}{2} \right) \bigg| \Psi_0^{(0)} \rangle + 2 dB \langle \Psi_0^{(0)} \bigg| \left( \frac{\hat{\sigma}_1 + \hat{\sigma}_2}{2} \right) \bigg| \Psi_0^{(1)} \rangle \right. + \\
+ dB^2 \left( 2 \langle \Psi_0^{(0)} \bigg| \left( \frac{\hat{\sigma}_1 + \hat{\sigma}_2}{2} \right) \bigg| \Psi_0^{(2)} \rangle + \langle \Psi_0^{(1)} \bigg| \left( \frac{\hat{\sigma}_1 + \hat{\sigma}_2}{2} \right) \bigg| \Psi_0^{(1)} \rangle \right) + \ldots \right] \\
= \frac{1}{dB \sin \vartheta} \left[ - \frac{(E_1^{(1)})^2}{(E_1^{(1)})^2 + \Delta^2 \sin^2 \vartheta} + dB^2 \frac{\Delta^4 \sin^4 \vartheta}{4 \delta \left( (E_1^{(1)})^2 + \Delta^2 \sin^2 \vartheta \right)} + \\
+ dB^2 \frac{\eta^2}{\Delta^2} \left( (E_1^{(1)})^2 + \Delta^2 \sin^2 \vartheta \right) \frac{(E_1^{(1)})^2 \times \Delta^2 \sin^2 \vartheta}{4 \delta \left( (E_1^{(1)})^2 + \Delta^2 \sin^2 \vartheta \right)^2} + \ldots \right] \\
\approx \frac{1}{dB \sin \vartheta} \left[ - \frac{1}{2} \left( 1 + \frac{\cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right) + dB^2 \frac{\sin^2 \vartheta}{8 \delta^2} \times \\
\times \left( 1 - \beta^2 \right) \left( 1 - \frac{\cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right) + 1 + \frac{\beta^2 \cos^2 \vartheta}{1 - \beta^2 \sin^2 \vartheta} + \frac{(1 + \beta^2) \cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} + \ldots \right] \\
\approx \frac{1}{dB \sin \vartheta} \left[ - \frac{1}{2} \left( 1 + \frac{\cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right) + \\
+ dB^2 \left( \frac{\sin^2 \vartheta}{8 \delta^2} \right) \left( 2 - \beta^2 + \frac{\beta^2 \cos^2 \vartheta}{1 - \beta^2 \sin^2 \vartheta} + \frac{2 \beta^2 \cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right) \right], \quad (F.17)
\]

where

\[
\beta^2 = \frac{g}{\delta} = \frac{g}{\sqrt{B_0^2 + g^2}}, \quad \frac{\eta^2}{\Delta^2} = \frac{1 + \beta^2}{1 - \beta^2}. \quad (F.18)
\]

In summary, one can write the Berry connection (magnetic vector potential) in spherical coordinates \( \vec{A}^{(S)}_+ (dB, \vartheta, \phi) = A_{\phi^+} \hat{\phi} \), with

\[
A_{\phi^+} \approx \frac{1}{dB \sin \vartheta} \left[ - \frac{1}{2} \left( 1 + \frac{\cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right) + \\
+ dB^2 \frac{\sin^2 \vartheta}{8 \delta^2} \left( 2 - \beta^2 + \frac{\beta^2 \cos^2 \vartheta}{1 - \beta^2 \sin^2 \vartheta} + \frac{2 \beta^2 \cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right) \right], \quad (F.19)
\]

and keeping only the leading order term for \( A_{\phi^+} \), we have

\[
A_{\phi^+} \approx - \frac{1}{2} \frac{1}{dB \sin \vartheta} \left( 1 + \frac{\cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right). \quad (F.20)
\]
Figure F.1: A density plot of the $y$ component of $\vec{\nabla} \times \vec{F}$ in Cartesian coordinates as a function of $B_x$ and $B_z$ is shown for $B_y = 0$, $g = 2$ and $B_0 = 1$. The curl of the Berry curvature has only a $y$ component in the plane defined by $B_y = 0$. Negative values indicate that the vectors point perpendicularly out of the plane and positive values indicate the vectors point perpendicularly into the plane. On the left panel we show the curl of the Berry curvature obtained by perturbation theory and on the right obtained by exact diagonalization.

