Universidade de São Paulo
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Fases geométricas e aplicações em sistemas quânticos de dois níveis

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“Geometric phases and applications in two-level quantum systems”

Abstract

Several formulations for the geometric phase for closed and open quantum systems are reviewed and are illustrated by two-level systems. In particular, using the result for non-unitary evolution in the context of interferometry, we obtain phase factors for a two-level quantum system considering relevant sources of decoherence.

The study of two-level quantum systems subjected to time-dependent perturbation is reviewed using the rotating wave approximation and a perturbative solution. For the later, we obtain the phase factors for a cyclic evolution in the parameter space of the Hamiltonian and also extend the results for two two-level quantum systems non-interacting and with interaction modeled by a delta function. The time-evolution operator used in our results are calculated up to first order in the Dyson series.

We furthermore investigate the limits of the implementation of a quantum gate using the rotating wave approximation and explore the possibility of implementing a quantum phase gate using the perturbative solution.

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Contents

Chapter 1

Introduction

Even though the grounds for Quantum Mechanics have been established for a while, new concepts and effects concerning quantum systems are constantly formulated, observed and, with luck, interpreted. This is the case for a fundamental property of quantum systems called geometric phase.

First noted in 1956 by Pancharatnam [52] in the context of classical interferometry, the geometric phase was later formulated as a fundamental quantum property by M. Berry [12]. Berry demonstrated that the state vector of a system with dynamics given by a Hamiltonian dependent on some parameters which vary adiabatically during a cyclic evolution is accompanied by an additional phase factor, and surprisingly this phase factor depends only on the path traced by the evolution on the parameter space. Succeeding Berry's work, several generalizations were made ([1], [58]) and countless formulations, applications and experimental observations of geometric phase have been made ([59] presents an extensive collection of works on the subject).

The important extension of geometric phase to open quantum systems, however, is still an open question. From the pioneering work by Uhlmann [74] on geometric phase through purification of the density operator to various approaches (in the context of interferometry [64] [53], the quantum jump approach [22], the quantum state diffusion [19], etc), there is no unique parallel transport condition for density operators, hence, an expression for geometric phase for mixed states with non-unitary evolution can be defined in different ways.

The study of geometric phases in open quantum systems is, in itself, a great and interesting task. Nevertheless, to increase the interest in the field, it was shown that geometric phase could be used to process quantum information [79] and due to its geometric properties, presents a inherent resilience to errors. Since quantum

computation must be performed on quantum physical systems that, in spite all experimental efforts, interacts with the environment, it is of crucial importance the understanding of geometric phases in open quantum systems.

Finally, in the interest of obtaining useful results in the field of quantum computation and also for the extensive applicability in several physical systems, studying two-level quantum systems is of great importance. Although they are simple, obtaining phase factors for two-level quantum systems opens up the possibility of using these factors to implement quantum gates and, if the phase factors are purely geometric, the resulting gate has the robustness of the geometric phase against several decoherence processes.

Outline of the work

This thesis is organised as follows. In Chapter 2 we investigate the various formulations of geometric phases in closed quantum systems. Chapter 3 presents an overview on the theory of open quantum systems and then we present some approaches to define geometric phase for mixed states with unitary and non-unitary evolution. Also, using the results obtained in [53] we obtain the phase factors for a two-level quantum system subjected to some decoherence processes. In Chapter 4 we discuss the theory of two-level quantum systems. Following the work of [29], we obtain the phase factors for a two-level quantum system subjected to a time-dependent perturbation using the rotating wave approximation. Next, we use the method developed in [9] and [10] that gives a solution for the time evolution of a two-level quantum system subjected to time-dependent perturbation, and we use this result to obtain the phase factors for a two-level quantum system and for two two-level quantum systems (we consider non-interacting systems and interactions given by a delta function). In Chapter 5 we define the basic ideas behind the theory of quantum information to understand what is needed for a reliable and functional quantum information processing and to illustrate how geometric quantum computation can achieve implementation of universal quantum gates, we study the work of Ekert et al. [29]. Finally, we propose a two-qubit gate implementation using the results obtained in Chapter 4. Although the resulting gate is not purely geometrical, we indicate future approaches to removing the dynamical contribution to the phase factor.

Notation

Throughout this work, we tried to introduce the notation in a natural way: the symbol is presented right after the associated concept is cited (for example, *given a self-adjoint operator A acting on a Hilbert space $\mathcal{H}$*). We also tried to maintain the notation for state vectors on a Hilbert space as $\psi \in \mathcal{H}$. However, Dirac's notation is used when dealing with projectors ($P_\psi = |\psi\rangle\langle\psi|$) and the states of the computational basis ($\{|0\rangle, |1\rangle\}$ and $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$). The Pauli matrices are indicated by σ_1, σ_2 and σ_3 and are defined by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The identity matrix is indicated by $\mathbb{1}$ and sometimes has a subscript indicating the dimension of the Hilbert space associated with it.

Since we are working with phase factors of quantum systems, we tried to be consistent with the following notation: α_{dyn} for dynamical phase, ϕ_{tot} for total phase and γ_{geo} for geometric phase.

In this work we adopt Planck's constant as $\hbar = 1$.

Chapter 2

Geometric phases in closed quantum systems

Although the formulation of Quantum Mechanics dates from the 1930's, the geometric phase passed almost unnoticed for nearly thirty years. It consists of a phase factor that depends on the path in the projective Hilbert space associated with a physical system. In 1956, Pancharatnam published a work [52] that preceded in thirty years the first formulation of geometric phase made by M. Berry. In this paper, Pancharatnam investigated whether polarized light would have acquired a phase after going through a cyclic series of changes in polarization. He realized that this phase factor could be measured by a simple interference experiment. Then this topic was relegated to oblivion until the publication of M. Berry [12] in 1984. In his study, Berry considered a quantum system evolving under a Hamiltonian dependent on a number of parameters which vary adiabatically, this evolution was cyclic, that is, the parameters returned to their initial values. He noticed that the final wave function presented a phase factor besides the well-known dynamic phase, this additional phase factor depends only on the path traversed in parameter space. After Berry's work, the interest in geometric phase resulted in numerous generalizations of his result: Aharonov and Anandan [1] removed the adiabaticity condition, Samuel and Bandhari [58] extended the result to non-cyclic evolutions and Simon [63] expressed the geometric phase in the language of differential geometry by showing that the geometric phase is the holonomy in a Hermitian line bundle.

Since then, there were various works regarding the observation of the geometric phase and even its appearance in classical mechanics [37]. For a comprehensive

understanding and great commentaries there is a collection of papers by Shapere and Wilczek [59] and Anandan et al. [4] provides an excellent guide through the literature on geometric phases (anticipations, foundations and formulations, books, review articles and theoretical and experimental applications).

Our aim in this chapter is to obtain useful expressions for the geometric phase in the context of closed quantum systems. The outline of the chapter is the following: in Section 2.1 we obtain the so called Pancharatnam's phase in the context of polarization of light, to achieve this it is necessary to define the phase difference between two different polarization states, we extend this notion to phase difference between two state vectors. This result will be used later in the quantum jump approach to define geometric phases for open quantum systems. In Section 2.2 we study the case of a cyclic evolution given by a Hamiltonian that depends on some parameters which vary adiabatically with time, as was done by M. Berry in his seminal paper [12]. In Section 2.3 we derive the non-adiabatic generalization made by Aharonov and Anandan [1] and, finally, in Section 2.4 we give the classic example of a spin-half particle interacting with a constant magnetic field and we calculate the geometric phase using Berry's and Aharonov and Anandan's expressions.

2.1 Pancharatnam phase

In an important paper on phase shifts in polarized light [52], S. Pancharatnam anticipated the geometric phase in quantum systems. His main result was that a beam of light whose state of polarization returned to its initial state after some changes presents a phase factor that depends on the path traversed on the Poincaré sphere. To obtain such a result, Pancharatnam had to go through the question about how to define a phase difference between distinct polarization states of light. In this section we are going to obtain such a definition in the context of light polarization and then we are going to extend it to state vectors in a Hilbert space.

Polarization of light and Pancharatnam phase

Let us recall the description of polarization states for an electromagnetic wave ([39]). A monochromatic plane wave traveling in a direction $\boldsymbol{k}$ is given by

$$\boldsymbol{E}(\boldsymbol{r},t) = (E_1\epsilon_1 + E_2\epsilon_2)e^{i(\boldsymbol{k}\boldsymbol{r}-\omega t)}, \tag{2.1.1}$$

where $\omega = k/c$ (c the velocity of light) and $\epsilon_{1,2}$ are the circular polarization vectors (orthogonal to $\boldsymbol{k}$). The amplitudes E_1 and E_2 are complex numbers and they determine the polarization of the wave:

(i) If $E_{1,2} \neq 0$ and $E_1/E_2 \in \mathbb{R}$, the wave is *linearly polarized*.

(ii) If $E_{1,2} \neq 0$ and $E_1/E_2 \in \mathbb{C}$, the wave is *elliptically polarized*.

(iii) If $E_1 = 0$ or $E_2 = 0$, the wave is *circular polarized*.

We define a complex unit vector $d \in \mathbb{C}^2$

$$d = (d_1, d_2) := \frac{(E_1, E_2)}{|\boldsymbol{E}|}, \tag{2.1.2}$$

d is called the polarization vector. We note that d obeys the normalization condition $\langle d, d\rangle = 1$, so $d \in S^3 \subset \mathbb{C}^2$. The polarization state is uniquely defined by the vector

$$\boldsymbol{s} := \langle d, \boldsymbol{\sigma} d\rangle, \tag{2.1.3}$$

where $\boldsymbol{s}$ is also normalized, so $\boldsymbol{s} \in S^2$. If we have two polarization vectors d and d' differing by a phase factor

$$d' = e^{i\lambda} d,$$

their respective polarization states $\boldsymbol{s}$ and $\boldsymbol{s'}$ are the same:

$$\boldsymbol{s} = \langle d, \boldsymbol{\sigma} d\rangle = \langle d', \boldsymbol{\sigma} d'\rangle = \boldsymbol{s'}.$$

Therefore, the space of polarization states is $S^3/U(1) \cong S^2$, this sphere that represents the space of polarization states is called *Poincaré sphere*[1] (Figure 2.1). Thus, for a monochromatic plane wave the space of polarization states is isomorphic to the phase space of pure states of a two-level quantum system (the surface of the Bloch sphere). Suppose we have two waves with different polarization vectors d_A and d_B, then the intensity I resulting from their interference is

$$\begin{aligned} I &:= \langle \boldsymbol{s}_A + \boldsymbol{s}_B, \boldsymbol{s}_A + \boldsymbol{s}_B\rangle \\ &= 2 + 2|\langle \boldsymbol{s}_A, \boldsymbol{s}_B\rangle| \cos(\arg\langle \boldsymbol{s}_A, \boldsymbol{s}_B\rangle) \end{aligned} \tag{2.1.4}$$

[1]The nomenclature Poincaré sphere is ambiguous: in the context of interferometry it follows the definition given here.

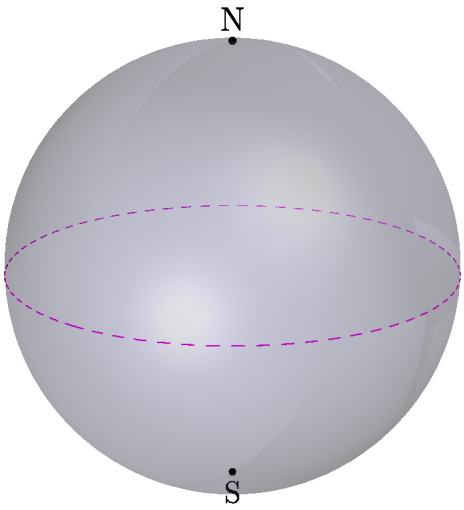


Figure 2.1: Poincaré sphere: representation of the space of polarization states of a monochromatic plane wave. The north (N) and south (S) are circular polarizations, the equator (dotted red line) represents linear polarizations and the remaining points correspond to elliptical polarizations.

Pancharatnam defined the relative phase between the two waves simply as $\arg\langle \boldsymbol{s}_A, \boldsymbol{s}_B \rangle$ and then considered them in phase when the interference intensity is maximum, that is, when

$$\langle \boldsymbol{s}_A, \boldsymbol{s}_B \rangle \text{ is real and positive.} \tag{2.1.5}$$

The term Pancharatnam connection is often used to refer to the term $\langle \boldsymbol{s}_A, \boldsymbol{s}_B \rangle$. The other main contribution from Pancharatnam's work is the observation that the connection is not transitive, that is, suppose a wave A is in phase with another wave B and B in its turn is in phase with C, then C need not to be in phase with A. In fact, if C is in phase with a wave A' corresponding to the same polarization state as A ($d_{A'} = e^{i\varphi} d_A$), then

$$\langle s_A, s_{A'} \rangle = e^{i\varphi} = e^{-i\Omega_{ABC}/2}, \tag{2.1.6}$$

where Ω_{ABC} is the solid angle of the geodesic triangle ABC on the sphere.

Formalization of Pancharatnam phase

Consider a physical system with an associated Hilbert space $\mathcal{H}$ and a pair of state vectors $\psi, \psi' \in \mathcal{H}$. Suppose ψ and ψ' represent the same quantum state, that is, $\psi' = e^{i\alpha}\psi$, $\alpha \in \mathbb{R}$. It is clear that α is the phase difference between ψ and ψ'.

However, a relative phase between state vectors representing different quantum states is not so obvious. To define such a phase difference we extend the notion of relative phase obtained for monochromatic plane waves in the previous subsection to state vectors in a Hilbert.

Definition 2.1.1 (Pancharatnam phase)**.** The phase difference or relative phase α_{12} between two state vectors ψ_1 and $\psi_2 \in \mathcal{H}$ is

$$\alpha_{12} := \arg\langle\psi_1, \psi_2\rangle. \tag{2.1.7}$$

Moreover, we say that ψ_1 and ψ_2 are in phase if

$$\langle\psi_1, \psi_2\rangle \text{ is real and positive.} \tag{2.1.8}$$

In the context of measurement processes, we can define a Pancharatnam phase. A measurement may be described by a projection operator onto the eigenstate corresponding to the eigenvalue of the measured state. If a system is initially in a state given by $\psi_i = \psi_0$ and we perform two measurements, the final state is given by a projection of the initial state onto the state ψ_1 associated to the first measurement, then another projection onto the state ψ_2 associated to the second measurement and, finally, a projection onto the initial state:

$$\psi_f = \psi_0\langle\psi_0, \psi_2\rangle\langle\psi_2, \psi_1\rangle\langle\psi_1, \psi_0\rangle,$$

where we ignored the time evolution of the system. We can obtain the Pancharatnam phase γ between ψ_i and ψ_f by taking the inner product of the above expression with the initial state

$$\begin{aligned}\langle\psi_i, \psi_f\rangle &= \langle\psi_0, \psi_0\rangle\langle\psi_0, \psi_2\rangle\langle\psi_2, \psi_1\rangle\langle\psi_1, \psi_0\rangle \\ |\langle\psi_i, \psi_f\rangle|e^{i\gamma} &= \langle\psi_0, \psi_2\rangle\langle\psi_2, \psi_1\rangle\langle\psi_1, \psi_0\rangle\end{aligned}$$

so the phase δ is given by

$$\gamma = \arg\langle\psi_0, \psi_2\rangle\langle\psi_2, \psi_1\rangle\langle\psi_1, \psi_0\rangle. \tag{2.1.9}$$

2.2 Berry's phase

In 1984, unaware of Pancharatnam's paper, M. Berry formulated the concept of geometric phase for quantum systems in his classical paper [12]. He considered a closed quantum system with dynamics governed by a parameter dependent Hamiltonian. The evolution of the system was taken to be cyclic and adiabatic, after Berry's work those conditions were generalized ([1], [58]).

In quantum mechanics, pure quantum states are represented by vectors in a complex Hilbert space $\mathcal{H}$. Given a self-adjoint operator A acting on $\mathcal{H}$, a quantum state is described by a vector $\psi \in \mathcal{H}$ and the collection of expectation values of A

$$A \to \frac{\langle \psi, A\psi \rangle}{\langle \psi, \psi \rangle}.$$

According to this, two vectors ψ and φ linearly dependent, $\psi = \lambda\varphi$ ($\lambda \in \mathbb{C}$), describe the same physical state. This motivates the definition of the so called projective Hilbert space.

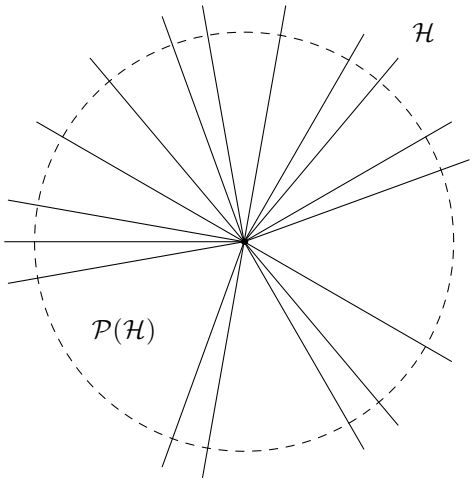


Figure 2.2: An illustration of the projective Hilbert space $\mathcal{P}(\mathcal{H})$, each line is a ray in $\mathcal{H}$ representing the same quantum state.

Definition 2.2.1 (Projective Hilbert space)**.** Let ψ and φ be vectors in a complex Hilbert space $\mathcal{H}$. The projective Hilbert space $\mathcal{P}(\mathcal{H})$ is a set of equivalence classes with respect to the following equivalence relation:

$$\psi \sim \varphi \iff \exists \lambda \in \mathbb{C}, \psi = \lambda\varphi.$$

The equivalence classes for the relation above are called *rays* or *projective rays*. So the projective Hilbert space is $\mathcal{P}(\mathcal{H}) := \mathcal{H}/\sim$. A simple representation is given in Figure 2.2.

If we choose normalized vectors, $\langle\psi,\psi\rangle = 1$, we can still have $\psi = e^{i\alpha}\varphi$ being physically equivalent. This phase factor was taken to have no physical meaning for almost 50 years, although Pancharatnam, in the context of interferometry, had already pointed out that this relative phase can be measured. It was not until Berry's work that this phase factor was taken into account as a physical quantity.

Consider a curve C on a manifold of external parameters M

$$t \to x_t \in M,$$

and a closed quantum system with an associated Hilbert space $\mathcal{H}$ and evolution given by a parameter dependent Hamiltonian $H(x_t)$ which evolves adiabatically along the curve C. The state of the system evolves according to Schrödinger equation

$$H(x_t)\psi(t) = i\dot{\psi}(t), \tag{2.2.1}$$

where we are taking $\hbar = 1$ and the dot stands for the time derivative. Then the time dependence of the Hamiltonian is given by the time dependence of the parameters x, $H(t) = H(x_t)$. Suppose that for any $x \in M$ the Hamiltonian has a purely discrete spectrum,

$$H(x)\psi_n(x) = E_n(x)\psi_n(x),$$

with

$$\langle\psi_n(x),\psi_m(x)\rangle = \delta_{nm},$$

where $\psi_n(x) \in \mathcal{H}, n \in \mathbb{N}$. Furthermore, let us assume that the spectrum is non-degenerate. So, there is a one-dimensional projector $P_n(x)$ onto the nth eigenspace $\mathcal{H}_n(x)$

$$\mathcal{H}_n(x) := \text{Range } P_n(x) = \{\lambda\psi_n(x), \lambda \in \mathbb{C}\}.$$

As was pointed out before, the states $\psi_n(x)$ are not uniquely defined, there is an ambiguity that allows us to write

$$\psi_n(x) \to \psi'_n(x) = e^{i\alpha_n(x)}\psi_n(x),$$

where $\alpha_n : M \to \mathbb{R}$ is a phase factor that depends on the external parameters x. If the initial state of the system is $\psi(0) = \psi_n(x_0)$, then by the adiabatic condition [42]

the evolution of the state will remain in the eigenspace correspondent to the initial condition:

$$\psi(0) = \psi_n(x_0) \to \psi(t) \in \mathcal{H}_n(x_t).$$

Besides, if the evolution is cyclic, i.e., a curve C on M is closed ($x_0 = x_T$ for some $T > 0$), then $\psi(0)$ and $\psi(T)$ both belong to $\mathcal{H}_n(x_0)$ and they may differ only by a phase factor

$$\psi(T) = e^{i\gamma}\psi(0).$$

This is the phase factor that until Berry's work was taken to be just the so called dynamic phase γ_{dyn}:

$$\alpha_{dyn} = -\int_0^T E_n(x_t)dt. \tag{2.2.2}$$

What Berry did was to consider that $\psi(T)$ could present an additional phase

$$\psi(T) = e^{i(\alpha_{dyn}+\gamma_n(t))}\psi_n(x_t). \tag{2.2.3}$$

The main result is that the phase factor $\gamma_n(t)$ is non-integrable, i.e., γ_n cannot be written as a function of the parameters x and in particular around a closed curve in M, $\gamma_n(T) \neq \gamma_n(0)$. Since $\psi(t)$ satisfies the Schrödinger equation, we can substitute 2.2.3 in 2.2.1 yielding

$$\dot{\gamma}_n(t) = i\langle\psi_n(x_t), \nabla_x\psi_n(x_t)\rangle\dot{x}_t$$

So the total phase of ψ round the curve C is given by

$$\psi(T) = \exp(i\gamma_n(C)) \exp\left(-i\int_0^T E_n(x_t)dt\right)\psi(0) \tag{2.2.4}$$

where

$$\gamma_n(C) = i\oint_C \langle\psi_n(x_t), \nabla_x\psi_n(x_t)\rangle dx \tag{2.2.5}$$

is a geometric phase factor accompanying the evolution of the system. As stated before, this phase factor is a non-integrable quantity and is not single-valued. It depends on the circuit integral in the parameter space M. Let us note that due to the normalization of $\psi(t)$, $\gamma_n(C)$ in 2.2.5 is real:

$$\begin{aligned} \langle\psi(t), \psi(t)\rangle = 1 &\implies \nabla_x\langle\psi_n(x_t), \psi_n(x_t)\rangle = 0 \\ \langle\nabla_x\psi_n(x_t), \psi_n(x_t)\rangle + \langle\psi_n(x_t), \nabla_x\psi_n(x_t)\rangle &= 0 \\ \mathfrak{Re}(\langle\psi_n(x_t), \nabla_x\psi_n(x_t)\rangle) &= 0 \\ \implies \gamma_n(C) &\in \mathbb{R}. \end{aligned} \tag{2.2.6}$$

Berry's geometric phase was later described by Simon [63] in the language of differential geometry as an holonomy of the parallel transport of eigenstates in the parameter space.