F.1.2 Berry curvature – Effective magnetic field

The Berry curvature $\vec{F}^{(S)}(dB, \vartheta, \phi)$ is obtained by taking the curl of (F.20). The curl operator in spherical coordinates $(dB, \vartheta, \phi)$ reads

$$\vec{F}^{(S)}(dB, \vartheta, \phi) = \vec{\nabla} \times \vec{A}^{(S)}(dB, \vartheta, \phi) = \frac{1}{dB \sin \vartheta} (\partial_\vartheta (A_\phi \sin \vartheta) - \partial_\phi A_\vartheta) dB +$$

$$+ \frac{1}{dB} \left( \frac{1}{\sin \vartheta} \partial_\phi A_{dB} - \partial_{dB} (dB A_\phi) \right) \hat{\vartheta} + \frac{1}{dB} (\partial_{dB} (dB A_\vartheta) - \partial_\vartheta A_{dB}) \hat{\phi},$$

where $\vec{A}^{(S)}(dB, \vartheta, \phi) = A_{dB} \hat{dB} + A_\vartheta \hat{\vartheta} + A_\phi \hat{\phi}$. The only non-vanishing component of $\vec{A}^{(S)}_+(dB, \vartheta, \phi)$ is $A_{\phi,+}$ and hence in the leading order of $dB$ we find

$$\vec{F}^{(S)}_+(dB, \vartheta, \phi) = \vec{\nabla} \times \vec{A}^{(S)}_+(dB, \vartheta, \phi) \approx \frac{1}{2} \frac{1}{\gamma^2 (1 - \beta^2 \sin^2 \vartheta)^{3/2}} \frac{1}{dB^2} \hat{dB},$$

where we introduced $\gamma \equiv 1/\sqrt{1 - \beta^2}$. 
F.1.3 Curl of Berry curvature

Finally, the curl of the Berry curvature to the leading order in $dB$ near the monopole $B^+_z$ can be calculated, and reads

$$\vec{n} \times \vec{F}^{(S)}_+ (dB, \vartheta, \phi) \approx -\frac{3}{4} \frac{\beta^2 \sin 2 \vartheta}{\gamma^2 (1 - \beta^2 \sin^2 \vartheta)^{5/2}} \frac{1}{dB^3} \hat{\theta} .$$  \hspace{1cm} (F.23)

Following exactly the same procedure described above, but applied to the degeneracy located at $B^-_z$, one finds that the leading order of $A_{\phi, -}$ is given by

$$A_{\phi, -} \approx \frac{1}{2} \frac{1}{dB \sin \vartheta} \left( 1 - \frac{\cos \vartheta}{\sqrt{1 - \beta^2 \sin^2 \vartheta}} \right) ,$$  \hspace{1cm} (F.24)

with respect to the coordinate system centered on $B^-_z$. The Berry curvature $\vec{F}^{(S)}_-(dB, \vartheta, \phi)$ and $\vec{n} \times \vec{F}^{(S)}_-(dB, \vartheta, \phi)$ can then be calculated accordingly.