Aharonov-Bohm effect

A simple but very important example of a geometric phase is the Aharonov-Bohm effect. In 1959, Aharonov and Bohm [1] showed that a charged particle is affected by an electromagnetic field despite being confined to a region in which both magnetic and electric fields are zero. The wave function of the particle acquires a phase shift that is immediately related to Berry's geometric phase.

Consider a particle with charge q and mass m in the presence of an external magnetic field. The non-relativistic Hamiltonian of the system is given by [39]

$$H = -\frac{1}{2m}\left(\nabla - iq\boldsymbol{A}\right)^2, \tag{2.2.7}$$

where $\boldsymbol{A}$ is the vector potential. It is possible to show that if $\psi_0(\boldsymbol{r})$ is an eigenstate of the Hamiltonian in 2.2.7 with $\boldsymbol{A} = 0$, then the eigenstate for a general vector potential $\boldsymbol{A} \neq 0$ $\psi(\boldsymbol{r})$ is

$$\psi(\boldsymbol{r_b}) = \exp\left(iq\int_{r_a}^{r_b} \boldsymbol{A}(\boldsymbol{r'})\cdot d\boldsymbol{r'}\right)\psi_0(\boldsymbol{r_b}), \tag{2.2.8}$$

where $\boldsymbol{r_a}$ and $\boldsymbol{r_b}$ are arbitrary points and the integral is along the path connecting them both. If we consider a cyclic trajectory C, that is, $\boldsymbol{r_a} = \boldsymbol{r_b}$, the wave function acquires the phase

$$\varphi = q\oint_C \boldsymbol{A}\cdot d\boldsymbol{r}. = q\int_{\Sigma(C)} \boldsymbol{B}\cdot d\boldsymbol{s} = q\Phi, \tag{2.2.9}$$

where we used Stokes theorem, $\Sigma(C)$ is a surface enclosing C and Φ is the flux of magnetic field that goes through $\Sigma(C)$. Therefore, particles with the same start and end points traveling along different paths will acquire a phase difference given by 2.2.9. An experimental configuration to observe this phase difference is shown in Figure 2.3: a very long solenoid generates a magnetic flux line between the slits of a double slit experiment, electrons pass through the two slits and the interference pattern is shifted due to the presence of the magnetic flux. If we use Berry's

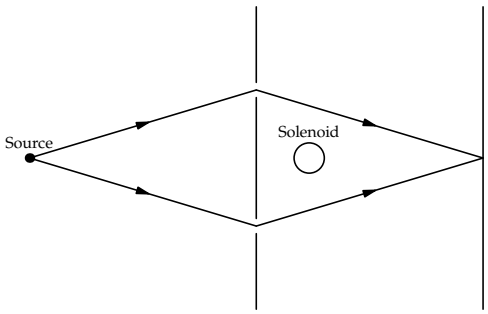


Figure 2.3: Experimental arrangement to observe the Aharonov-Bohm effect. A very long solenoid is placed between the two slits of a double slit experiment. A beam of electrons passes through the two slits interfering at an observation scree. The interference pattern shifts due to the presence of the magnetic flux generated by the solenoid.

expression 2.2.5 for the wave function 2.2.9 we get

$$\begin{aligned}\langle \psi(\boldsymbol{r}), \nabla_{\boldsymbol{r}}\psi(\boldsymbol{r})\rangle &= \langle \psi(\boldsymbol{r}), iq\boldsymbol{A}(\boldsymbol{r})\psi(\boldsymbol{r}) + e^{iq\oint_C \boldsymbol{A}(\boldsymbol{r})\cdot d\boldsymbol{r}}\nabla_{\boldsymbol{r}}\psi_0(\boldsymbol{r})\rangle \\ &= iq\boldsymbol{A}(\boldsymbol{r})\langle \psi(\boldsymbol{r}), \psi(\boldsymbol{r})\rangle + \langle \psi_0(\boldsymbol{r}), \nabla_{\boldsymbol{r}}\psi_0(\boldsymbol{r})\rangle \\ &= iq\boldsymbol{A}(\boldsymbol{r}),\end{aligned}$$

where the second term vanishes due to the normalization of $\psi_0(\boldsymbol{r})$. Finally, Berry's geometric phase is

$$\begin{aligned}\gamma(C) &= i\oint_C \langle \psi(\boldsymbol{r}), \nabla_{\boldsymbol{r}}\psi(\boldsymbol{r})\rangle \cdot d\boldsymbol{r} \\ &= -q\oint_C \boldsymbol{A}(\boldsymbol{r})\cdot d\boldsymbol{r} \\ &= -q\Phi.\end{aligned}$$

The expression above is the same obtained in 2.2.9. Although the phase shift obtained by Aharonov and Bohm may be interpreted as a geometric phase, from 2.2.9 we note that it does not depend on the detailed shape of the path C, but depends on the topology of the space enclosed by C, for this reason the phase factor from the Aharonov-Bohm effect is called a *topological phase*. To visualize the topological nature of the Aharonov-Bohm phase, we represent the parameter space M as the space of magnetic flux associated to the situation in Figure 2.3 and the phase is related to the parallel transport of a vector in M. In this case, M is a cone where the region of space with non-zero magnetic flux (inside the solenoid) is represented by the tip of the cone and the magnetic flux is defined by the angle

α, the flat space around the tip represents the absence of magnetic flux. When a vector is transported on the cone along a closed curve without encircling the tip, no holonomy is observed, on the other hand when the vector encircles the tip, the final vector will be rotated in respect to the initial vector and this difference is analogous to the Aharonov-Bohm effect (Figure 2.4).

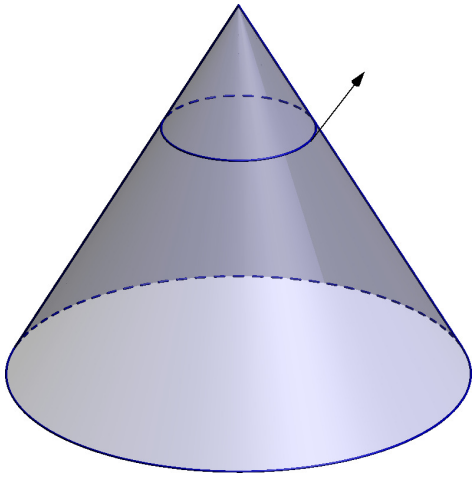


Figure 2.4: Parallel transport of a vector on a cone along a closed curve. The cone represents the parameter space associated to the Aharonov-Bohm effect: the parameter is the value of the magnetic flux. The tip is the region inside the solenoid and the value of magnetic flux generated by the solenoid is associated to the angle α. The flat region around the tip is the region with no magnetic flux. A beam of electrons going round the solenoid as depicted in Figure 2.3 is analogous to the parallel transport of a vector along a closed curve enclosing the tip.

We must note that if we add a gradient of a scalar field f to the vector potential

$$\boldsymbol{A} \to \boldsymbol{A} + \nabla f, \text{ and } V \to V - \dot{f},$$

where V is the electric potential and the dot represents the time derivative, the phase factor 2.2.9 does not change. The phase shift due to the Aharonov-Bohm effect was experimentally detected ([23]). The electric dual phenomenon to the Aharonov-Bohm effect is the Aharonov-Casher effect, predicted in 1984 [2]. Aharonov and Casher showed that a particle with a magnetic dipole moment μ traveling along a path C is affected by an electric field $\boldsymbol{E}(\boldsymbol{r})$ by also presenting a phase shift γ_{AC} given by

$$\gamma_{AC} = \oint_C (\boldsymbol{E}(\boldsymbol{r}) \times \mu) \cdot d\boldsymbol{r}. \tag{2.2.10}$$

The above phase factor, as the one in 2.2.9 is a non-integrable phase and is referred to as a topological phase, since it does not depend on the geometry of the path C, but on the topology of the space enclosed by C.

2.3 Aharonov-Anandan's phase

After Berry's work [12], many generalizations of the geometric phase were made. In 1987 Aharonov and Anandan [1] proposed an important generalization of Berry's phase: they consider cyclic evolutions that are not restricted by an adiabatic condition. This generalization was obtained by describing a cyclic evolution as a closed curve in the projective Hilbert space, and not as a closed curve in a parameter space. This generalization is of great importance, since the adiabatic condition is a rather restrictive condition for physical systems to fulfill.

Derivation

The solution of the Schrödinger equation

$$i\dot{\psi}(t) = H\psi(t), \quad \psi(0) = \psi_0,$$

defines a trajectory in the Hilbert space $\mathcal{H}$:

$$t \to \psi(t) \in \mathcal{H}.$$

Such a trajectory projects onto a trajectory in the associated projective Hilbert space $\mathcal{P}(\mathcal{H})$. We can define a projection map π from the Hilbert space into the projective Hilbert space by

$$\begin{aligned} &\pi : \mathcal{H} \to \mathcal{P}(\mathcal{H}) \\ &\pi(\psi) = \{\psi' : \psi' = c\psi, c \in \mathbb{C}\} \end{aligned} \tag{2.3.1}$$

A cyclic evolution of a state vector $\psi(t)$ with a period T in the projective Hilbert space means the evolution traces out an arbitrary curve C in $\mathcal{H}$ but the projection of this curve gives a closed curve C' in $\mathcal{P}(\mathcal{H})$ (Figure 2.5). This closed curve is

$$t \to C'(t) \in \mathcal{P}(\mathcal{H}),$$

that is,

$$C'(t) := \pi(\psi(t)).$$

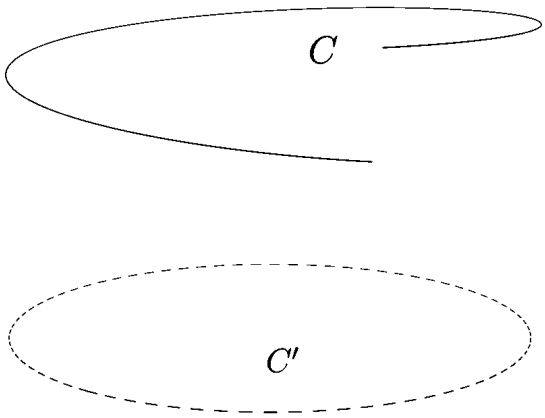


Figure 2.5: An open curve $C : \psi(T) = e^{i\gamma}\psi(0)$ in Hilbert space $\mathcal{H}$ projected with the map π to a closed curve C' in the projective Hilbert space $\mathcal{P}(\mathcal{H})$.

This defines a solution to the Heisenberg equation

$$i\dot{C}'(t) = [H, C'], \quad C'(0) = P_{\psi_0}, \tag{2.3.2}$$

where P_{ψ_0} is the spectral projector associated to the state vector ψ_0. Since C' is closed, i.e., $C'(T) = C'(0)$ for some $T > 0$, $\psi(T)$ and $\psi(0)$ define the same quantum state, they must differ only by a phase factor

$$\psi(T) = e^{i\varphi}\psi(0), \tag{2.3.3}$$

for some $\varphi \in [0, 2\pi)$. We want to find the phase shift φ knowing that the system performs a cyclic evolution in $\mathcal{P}(\mathcal{H})$. We first note that the following transformation leaves the solution $C'(t)$ of 2.3.2 invariant:

$$H' = H + a(t)\mathbb{1}, \tag{2.3.4}$$

where $\mathbb{1}$ is the identity operator in $\mathcal{H}$ and $a(t)$ is a real function of time. The solution of the Schrödinger equation with this new Hamiltonian is

$$\psi'(t) = \exp\left(-i\int_0^t a(\tau)d\tau\right)\psi(t),$$

and since $\psi'(T)$ and $\psi'(0)$ still define the same physical state, we have

$$\begin{aligned}
\psi'(T) &= e^{i\varphi'}\psi'(0) \\
e^{-i\int_0^T a(\tau)d\tau}\psi(T) &= e^{i\varphi'}\psi(0) \\
e^{-i\int_0^T a(\tau)d\tau}e^{i\varphi}\psi(0) &= e^{i\varphi'}\psi(0),
\end{aligned}$$

so

$$\varphi' = \varphi - \int_0^T a(\tau)d\tau.$$

What we get is that an arbitrary transformation in the Hamiltonian changes completely the phase shift φ. However, the total phase φ may be divided into two parts

$$\varphi = \alpha_{dyn} + \gamma_{geo}, \tag{2.3.5}$$

where we take the geometric part γ_{geo} to be invariant under transformations like 2.3.4 and to be dependent only on the closed curve $C'(t)$ in the projective Hilbert space $\mathcal{P}(\mathcal{H})$. To obtain γ_{geo} we consider a function $a(t)$ such that $\varphi'(0) = 0$:

$$\varphi = \int_0^T a(\tau)d\tau, \tag{2.3.6}$$

which means that $\psi'(T) = \psi'(0)$. The Schrödinger's equation for $\psi'(t)$ is

$$i\dot{\psi}'(t) = (H + a(t)\mathbb{1})\psi'(t),$$

we take a inner product of the expression above with $\psi'(t)$ and integrate over time from 0 to T

$$\int_0^T \langle\psi'(t), i\dot{\psi}'(t)\rangle dt = \int_0^T \langle\psi'(t), H\psi'(t)\rangle dt + \int_0^T a(t)dt,$$

using the specific function $a(t)$ for which 2.3.6 holds, we get

$$\varphi = \int_0^T \langle\psi'(t), i\dot{\psi}'(t)\rangle dt - \int_0^T \langle\psi'(t), H\psi'(t)\rangle dt.$$

Finally, we divide φ into two parts:

$$\alpha_{dyn} := -\int_0^T \langle\psi'(t), H\psi'(t)\rangle dt = -\int_0^T \langle\psi(t), H\psi(t)\rangle dt, \tag{2.3.7}$$

that explicitly depends on the system Hamiltonian and we call dynamic phase, and the geometric phase

$$\gamma_{geo} := \int_0^T \langle\psi'(t), i\dot{\psi}'(t)\rangle dt, \tag{2.3.8}$$

that we shall show that depends only on the closed curve traversed in the projective Hilbert space $\mathcal{P}(\mathcal{H})$. Let us consider a state vector given by

$$\phi(t) = e^{if(t)}\psi'(t), \tag{2.3.9}$$

such that $f(T) = f(0)$, that is, $\phi(t)$ describes a closed curve in $\mathcal{P}(\mathcal{H})$. We can calculate

$$\begin{aligned}\int_0^T \langle \phi(t), i\dot{\phi}(t)\rangle dt &= \int_0^T \left(\langle \psi'(t), \dot{f}(t)\psi'(t)\rangle + \langle \psi'(t), i\dot{\psi}'(t)\rangle\right) dt \\ &= -(f(T) - f(0)) + \int_0^T \langle \psi'(t), i\dot{\psi}'(t)\rangle dt \\ &= \gamma_{geo},\end{aligned}$$

proving that the geometric phase γ_{geo} is characteristic of the closed curve $C'(t)$ in the projective Hilbert space $\mathcal{P}(\mathcal{H})$. The phase factor obtained in 2.3.8 by Aharonov and Anandan does not depend on the form of the Hamiltonian. The parametrization of the curve C' has no effect on the value of the geometric phase, it only depends on the geometry of the projective Hilbert space. Berry's phase depends on the parameter space that defines the Hamiltonian and so is a special case of Aharonov and Anandan's phase.

2.4 Spin-half particle in a magnetic field

An illustration of the appearance of the geometric phase is the simple example of a spin-half particle subjected to an external magnetic field. The Hamiltonian of the system is given by

$$H(\boldsymbol{B}) = \frac{1}{2}\mu\boldsymbol{\sigma}\cdot\boldsymbol{B}, \tag{2.4.1}$$

where $\boldsymbol{B}$ is the magnetic field, μ is the magnetic dipole moment and $\boldsymbol{\sigma}$ is the vector of Pauli matrices. In this case, the parameter is the magnetic field, $\boldsymbol{B} \in \mathbb{R}^3$. Since we are considering a two-level quantum system, we shall define its geometrical representation.

Definition 2.4.1 (Bloch sphere)**.** The Bloch sphere is the geometrical representation of a two-level quantum system. Points on the surface of the sphere correspond to pure states and points in its interior correspond to mixed states. We choose a vector basis $\{\psi_+, \psi_-\}$ to correspond to the north and south poles, respectively. A pure state ψ can be written as a superposition of ψ_+ and ψ_-

$$\psi = \cos\left(\frac{\theta}{2}\right)\psi_+ + e^{i\phi}\sin\left(\frac{\theta}{2}\right)\psi_-, \tag{2.4.2}$$

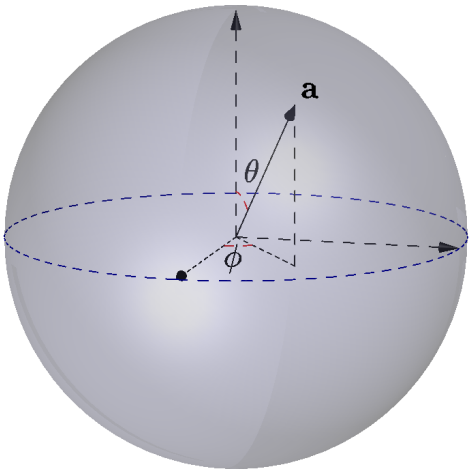


Figure 2.6: Bloch sphere: representation of a two-level quantum system. Pure and mixed states are represented by points on the surface and in the interior of the sphere, respectively. The north and south poles are chosen to represent the vectors ψ_+ and ψ_-. The Bloch vector is a vector that defines points in the sphere.

with $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$. The parameters θ and ϕ define the *Bloch vector* $\boldsymbol{a} \in \mathbb{R}^3$

$$\boldsymbol{a} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \tag{2.4.3}$$

For mixed states, we have to consider density matrices. Any density matrix in $\mathbb{C}^2$ can be written as

$$\rho = \frac{1}{2}(\mathbb{1}_2 + \boldsymbol{a}\cdot\boldsymbol{\sigma}), \tag{2.4.4}$$

where $\mathbb{1}_2$ is the identity matrix in $\mathbb{C}^2$ and $\boldsymbol{\sigma}$ is the three-vector of Pauli matrices. Due to the positiveness of ρ, we have $|\boldsymbol{a}| \leq 1$ (the equality holding for pure states).

Writing the magnetic field in spherical coordinates, we get

$$\boldsymbol{B} = B\begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}, \tag{2.4.5}$$

where $\phi = \omega t$ for a particle in a rotating magnetic field with angular frequency ω. The eigenvalues $E_{1,2}$ of 2.4.1 are

$$E_{1,2} = \pm\frac{1}{2}\mu B, \tag{2.4.6}$$

from 2.4.5 we see that we can take the parameter space M to be a two-dimensional sphere S^2, not including the case in which $\boldsymbol{B} = 0$. The correspondent eigenvectors $\psi_{1,2}$ are

$$\psi_1(\theta,\phi) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ e^{i\phi}\sin\left(\frac{\theta}{2}\right) \end{pmatrix}, \quad \psi_2(\theta,\phi) = \begin{pmatrix} -\sin\left(\frac{\theta}{2}\right) \\ e^{i\phi}\cos\left(\frac{\theta}{2}\right) \end{pmatrix}, \tag{2.4.7}$$

written in the basis of the eigenvectors of the Pauli matrix σ_3. We can interpret

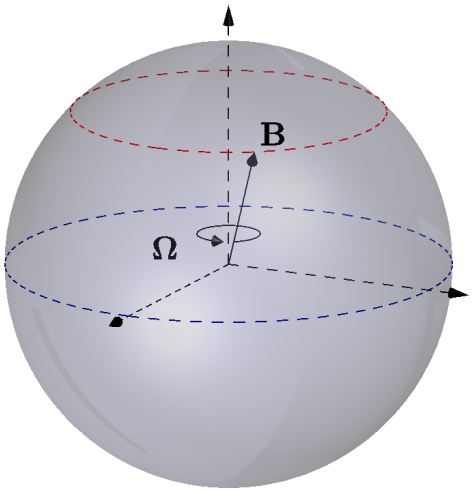


Figure 2.7: Parameter space associated to the Hamiltonian 2.4.1 with magnetic field given by 2.4.5.

these eigenvectors as the analogous to spin-up and spin-down along the $\boldsymbol{B}$-direction. We will obtain the geometric phase for this situation using the expressions derived by Berry and Aharonov and Anandan.