The curl of the Berry curvature with respect to the original Cartesian coordinate system $(B_x, B_y, B_z)$ takes then the form

$$\vec{n} \times \vec{F}^{(C)}_\pm \approx -\frac{3}{2} \frac{\beta^2 B_z}{\gamma^2 \left( (1 - \beta^2) B_x^2 + (B_z - B_z^{(\pm)})^2 \right)^{5/2}} \left( \frac{-B_y \hat{x} + B_x \hat{y}}{\sqrt{B_x^2 + B_y^2}} \right) .$$  \hspace{1cm} (F.25)

In the $B_x - B_z$ plane, corresponding to $B_y = 0$, only the $y$-component of $\vec{n} \times \vec{F}^{(C)}_\pm$ is non-zero. This scenario is plotted in Fig. F.1. For comparison, we also plot the $y$-component of the curl of the Berry curvature calculated numerically by using exact diagonalization.
Appendix G

Location of the Two-qubit Charges

G.1 Locations of effective charges for the interacting two-qubit system

In Chapter 5, we explore and plot the Berry curvature and its curl for the ground-state $|\Psi_0\rangle$ to illustrate the locations of the ground-state degeneracies in parameter space. We use the analogy with electromagnetism, pointed out by M. V. Berry (Berry, 1984), that identifies the Berry curvature $\vec{F}$ with an effective magnetic field in parameter space whose vector potential is the Berry connection $\vec{A} = i\langle\Psi_0|\hat{\nabla}|\Psi_0\rangle$. The locations of the associated magnetic charges are given by the ground-state degeneracies, and their charge is determined by the first Chern number. The fact that degeneracies of the ground-state act as magnetic charges can be seen by the following reasoning: the vector identity $\hat{\nabla} \cdot (\hat{\nabla} \times \vec{A}) = 0$ holds only if $\vec{A}$ has continuous derivatives. This is no longer the case when the ground-state becomes degenerate, since at these points $|\Psi_0\rangle$ undergoes a discontinuous change and so the derivatives of $\vec{A}$ become discontinuous. As a result, at the degeneracies we have $\vec{\nabla} \cdot (\vec{\nabla} \times \vec{A}) \neq 0$, and in analogy with Maxwell’s equations we can write an equivalent Gauss’s law for the Berry curvature

$$\vec{\nabla} \cdot \vec{F} = 2\pi \rho_m,$$  \hspace{1cm} (G.1)

where $\rho_m$ is the effective magnetic charge density. The volume integral of (G.1) yields

$$\iiint_{\Sigma} \vec{F} \cdot d\vec{S} = 2\pi \iiint_{V} \rho_m dV,$$ \hspace{1cm} (G.2)
where the divergence theorem was applied to the left hand side of the equation. According to the Chern theorem (Nakahara, 2003), the integral of the Berry curvature over a closed manifold $\Sigma$ is quantized in units of $2\pi$, and this number defines the first Chern number

$$\text{ch}_1 = \frac{1}{2\pi} \iint_{\Sigma} \vec{F} \cdot d\vec{S}. \quad (G.3)$$

The comparison of the previous two equations implies the quantization of $\iiint_V \rho_m dV$, which also defines the effective charge enclosed by the manifold $\Sigma$.

For a single magnetic monopole charge $q_m$, the magnetic charge density is $\rho_m = q_m \delta(\vec{r})$ and the associated magnetic field is then given, in view of Eq. (G.2), by

$$\vec{F} = \frac{1}{2} q_m \frac{\hat{\vec{r}}}{|\vec{r}|^2}, \quad (G.4)$$

where the prefactor of $1/2$ sets the units such that the charge $q_m$ is equal to the Chern number. This example is realized by a single qubit (spin-1/2) in an external magnetic field $\vec{B}$, where the resulting Berry curvature is given by (G.4) and therefore analogous to an effective magnetic field in parameter space $(B_x, B_y, B_z)$, or $\vec{r} \equiv \vec{B}$, created by a magnetic monopole sitting at $B = 0$ and carrying a charge $q_m = 1$.