Berry's phase

Considering a closed curve C in the parameter space $M = S^2$ as the one represented in Figure 2.7, we can calculate Berry's phase given by 2.2.5 for the eigenvectors:

$$\gamma(C) = i \oint_C \langle \psi_{1,2}, \nabla \psi_{1,2} \rangle \cdot d\boldsymbol{B},$$

we have

$$\nabla\psi_1 = \frac{1}{B}\begin{pmatrix} -\frac{1}{2}\cos\left(\frac{\theta}{2}\right) \\ -\frac{1}{2}e^{i\phi}\sin\left(\frac{\theta}{2}\right) \end{pmatrix}\hat{\theta} + \frac{1}{B\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\cos\left(\frac{\theta}{2}\right) \end{pmatrix}\hat{\phi},$$
$$\nabla\psi_2 = \frac{1}{B}\begin{pmatrix} -\frac{1}{2}\sin\left(\frac{\theta}{2}\right) \\ -\frac{1}{2}e^{i\phi}\cos\left(\frac{\theta}{2}\right) \end{pmatrix}\hat{\theta} + \frac{1}{B\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\sin\left(\frac{\theta}{2}\right) \end{pmatrix}\hat{\phi},$$

so

$$\langle\psi_1, \nabla\psi_1\rangle = i\frac{\cos^2\left(\frac{\theta}{2}\right)}{B\sin\theta}\hat{\phi},$$
$$\langle\psi_2, \nabla\psi_2\rangle = i\frac{\sin^2\left(\frac{\theta}{2}\right)}{B\sin\theta}\hat{\phi}.$$

Integrating along a curve C:

$$C : B, \theta \text{ constant}, \phi \in [0, 2\pi],$$

we get

$$\gamma(C) = i\oint_C \langle\psi_{1,2}, \nabla\psi_{1,2}\rangle B\sin\theta d\theta d\phi = -\pi(1 \pm \cos\theta), \tag{2.4.8}$$

in terms of the solid angle $\Omega = \int_0^{2\pi}(1-\cos\theta)d\phi$ the geometric phase can be written as

$$\gamma_{1,2}(C) = \pm\frac{1}{2}\Omega(C), \tag{2.4.9}$$

where $\Omega(C)$ is the solid angle subtended by the curve C on S^2.

Aharonov and Anandan's phase

We consider the general evolution of an arbitrary state $\psi(t)$ by the time dependent Schrödinger equation

$$H(t)\psi(t) = i\dot{\psi}(t).$$

To solve the above equation we make the following ansatz[2]

$$\eta(t) = e^{i\frac{\omega}{2}\sigma_3 t}\psi(t), \tag{2.4.10}$$

[2]We follow the directions of A. Bohm [15].

with the initial condition $\eta(0) = \psi(0)$. The state vector $\eta(t)$ satisfy a Schrödinger equation

$$\bar{H}\eta(t) = i\dot{\eta}(t). \tag{2.4.11}$$

We can determine $\bar{H}$ by taking the time derivative of 2.4.10

$$\begin{aligned} i\dot{\eta}(t) &= -\frac{\omega}{2}\sigma_3 e^{i\frac{\omega}{2}\sigma_3 t}\psi(t) + e^{i\frac{\omega}{2}\sigma_3 t} i\dot{\psi}(t) \\ \bar{H}(t)\eta(t) &= -\frac{\omega}{2}\sigma_3\eta(t) + e^{i\frac{\omega}{2}\sigma_3 t} H(t) e^{-i\frac{\omega}{2}\sigma_3 t}\eta(t) \end{aligned}$$

using the explicit form of the Hamiltonian in 2.4.1 and the commutator relations between Pauli matrices, it is possible to see that

$$\begin{aligned} e^{i\frac{\omega}{2}\sigma_3 t} H(t) e^{-i\frac{\omega}{2}\sigma_3 t} &= e^{i\frac{\omega}{2}\sigma_3 t}\frac{1}{2}\mu \boldsymbol{B}\cdot\boldsymbol{\sigma} e^{-i\frac{\omega}{2}\sigma_3 t} \\ &= \frac{1}{2}\mu B \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}, \end{aligned}$$

it follows that the Hamiltonian $\bar{H}$ is time independent

$$\begin{aligned} \bar{H} &= H(t=0) - \frac{\omega}{2}\sigma_3 \\ &= \frac{1}{2}\begin{pmatrix} \mu B\cos\theta - \omega & \mu B\sin\theta \\ \mu B\sin\theta & -\mu B\cos\theta + \omega \end{pmatrix}. \end{aligned} \tag{2.4.12}$$

We can write the Hamiltonian $\bar{H}$ as

$$\bar{H} = \frac{1}{2}\mu\bar{\boldsymbol{B}}\cdot\boldsymbol{\sigma}. \tag{2.4.13}$$

Considering a magnetic field $\bar{B}$ in the form

$$\bar{B} = \begin{pmatrix} \bar{B}_1 \\ \bar{B}_2 \\ \bar{B}_3 \end{pmatrix},$$

using the above expression in the 2.4.13 and comparing with 2.4.12 we get

$$\frac{1}{2}\begin{pmatrix} \mu B\cos\theta - \omega & \mu B\sin\theta \\ \mu B\sin\theta & -\mu B\cos\theta + \omega \end{pmatrix} = \frac{1}{2}\mu\begin{pmatrix} \bar{B}_3 & \bar{B}_1 - i\bar{B}_2 \\ \bar{B}_1 + i\bar{B}_2 & -\bar{B}_3 \end{pmatrix},$$

we conclude that $\bar{B}_2 = 0$ and, if we write $\bar{B}$ as

$$\bar{B} = \bar{B} \begin{pmatrix} \sin\bar{\theta} \\ 0 \\ \cos\bar{\theta} \end{pmatrix},$$

where the factors $\bar{B}$ and $\bar{\theta}$ are given by

$$\begin{aligned} \bar{B} &= B\Delta \\ \sin\bar{\theta} &= \frac{\sin\theta}{\Delta} \\ \cos\bar{\theta} &= \frac{\cos\theta}{\Delta} - \frac{\omega}{2B\mu\Delta} \end{aligned}$$

with the scaling factor Δ

$$\Delta = \left[1 - \frac{\omega}{\mu B}\cos\theta + \frac{\omega^2}{4\mu^2 B^2}\right]^{\frac{1}{2}}.$$

The eigenvalues of the Hamiltonian $\bar{H}$ in 2.4.12 are

$$E_\pm = \pm\frac{1}{2}\mu\bar{B}, \tag{2.4.14}$$

with the respective eigenvectors

$$\eta_+ = \cos\left(\frac{\bar{\theta}}{2}\right)\psi_+ + \sin\left(\frac{\bar{\theta}}{2}\right)\psi_- \tag{2.4.15}$$

$$\eta_- = \sin\left(\frac{\bar{\theta}}{2}\right)\psi_+ - \cos\left(\frac{\bar{\theta}}{2}\right)\psi_- \tag{2.4.16}$$

where $\psi_\pm$ are the eigenvalues of the Pauli matrix σ_3. Since the Hamiltonian $\bar{H}$ is time independent, we have

$$\eta(t) = e^{-i\bar{H}t}\eta(0),$$

using this in 2.4.10 we get the solution of the Schrödinger equation

$$\psi(t) = e^{-i\frac{\omega}{2}\sigma_3 t}e^{-i\bar{H}t}\psi(0).$$

if we consider that the initial state is one of the eigenvectors of $\bar{H}$ 2.4.15 or 2.4.16, $\psi(0) = \eta(0) = \eta_\pm$ we have

$$\psi(t) = e^{-i\frac{\omega}{2}\sigma_3 t}e^{-iE_\pm t}\eta_\pm. \tag{2.4.17}$$

Considering a cyclic evolution with a period $T = \frac{2\pi}{\omega}$ we can compute the final state. If $\psi(0) = \eta_+$:

$$\begin{aligned}
\psi(T) &= e^{-i\frac{\omega}{2}\sigma_3 T} e^{-iE_+ T} \eta_+ \\
&= e^{-iE_+ T} e^{-i\frac{\omega}{2}\sigma_3 T} (\cos\left(\frac{\bar{\theta}}{2}\right) \psi_+ + \sin\left(\frac{\bar{\theta}}{2}\right) \psi_-) \\
&= e^{-iE_+ T} (e^{-i\frac{\omega}{2}T} \cos\left(\frac{\bar{\theta}}{2}\right) \psi_+ + e^{i\frac{\omega}{2}T} \sin\left(\frac{\bar{\theta}}{2}\right) \psi_-) \\
&= e^{-iE_+ T} (e^{-i\pi} \cos\left(\frac{\bar{\theta}}{2}\right) \psi_+ + e^{i\pi} \sin\left(\frac{\bar{\theta}}{2}\right) \\
&= e^{-iE_+ T} e^{-i\pi} \eta_+,
\end{aligned}$$

and if $\psi(0) = \eta_-$:

$$\begin{aligned}
\psi(T) &= e^{-i\frac{\omega}{2}\sigma_3 T} e^{-iE_+ T} \eta_- \\
&= e^{-iE_+ T} e^{-i\frac{\omega}{2}\sigma_3 T} (\sin\left(\frac{\bar{\theta}}{2}\right) \psi_+ - \cos\left(\frac{\bar{\theta}}{2}\right) \psi_-) \\
&= e^{-iE_+ T} (e^{-i\frac{\omega}{2}T} \sin\left(\frac{\bar{\theta}}{2}\right) \psi_+ - e^{i\frac{\omega}{2}T} \cos\left(\frac{\bar{\theta}}{2}\right) \psi_-) \\
&= e^{-iE_+ T} (e^{-i\pi} \sin\left(\frac{\bar{\theta}}{2}\right) \psi_+ - e^{i\pi} \cos\left(\frac{\bar{\theta}}{2}\right) \\
&= e^{-iE_+ T} e^{-i\pi} \eta_-.
\end{aligned}$$

Collecting the results above we have that

$$\psi(T) = e^{i(\mp\pi - E_\pm T)} \eta_\pm,$$

and the total phase $\varphi(T)$ acquired by $\psi(t)$ during the evolution is

$$\varphi(T) = \mp\pi - E_\pm T. \tag{2.4.18}$$

The corresponding dynamical part of the total phase can be calculated using 2.3.7 and 2.4.17 and the explicit forms of $\eta_\pm$ in 2.4.15 and 2.4.16, we get

$$\begin{aligned}
\alpha_{dyn}(T) &= -\int_0^T \langle \psi(t), H(t)\psi(t)\rangle dt \\
&= -\int_0^T \langle \eta_\pm e^{-i\frac{\omega}{2}\sigma_3 t}, (\bar{H} + \frac{\omega}{2}\sigma_3) e^{-i\frac{\omega}{2}\sigma_3 t}\eta_\pm\rangle dt \\
&= -\int_0^T \langle \eta_\pm, \bar{H}\eta_\pm\rangle dt - \frac{\omega}{2}\int_0^T \langle \eta_\pm, \sigma_3\eta_\pm\rangle dt \\
&= -E_\pm T \mp \frac{\omega}{2}\cos\bar{\theta}T \\
&= -E_\pm T \mp \pi\cos\bar{\theta}.
\end{aligned}$$

Finally, the geometric phase is given by

$$\begin{aligned}
\gamma_{geo} &= \varphi(T) - \alpha_{dyn}(T) \\
&= \mp\pi - E_\pm T + E_\pm T - \pm\pi\cos\bar{\theta} \\
&= \mp\pi(1 - \cos\bar{\theta}).
\end{aligned} \tag{2.4.19}$$

Taking the limit that corresponds to the adiabatic approximation, $\omega \ll \mu B$, the geometric phase obtained above tends to $\mp\pi(1-\cos\theta)$, which is the phase factor in 2.4.8 using Berry's expression. The adiabatic limit corresponds to the case in which the angular frequency of the precession of the external magnetic field ω is very slow compared to the internal frequency μB with which the state rotates due to the strength of the magnetic field.

Chapter 3

Geometric phases in open quantum systems

In Chapter 2 we studied various formulations of geometric phase, but all concerning the evolution of a pure state undergoing unitary evolutions. Hence, the state of the system was described by state vectors in a Hilbert space and the unitary evolution was associated with a group of unitary transformations acting in the same Hilbert space. The question about a further generalization for mixed states, non-unitary evolution or both, comes naturally. Motivated by the possibility of using geometric phases for processing quantum information ([29], [65]), the interest of formulating geometric phase for density operators undergoing unitary and non-unitary evolutions increased, since the basic unit of quantum information is the qubit, a two-level quantum system, that is in contact with an environment, therefore, an open quantum system.

Defining a proper parallel transport condition for density operators is not a straightforward task, since it depends on the connection used to perform such parallel transport and in the context of mixed states there is an uncountable set of connections. The first attempt of defining geometric phase for mixed state was made by A. Uhlmann [74]. His method was based on the idea of purification: any mixed state can be obtained by tracing out some degrees of freedom of a larger system which is in a pure state. Uhlmann then obtained a parallel transport condition for these purifications. However, Uhlmann's geometric phase and parallel transport condition are very abstract and hard to come by experimentally. In a more experimental approach, Sjöqvist et al. [64] and Peixoto de Faria et al. [53]

proposed a formulation of geometric phases in the context of interferometry for unitary and non-unitary evolutions, respectively. Through the method known as the Quantum Jump Approach, already vastly used in quantum optics [54], Carollo et al. [22] showed that it is possible to define geometric phase for an open system. This method avoids the problem of defining a proper parallel transport condition for mixed states, since it is based on the idea that the system can be described by pure states associated to generalized measurements, hence, the expressions for geometric phase for pure states obtained in Chapter 2 can be used. The quantum state diffusion method [19] also tackles the problem of defining geometric phases for mixed states through the use of pure states undergoing stochastic evolution. Mukunda and Simon [48] proposed a quantum kinematic approach in which the geometric phase is expressed exclusively in terms of density operators.

In this chapter we wish to study some approaches to the problem of defining a proper parallel transport condition for mixed states and the respective geometric phase of the system. In Section 3.1 we start with the mathematical background of open quantum systems. In Section 3.2 we present Uhlmann's formulation of geometric phases for mixed states. In Section 3.3 we present the operational approach in the context of interferometry proposed by Sjöqvist et al. and Peixoto de Faria et al.. Section 3.4 is devoted to the quantum jump approach. The quantum state diffusion method and the kinematic approach are not covered.

3.1 Theory of open quantum systems

The mathematical formulation of Quantum Mechanics dates from the 1930's with E. Schrödinger, W. Heisenberg, M. Born, P. Dirac and J. von Neumann. The last one published in 1932 the book *Mathematische Grundlagen der Quantenmechanik* [75] where a rigorous mathematical description of Quantum Mechanics was developed using Functional Analysis. This formalism can be described as follows: every quantum system is related to a separable Hilbert space in which a set of self-adjoint operators act and are related to the observables of the system. The dynamics of the system is described by a self-adjoint operator called Hamiltonian.

The processes that occur in closed quantum systems are described by operators that form a group of unitary transformations. Therefore, the existence of the inverse element of the group is related to the reversibility of processes. However, in open quantum systems the reversibility of processes is not binding. To describe

such systems we consider that the system interacts with a reservoir so that the total system can be described using the theory of closed quantum systems, the reduced dynamics of the first system is then described not as a group of unitary transformations, but as a semigroup. The theory of semigroups is substantiated on the Hille-Yosida theorem and on the works about dynamical semigroups and its generators.

We shall make a brief survey of the theory of open quantum systems. We begin by defining the global dynamics of the system and reservoir, then we proceed to the identification of an important characteristic of the system's density operator, complete positivity, and finally we define quantum dynamical semigroups and its generators. For a more complete and detailed description and formalization of the theory of open quantum systems see, e.g., [26], [3], [6].

Reduced dynamics

As was stated before in Section 2.2, in Quantum Mechanics a physical system is associated to a separable Hilbert space $\mathcal{H}$ and the state of the system is univocally associated to a density operator ρ.

Definition 3.1.1 (State space)**.** A density operator is a self-adjoint, positive[1], trace class operator of trace one[2]. The set of density operators form a Banach space with the trace norm $\|\cdot\|_{\mathrm{Tr}} := \mathrm{Tr}\,|\cdot|$ that is called state space of $\mathcal{H}$ and is denoted by $V(\mathcal{H})$.

An open quantum system is a quantum system which is found to be interacting with an external system. Let us consider an open quantum system S with a Hilbert space $\mathcal{H}_S$ and a reservoir with a Hilbert space $\mathcal{H}_R$, so that the global system $S + R$ is closed. The dynamics of the global system is governed by a unitary operator $U : \mathcal{H}_S \otimes \mathcal{H}_R \mapsto \mathcal{H}_S \otimes \mathcal{H}_R$. If we assume that the systems are weakly coupled, we may assume that the initial state of the global system is given by $\rho_S \otimes \rho_R$ where ρ_S and ρ_R are the initial states of the system S and the reservoir R, respectively. The

[1] **Definition** (Positive operator) Let A be a bounded operator acting on a Hilbert space $\mathcal{H}$. We call A a positive operator if $\langle A\psi, \psi\rangle \geq 0$ for all $\psi \in \mathcal{H}$ ([57]).

[2] **Definition** (Trace class) Let $\mathcal{H}$ be a separable Hilbert space, $\{\varphi_n\}_{n=1}^{\infty}$ an orthonormal basis of $\mathcal{H}$. Then for any positive and bounded operator A we define the trace of A as $\mathrm{Tr}\,A = \sum_{n=1}^{\infty}\langle\varphi_n, A\varphi_n\rangle$ if this series converges and is independent of the orthonormal basis chosen. A bounded operator A is called of trace class if and only if $\mathrm{Tr}\,|A| < \infty$ ([57]).

reduced dynamics of the system S is given by the linear map Φ :

$$\rho_S \mapsto \Phi(\rho_S) := \mathrm{Tr}_{\mathcal{H}_R} U(\rho_S \otimes \rho_R)U^*, \tag{3.1.1}$$

where $\mathrm{Tr}_{\mathcal{H}_R}$ stands for the partial trace with respect to the reservoir. In general, the reservoir is taken to be a finite-dimensional system, for the case of an infinite system, the state of the reservoir is constructed using the GNS representation ([3], [26]).

Complete positivity

We now consider the case in which the system S represents a particle in a box with an associated Hilbert space $\mathcal{H}_S$, and the reservoir R is represented by a particle with n degrees of freedom ($\mathcal{H}_R \cong \mathbb{C}^n$). The latter is taken to be very distant from the former in a way that there is no interaction between the two. The total Hilbert space is $\mathcal{H}_S \otimes \mathbb{C}^n$. Let us assume that the dynamics of the system S is given by a family of positive maps $T : \mathcal{B}(\mathcal{H}_S) \to \mathcal{B}(\mathcal{H}_S)$ where $\mathcal{B}(\mathcal{H}_S)$ stands for the set of bounded operators acting on $\mathcal{H}_S$. Since the systems do not interact, we can extend T to the global system as the action of an operator $T_n : \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_R) \to \mathcal{B}(\mathcal{H}_S \otimes \mathcal{H}_R)$ such that

$$T_n(A \otimes B) = T(A) \otimes B, \tag{3.1.2}$$

for all $A \in \mathcal{B}(\mathcal{H}_S)$ and $B \in \mathcal{B}(\mathcal{H}_R)$. But $\mathcal{B}(\mathcal{H}_R) \cong \mathcal{B}(\mathbb{C}^n) \cong \mathcal{M}_n(\mathbb{C})$[3] and we have that $\mathcal{B}(\mathcal{H}_S \otimes \mathbb{C}^n)$ is isomorphic to $\mathcal{M}_n(\mathcal{B}(\mathcal{H}_S))$. Since the map T is positive on $\mathcal{B}(\mathcal{H}_S)$, the map T_n is positive for all n.

The positivity of 3.1.2 for all n is not obvious from a mathematical point of view, but necessary from a physical one: we expect that the dynamics of an isolated system such as S is not disturbed by the presence of a second system wherewith S does not even interact. This property is called complete positivity. We define complete positivity below using the formalism of C^* algebra[4].

[3] $\mathcal{M}_n(\mathbb{C})$ is the $n \times n$ matrix algebra with complex entries.

[4] The study of C^* algebras is of great importance to a better understanding of Quantum Mechanics from an algebraic point of view. We chose to formulate our results in terms of the usual Hilbert space description, but a rough definition is that a C^* algebra with identity is a Banach space $\mathscr{B}$ which is also an algebra with identity and an involution satisfying $\|AB\| \leq \|A\| \, \|B\|$ and $\|A^*A\| = \|A\|^2 = \|A^*\|^2$ for all $A, B \in \mathscr{B}$. For a good algebraic formulation of Quantum Mechanics using C^* algebras see [18].

Definition 3.1.2 (Complete positivity)**.** Let $\mathscr{A}$ and $\mathscr{B}$ be C^* algebras, $\mathcal{M}_n(\mathbb{C})$ the $n \times n$ matrix algebra with complex entries and $\mathrm{id}_n : \mathcal{M}_n(\mathbb{C}) \to \mathcal{M}_n(\mathbb{C})$ the identity map in $\mathcal{M}_n(\mathbb{C})$. A linear map $T : \mathscr{A} \to \mathscr{B}$ is completely positive if $T \otimes \mathrm{id}_n : \mathscr{A} \otimes \mathcal{M}_n(\mathbb{C}) \to \mathscr{B} \otimes \mathcal{M}_n(\mathbb{C})$ is positive for any $n \in \mathbb{N}$.

Complete positivity is a stronger condition than mere positivity, it means that a transformation acting on a Hilbert space is robust against coupling with another Hilbert space. This is crucial for the description of open quantum systems, since we couple the open system to a larger system and we wish that positive maps acting on the former remain positive.

Before featuring as a subject of interest for the description of open quantum systems, completely positive maps were a topic of study for its mathematical importance. For this reason there are works exploring the various properties of completely positive maps, for example M. Choi obtained a necessary and sufficient condition for a map to be completely positive in a matrix algebra of finite dimension [24]. Next, W. Stinespring formulated a generalization of the GNS representation that relates completely positive maps on a C^* algebra with operators acting on a Hilbert space [71]. At last, K. Kraus characterized completely positive maps acting on the set of bounded operators on a Hilbert space [44]. This last result is known as Kraus theorem and we shall state it bellow.