Finally, we note that the Berry curvature $\vec{F}$ associated with the ground-state can also be rewritten, using the resolution of the identity $\sum_m |\Psi_m\rangle\langle\Psi_m| = 1$, as a sum over all other eigenstates

$$\vec{F} = \ii \sum_{m \neq 0} \frac{\langle\Psi_0|\vec{\nabla} H|\Psi_m\rangle \times \langle\Psi_m|\vec{\nabla} H|\Psi_0\rangle}{(E_0 - E_m)^2}. \quad (G.5)$$

This equation highlights that degeneracies in the ground-state, $E_0 = E_m$, act as charges for $\vec{F}$. In particular, the expression (G.5) is useful to compute the Berry curvature numerically, if the Hamiltonian is not analytically diagonalizable.

In the following, we illustrate the calculations that lead to the localization of the ground-state degeneracies in parameter space for the two-qubit systems considered in Chapter 5. We also calculate the corresponding Berry connection, curvature and its curl. First, however, let us review some important properties of the system studied in Chapter 5, consisting of two interacting qubits, with each qubit separately coupled to external magnetic fields. The
Hamiltonian of this system is given by

\[ H = \vec{B} \cdot (\gamma_1 \vec{\sigma}_1 + \gamma_2 \vec{\sigma}_2) + \frac{g}{2} (\sigma^x_1 \sigma^x_2 + \sigma^y_1 \sigma^y_2) + g_z \sigma^z_1 \sigma^z_2 + B_0 \sigma^z_1, \]

where \( \vec{\sigma}_i \equiv (\sigma^x_i, \sigma^y_i, \sigma^z_i)^T \) are the usual Pauli matrices for the \( i \)-th spin

\[ \sigma^x_i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y_i = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z_i = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]

with \( i = 1, 2 \). The external magnetic field is \( \vec{B} = (B_x, B_y, B_z)^T \equiv (x, y, z)^T \), which acts isotropically on both spins if \( \gamma_1 = \gamma_2 \), and anisotropically if \( \gamma_1 \neq \gamma_2 \). The field \( B_0 \) is a local magnetic field applied only to the first spin in the \( z \) direction, and allows us to break the exchange symmetry between the two spins. The term \( g \) is the energy scale of the interaction between the two spins in the \( x \) and \( y \) direction, and \( g_z \) indicates the interaction in the \( z \) direction.

As mentioned in Chapter 5, we consider the parameters \( \gamma_1, \gamma_2, g, B_0 \) and \( g_z \) as fixed and restrict ourselves to the case of an adiabatically varying external magnetic field \( \vec{B} \) that spans the parameter space \( \mathcal{M} \equiv \mathbb{R}^3 \). The magnetic field \( \vec{B} \) in spherical coordinates \( (B, \theta, \phi) \) reads \( \vec{B} = B (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T = B \hat{B}(\theta, \phi) \), where \( \hat{B}(\theta, \phi) \) is the unit vector in the radial direction. The Hamiltonian in spherical coordinates can be rewritten as

\[ H(B, \theta, \phi) = B \hat{B}(\theta, \phi) \cdot (\gamma_1 \vec{\sigma}_1 + \gamma_2 \vec{\sigma}_2) + \frac{g}{2} (\sigma^x_1 \sigma^x_2 + \sigma^y_1 \sigma^y_2) + g_z \sigma^z_1 \sigma^z_2 + B_0 \sigma^z_1, \]

and written in this form, it is evident that the Hamiltonian at arbitrary \( \phi \) can be obtained from the one at \( \phi = 0 \) by

\[ H(B, \theta, \phi) = R^\dagger(\phi) H(B, \theta, 0) R(\phi), \]

where \( R(\phi) = \exp(i \phi \sigma^z_{\text{tot}}/2) \) and \( \sigma^z_{\text{tot}} = \sigma^z_1 + \sigma^z_2 \). Equation (G.9) implies that the eigenstates of \( H(B, \theta, \phi) \) are simply given by a rotation of the eigenstates of \( H(B, \theta, 0) \),

\[ |\Psi_m(B, \theta, \phi)\rangle = R^\dagger(\phi) |\Psi_m(B, \theta, 0)\rangle, \]