Theorem 3.1.1 (Kraus)**.** *A completely positive map $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ is of the form*

$$\Phi(A) = \sum_{k \in N} W_k^* A W_k, \tag{3.1.3}$$

where $W_k \in \mathcal{B}(\mathcal{H})$ and the sum converges in the strong operator sense[5]*. If $\mathcal{H}$ is separable then the indexing set N may be taken to be countable.*

The Kraus Representation Theorem 3.1.1 is directly related to the measurement theory in Quantum Mechanics. The foundations of measurement theory were established by J. von Neumann [75] and later vastly studied ([76], [17]). We will give a brief approach to the subject to justify the relation between Kraus operators and the outcomes of a measurement process.

We consider a system S with an associated Hilbert space $\mathcal{H}_S$ interacting with another system called *apparatus*, that in its turn is described by a Hilbert space

[5] A sequence of bounded operators $\{A_n\} \in \mathcal{B}(\mathcal{H})$ converges strongly to A if $\|A_n\psi - A\psi\| \to 0$ for all $\psi \in \mathcal{H}$ [57].

$\mathcal{H}_A$. We consider the simple case of an observable A with a discrete set of possible outcomes $\{\lambda_j\}$, associated to this observable is a self-adjoint operator acting on $\mathcal{H}_S$ of the form

$$A := \sum_j \lambda_j P_j, \tag{3.1.4}$$

where P_j are the spectral projectors of A [6]. We assume that $\mathcal{H}_A$ is a separable Hilbert space with an orthonormal basis $\{\varphi_k\}$ and that each element of the basis corresponds to an outcome of the measurement process

$$\varphi_j \iff \lambda_j.$$

If the initial state of the system S is ρ_0 and we prepare the apparatus in the pure state $|\varphi_0\rangle\langle\varphi_0|$ ($\varphi_0 \in \{\varphi_k\}$), then the initial state ϱ_0 of the composite system can be written as

$$\varrho_0 = \rho_0 \otimes |\varphi_0\rangle\langle\varphi_0|.$$

The interaction between the system S and the apparatus is described by the action of an unitary operator U acting of the Hilbert space of the composite system $\mathcal{H}_S \otimes \mathcal{H}_A$. After the measurement process, the state of the global system is

$$\varrho_f = U\varrho_0 U^*,$$

and the reduced dynamics of the system S is obtained by taking the partial trace of the final state in respect to the apparatus:

$$\begin{aligned}
\varrho_{S,f} &= \mathrm{Tr}_{\mathcal{H}_A}\, U\varrho_0 U^* \\
&= \sum_k \langle\varphi_k, U(\rho_0 \otimes |\varphi_0\rangle\langle\varphi_0|U^*)\varphi_k\rangle_{\mathcal{H}_A} \\
&= \sum_k \langle\varphi_k, U\varphi_0\rangle_{\mathcal{H}_A}\, \rho_0\, \langle\varphi_0, U^*\varphi_k\rangle_{\mathcal{H}_A} \\
&= \sum_k W_k\, \rho_0\, W_k^*,
\end{aligned}$$

where we defined the operator $W_k : V(\mathcal{H}_S) \to V(\mathcal{H}_S)$ as

$$W_k := \langle\varphi_k, U\varphi_0\rangle_{\mathcal{H}_A}. \tag{3.1.5}$$

[6] Spectral projectors satisfy the following conditions $P_iP_j = \delta_{ij}P_i$ and $\sum_j P_j = \mathbb{1}$ [57]

It follows from the unitarity of U that the operators $\{W_k\}$ satisfy the property

$$\begin{aligned}\sum_k W_k^* W_k &= \sum_k \langle \varphi_0, U^* \varphi_k \rangle_{\mathcal{H}_A} \langle \varphi_k, U\varphi_0 \rangle_{\mathcal{H}_A} \\ &= \sum_k \langle U\varphi_0, P_{\varphi_k} U\varphi_0 \rangle_{\mathcal{H}_A} \\ &= \|U\varphi_0\|_{\mathcal{H}_A} \\ &= \mathbb{1}_{\mathcal{H}_S},\end{aligned}$$

where $P_{\varphi_k} = |\varphi_k\rangle\langle\varphi_k|$ is the one-dimensional projector along $\varphi_k \in \mathcal{H}_A$ and satisfies $\sum_k P_{\varphi_k} = \mathbb{1}_{\mathcal{H}_A}$. If we define the map

$$\Phi_k(\rho) := W_k \, \rho_0 \, W_k^*,$$

the state ρ_k of the system S corresponding to the outcome λ_k of the observable A is

$$\rho_k = \frac{\Phi_k(\rho)}{\operatorname{Tr} \Phi_k(\rho)}.$$

The probability of obtaining the value λ_k in a measurement of the observable A is $\operatorname{Tr} \Phi_k(\rho)$ and the mean value of A is

$$\langle A \rangle = \sum_k \lambda_k \operatorname{Tr} \Phi_k(\rho).$$

The measurement process of an observable is represented by the unitary operator U in the global system. In the open system S each possible outcome λ_k is directly related to the map Φ_k. In a non-selective measurement, i.e., without recording the result, the state of S is given by the mapping

$$\rho_S \mapsto \Phi(\rho), \quad \Phi := \sum_k \Phi_k,$$

that is,

$$\rho \mapsto \Phi(\rho) := \sum_k W_k \rho W_k^*, \tag{3.1.6}$$

with

$$\sum_k W_k^* W_k = \mathbb{1}_{\mathcal{H}_S}. \tag{3.1.7}$$

The map Φ in 3.1.6 takes elements of the state space $V(\mathcal{H}_S)$ into itself, is trace-preserving and, according to Kraus representation theorem 3.1.1, presents the general form of a completely positive map. For this reason, Kraus operators are often referred to as *measurement operators* in the context of quantum measurement theory.

Quantum Dynamical Semigroups

The evolution of a closed quantum system with a Hilbert space $\mathcal{H}$ is determined by a self-adjoint operator H acting on $\mathcal{H}$ called Hamiltonian through the equation

$$\frac{d}{dt}\rho(t) = -i[H, \rho(t)],$$

where the density operator ρ describes the state of the system. If the Hamiltonian is time-independent, it is possible to show that the state of the system at a time t is

$$\rho(t) = U_t \rho(t_0) U_t^*,$$

where $\rho(t_0)$ is the initial state of the system and $U_t = e^{-itH}$. Thus, the dynamics of the closed system is characterized by a one-parameter group of unitary transformations $\{U_t\}$ with the infinitesimal generator $-iH$ (according to Stone's Theorem [57]).

The existence of the inverse element of a group is related to the reversibility of processes in the physical system. However, when dealing with open quantum systems reversibility is not a guaranteed feature. The approach to describe such systems is to couple them with larger systems, the so called reservoir or environment. From there on we have two paths: the Hamiltonian approach and the Markovian approach. The former deals directly with the dynamics of the total system, the rough idea behind it is to quantisize the reservoir, then we would have a Hamiltonian for the total system which would include terms describing the interaction between the open system and the reservoir (the mathematical framework of the Hamiltonian approach is nicely developed in [5]). The latter tries to describe the effective dynamics induced on the open system by the environment ([6] presents a great review on Markov processes in Quantum Mechanics and its applications in the theory of open quantum systems). The description of the joint system on which relies the Hamiltonian approach is usually very complicated, since the environment generally has an almost infinite number of degrees of freedom. Hence, the Markovian approach is of great use to the description of open quantum systems.

As was stated before, the time evolution of a closed quantum system is given by a group of unitary transformations. For an open quantum system, we will assume that its evolution is given by a semigroup that we shall call *quantum dynamical semigroup* ([26], [3]).

Definition 3.1.3 (Quantum dynamical semigroup)**.** Given a Hilbert space $\mathcal{H}$ with state space $V(\mathcal{H})$ we define a quantum dynamical semigroup to be a one-parameter family of linear operators $T_t : V(\mathcal{H}) \to V(\mathcal{H})$ defined for all $t \geq 0$ and satisfying

(i) if $\rho \geq 0$ then $T_t\rho \geq 0$;

(ii) $\operatorname{Tr} T_t\rho = \operatorname{Tr} \rho$;

(iii) $T_t T_s \rho = T_{t+s}\rho$;

(iv) $\lim_{t\to 0} \|T_t\rho - \rho\|_{\mathrm{Tr}} = 0$,

for all $\rho \in V(\mathcal{H})$ and $s, t \geq 0$.

The first condition means that the semigroup preserves positivity. The second one stands for the trace-preserving property of the semigroup. The third condition is the Markovicity condition: we expect that if we know the state of the system in a determined instant t_0, we can obtain the state of the system at all times $t \geq t_0$, that is, the memory effects are neglected. The last condition allows us to use the Hille-Yosida Theorem ([38], [78]) to ensure the existence and to characterize the generator of the semigroup[7]. As was discussed before, the positivity-preserving condition must be extended to the notion of complete positivity, i.e., the operators T_t must be completely positive.

The explicit form of the generator of quantum dynamical semigroups for a finite dimensional Hilbert space was obtained independently in 1976 by G. Lindblad [47] and V. Gorini et al. [35] and is presented in the Gorini-Kossakowski-Lindblad-Sudarshan Theorem.

Theorem 3.1.2 (Gorini-Kossakowski-Lindblad-Sudarshan Theorem)**.** *Let H be a self-adjoint operator on $\mathcal{H}$ and Γ_k a positive linear map on the state space $V(\mathcal{H})$. Then the operator $\mathscr{L}$ on $V(\mathcal{H})$ defined by*

$$\mathscr{L}(\rho) = -i[H, \rho] + \frac{1}{2}\sum_k (\Gamma_k \rho \Gamma_k^* - \Gamma_k^* \Gamma_k \rho - \rho \Gamma_k^* \Gamma_k), \tag{3.1.8}$$

is the generator of the quantum dynamical semigroup on $V(\mathcal{H})$. The summation is finite.

[7] Quantum dynamical semigroups are a special case of strongly continuous one-parameter semigroups or C_0 semigroups, for which the Hille-Yosida Theorem holds.

The Hille-Yosida Theorem ensures the existence of the generator of a strongly continuous one-parameter semigroup and the Theorem 3.1.2 gives the form for the generators of a quantum dynamical semigroup, so the time evolution for the states of the system can be summarized into

$$\frac{d}{dt}\rho_t = \mathscr{L}(\rho_t). \tag{3.1.9}$$

The equation 3.1.9 is called *quantum master equation*. We note that the second term of $\mathscr{L}$ in 3.1.8 corresponds to the introduction of non-unitarity in the evolution of the system, that is, the operators Γ_k are related to the interaction between the system and the environment. If $\Gamma_k = 0$ for all k, 3.1.8 reduces to the usual Hamiltonian evolution correspondent to a closed quantum system.

Generalized measurement and Lindblad equation

In the context of generalized measurement process, there is an intrinsic relation between Kraus operators and the terms in Lindblad equation. Let us consider a system with an associated Hilbert space $\mathcal{H}$ undergoing a completely positive non-unitary evolution. The state of the system is represented by the density operator $\rho(t) \in V(\mathcal{H})$. We obtained in 3.1.6 the relation between Kraus operators W_k and a non-selective measurement given by a completely positive map Φ:

$$\rho \to \Phi(\rho) = \sum_k W_k \rho W_k^*,$$

so if we consider that the system at an instant of time t is in the state $\rho(t)$ and suffers a non-selective measurement process, after dt the state of the system will be

$$\rho(t+dt) = \sum_k W_k(dt)\rho(t)W_k^*(dt), \tag{3.1.10}$$

where each W_k is related to a different outcome of the measurement process. In particular the W_0 is associated to a null outcome, this motivates us to define $W_0(t)$ as a time evolution operator associated with an effective Hamiltonian, $\tilde{H}$, that is not necessarily self-adjoint:

$$W_0(t) := e^{-i\tilde{H}t}. \tag{3.1.11}$$

We can formally expand $\rho(t+dt)$ as [8]

$$\rho(t+dt) = \sum_{n=0}^{\infty} \frac{\rho^{(n)}(t)}{n!}(dt)^n, \tag{3.1.12}$$

[8] A more rigorous study on this expansion is yet to be done.

where $\rho^{(n)}(t)$ denotes the nth time derivative of $\rho(t)$. Using the fact that $\rho(t)$ undergoes a completely positive map and using the Lindblad equation 3.1.8 in the expansion 3.1.12, we get

$$\sum_k W_k(dt)\rho(t)W_k^*(dt) = \rho(t) + \mathscr{L}((\rho(t))dt + \frac{1}{2!}\dot{\mathscr{L}}(\rho(t))(dt)^2 + \dots$$

For the sake of notation, we express $\mathscr{L}(\rho(t))$ as

$$\mathscr{L}(\rho(t)) = -i[H(t), \rho(t)] + \mathscr{D}(\rho(t)), \tag{3.1.13}$$

where $\mathscr{D}$ represents the dissipative part of the evolution:

$$\mathscr{D}(\rho(t)) := \frac{1}{2}\sum_k (2\Gamma_k\rho(t)\Gamma_k^* - \Gamma_k^*\Gamma_k\rho(t) - \rho(t)\Gamma_k^*\Gamma_k). \tag{3.1.14}$$

From 3.1.8 we have that

$$\rho^{(n)} = -i\sum_{p=0}^{n-1}\binom{n-1}{p}[H^{(p)}, \rho^{(n-1-p)}] + \mathscr{D}(\rho^{(n-1)}). \tag{3.1.15}$$

where we omitted the time dependence. The expression 3.1.15 is a recursive relation, since the time derivatives of ρ in the right side are also expressions involving the commutator with $H(t)$ and the dissipative part $\mathscr{D}$.

We take the expansion 3.1.12 up to first order::

$$\begin{aligned}
&\rho(t+dt) = \rho(t) + \dot{\rho}(t)dt \\
&\sum_k W_k(dt)\rho(t)W_k^* = \rho(t) + \mathscr{L}(\rho(t))dt \\
&W_0(dt)\rho(t)W_0^*(dt) + \sum_{k\geq 1} W_k(dt)\rho(t)W_k^*(dt) = \\
&\rho(t) - i[H(t), \rho(t)] + \frac{1}{2}\sum_k (2\Gamma_k\rho(t)\Gamma_k^* - \Gamma_k^*\Gamma_k\rho(t) - \rho(t)\Gamma_k^*\Gamma_k).
\end{aligned}$$

We expand the operator $W_0(dt)$ up to first order as well, $W_0(dt) \approx \mathbb{1} - i\tilde{H}dt$. The above expression yields

$$\begin{aligned}
&\rho(t) - i(\tilde{H}(t)\rho(t) - \rho(t)\tilde{H}^*(t))dt + \sum_{k\geq 1} W_k(dt)\rho(t)W_k^*(dt) = \\
&\rho(t) - i\left[\left(H(t) - \frac{i}{2}\sum_k \Gamma_k^*\Gamma_k\right)\rho(t) - \rho(t)\left(H(t) + \frac{i}{2}\sum_k \Gamma_k^*\Gamma_k\right)\right]dt + \\
&\sum_k \Gamma_k\rho(t)\Gamma_k^* dt.
\end{aligned}$$

We define the measurement operators $W_k(dt)$ so that the expression above holds:

$$W_0(dt) := \mathbb{1} - i\tilde{H}(t)dt, \tag{3.1.16}$$

$$W_k(dt) := \sqrt{dt}\,\Gamma_k, \quad k = 1, 2, \ldots \tag{3.1.17}$$

where the effective Hamiltonian is given by

$$\tilde{H}(t) := H(t) - \frac{i}{2}\sum_k \Gamma_k^*\Gamma_k, \tag{3.1.18}$$

and is clearly not self-adjoint.

3.2 Uhlmann's geometric phase

Since its introduction by Pancharatnam [52], the concept of geometric phase was vastly studied: from the formulation by Berry [12] up to the generalizations for non cyclic evolutions by Aharonov and Anandan [1] and for non adiabatic evolutions by Samuel and Bandhari [58]. However, the first generalization of geometric phases concerning mixed states was made by A. Uhlmann [74]. Uhlmann's approach is based on the purification of the density operator describing the quantum system: he considered a lift of the density operator to an extended Hilbert space where it is possible to define a parallel transport condition and to obtain an expression for the geometric phase.

Let us consider a system S with an associated Hilbert space $\mathcal{H}$ and a state space $V(\mathcal{H})$. The state of the system is represented by a density operator $\rho \in V(\mathcal{H})$ that might be a pure or a mixed state. The idea is to couple the system S to a system S' with an associated Hilbert space $\mathcal{H}'$ in a way that the state of the composite system $S + S'$ is a pure state. The Hilbert space of the composite system is $\mathcal{H}^{comp} := \mathcal{H} \otimes \mathcal{H}'$, we shall consider that $\mathcal{H}' = \mathcal{H}$. If $\dim < \infty$, it is possible to show that $\mathcal{H}^{comp}$ is isomorphic to the space of Hilbert-Schmidt operators $\mathcal{H}^{HS}$. We define $\mathcal{H}^{HS}$ bellow[9].

Definition 3.2.1 (Space of Hilber-Schmidt operators)**.** Let $\mathcal{H}$ be a separable Hilbert space and $\mathcal{B}(\mathcal{H})$ the space of bounded operators acting in $\mathcal{H}$. The space of Hilbert-Schmidt operators is defined as

$$\mathcal{H}^{HS} := \{A \in \mathcal{B}(\mathcal{H}) | \operatorname{Tr}(A^*A) < \infty\},$$

[9]The proof that $\mathcal{H} \otimes \mathcal{H} \cong \mathcal{H}^{HS}$ is presented in many books on Functional Analysis, e.g., [41] and [7].

The expression

$$\langle A, B\rangle_{HS} := \mathrm{Tr}(A^* B), \quad A, B \in \mathcal{H}^{HS} \tag{3.2.1}$$

defines an inner product in $\mathcal{H}^{HS}$ and induces a norm $\|\cdot\|_{HS}$ and $\mathcal{H}^{HS}$ is complete in this norm. Hence, $\mathcal{H}^{HS}$ is a Hilbert space equipped with the inner product $\langle\ ,\ \rangle_{HS}$ defined in 3.2.1.

Next we define the purification of a density operator in $V(\mathcal{H})$ in terms of Hilbert-Schmidt operators.

Definition 3.2.2 (Purification)**.** Let $\rho \in V(\mathcal{H})$ and $W \in \mathcal{H}^{HS}$. W is a *purification* of ρ iff

$$\rho = WW^* \tag{3.2.2}$$

is valid.

It is clear that a purification W of a density operator is by no means unique. Any element of the form $W' = WU$, where U is a unitary operator on $\mathcal{H}$, purifies the same ρ. Pancharatnam defined when two state vectors representing different quantum states are in phase (Definition 2.1.1), analogously, Uhlmann defined when two pairs of purifications are parallel[10].

Definition 3.2.3 (Uhlmann's Parallelity)**.** Let be W_1 and W_2 Hilbert-Schmidt operators that purify different density operators ρ_1 and ρ_2, respectively. We say that W_1 and W_2 are *parallel* if

$$W_1^* W_2 = W_2^* W_1 > 0. \tag{3.2.3}$$

An important observation is that if ρ_1 and ρ_2 are purified by another pair $\tilde{W}_1$ and $\tilde{W}_2$, then we can write $\tilde{W}_i = W_i U_i$ $(i = 1, 2)$ for some unitary operators U_i. From the parallelity condition 3.2.3 we have

$$\begin{aligned} \tilde{W}_1^* \tilde{W}_2 &= \tilde{W}_2^* \tilde{W}_1 \\ U_1 W_1^* W_2 U_2 &= U_2 W_2^* W_1 U_1 \\ U_1 W_2^* W_1 U_2 &= U_2 W_2^* W_1 U_1 \\ \Longrightarrow\ U_1 &= U_2 \end{aligned}$$

[10] Chruściński and Jamiolkowski [25] develops a justification for Uhlmann's parallelity condition in terms of Differential Geometry by considering a connection in the appropriate bundle and obtaining the respective parallel transport condition.

This means that if (W_1, W_2) are parallel purifications of (ρ_1, ρ_2), then all other parallel purifications can be obtained by the simultaneous replacement $W_i \to W_i U$ $(i = 1, 2)$ where U runs through all the unitary operators in $\mathcal{H}$.

Now we consider a curve

$$t \to \rho(t) \in V(\mathcal{H}),$$

sufficiently regular and differentiable, and let

$$t \to W(t) \in \mathcal{H}^{HS}$$

be a purification of $\rho(t)$. We want that $\rho(t)$ and $\rho(t + dt)$ be parallel, so we use the parallelity condition 3.2.3 for infinitesimal intervals of t and we obtain

$$W^* \dot{W} = \dot{W}^* W, \tag{3.2.4}$$

where the dot stands for derivation relative to t. We can define a phase factor between two purifications $W(0)$ and $W(t)$ as

$$\varphi_{Uhlmann} := \arg\langle W(0), W(t)\rangle_{HS} = \arg \mathrm{Tr}(W^*(t)W(0)). \tag{3.2.5}$$

In spite its importance as a mathematical treatment for mixed states, Uhlmann's geometric phase is difficult to be realized experimentally. Tidström and Sjöqvist [73] proposed an experimental setting to study Uhlmann's geometric phase in the context of interferometry, but they concluded that Uhlmann's phase is not as robust to reduction in the length of the Bloch vector as the geometric phase proposed by Sjöqvist et al. [64] (this approach will be presented in Section 3.3).

3.3 Geometric phases in the context of interferometry

In Section 3.2 we described Uhlmann's approach to mixed state geometric phase. However, it is a very abstract approach and it is not clear how to realize an experiment to measure it. Although formulated in a classical setting by Pancharatnam, geometric phase was first defined in the context of interferometry, as we saw in Section 2.1. Following this motivation, Sjöqvist et al. [64] and Faria et al. [53] proposed a new approach to geometric phase for mixed states, the former considered systems undergoing unitary evolutions and the latter considered mixed states undergoing completely positive non-unitary evolution. First we state the geometric phase in the context of quantum interferometry and then we will present both approaches and then show how Faria's results reduce to the ones obtained by Sjöqvist et al.

Quantum interferometry: phases and measurements

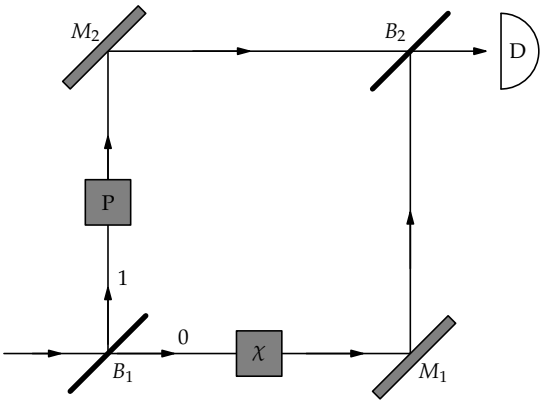


Figure 3.1: A conventional Mach-Zehnder interferometer: M_1 and M_2 are perfect mirrors, B_1 and B_2 are beam-splitters, χ is the phase difference between the beam in the 0 arm and in the 1 arm, D is a detector that measures the intensity of the beam in the 0 arm and, finally, P is the device introduced in the interferometer to cause non-unitarity in the evolution.

A Mach-Zehnder interferometer is a device used to determine the relative phase between two beams from a single source (Figure 3.1). A beam of particles moves in two given directions defined by the geometry of the interferometer, the so called arms of the interferometer, that we shall label as 0 and 1. We associate to these paths a two dimensional Hilbert space $\tilde{\mathcal{H}} = \{|\tilde{0}\rangle, |\tilde{1}\rangle\}$. The state vectors $|\tilde{0}\rangle$ and $|\tilde{1}\rangle$ represent the wave packets moving along the arms of the interferometer. In this basis, the action of the elements of the interferometer (beam-splitters, mirrors and shift phase) are represented by the following unitary operators:

$$\tilde{U}_M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{U}_B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}, \quad \tilde{U}(1) = \begin{pmatrix} e^{i\chi} & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.3.1}$$

respectively. We consider that the beam enters in the arm associated to $|\tilde{0}\rangle$, so the input state of the beam is the pure state

$$\tilde{\rho}_{in} = |\tilde{0}\rangle\langle\tilde{0}|. \tag{3.3.2}$$

After passing through the elements of the interferometer, the output state measured by the detector D is

$$\begin{aligned} \tilde{\rho}_{out} &= \tilde{U}_B \tilde{U}_M \tilde{U}(1) \tilde{U}_B \tilde{\rho}_{in} \tilde{U}_B^* \tilde{U}(1)^* \tilde{U}_M^* \tilde{U}_B^* \\ &= \frac{1}{2} \begin{pmatrix} 1+\cos\chi & i\sin\chi \\ -i\sin\chi & 1-\cos\chi \end{pmatrix}. \end{aligned} \tag{3.3.3}$$

The intensity measured by the detector is given by

$$\begin{aligned} I &\propto \langle \tilde{0}, \tilde{\rho}_{out} \tilde{0} \rangle \\ &\propto 1 + \cos\chi, \end{aligned} \tag{3.3.4}$$

so the phase shift χ can be observed in the output signal of the interferometer.

We recall the Pancharatnam's definition in 2.1.7 for a relative phase between two state vectors ψ_a and ψ_b in a Hilbert space $\mathcal{H}$:

$$\phi := \arg\langle \psi_a, \psi_b \rangle.$$

If we shift the phase of ψ_a by χ

$$\psi_a \to \psi_a' = e^{i\chi}\psi_a,$$

the intensity of the interference between the two is

$$\begin{aligned} I &\propto \langle \psi_a' + \psi_b, \psi_a' + \psi_b \rangle \\ &\propto 1 + |\langle \psi_a, \psi_b \rangle| \cos[\chi - \arg\langle \psi_a, \psi_b \rangle]. \end{aligned} \tag{3.3.5}$$

We identify the visibility $\nu := |\langle \psi_a, \psi_b \rangle|$ and the shift $\phi := \arg\langle \psi_a, \psi_b \rangle$. We note that the intensity is maximum when $\chi = \phi$, as was defined by Pancharatnam We identify the visibility $\nu := |\langle \psi_a, \psi_b \rangle|$ and the shift $\phi := \arg\langle \psi_a, \psi_b \rangle$. We note that the intensity is maximum when $\chi = \phi$, as was defined by Pancharatnam.

Unitary evolution

Now we consider that the particles carry additional internal degrees of freedom, e.g., polarization or spin. The space associated to these internal degrees of freedom is $\mathcal{H}_i$ and we consider $\mathcal{H}_i \cong \mathbb{C}^N$ spanned by the vectors $\{\psi_k\}$, $k = 1, 2, \ldots, N$. Suppose that the initial state in $\mathcal{H}_i$ is

$$\rho_0 = \sum_k w_k |\psi_k\rangle\langle\psi_k|, \tag{3.3.6}$$

where w_k is the probability of finding the quantum system in the pure state ψ_k. We consider that ρ_0 undergoes a unitary evolution inside the interferometer, such that

$$\rho_0 \to U_i \rho_0 U_i^*, \tag{3.3.7}$$

where U_i is a unitary operator acting only in $\mathcal{H}_i$. The total Hilbert space associated to the beam is the product space $\tilde{\mathcal{H}} \otimes \mathcal{H}_i$. Assuming the mirrors and beam-splitters act only in $\tilde{\mathcal{H}}$, we can rewrite their action in the total Hilbert space, $U_M = \tilde{U}_M \otimes \mathbb{1}_i$ and $U_M = \tilde{U}_B \otimes \mathbb{1}_i$, where $\mathbb{1}_i$ is the identity operator in $\mathcal{H}_i$. The evolution of the system particles + internal degrees of freedom after the first beam-splitter is given by the operator

$$U = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes U_i + \begin{pmatrix} e^{i\chi} & 0 \\ 0 & 0 \end{pmatrix} \otimes \mathbb{1}_i. \tag{3.3.8}$$

The operator U generalizes the notion of phase to mixed states evolving unitarily. The total output state ϱ_{out} detected by the D is

$$\varrho_{out} = U_B U_M U U_B \varrho_{in} U_B^* U^* U_M^* U_B^* \tag{3.3.9}$$

$$= \frac{1}{4}\left[\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes U_i \rho_0 U_i^* + e^{i\chi} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \otimes \rho_0 U_i^* \right. \tag{3.3.10}$$

$$\left. + e^{-i\chi} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \otimes U_i \rho_0 \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \otimes \rho_0 \right]. \tag{3.3.11}$$

Analogously to 3.3.4, the intensity measured by the detector is

$$\begin{aligned} I &\propto \sum_k (\langle \tilde{0}| \otimes \langle \psi_k|)\varrho_{out}(|\tilde{0}\rangle \otimes |\psi_k\rangle) \\ &\propto \mathrm{Tr}_{\mathcal{H}_i}(U_i \rho U_i^* + e^{i\chi}\rho_0 U_i^* + e^{-i\chi} U_i \rho_0 + \rho_0) \\ &\propto 1 + |\,\mathrm{Tr}_{\mathcal{H}_i}(U_i\rho_0)| \cos[\chi - \arg \mathrm{Tr}_{\mathcal{H}_i}(U_i\rho_0)]. \end{aligned} \tag{3.3.12}$$

As in 3.3.5, we identify the visibility $\nu = |\,\mathrm{Tr}_{\mathcal{H}_i}(U_i\rho_0)|$ and the phase shift $\phi = \arg \mathrm{Tr}_{\mathcal{H}_i}(U_i\rho_0)$. The phase shift is valid for pure or mixed states of $\mathcal{H}_i$. Considering pure states ψ_k, we have that $\psi_k(t) = U_i\psi_k$. As in 3.3.5, we perform a phase shift $\psi_k \to \psi_k' = e^{i\chi}\psi_k$, so the interference profile I_k relative to the state ψ_k is weighted by the probabilities w_k in 3.3.6 and is given by

$$\begin{aligned} I_k &= w_k \langle \psi_k' + \psi(t), \psi_k' + \psi_k(t)\rangle \\ &= w_k(2 + 2|\langle \psi_k, \psi_k(t)\rangle| \cos[\chi - \arg\langle \psi_k, \psi_k(t)\rangle]), \end{aligned} \tag{3.3.13}$$

We define $\nu_k := |\langle \psi_k, \psi_k(t)\rangle| = |\langle \psi_k, U_i\psi_k\rangle|$ and $\phi_k := \arg\langle \psi_k, \psi_k(t)\rangle = \arg\langle \psi_k, U_i\psi_k\rangle$. We can interpret the total intensity as an incoherent average of the interference

profiles I_k:

$$\begin{aligned} I &= \sum_k I_k \\ &= 2 + 2\sum_k w_k |\langle \psi_k, \psi_k(t)\rangle| \cos[\chi - \arg\langle \psi_k, \psi_k(t)\rangle] \\ &= 2 + 2\left[\cos\chi \left(\sum_k w_k \nu_k \cos\phi_k\right) + \sin\chi \left(\sum_k w_k \nu_k \sin\phi_k\right)\right], \end{aligned}$$

defining

$$\phi := \arg\left(\sum_k w_k \nu_k e^{i\phi_k}\right) = \arg \mathrm{Tr}_{\mathcal{H}_i}(U_i \rho_0) \tag{3.3.14}$$

and

$$\nu := \left|\sum_k w_k \nu_k e^{i\phi_k}\right| = |\,\mathrm{Tr}_{\mathcal{H}_i}(U_i \rho_0)|. \tag{3.3.15}$$

we can rewrite the intensity as

$$I \propto 1 + \nu \cos(\chi - \phi), \tag{3.3.16}$$

in accordance with the expression obtained using Pancharatnam's definition 3.3.5. From now on we will omit the subscript $\mathcal{H}_i$, since we will deal only with the Hilbert space $\mathcal{H}_i$ associated to the internal degrees of freedom of the beam and its respective state space. Besides, we consider that U_i is a continuous unitary transformation acting in $\mathcal{H}_i$ and we will denote it by $U(t)$.

Phase difference and parallel transport condition

According to Sjöqvist et al. [64], a necessary condition for the parallel transport of a density operator $\rho(t)$ along an arbitrary path in the state space is that at each instant of time the state $\rho(t)$ must be *in phase* with the state $\rho(t + dt)$ at an infinitesimal time. The density operator $\rho(t + dt)$ is

$$\begin{aligned} \rho(t + dt) &= U(t + dt)\rho_0 U^*(t + dt) \\ &= U(t + dt)U^*(t)\rho(t)U(t)U^*(t + dt). \end{aligned}$$

The phase difference between $\rho(t)$ and $\rho(t + dt)$ is given by

$$d\phi = \arg\left\{\mathrm{Tr}\left[U(t + dt)U^*(t)\rho(t)\right]\right\},$$

following Pancharatnam's definition (Definition 2.1.1) that two state vectors are in phase if their relative phase is real and positive, we can say that $\rho(t)$ and $\rho(t+dt)$ are in phase if

$$\mathrm{Tr}[U(t+dt)U^*(t)\rho(t)] \text{ is real and positive.}$$

We have that

$$\begin{aligned}\mathrm{Tr}[U(t+dt)U^*(t)\rho(t)] &= \mathrm{Tr}[(U(t)+\dot{U}(t)dt)U^*(t)\rho(t)] \\ &= 1+\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)]dt,\end{aligned}$$

where we used that $\mathrm{Tr}\,\rho(t)=1$. We can also use the trace property that $\overline{\mathrm{Tr}\,A}=\mathrm{Tr}\,A^*$ (if A is a trace class operator [57]):

$$\begin{aligned}&\overline{\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)]} = \mathrm{Tr}[\rho(t)U(t)\dot{U}^*(t)] \\ &\overline{\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)]} = -\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)] \\ &\implies \mathfrak{Re}(\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)])=0,\end{aligned}$$

where we used the unitarity of $U(t)$ (omitting briefly the dependence in t, $U^*U=\mathbb{1} \implies \dot{U}^*U+U^*\dot{U}=0$). The expression $\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)]$ is purely imaginary. Therefore, for the condition of parallel transport to be fulfilled we must have

$$\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)]=0. \tag{3.3.17}$$

If we consider an N-dimensional Hilbert space, the density operator is then a $N\times N$ density matrix as well as the operator $U(t)$. The condition 3.3.17 determines $U(t)$ up to N phase factors, they can be fixed by

$$\langle\psi_k,\dot{\psi}_k\rangle=0, \quad k=1,2,\ldots,N. \tag{3.3.18}$$

Now, 3.3.18 is a necessary and sufficient condition to determine the operator $U(t)$ responsible for the parallel transport of $\rho(t)$ in the state space.

Thus, in Sjöqvist et al. formulation of geometric phase in the context of quantum interferometry, the phase difference between the initial state of the beam and the final one is given by 3.3.14:

$$\phi=\arg\mathrm{Tr}(U(t)\rho_0),$$

and the parallel transport condition is given by 3.3.17:

$$\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)]=0.$$

We can check that the geometric phase and parallel transport condition obtained by Sjöqvist et al. recovers the results already known for pure states. Let us consider that the system is initially in a pure state $\rho_o = |\psi_0\rangle\langle\psi_0|$ and the state vector undergoes a unitary evolution $\psi(t) = U(t)\psi_0$, according to 3.3.14 the geometric phase is

$$\begin{aligned}\phi &= \arg \mathrm{Tr}(U(t)\rho_0) \\ &= \arg \sum_k \langle\psi_k, U(t)\psi_0\rangle\langle\psi_0, \psi_k\rangle \\ &= \arg\langle\psi_0, \psi(t)\rangle,\end{aligned}$$

that is exactly the expression obtained in 2.1.7. For the parallel transport condition we use that $\psi(t) = U(t)\psi_0$ and $\dot{\psi}(t) = \dot{U}(t)\psi_0 = \dot{U}(t)U^*(t)\psi(t)$:

$$\begin{aligned}\mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)] &= 0 \\ \sum_k \langle\psi_k, \dot{U}(t)U^*(t)\psi(t)\rangle\langle\psi(t), \psi_k\rangle &= 0 \\ \langle\psi(t), \dot{\psi}(t)\rangle &= 0,\end{aligned}$$

which is precisely the condition obtained in 2.2.6.

Finally, we consider a system with an initial state ρ_0 and its unitary evolution given by a curve C in the state space

$$C : t \in [0, T] \to \rho(t) = U(t)\rho_0 U^*(t), \quad \rho_0, \rho(t) \in V(\mathcal{H}).$$

We can define a geometric phase γ_g to this curve. Considering that 3.3.17 is valid, that is, that the density operator is parallel transported along the curve C, we can calculate the dynamical phase associated to this evolution. This phase γ_{dyn} is given

by the time integral of the Hamiltonian's average:

$$\begin{aligned}
\alpha_{dyn} &= -\int_0^T dt\, \mathrm{Tr}[\rho(t)H(t)] \\
&= -\int_0^T dt\, \mathrm{Tr}[U(t)\rho_0 U^*(t)H(t)] \\
&= -\int_0^T dt\, \mathrm{Tr}[U^*(t)U(t)\rho_0 U^*(t)H(t)U(t)] \\
&= -\int_0^T dt\, \mathrm{Tr}[\rho_0 U^*(t)(i\dot{U}(t))] \\
&= -i\int_0^T dt\, \mathrm{Tr}[U^*(t)\rho(t)U(t)U^*(t)\dot{U}(t)] \\
&= -i\int_0^T dt\, \mathrm{Tr}[\dot{U}(t)U^*(t)\rho(t)] \\
&= 0,
\end{aligned}$$

where we used that $\mathrm{Tr}\, A = \mathrm{Tr}\, U^* A U$ for a trace class operator A and U unitary ([57]), and that $\dot{U}(t) = iH(t)$. Besides, in the last step we used the parallel transport condition 3.3.17. So, the dynamical phase vanishes identically and we can define the geometric phase along C using 3.3.14, $\gamma_g(C)$:

$$\gamma_g(C) = \phi = \arg \mathrm{Tr}[U(t)\rho_0] \arg\left(\sum_k w_k \nu_k e^{i\phi_k}\right)$$

where w_k, ν_k and ϕ_k are respectively the probability, visibility and geometric phase factors associated with the individual pure states $\psi_k \in \mathcal{H}_i$.

Purification

The phase factor 3.3.14 can be obtained by a purification procedure (as made by Uhlmann). We will briefly describe this procedure. Any mixed state ρ_0 can be obtained by tracing out some degrees of freedom of a larger system which is in a pure state

$$\Psi_0 = \sum_k \sqrt{w_k}\, \psi_k \otimes \eta_k,$$

where $\{\eta_k\} \in \mathcal{H}_a$ is a basis for the Hilbert space $\mathcal{H}_a$ of the auxiliary system. So $\rho_0 = \mathrm{Tr}_a\, |\Psi_0\rangle\langle\Psi_0|$. Considering a time evolution of Ψ given by an unitary operator $\mathcal{U}(t) = U(t) \otimes \mathbb{1}_a$ where $U(t)$ is an unitary operator acting in the Hilbert space of

the system and $\mathbb{1}_a$ is the identity operator in $\mathcal{H}_a$. Then, for an instant of time t we have

$$\Psi(t) = \sum_k \sqrt{w_k}\, U(t)\psi_k \otimes \eta_k,$$

taking the inner product with Ψ_0

$$\begin{aligned}\langle \Psi_0, \Psi(t)\rangle &= \sum_k w_k \langle \psi_k, U(t)\psi_k\rangle \\ &= \mathrm{Tr}[U(t)\rho_0],\end{aligned}$$

so the relative phase φ between the purifications Ψ_0 and $\Psi(t)$ is $\varphi = \arg \mathrm{Tr}[U(t)\rho_0]$, as obtained by Sjöqvist et al. (equation 3.3.14). The question if Uhlmann's mathematical treatment and Sjöqvist et al. interferometric approach always coincide comes naturally. In [66] Slater studied this question and the answer is that, except for pure states, they are not equivalent.

Example: Qubit

To illustrate the use of the expression 3.3.14 we consider a qubit, i.e., a two-level quantum system. As we saw in 2.4.4, a density matrix for such a system can be written as

$$\rho = \frac{1}{2}(\mathbb{1}_2 + \boldsymbol{a}\cdot\sigma),$$

where $\mathbb{1}_2$ is the identity matrix in $\mathbb{C}^2$, $\boldsymbol{a} \in \mathbb{R}^3$ is the Bloch vector and σ is the three-vector of Pauli matrices. Writing the Bloch vector as $\boldsymbol{a} = a\boldsymbol{n}$ where $\boldsymbol{n} = \boldsymbol{a}/a$ and denoting the eigenvectors of ρ as $\psi_\pm(\boldsymbol{n})$, we have that

$$\rho\ \psi_\pm(\boldsymbol{n}) = \frac{1 \pm a}{2}\psi_\pm(\boldsymbol{n}).$$

We consider the case in which $\rho(t)$ undergoes an unitary evolution and the corresponding unit vector $\boldsymbol{n}(t)$ traces out a geodesically closed curve on the Bloch sphere that encloses a solid angle Ω. The eigenvectors $\psi_\pm(\boldsymbol{N})$ acquire phase factors $\varphi_\pm = \mp\frac{1}{2}\Omega$ (as obtained in 2.4.9). We can write $\rho(t)$ as

$$\rho(t) = \frac{1+a}{2}|\psi_+(\boldsymbol{n}(t))\rangle\langle\psi_+(\boldsymbol{n}(t))| + \frac{1-a}{2}|\psi_-(\boldsymbol{n}(t))\rangle\langle\psi_-(\boldsymbol{n}(t))|,$$

so $w_\pm = \frac{1\pm a}{2}$. From 3.3.15 the corresponding visibilities are identical $\nu_\pm := \eta$. Finally we can calculate the phase factor acquired by $\rho(t)$, from 3.3.14:

$$\begin{aligned}\phi &= \arg\left(w_+\nu_+e^{i\phi_+} = w_-\nu_-e^{i\phi_-}\right)\\ &= \arg\left\{\frac{\eta}{2}\left[(1+a)e^{-i\Omega/2} + (1-a)e^{i\Omega/2}\right]\right\}\\ &= \arg\left\{\eta\left[\cos\left(\frac{\Omega}{2}\right) - ia\sin\left(\frac{\Omega}{2}\right)\right]\right\}\\ &= -\arctan\left(a\tan\left(\frac{\Omega}{2}\right)\right).\end{aligned}$$

When $a = 1$ we have a pure state and the expression above recovers the result obtained before.

Non-unitary evolution

In this section we follow the work of Peixoto de Faria et al. [53] in which an operational definition of phases between mixed states is defined in the context of interferometry. The difference between this work and the one presented previously elaborated by Sjöqvist et al. is that now the system undergoes a non-unitary evolution.