and the eigenenergies of \( H(B, \theta, \phi) \) are the same for \( H(B, \theta, 0) \), \( E_m(B, \theta, \phi) = E_m(B, \theta, 0) \). Note that Eq. (G.9) does not provide any additional conservation laws but it is useful for the calculation of the Berry connection and curvature.
The relation $|\Psi_0(B, \theta, \phi)\rangle = R^\dagger(\phi)|\Psi_0(B, \theta, 0)\rangle$, where $R(\phi) = \exp(i \phi \sigma^z_{\text{tot}}/2)$, allows us to calculate the Berry connection in spherical coordinates straightforwardly. First, observe that the quantities $\langle \Psi_0|\partial_\mu|\Psi_0\rangle$, for $\mu = \{B, \theta, \phi\}$, must be purely imaginary numbers. This can be seen by differentiating the normalization condition $\langle \Psi_0|\Psi_0\rangle = 1$ with respect to either $B, \theta$ or $\phi$. A gauge choice allows us to choose the eigenstates of the Hamiltonian (G.6) to be real at $\phi = 0$, and therefore, for any $B$ and $\theta$, writing $|\Psi_0(B, \theta, \phi)\rangle \equiv |\tilde{\Psi}_0(\phi)\rangle$, we have

$$\langle \tilde{\Psi}_0(\phi)|\partial_B|\tilde{\Psi}_0(\phi)\rangle = \langle \tilde{\Psi}_0(0)|\partial_B|\tilde{\Psi}_0(0)\rangle = 0. \quad (G.11)$$

A similar reasoning holds for $\langle \Psi_0(B, \theta, \phi)|\partial_\theta|\Psi_0(B, \theta, \phi)\rangle$. The only non-vanishing component is $A_\phi$, which reads

$$A_\phi = i \frac{1}{B \sin \theta} \langle \tilde{\Psi}_0(\phi)|\partial_\phi|\tilde{\Psi}_0(\phi)\rangle = \frac{1}{B \sin \theta} \langle \tilde{\Psi}_0(0)|i R(\phi)\partial_\phi R^\dagger(\phi)|\tilde{\Psi}_0(0)\rangle, \quad (G.12)$$

and since

$$i R(\phi)\partial_\phi R^\dagger(\phi) = i e^{i \phi \sigma^z_{\text{tot}}/2} \partial_\phi e^{-i \phi \sigma^z_{\text{tot}}/2} = \frac{\sigma^z_{\text{tot}}}{2}, \quad (G.13)$$

the Berry connection in spherical coordinates is finally given by

$$\vec{A}^{(S)}(B, \theta, \phi) = \frac{1}{B \sin \theta} \langle \tilde{\Psi}_0(0)|\sigma^z_{\text{tot}}|\tilde{\Psi}_0(0)\rangle \hat{\phi} = \frac{1}{B \sin \theta} \frac{\langle \sigma^z_{\text{tot}}\rangle}{2} \hat{\phi}, \quad (G.14)$$

where $\langle \sigma^z_{\text{tot}}\rangle$ is the ground-state expectation value of the total magnetization in the $z$-direction at $\phi = 0$. In Cartesian coordinates, we have

$$\vec{A}^{(C)}(x, y, z) = \frac{\langle \sigma^z_{\text{tot}}\rangle}{2} \left( \frac{-y \hat{x} + x \hat{y}}{x^2 + y^2} \right), \quad (G.15)$$

with $\langle \sigma^z_{\text{tot}}\rangle$, the ground-state expectation value of the total magnetization in the $z$-direction given in Cartesian coordinates at $B_y = 0$. 
Bibliography


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EDUCATION

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• 2010, M.A. in Physics (Cum Laude), Federal University of Pernambuco, Recife, PE, Brazil
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RESEARCH AND TEACHING EXPERIENCE

• Sep. 2010 – Dec. 2015, Teaching assistant in several courses, including General Physics I, General Physics II and Advanced General Physics I at Boston University, Boston MA, USA.
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PUBLICATIONS