As before, we consider a conventional Mach-Zehnder interferometer (Figure 3.1), with an incoming beam of particles with internal degrees of freedom, but now a meter P is introduced in the arm 1 of the interferometer, so we have to consider a third system, the probe. The total Hilbert space associated to this configuration is

$$\mathcal{H} = \tilde{\mathcal{H}} \otimes \mathcal{H}_i \otimes \mathcal{H}_p,$$

where $\tilde{\mathcal{H}}$ is the two-dimensional Hilbert space associated with the geometry of the interferometer, $\mathcal{H}_i$ is a N-dimensional Hilbert space associated with the internal degrees of freedom of the particles that compose the beam and $\mathcal{H}_p$ is the Hilbert space associated with the probe. The role of this meter is to perform continuous generalized measurements in order to introduce non-unitarity in the evolution of the state $\rho_i \in V(\mathcal{H}_i)$. The unitary operators corresponding to the action of the elements of the interferometer (beam-splitters and mirrors) is given by

$$U_B = \tilde{U}_B \otimes \mathbb{1}_i \otimes \mathbb{1}_p, \tag{3.3.19}$$

$$U_M = \tilde{U}_M \otimes \mathbb{1}_i \otimes \mathbb{1}_p, \tag{3.3.20}$$

where $\tilde{U}_B$ and $\tilde{U}_M$ are defined in 3.3.1 and only act in $\tilde{H}$, $\mathbb{1}_i$ and $\mathbb{1}_p$ are the identity operators in $\mathcal{H}_i$ and $\mathcal{H}_p$, respectively. The action of the meter and the introduction of the phase shift χ in the arm 0 is given by the operator

$$U = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes U_{ip} + \begin{pmatrix} e^{i\chi} & 0 \\ 0 & 0 \end{pmatrix} \otimes \mathbb{1}_i \otimes \mathbb{1}_p, \tag{3.3.21}$$

where U_{ip} is an unitary operator acting in $\mathcal{H}_i \otimes \mathcal{H}_p$ and is related to the measurement process. Let $\{\eta_n\}_{n=0,1,\dots}$ be a basis of $\mathcal{H}_p$, we assume that the probe is prepared in the pure state $|\zeta_)\rangle\langle\zeta_0|$. Then the initial state ϱ_0 of the composite system is

$$\varrho_0 = |\tilde{0}\rangle\langle\tilde{0}| \otimes \rho_{i,0} \otimes |\zeta_0\rangle\langle\zeta_0|, \tag{3.3.22}$$

where $\rho_{i,0}$ is the initial state of the internal degrees of freedom of the particles in the beam. Assuming that the probe performs one measurement process, the state ϱ' of the composite system after passing through the elements of the interferometer is

$$\begin{aligned}\varrho' = \frac{1}{4}\Bigg[& \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes U_{ip}(\rho_{i,0} \otimes |\zeta_0\rangle\langle\zeta_0|)U_{ip}^* \\ & + e^{i\chi} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \otimes (\rho_{i,0} \otimes |\zeta_0\rangle\langle\zeta_0|)U_{ip}^* + e^{-i\chi} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \otimes U_{ip}(\rho_{i,0} \otimes |\zeta_0\rangle\langle\zeta_0|) \\ & + \quad \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \otimes (\rho_{i,0} \otimes |\zeta_0\rangle\langle\zeta_0|) \Bigg].\end{aligned}$$

The intensity I_k of the interference pattern for each outcome of the measurement process is

$$\begin{aligned} I_k &\propto \sum_i (\langle\tilde{0}| \otimes \langle\psi_i| \otimes \langle\zeta_k|)\varrho_0(|\tilde{0}\rangle \otimes |\psi_i\rangle \otimes |\zeta_k\rangle) \\ &\propto \operatorname{Tr}_{\mathcal{H}_i}(W_k^* W_k \rho_{i,0}) + \delta_{k,0}\left[e^{i\chi}\operatorname{Tr}_{\mathcal{H}_i}(\rho_{i,0}W_0^*) + e^{-i\chi}\operatorname{Tr}_{\mathcal{H}_i}(W_0\rho_{i,0}) + 1\right] \\ &\propto \operatorname{Tr}_{\mathcal{H}_i}(W_k^* W_k \rho_{i,0}) + \delta_{k,0}\left\{1 + 2|\operatorname{Tr}_{\mathcal{H}_i}(W_0\rho_{i,0})|\cos[\chi - \arg\operatorname{Tr}_{\mathcal{H}_i}(W_0\rho_{i,0})]\right\} \end{aligned}$$

where $\{\psi_i\}_{i=1}^N$ is a basis of $\mathcal{H}_i$ and we defined the operator W_k acting on $\mathcal{H}_i$ as

$$W_k := \langle\zeta_k, U_{ip}\zeta_0\rangle, \quad n = 1, 2, \dots \tag{3.3.23}$$

For $k \neq 0$ we have

$$I_k \propto \operatorname{Tr}_{\mathcal{H}_i}(W_k^* W_k \rho_{i,0}), \tag{3.3.24}$$

so there is no interference pattern. For $k = 0$ we have

$$I_0 \propto 1 + \mathrm{Tr}_{\mathcal{H}_i}(W_0^* W_0 \rho_{i,0}) + 2|\,\mathrm{Tr}_{\mathcal{H}_i}(W_0 \rho_{i,0})|\cos[\chi - \arg \mathrm{Tr}_{\mathcal{H}_i}(W_0 \rho_{i,0})],$$

Analogously to 3.3.4, we define the visibility ν_0 and shift ϕ_0:

$$\nu_0 := |\,\mathrm{Tr}_{\mathcal{H}_i}(W_0^* W_0 \rho_{i,0})| \tag{3.3.25}$$

$$\phi_0 := \arg \mathrm{Tr}_{\mathcal{H}_i}(W_0^* W_0 \rho_{i,0}), \tag{3.3.26}$$

so the expression for I_0 yields

$$I_0 \propto 1 + \mathrm{Tr}_{\mathcal{H}_i}(W_0^* W_0 \rho_{i,0}) + 2\nu_0 \cos(\chi - \phi_0), \tag{3.3.27}$$

The total intensity for a non-selective measurement process is given by an averaged sum of the intensities I_k's:

$$I = \sum_k I_k \propto 1 + \nu_0 \cos(\chi - \phi_0), \tag{3.3.28}$$

in a result analogous to 3.3.12 obtained by Sjöqvist et al.

Continuous generalized measurement process

As was said before, the non-unitarity comes from generalized measurements performed by the meter P in $\mathcal{H}_i$. Considering that each measurement takes a time interval δt in which the internal degrees of freedom interacts with the probe "through" the operator $U_{ip}(\Delta t)$. After the measurement, the state of the composite system is projected onto a state ζ_n of the basis of $\mathcal{H}_p$. Then, the state is restored in relation to the initial state of the probe ($|\zeta_0\rangle\langle\zeta_0|$) and the process is repeated. A "pseudoalgorithm" is the following:

1. The initial state ϱ_0 of the composite system is

$$\varrho_0 = |\tilde{0}\rangle\langle\tilde{0}| \otimes \rho_i(0) \otimes |\zeta_0\rangle\langle\zeta_0|.$$

2. After a time interval δt the operator $U_{ip}(\Delta t)$ acts on $\rho_i(0) \otimes |\zeta_0\rangle\langle\zeta_0|$ resulting in a state of the composite system ϱ_0':

$$\varrho_0 \xrightarrow{U_{ip}(\Delta t)} \varrho_0'.$$

3. Then the resulting state ϱ_0' is projected onto an element ζ_n of the basis of $\mathcal{H}_p$ in order to record the outcome of the measurement, but since we are considering a non-selective measurement process, we sum over all the possible outcomes, resulting in a state of the system of particles + degrees of freedom that we shall indicate as $\tilde{\varrho}_0$:

$$\begin{aligned}\tilde{\varrho}_0 &= \sum_n \langle \zeta_n, \varrho_0' \zeta_n \rangle \\ &= \mathrm{Tr}_{\mathcal{H}_p}\, \varrho_0'.\end{aligned}$$

This is the step in which the non-unitarity is properly introduced.

4. Finally, we restore the probe to its initial state:

$$\varrho_1 = \tilde{\varrho}_0 \otimes |\zeta_0\rangle\langle\zeta_0|.$$

5. The process is then repeated for ϱ_1.

These steps are performed N times and the limit of continuous generalized measurement is obtained by taking $N \to \infty$ and $\Delta t \to 0$. After this proceeding, the outcome state $\tilde{\varrho}_{out}$ of the system of particles + degrees of freedom measured bu the detector is given by

$$\begin{aligned}\tilde{\varrho}_{out}(t) = \frac{1}{4}\Bigg[&\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \rho_i(t) + e^{i\chi} \begin{pmatrix} 1 & -i \\ -i & -1 \end{pmatrix} \otimes [\rho_i(0) S^*(t)] \\ &+ e^{-i\chi} \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix} \otimes [S(t)\rho_i(0)] + \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \otimes \rho_i(0) \Bigg].\end{aligned} \tag{3.3.29}$$

where the operator $S(t)$ is defined as

$$S(t) := e^{-i\tilde{H}t} = \exp\left\{ -i \left(H(t) - \frac{i}{2} \sum_n \Gamma_n^* \Gamma_n \right) t \right\}, \tag{3.3.30}$$

and is obtained through the limit of the previous "pseudoalgorithm".

Phase difference and parallel transport condition

The intensity of the interference pattern is given by

$$\begin{aligned} I &\propto \sum_i (\langle\tilde{0}| \otimes \langle\psi_i|)\tilde{\varrho}_{out}(|\tilde{0}\rangle \otimes |\psi_i\rangle) \\ &\propto 2 + e^{i\chi}\,\mathrm{Tr}_{\mathcal{H}_i}[\rho_i(0)S^*(t)] + e^{-i\chi}\,\mathrm{Tr}_{\mathcal{H}_i}[S(t)\rho_i(0)] \\ &\propto 2 + 2|\,\mathrm{Tr}_{\mathcal{H}_i}[S(t)\rho_i(0)]|\cos\left\{\chi - \arg\mathrm{Tr}_{\mathcal{H}_i}[S(t)\rho_i(0)]\right\} \\ &\propto 1 + \nu\cos[\chi - \phi(0,t)], \end{aligned}$$

where we defined the visibility ν and the phase difference between $\rho_i(0)$ and $\rho_i(t)$ as

$$\nu := |\,\mathrm{Tr}_{\mathcal{H}_i}[S(t)\rho_i(0)]|, \tag{3.3.31}$$

$$\phi(0,t) := \arg\mathrm{Tr}_{\mathcal{H}_i}[S(t)\rho_i(0)] \tag{3.3.32}$$

Thus, the total phase difference $d\phi(t)$ between $\rho_i(t)$ and $\rho_i(t+dt)$ is given by (up to first order of approximation):

$$\begin{aligned} d\phi(t) &= \arg\mathrm{Tr}_{\mathcal{H}_i}\left\{\left[\mathbb{1}_i - i\left(H(t) - \frac{i}{2}\sum_n \Gamma_n^*\Gamma_n\right)dt\right]\rho_i(t)\right\} \\ &= \arg\left\{1 - \frac{dt}{2}\sum_n \mathrm{Tr}_{\mathcal{H}_i}[\Gamma_n^*\Gamma_n\rho_i(t)] - idt\,\mathrm{Tr}_{\mathcal{H}_i}[H(t)\rho_i(t)]\right\} \\ &= \arctan\left\{-\frac{dt\,\mathrm{Tr}_{\mathcal{H}_i}[H(t)\rho_i(t)]}{1 - \frac{dt}{2}\sum_n \mathrm{Tr}_{\mathcal{H}_i}[\Gamma_n^*\Gamma_n\rho_i(t)]}\right\}. \end{aligned}$$

Using that the Kraus operators W_k satisfy $\sum_k W_k^*W_k = \mathbb{1}$, we have that

$$0 \leq \sum_n \Gamma_n^*\Gamma_n dt \leq \sum_k W_k^*(dt)W_k(dt) = \mathbb{1}_i,$$

so

$$1 - \frac{dt}{2}\sum_n \mathrm{Tr}_{\mathcal{H}_i}[\Gamma_n^*\Gamma_n\rho_i(t)] \geq 0.$$

We say that $\rho_i(t)$ is in phase with $\phi_i(t+dt)$ when $d\phi(t) = 0$, therefore, we must have

$$\mathrm{Tr}_{\mathcal{H}_i}[H(t)\rho_i(t)] = 0, \tag{3.3.33}$$

The above condition is the parallel transport condition. That is, if we consider that the evolution of the system is given by a curve C in the state space

$$C : \tau \in [0, t] \to \rho_i(\tau) \in V(\mathcal{H}_i),$$

and that ϕ_i undergoes a non-unitary evolution characterized by completely positive maps, the associated dynamical phase γ_{dyn} is

$$\alpha_{dyn} = -\int_0^t d\tau \, \mathrm{Tr}_{\mathcal{H}_i}[H(t)\rho_i(t)], \tag{3.3.34}$$

that vanishes for a parallel transport of $\rho_i(\tau)$ along C. So the total phase difference 3.3.32 is purely geometrical:

$$\gamma_{geo} = \phi(0, t). \tag{3.3.35}$$

Example: spin-$\frac{1}{2}$ particle in a magnetic field

Once again we consider a two-level quantum system: a spin-$\frac{1}{2}$ particle in a magnetic field. The Hamiltonian of the system is given by

$$H = \frac{\omega}{2}\sigma_3, \tag{3.3.36}$$

and we consider that initially the system is in a pure state described by the density matrix $\rho_i(0)$:

$$\rho_i(0) = \frac{1}{2}(\mathbb{1}_2 + \boldsymbol{a} \cdot \boldsymbol{\sigma}), \tag{3.3.37}$$

where $\mathbb{1}_2$ is the identity matrix in $\mathbb{C}^2$ and

$$\boldsymbol{a} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta) \tag{3.3.38}$$

is the unit Bloch vector representing the pure state. We will calculate the geometric phase using 3.3.32 for the following cases: unitary evolution, evolution characterized by dephasing, evolution associated to bit-flip and phase-flip. For each case, we present the Lindblad equation (equation 3.1.8), the dynamical phase given by equation 3.3.34, the total phase given by equation 3.3.32, the geometrical phase given by the difference between the previous phase factors, the expression for the Bloch vector and the graphical representation of the respective evolution on the Bloch sphere. For all cases, we consider that the system is in a general superposition of the eigenstates of the Hamiltonian determined by the Bloch vector

$$\boldsymbol{a}(0) = (\sin\theta_0\cos\varphi_0, \sin\theta_0\sin\varphi_0, \cos\theta_0), \tag{3.3.39}$$

where θ_0 and φ_0 are angles on the Bloch sphere.

Unitary evolution In the case of unitary evolution, we consider $\Gamma_n = 0$ for all n. The operator $S(t)$ is given by

$$\begin{aligned} S(t) &= e^{-i\frac{\omega t}{2}\sigma_3 t} \\ &= \cos\left(\frac{\omega t}{2}\right)\mathbb{1}_2 - i\sin\left(\frac{\omega}{2}\right)\sigma_3, \end{aligned}$$

and the evolution of the density matrix ρ is simply given by

$$\dot{\rho}(t) = -i\frac{\omega}{2}[\sigma_3, \rho(t)].$$

Using equation 3.3.37, we obtain the Bloch vector $\boldsymbol{a}(t)$:

$$\mathbf{a}(t) = (\sin\theta_0\cos(\varphi_0 + \omega t), \sin\theta_0\sin(\varphi_0 + \omega t), \cos\theta_0),$$

where θ_0 and φ_0 are constants determined by the initial state of the system (equation 3.3.39. The dynamical phase α_{dyn} is given by

$$\alpha_{dyn}(t) = -\frac{\omega}{2}t\cos\theta_0, \tag{3.3.40}$$

and the total phase is

$$\phi_{total}(t) = \arctan\left[-\tan\left(\frac{\omega t}{2}\right)\cos\theta_0\right]. \tag{3.3.41}$$

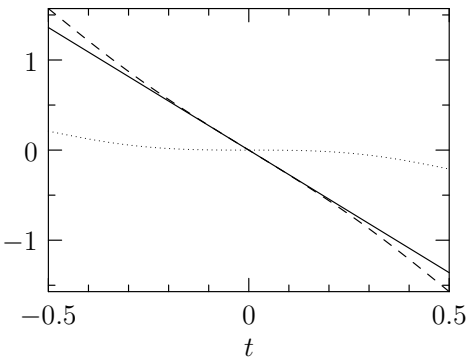
Figure 3.2a shows the values of the phase factors for a system with $\omega = 1.0$. Figure 3.2b shows the evolution of the Bloch vector. As expected, for $t = t_\omega = 2\pi/\omega$ the usual Berry's phase (equation 2.4.9) is recovered, since the evolution considered is unitary.

Dephasing Dephasing is one of the processes of decoherence and is characterized by the decaying of the off-diagonal terms of the density matrix that represents the physical system. In our case, a two-level quantum system, the decoherence is represented by the operator Γ_3:

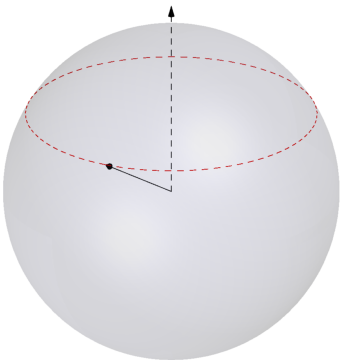
$$\Gamma_3 = \sqrt{\gamma}\sigma_3, \tag{3.3.42}$$

where γ is the dephasing rate. The corresponding Lindblad equation for the density matrix $\rho(t)$ is

$$\dot{\rho}(t) = -i\frac{\omega}{2}[\sigma_3, \rho(t)] + \gamma(\sigma_3\rho(t)\sigma_3 - \rho(t)). \tag{3.3.43}$$



(a) Phase factors.



(b) Evolution of the Bloch vector.

Figure 3.2: Figure 3.2a presents values of the dynamical phase α_{dyn} (full line), total phase ϕ_{tot} (dashed line) and geometric phase γ_{geo} (dotted line) for a two-level system described by the Hamiltonian in 3.3.36 (with $\omega = 1.0$) as a function of time (measured in units of $t_\omega = 2\pi/\omega$). Figure 3.2b shows the evolution of the Bloch vector on the Bloch sphere.

The corresponding Bloch vector $\boldsymbol{a}(t)$ is

$$\mathbf{a}(t) = (e^{-2\gamma t}\sin\theta_0\cos(\varphi_0+\omega t), e^{-2\gamma t}\sin\theta_0\sin(\varphi_0+\omega t), \cos\theta_0),$$

where θ_0 and φ_0 are constants determined by the initial state of the system (equation 3.3.39. We note that the Bloch vector for a system undergoing dephasing is the same as the one for a system evolving unitarily with a phase factor on the first and second coordinates, as can be seen in Figure 3.3.. Because Γ_3 is proportional to the Hamiltonian (equation 3.3.36, the total, dynamical and geometrical phases are the same as for the unitary evolution (equations 3.3.40 and 3.3.41).

Bit-flip In the context of quantum computation and information, an important operation is the bit-flip, a process that flips the states of the computational basis. This process is characterized by the operator Γ_1:

$$\Gamma_1 = \sqrt{\alpha}\sigma_1, \tag{3.3.44}$$

where α is a real constant. The corresponding Lindblad equation for the density matrix is

$$\dot{\rho}(t) = -i\frac{\omega}{2}[\sigma_3, \rho(t)] + \alpha(\sigma_1\rho(t)\sigma_1 - \rho(t)). \tag{3.3.45}$$

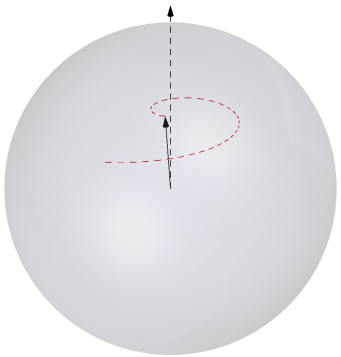


Figure 3.3: Graphical representation of the evolution of the Bloch vector on the Bloch sphere undergoing a dephasing process.

The Bloch vector associated with the solution of equation 3.3.45 is

$$
\begin{aligned}
a_x(t) &= \frac{\alpha}{\omega} e^{-\alpha t} \left\{ \left(A + B \left(\sqrt{\frac{\omega^2}{\alpha^2} - 1} \right) \right) \cos \left[\alpha \left(\sqrt{\frac{\omega^2}{\alpha^2} - 1} \right) t \right] \right. \\
&\quad \left. + \left(B - A \left(\sqrt{\frac{\omega^2}{\alpha^2} - 1} \right) \right) \sin \left[\alpha \left(\sqrt{\frac{\omega^2}{\alpha^2} - 1} \right) t \right] \right\}, \\
a_y(t) &= e^{-\alpha t} \left\{ A \cos \left[\alpha \left(\sqrt{\frac{\omega^2}{\alpha^2} - 1} \right) t \right] + B \sin \left[\alpha \left(\sqrt{\frac{\omega^2}{\alpha^2} - 1} \right) t \right] \right\}, \\
a_z(t) &= e^{-2\alpha t} \cos \theta_0,
\end{aligned}
$$

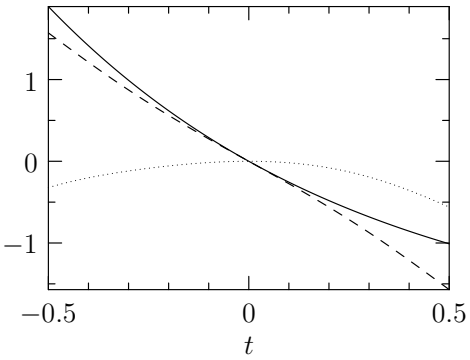
where $A = \sin\theta_0 \sin\varphi_0$ and $B = \sin\theta_0 \left(\frac{\omega^2}{\alpha^2} - 1 \right)^{-2} \left(\frac{\omega}{\alpha} \cos\varphi_0 - \sin\varphi_0 \right)$ are constants determined by the initial conditions of the system. The dynamical phase α_{dyn} is

$$
\alpha_{dyn}(t) = -\frac{\omega}{4\alpha} \cos\theta_0 (1 - e^{-2\alpha t}), \tag{3.3.46}
$$

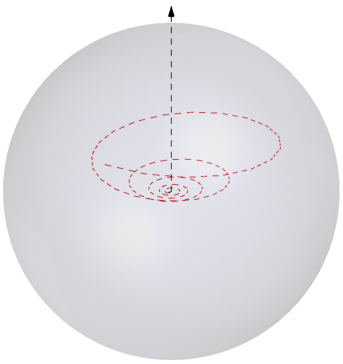
and the total phase ϕ_{tot}

$$
\phi_{total}(t) = \arctan \left[-\tan \left(\frac{\omega t}{2} \right) \cos\theta_0 \right]. \tag{3.3.47}
$$

Figure 3.4a shows the values of the phase factors for a system with $\omega = 1.0$ and $\alpha = 0.1$. As we can see from Figure 3.4b, the introduction of the bit-flip as an interaction of the system with the environment result in a decrease on the norm of the Bloch vector.



(a) Phase factors.



(b) Evolution of the Bloch vector.

Figure 3.4: Figure 3.4a presents values of the dynamical phase α_{dyn} (full line), total phase ϕ_{tot} (dashed line) and geometric phase γ_{geo} (dotted line) for a two-level system described by the Hamiltonian in 3.3.36 (with $\omega = 1.0$) and affected by the process of bit-flip characterized by Γ_1 (equation 3.3.48). The time is measured in units of $t_\omega = 2\pi/\omega$. Figure 3.4b shows the evolution of the Bloch vector on the Bloch sphere.

Decay The process of decaying is characterized by the operator

$$\Gamma_- = \sqrt{\lambda}\sigma_-, \tag{3.3.48}$$

where λ is a real constant. The corresponding Lindblad equation for the density matrix is

$$\dot{\rho}(t) = -\frac{1}{2}(i\omega + \lambda)[\sigma_3, \rho(t)] + \frac{\lambda}{2}(2\sigma_-\rho(t)\sigma_+ - \rho(t)), \tag{3.3.49}$$

and the correspondent Bloch vector is

$$\begin{aligned}\mathbf{a}(t) = \Big(&e^{-\frac{\lambda}{2}t}\sin\theta_0\cos(\varphi_0 + \omega t), e^{-\frac{\lambda}{2}t}\sin\theta_0\sin(\varphi_0 + \omega t),\\ &e^{-\lambda t}(1 + \cos\theta_0) - 1\Big),\end{aligned} \tag{3.3.50}$$

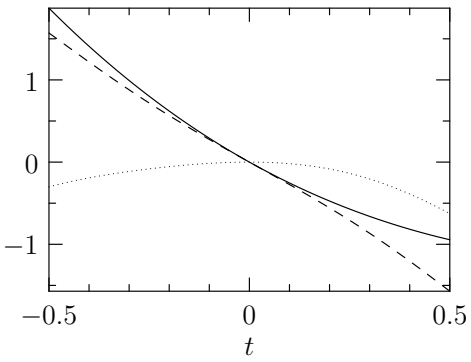
where θ_0 and φ_0 determine the initial state of the system (equation 3.3.39). The dynamical phase α_{dyn} is given by

$$\alpha_{dyn}(t) = -\frac{\omega}{2}\left(\frac{1}{\lambda}(1 + \cos\theta_0)(1 - e^{-\lambda t}) - t\right), \tag{3.3.51}$$

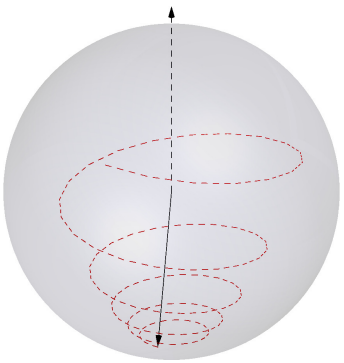
and the total phase ϕ_{tot} is given by

$$\phi_{total}(t) = -\arctan\left[\tan\left(\frac{\omega t}{2}\right)\frac{\sinh\left(\frac{\lambda t}{4}\right) - \cos\theta_0\cosh\left(\frac{\lambda t}{4}\right)}{\cosh\left(\frac{\lambda t}{4}\right) - \cos\theta_0\sinh\left(\frac{\lambda t}{4}\right)}\right]. \tag{3.3.52}$$

Figure 3.5a shows the values of the phase factors for a system with $\omega = 1.0$ and $\lambda = 0.2$. As we can see from Figure 3.5b, this interaction with the environment not only decreases the norm of the Bloch vector, but also takes an arbitrary state and to the state $|1\rangle$ (the eigenstate of Hamiltonian 3.3.36 with negative eigenvalue).



(a) Phase factors.



(b) Evolution of the Bloch vector.

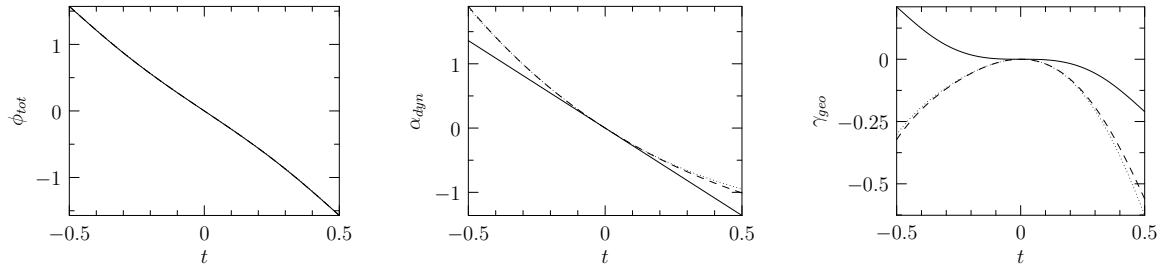
Figure 3.5: Figure 3.5a presents values of the dynamical phase α_{dyn} (full line), total phase ϕ_{tot} (dashed line) and geometric phase γ_{geo} (dotted line) for a two-level system described by the Hamiltonian in 3.3.36 (with $\omega = 1.0$) and affected by the process of bit-flip characterized by Γ_- (equation 3.3.48). The time is measured in units of $t_\omega = 2\pi/\omega$. Figure 3.5b shows the evolution of the Bloch vector on the Bloch sphere.

Figure 3.6 phase factors for the previously considered interactions of the system with the environment. We note that the total phase is almost unaffected by the interactions and the geometric phase for the bit-flip and the decaying present similar behaviors.

3.4 The Quantum Jump Approach

Firstly conceived in the context of quantum optics, the Quantum Jump Approach (QJA)[11] has been used to obtain an expression for geometric phases of open quantum systems [22] [21]. The main feature of QJA is to describe the state of the system via wave functions instead of density operators.

[11] The Quantum Jump Approach also appears in the literature as quantum trajectory method or Monte Carlo wave function method.



(a) Total phase. (b) Dynamical phase. (c) Geometric phase.

Figure 3.6: Plots of the phase factors for an initial state given by the Bloch vector 3.3.39, with dynamics given by 3.3.36 (with $\omega = 1.0$) and different interactions with the environment. The time is presented in units of $t_\omega = 2\pi/\omega$. The full line is associated with the unitary evolution of the system. The dashed line represents the phase factors for a system subjected to bit-flip interactions ($\Gamma_1 = \sqrt{\alpha}\sigma_1$ and $\alpha = 0.1$). The dotted line is associated with the decaying process ($\Gamma_- = \sqrt{\lambda}\sigma_-$ with $\lambda = 0.2$).

An illustration of the method is the following: consider an atom (open quantum system) interacting with a radiation field (environment). Suppose we perform measurements in the environment by detecting photons. When there is an electronic transition[12] in the atom, a photon is detected. Therefore, a change in the wave function representing the state of the atom occurs. The knowledge of the wave function of the system and its changes is due to the detections of such jumps as well as the detection of no jumps. Considering that the environment is monitored in rapid time intervals, the dynamics of the system is recovered by summing over all possible outcomes of the measurement process. In [54] Plenio and Knight present a thorough description of QJA and its applications in a number of problems in quantum optics.

Coarse graining of the evolution

Let us consider a system with an associated Hilbert space $\mathcal{H}$ that undergoes a non-unitary evolution described by the master equation 3.1.9

$$\frac{d}{dt}\rho(t) = \mathscr{L}(\rho(t)),$$

We consider that the total evolution time of the system is T. If we divide it in N equal intervals, we have $\Delta t = \frac{T}{N}$. The dynamics of the system is given by a

[12] When an electron "jumps"from one energy level to another, hence the name: quantum jump approach.

completely positive map, hence, from 3.1.6 we can write

$$\rho(t_{m+1}) = \sum_{k=0}^{N} W_k(\Delta t)\rho(t_m)W_k^*(\Delta t), \tag{3.4.1}$$

where $t_m = m\Delta t$. When $N \to \infty$ and $\Delta t \to 0$ in a way that $T = N\Delta t$ remains constant we get

$$\rho(T) = \lim_{\substack{N\to\infty \\ \Delta t\to 0}} \left(\sum_{k=0}^{N} W_k(\Delta t)\rho(t_0)W_k^*(\Delta t) \right)^N. \tag{3.4.2}$$

We can think that at each time interval Δt the system suffers a measurement process represented by the action of a Kraus operator W_k, where W_0 and $W_k(k \neq 0)$ are called "no-jump" and jump operators, respectively. To recover $\rho(t)$ we sum incoherently over all the possible processes.

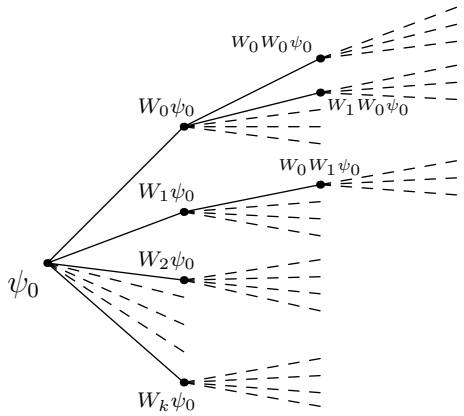


Figure 3.7: Possible trajectories for a system with initial state ψ_0. Each Kraus operator W_k indicates a different outcome of a measurement process.

In particular, if the initial state is a pure state, $\rho(0) = |\psi_0\rangle\langle\psi_0|$, after a time interval Δt the probability of $\rho(\Delta t)$ being $\rho(\Delta t) = W_k\rho(0)W_k^*$ is $\mathrm{tr}(W_k\rho(0)W_k^*)$, that is, $\psi(\Delta t) = W_k(\Delta t)\psi(0) = W_k(\Delta t)\psi_0$. The Figure 3.7 represents some possible trajectories of such a system. So after a time interval $t_m = m\Delta t$, the corresponding state vector for a particular trajectory i is given by

$$\psi^i(t_m) = \prod_{l=1}^{m} W_{i(l)}(\Delta t)\psi_0, \tag{3.4.3}$$

where $W_{i(l)}$ is the Kraus operator correspondent to the l-th step of the trajectory i. If the system is in a pure state, then at each step of every trajectory, it will

remain a pure state. i. So a trajectory i is represented by a sequence of pure states $\{\psi(t_0), \psi(t_1), \psi(t_2), \ldots, \psi(t_N)\}$. To recover the dynamics given by 3.1.9 we sum over all possible trajectories. Since we are dealing with pure states, we can use the Pancharatnam formula 2.1.9 to obtain the geometric phase for a given trajectory i

$$\begin{aligned}\gamma_i = -\arg\{&\langle\psi(0), \psi(t_1)\rangle\langle\psi(t_1), \psi(t_2)\rangle \ldots \\ &\langle\psi(t_{N-1}), \psi(t_N)\rangle\langle\psi(t_N), \psi(0)\rangle\}. \end{aligned} \tag{3.4.4}$$

To illustrate this situation, let us consider an atom interacting with the normal modes of an electromagnetic field. The photons emitted by the atom can be measured and each Kraus operator W_k is related to a different outcome of the measurement process, in this case, the measurement is the number of photons emitted due to the quantum jumps of the electron within the energy levels of the atom. A trajectory i_0 with N steps and without any photons detected and with initial state ψ_0 is represented as a chain of pure states of the form

$$i_0 : (\psi_0, W_0\psi_0, W_0W_0\psi_0, \ldots, (W_0)^N\psi_0) \tag{3.4.5}$$

For the trajectory above, the state vector $\psi_m^{i_0}(t)$ at a time $t = m\Delta t$ is given by

$$\begin{aligned}\psi_m^{i_0}(t) &= (W_0(\Delta t))^m\psi_0 \\ &= (W_0(\Delta t))^{(t/\Delta t)}\psi_0 \\ &= (\exp(-i\tilde{H}\Delta t))^{(t/\Delta t)}\psi_0 \\ &= \exp(-i\tilde{H}t)\psi_0.\end{aligned}$$

From the expression above, we can say that the dynamics of the vector state in the "no-jump" trajectory is determined by the effective Hamiltonian $\tilde{H}$:

$$i\frac{d}{dt}\psi^{i_0}(t) = \tilde{H}(t)\psi^{i_0}(t), \tag{3.4.6}$$

with initial condition $\psi^{i_0}(0) = \psi_0$. Using 3.4.4 we obtain the following geometric phase for the trajectory i_0

$$\gamma_{i_0} = -\mathfrak{Im}\int_0^T \frac{\langle\psi_{i_0}(t), \frac{d}{dt}\psi_{i_0}(t)\rangle}{\langle\psi_{i_0}(t), \psi_{i_0}(t)\rangle}dt - \arg\langle\psi_{i_0}(T), \psi_{i_0}(0)\rangle,$$

substituting 3.4.6 in the expression above we get

$$\gamma_{i_0} = -\mathfrak{Im}\int_0^T \frac{\langle\psi_{i_0}(t), H(t)\psi_{i_0}(t)\rangle}{\langle\psi_{i_0}(t), \psi_{i_0}(t)\rangle}dt - \arg\langle\psi_{i_0}(T), \psi_{i_0}(0)\rangle. \tag{3.4.7}$$

Clearly the first term on the right is opposite of the well known dynamical phase and the second one the phase difference between the final and initial state. Hence, the geometric phase for a "no-jump" trajectory is the difference between the total phase difference and the dynamic phase, as expected.

Now let us consider a trajectory in which a jump associated to a Kraus operator W_k occurs at an arbitrary time t_1 as represented in Figure 3.8. We denote by $\psi'(t)$ and $\psi''(t)$ the state vectors before and after the jump, respectively. Up to the instant

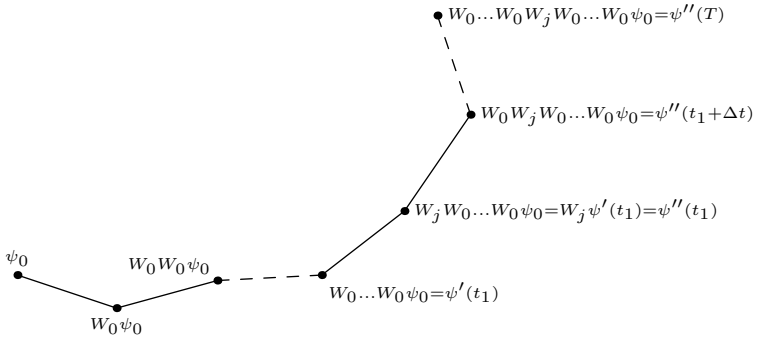


Figure 3.8: Representation of a trajectory in which a jump associated to the Kraus operator W_j occurs at a time t_1. The state vectors before and after the jump are represented by $\psi'(t)$ and $\psi''(t)$, respectively.

in which the jump occurs, the dynamics of the state vector is given by 3.4.6. After the jump, we have a new "no-jump" trajectory but with a new initial condition. Hence, we can write the dynamics of the state vectors before and after the jump as

$$i\frac{d}{dt}\psi'(t) = \tilde{H}(t)\psi'(t), \quad \psi'(0) = \psi_0, \tag{3.4.8}$$

$$i\frac{d}{dt}\psi''(t) = \tilde{H}(t)\psi''(t), \quad \psi''(t_1) = W_j(\Delta t)\psi'(t_1). \tag{3.4.9}$$

From the continuous limit of 3.4.4 for the evolution above, the geometric phase for the trajectory with one jump is given by

$$\begin{aligned}\gamma_{i_1} = &-\mathfrak{Im}\int_0^{t_1}\frac{\langle\psi'(t),\tilde{H}(t)\psi'(t)t\rangle}{\langle\psi'(t),\psi'(t)\rangle}dt - \arg\langle\psi'(t_1),\Gamma_j\psi'(t_1)\rangle \\ &-\mathfrak{Im}\int_{t_1}^{T}\frac{\langle\psi''(t),\tilde{H}(t)\psi''(t)t\rangle}{\langle\psi''(t),\psi''(t)\rangle}dt - \arg\langle\psi''(T),\psi'(0)\rangle\end{aligned} \tag{3.4.10}$$

For a trajectory with more jumps, we can generalize the above argument to obtain the respective dynamics and geometric phase.

Example: two-level quantum system

Once more we consider a two-level quantum system with dynamics given by the Hamiltonian

$$H = \frac{\omega}{2}\sigma_3. \tag{3.4.11}$$

Consider that the system is initially in the state given by

$$\psi(0) = \cos\left(\frac{\theta}{2}\right)\psi_- + e^{i\phi}\sin\left(\frac{\theta}{2}\right)\psi_+, \tag{3.4.12}$$

where $\psi_\pm$ are the eigenvectors of $\frac{\sigma_3}{2}$ and θ and ϕ are the spherical coordinates in the Bloch sphere (Definition 2.4.1).Following [22] we consider three models of interaction between the system and the environment: evolution given by a dephasing Lindblad operator with no jumps, with one jump and an evolution characterized by decaying.

Decoherence is an effect of the interaction between an open quantum system and the environment. There are many kinds of decoherence processes, but one in particular is the dephasing, in which the interference pattern is destroyed but the energy of the system is conserved. Therefore, the operators $\mathscr{L}^{deph}$ that characterize this process must satisfy

$$[\mathscr{L}^{deph}, H] = 0 \implies [\Gamma_k, H] = 0. \tag{3.4.13}$$

We consider an evolution from $t = 0$ to $T = \frac{2\pi}{\omega}$. The geometric phases and the interpretation in terms of the evolution of the Bloch vector for for the three cases are the following.

(a) *Dephasing Lindblad operators: no jumps*

We consider that the non-unitarity is given by a Lindblad operator with

$$\begin{aligned} \Gamma_1 &= \lambda\sigma_3, \\ \Gamma_k &= 0, \quad k \neq 0 \end{aligned} \tag{3.4.14}$$

The corresponding effective Hamiltonian is

$$\tilde{H}(t) = \frac{\omega}{2}\sigma_3 - \frac{i}{2}\mathbb{1}, \tag{3.4.15}$$

With 3.4.6 we can calculate the state vector $\psi_{i_0}(t)$ for this evolution:

$$\psi_{i_0}(t) = \cos\left(\frac{\theta}{2}\right) e^{-\frac{i}{2}(\omega - i|\lambda|^2)}\psi_- + e^{i\phi}\sin\left(\frac{\theta}{2}\right) e^{\frac{i}{2}(\omega + i|\lambda|^2)}\psi_+, \tag{3.4.16}$$

Then the geometric phase γ_{i_0} is obtained through 3.4.7:

$$\gamma_{i_0} = \pi(\cos\theta - 1), \tag{3.4.17}$$

which is precisely the geometric phase for an unitary evolution (calculated through Berry's and Aharonov and Anandan's definition). In this case, the Bloch vector simply traces out a curve on the Bloch sphere with a fixed azimuthal angle θ.

(b) *Dephasing Lindblad operators: one jump*
Now we consider the same evolution but with the occurrence of a jump at an instant of time t_1. The state vector after the jump is given by 3.4.9 in which the Kraus operator, according to 3.1.17, is

$$W_1 = \sqrt{\Delta t}\Gamma_1 = \sqrt{\Delta t}\lambda\sigma_3,$$

and the state vector $\psi''(t)$ is

$$\psi''(t) = \lambda\sqrt{\Delta t}\cos\left(\frac{\theta}{2}\right) e^{-\frac{i}{2}(\omega - i|\lambda|^2)}\psi_- + \lambda\sqrt{\Delta t}e^{i\phi}\sin\left(\frac{\theta}{2}\right) e^{\frac{i}{2}(\omega + i|\lambda|^2)}\psi_+, \tag{3.4.18}$$

and the geometric phase can be obtained through 3.4.10

$$\gamma_{i_1} = \pi(\cos\theta - 1). \tag{3.4.19}$$

It is possible to demonstrate that for any finite number of jumps, the geometric phase will be robust against dephasing. The Bloch vector related to this evolution traces a curve on the Bloch sphere with a fixed azimuthal angle, in the instant for which the jump occurs, the Bloch vector is flipped and then continues to trace such a curve. In the context of quantum information, this source of decoherence is called *phase flip*. The geometric phase can be interpreted as the area enclosed by the curved traced by the evolution of the Bloch vector is the same as the unitary case.

(c) *Decaying: no jumps*
Now we consider the following operators as source of decoherence

$$\Gamma_1 = \lambda\sigma_3, \tag{3.4.20}$$

$$\Gamma_2 = \alpha\sigma_-, \quad \sigma_- := \frac{1}{2}(\sigma_1 - i\sigma_2) \tag{3.4.21}$$

$$\Gamma_k = 0, \quad k \neq 1 \text{ or } k \neq 2. \tag{3.4.22}$$

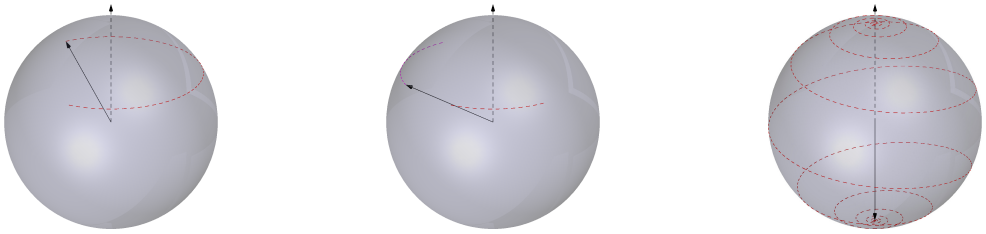
The corresponding state vector is given by 3.4.6:

$$\begin{aligned}\psi(t) = \lambda\sqrt{\Delta t}\cos\left(\frac{\theta}{2}\right) e^{-\frac{i}{2}(\omega - i|\lambda|^2) - i|\alpha|^2}\psi_- \\ + \lambda\sqrt{\Delta t}e^{i\phi}\sin\left(\frac{\theta}{2}\right) e^{\frac{i}{2}(\omega + i|\lambda|^2) + i|\alpha|^2}\psi_+,\end{aligned} \tag{3.4.23}$$

and the geometric phase given by 3.4.7

$$\gamma = \pi(\cos\theta - 1) + \frac{|\alpha|^2}{\omega}\pi^2\sin^2\theta + \mathcal{O}\left(\frac{|\alpha|^4}{\omega^2}\right). \tag{3.4.24}$$

As we can see from the Figure 3.9c, this kind of evolution causes a decaying of the state vector.



(a) Phase-flip: no jumps. (b) *Phase-flip: one jump.* (c) *Decaying.*

Figure 3.9: Representation of the evolution if a two-level quantum system subjected to different interactions with the environment. The dotted line represents the evolution of the Bloch vector. Figure 3.9a represents the unitary evolution or an evolution with no jumps given by a dephasing Lindblad operator. Figure 3.9b represents the evolution of the system when the interaction is given by a dephasing Lindblad operator ($\Gamma \propto \sigma_3$). Figure 3.9c represents the evolution of the system with a decoherence source that causes decaying of the state ($\Gamma \propto \sigma_-$).

Chapter 4

Two-level quantum systems

The previous chapters featured some examples of two-level quantum systems. Not only because the concepts presented have a straightforward application in such systems, but also because many applications of Quantum Mechanics involve systems that can be treated as a two-level system. Examples of two-level systems include spin-half particles, photon polarization, the path of a photon through a beam splitter and the transition of an atom between an excited state and the ground state. Two-level systems are of great importance in the field of quantum computation and information, since the unit of information of a quantum computer — the qubit— is, in fact, a two-level system.

Two-level systems are the simplest quantum systems to study, since its corresponding Hilbert Space is two-dimensional and for a large collection of systems its properties can be obtained analytically. Understanding which model is being used, the resulting evolution and its restraints is crucial when it comes to the physical realization of such systems.

In the following sections, we review the formalism of two-level quantum systems. Next, we address the widely used Rotating Wave Approximation (RWA), its limitations and, as obtained by [29], we derive the expression for the geometric phase for the case in which the RWA is valid. Lastly, we make a brief overview of the method described in [9] and [10] and we use it to compute the total, dynamic and geometric phases for a two-level system and two two-level systems.

4.1 A brief overview of the formalism of two-level quantum systems

As seen in Section 2.4, the geometrical representation of a two-level quantum system is the Bloch sphere and its state can be expressed by the density operator ρ (equation 2.4.4):

$$\rho = \frac{1}{2}(\mathbb{1}_2 + \boldsymbol{a} \cdot \boldsymbol{\sigma}),$$

where $\boldsymbol{a} \in \mathbb{R}^3$ is the Bloch vector and $\boldsymbol{\sigma}$ is the three-vector of Pauli matrices. In the same direction, a general Hamiltonian of the system can be written as

$$H = \frac{1}{2}(\Omega_0 \mathbb{1} + \boldsymbol{\Omega} \cdot \boldsymbol{\sigma}), \tag{4.1.1}$$

where $\Omega_0 \in \mathbb{R}$ and $\boldsymbol{\Omega}$ is called Rabi vector. The evolution of a density operator for a closed system is given by

$$\frac{d}{dt}\rho(t) = -i[H, \rho(t)].$$

Using the expressions for the density operator 2.4.4 and for the Hamiltonian 4.1.1 in the expression above we get

$$\begin{aligned} \frac{1}{2}\dot{\boldsymbol{a}} \cdot \boldsymbol{\sigma} &= -i\left[\frac{1}{2}(\Omega_0 \mathbb{1} + \boldsymbol{\Omega} \cdot \boldsymbol{\sigma}), \frac{1}{2}(\mathbb{1} + \boldsymbol{a} \cdot \boldsymbol{\sigma})\right] \\ \dot{\boldsymbol{a}} \cdot \boldsymbol{\sigma} &= -\frac{i}{2}[\boldsymbol{\Omega} \cdot \boldsymbol{\sigma}, \boldsymbol{a} \cdot \boldsymbol{\sigma}], \end{aligned}$$

where the dot stands for time derivation. Now we use the identity

$$(\boldsymbol{A} \cdot \boldsymbol{\sigma})(\boldsymbol{B} \cdot \boldsymbol{\sigma}) = (\boldsymbol{A} \cdot \boldsymbol{B})\mathbb{1} + i(\boldsymbol{A} \times \boldsymbol{B}) \cdot \boldsymbol{\sigma},$$

and we obtain

$$\frac{d}{dt}\boldsymbol{a} = \boldsymbol{\Omega} \times \boldsymbol{a}. \tag{4.1.2}$$

The geometric interpretation of this equation is that the Bloch vector $\boldsymbol{a}$ revolves around $\boldsymbol{\Omega}$ with an angular frequency $|\boldsymbol{\Omega}|$. Its classical analogue is the Larmor precession, a phenomenon exhibited by any object with a magnetic moment subjected to an external magnetic field [39]. This observation follows from [32] and was later explored in [9], [8] and [10].

4.2 Rotating Wave Approximation

The Hamiltonian of a two-level quantum system (equation 4.1.1) has numerous expressions, depending on the physical system it represents. But among this infinity of systems, the oscillatory driven two-level quantum system is of great relevance. Its properties were investigated in the early years of Quantum Mechanics by I. I. Rabi [56]. In this work, Rabi obtained the probability that an atom subjected to a rotating magnetic field undergoes a transition from one of its states to the other. Rabi's "flopping formula", as it became known, had immediate applications in the fields of quantum optics, magnetic resonance and, recently, in quantum computing.

Although a two-level system is a simple system, there are many situations in which its equations of motion have no simple or even analytical solutions. In particular, the case of an oscillatory driven two-level system has been treated by various methods, from which we can mention the rotating wave approximation, widely used in quantum optics, the method of averaging [11] and a method developed in [9] and [10] that gives an exact solution through perturbative expansions. In this section we will give an overview of the rotating wave approximation and we will use it to obtain the geometric phase for a two-level quantum system and two two-level quantum systems.

The underlying physical idea of the rotating wave approximation, in simple terms, is that the oscillation can be decomposed into two parts: one which will be near the resonance frequency of the system and the other, antiresonant. The approximation is to neglect the so called antiresonant terms. It will become clear what this means in the derivation of the equations of motion using the rotating wave approximation.

Neglecting the antiresonant terms has consequences. Bloch and Siegert [13] were the first to present some considerations about the theoretical effects of the rotating wave approximation, Stevenson [70] followed. Both works point that the resonance curve of the system presents a shift. In this direction, Silverman [62] developed a method that demonstrates that, not only the resonance curve is shifted, but also for the case of decaying states, the difference in level decay rates also changes. The validity and applicability of the rotating wave approximation has been studied in depth by many authors. We can mention the study carried out in [33] in the context of open quantum systems, the review in [34], the study of the limitations of RWA for many-level quantum systems in [16] and for non-adiabatic evolution in [68].

Derivation

We consider a quantum system with the following Hamiltonian:

$$H_0 = \frac{\omega_0}{2}\sigma_3, \tag{4.2.1}$$

where ω_0 is the transition frequency of the system. Now we consider the system interacting with a periodic field. The component of the Hamiltonian that models this interaction can be written, without loss of generality, as:

$$V(t) = V_0 \cos(\omega t + \phi)\sigma_1, \tag{4.2.2}$$

where V_0 and ω are the amplitude and the frequency of the interaction, respectively, and ϕ is a phase factor. So, the total Hamiltonian of the system is

$$\begin{aligned} H(t) &= H_0 + V(t) \\ &= \frac{1}{2}\begin{pmatrix} \omega_0 & 2V_0\cos(\omega t+\phi) \\ 2V_0\cos(\omega t+\phi) & -\omega_0 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} \omega_0 & V_0(e^{i(\omega t+\phi)} + e^{-i(\omega t+\phi)}) \\ V_0(e^{i(\omega t+\phi)} + e^{-i(\omega t+\phi)}) & -\omega_0 \end{pmatrix} \end{aligned} \tag{4.2.3}$$

At this point, we transform the above Hamiltonian to the interaction representation characterized by the transformation

$$\psi = U_0(t)\psi_I, \tag{4.2.4}$$

where $U_0(t) = e^{iH_0 t}$ is the usual evolution operator of the unperturbed Hamiltonian and ψ_I is the state vector in the interaction representation. The interaction Hamiltonian is obtained through the following transformation

$$H_I(t) = U_0^*(t)H(t)U_0(t). \tag{4.2.5}$$

Applying this transformation to the Hamiltonian 4.2.3, we get

$$H_I(t) = \frac{1}{2}\begin{pmatrix} \omega_0 & V_0(e^{i(\tilde{\omega}' t+\phi)} + e^{-i(\omega' t+\phi)}) \\ V_0(e^{-i(\tilde{\omega}' t+\phi)} + e^{i(\omega' t+\phi)}) & -\omega_0 \end{pmatrix}, \tag{4.2.6}$$

where $\omega' = \omega - \omega_0$ and $\tilde{\omega}' = \omega + \omega_0$. The off-diagonal matrix elements presents phase factors proportional to ω' and $\tilde{\omega}'$. The rotating wave approximation (RWA)

consists on neglecting the terms proportional to $\tilde{\omega}'$ and the justification is that, for situations near the resonance, i.e., $\omega \approx \omega_0$, the factor proportional to $\tilde{\omega}'$, sometimes referred to as the counter-rotating term, varies much more rapidly than any changes of the system. Hence, they will average to zero in the time scale of the system and, therefore, can be neglected. Upon taking the approximation, the Hamiltonian in the original representation is reduced to

$$H(t) = \frac{1}{2}\begin{pmatrix} \omega_0 & V_0 e^{-i(\omega t+\phi)} \\ V_0 e^{i(\omega t+\phi)} & -\omega_0 \end{pmatrix}. \tag{4.2.7}$$

The system evolving according to the Hamiltonian 4.2.7 obeys the Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H(t)\psi(t).$$

To solve this equation, we apply the transformation given by

$$\psi_R(t) = R_z(\omega t + \phi)\psi(t), \tag{4.2.8}$$

where $R_z(\omega t)$ is the rotation around the z-axis by ωt. In other words, we are considering the evolution of the system in a frame that rotates with frequency ω around the z-axis. The Schrödinger equation becomes

$$i\frac{d}{dt}\psi_R(t) = \frac{1}{2}\begin{pmatrix} \omega_0 - \omega & V_0 \\ V_0 & -\omega_0 + \omega \end{pmatrix}\psi_R(t). \tag{4.2.9}$$

Using the relation 4.1.1 and the Hamiltonian in the rotating frame 4.2.9, the expression of the Rabi vector for the system is

$$\mathbf{\Omega}_R = (V_0\cos(\phi),\ V_0\sin(\phi),\ \omega_0 - \omega), \tag{4.2.10}$$

where the subscript R indicates that the expression is valid for the rotating frame. The solution for the equation 4.2.9 is given by the state vector $\psi(t)$, rotating back to the original frame, i.e., applying the rotation $\psi(t) = R_z^*(\omega t + \phi)\psi_R(t)$, and considering the initial condition $\psi(0) = |0\rangle$, the state vector in the original frame is

$$\begin{aligned}\psi(t) = e^{-\frac{i}{2}(\omega t+\phi)}&\left(\cos\left(\frac{\Omega_R t}{2}\right) - i\frac{\Delta\omega}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)\right)|0\rangle \\ &- i\frac{V_0}{\Omega_R}e^{\frac{i}{2}(\omega t+\phi)}\sin\left(\frac{\Omega_R t}{2}\right)|1\rangle\end{aligned} \tag{4.2.11}$$

where $\Omega_R = |\mathbf{\Omega}_R|$. Since the system is closed, the density matrix is simply given by $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$. Using the expression 2.4.4 for the density operator of a two-level quantum system and the solution 4.2.11 for the state vector considering the rotating wave approximation, the corresponding expression for the Bloch vector $\boldsymbol{a}(t) = (a_x(t), a_y(t), a_z(t))$ is

$$a_x(t) = \frac{2V_0}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)\left[\cos\left(\frac{\Omega_R t}{2}\right)\sin(\omega t+\phi) + \frac{\Delta\omega}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)\cos(\omega t+\phi)\right], \tag{4.2.12}$$

$$a_y(t) = -\frac{2V_0}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)\left[\cos\left(\frac{\Omega_R t}{2}\right)\cos(\omega t+\phi) - \frac{\Delta\omega}{\Omega_R}\sin\left(\frac{\Omega_R t}{2}\right)\sin(\omega t+\phi)\right], \tag{4.2.13}$$

$$a_z(t) = 1 - \frac{2V_0^2}{\Omega_R^2}\sin^2\left(\frac{\Omega_R t}{2}\right). \tag{4.2.14}$$

The evolution of the Bloch vector with coordinates given by 4.2.12, 4.2.13 and 4.2.14 is graphically represented in Figure 4.1. We note that $\Delta\omega = \omega_0 - \omega$ must be sufficiently small, since the rotating wave approximation is valid for near resonant regions.

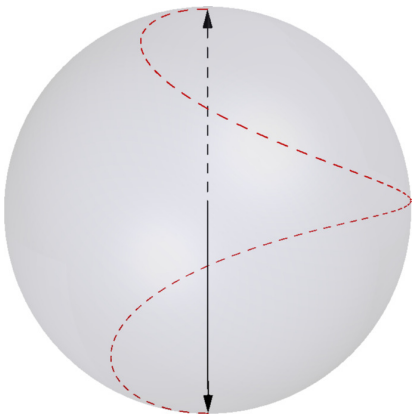


Figure 4.1: Graphical representation of the evolution of the Bloch vector (indicated by the arrow) initially aligned with the z-axis. The trajectory of the Bloch vector considering the RWA is indicated by the dotted red line and is given by 4.2.12, 4.2.13 and 4.2.14.

RWA and geometric phase

The relation expressed in 4.2.10 for the Rabi vector $\mathbf{\Omega}_R$ in the rotating frame and the parameters V_0 and ω of the external field gives the angle θ between $\mathbf{\Omega}_R(t)$ and the z-axis

$$\begin{aligned}\cos\theta &= \frac{\Omega_R^{(z)}(t)}{|\mathbf{\Omega}_R(t)|} \\ &= \frac{\omega_0 - \omega}{[(\omega_0 - \omega)^2 + V_0^2]^{\frac{1}{2}}}.\end{aligned} \tag{4.2.15}$$

Now we consider the context of Berry's phase: a cyclic, adiabatic evolution in the parameter space of the Hamiltonian. In this case, the parameter space is the frequency ω, the amplitude V_0 and the phase ϕ of the external field. In the absence of the external field, the Rabi vector lies on the z-axis, as the amplitude of the external field increases, the Rabi vector rotates and when the amplitude of the applied field reaches V_0, the phase between the Rabi vector and the z-axis is given by 4.2.15. If the Bloch vector $\boldsymbol{a}$ of the system is initially aligned with the Rabi vector and the evolution of the system is adiabatic, then the angle between the Bloch vector and the z-axis will also be given by 4.2.15.

We have fixed two of the three parameters of the external field: the and the frequency ω and the amplitude V_0. The former is chosen to be near the resonance. Thus, we are left with the phase ϕ. Let us consider a curve C in the parameter space such that

$$C : \phi \to \alpha \in [0, 2\pi].$$

We represent the state of the system associated to this curve in the parameter space as

$$|\psi(t)\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\alpha}\sin\left(\frac{\theta}{2}\right)|1\rangle, \tag{4.2.16}$$

where $|0\rangle$ and $|1\rangle$ are the eigenvectors of σ_3. Finally, we can use Berry's definition

2.2.5 to calculate the geometric phase associated to this evolution:

$$\begin{aligned}\gamma_{geo} &= i\oint_C \langle\psi(t), \frac{d}{d\alpha}\psi(t)\rangle d\alpha \\ &= i\oint_C \left(\cos\left(\frac{\theta}{2}\right)\langle 0| + \sin\left(\frac{\theta}{2}\right)e^{-i\alpha}\langle 1|\right)\frac{d}{d\alpha}\left(\cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)e^{-i\alpha}|1\rangle\right)d\alpha \\ &= i\oint_C \left(\cos\left(\frac{\theta}{2}\right)\langle 0| + \sin\left(\frac{\theta}{2}\right)e^{-i\alpha}\langle 1|\right) i\sin\left(\frac{\theta}{2}\right)e^{i\alpha}|1\rangle d\alpha \\ &= -\frac{1}{2}(1-\cos\theta)\int_0^{2\pi} d\alpha \\ &= \pi(1-\cos\theta) \end{aligned} \tag{4.2.17}$$

which is the same expression found in 2.4.8. This was expected, since the physical system is the same (a two-level quantum system interacting with a Hamiltonian given by 4.1.1) and the parameters are the same). The process of eliminating the dynamic phase used by Ekert et al. is the spin-echo technique. The idea is to apply the cyclic evolution twice in a way that the dynamic phase accumulated in the evolution cancels out, remaining only the geometric phase. This process to remove the dynamic phase will be reviewed in Section 5.2.

Two two-level quantum systems under RWA

Let us now consider two two-level quantum systems with individual Hamiltonians H_0 given by 4.2.1. The Hamiltonian of the composite system when no interaction between the two systems is considered is given by

$$\begin{aligned} H_0 &= H_0^{(a)} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes H_0^{(b)} \\ &= \frac{1}{2}\omega_a \sigma_3^{(a)} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \frac{1}{2}\omega_b \sigma_3^{(b)} \end{aligned} \tag{4.2.18}$$

where a and b indicates the two systems and $\omega_{a,b}$ are the transition frequencies of each system.. The subscript on operators indicates operators acting on the Hilbert space associated with each system and $\mathbb{1}_2$ is the identity operator on a two-dimensional Hilbert space. Writing the Hamiltonian 4.2.18 in the basis $\{|0\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle\}$, also known as the computational basis, we

obtain

$$H_0 = \frac{1}{2}\begin{pmatrix} \omega_a+\omega_b & 0 & 0 & 0 \\ 0 & \omega_a-\omega_b & 0 & 0 \\ 0 & 0 & -\omega_a+\omega_b & 0 \\ 0 & 0 & 0 & -\omega_a-\omega_b \end{pmatrix}. \tag{4.2.19}$$

For the case in which the systems are sufficiently close to each other, they will interact and the energy levels will be affected. Let us consider, for example, two spin half particles. The magnetic field of one particle may affect the other one, the result is that if the spins are parallel the total energy of the system is increased by πJ and if they are antiparallel it is decreased by πJ. The Hamiltonian describing this interaction is

$$H = H_0 + 2\pi J S_3^{(a)} \otimes S_3^{(b)}, \tag{4.2.20}$$

and its matrix representation in the basis used before is

$$H = \frac{1}{2}\begin{pmatrix} \omega_a+\omega_b+\pi J & 0 & 0 & 0 \\ 0 & \omega_a-\omega_b-\pi J & 0 & 0 \\ 0 & 0 & -\omega_a+\omega_b-\pi J & 0 \\ 0 & 0 & 0 & -\omega_a-\omega_b+\pi J \end{pmatrix}. \tag{4.2.21}$$

Due to the interaction between the particles, the energy levels of the system suffers

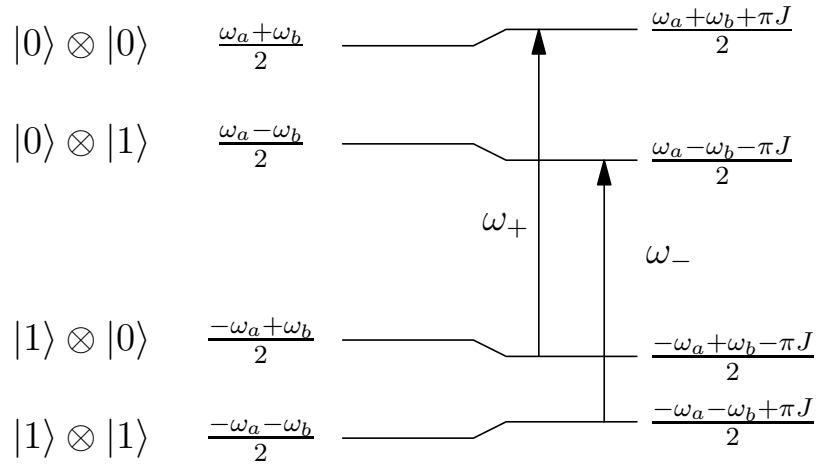


Figure 4.2: Diagram of the energy levels of two spin half particles. The shift is due to the interaction between them.

a change (Figure 4.2). If we consider the particle b as the control system, we have that the transition frequency for the particle a is given by

$$\omega_{\pm} = \omega_a \pm \pi J, \tag{4.2.22}$$

the plus sign is when particle b is in the state $|0\rangle$ and the minus sign when particle b is in the state $|1\rangle$.

For the situation in which the spin-half particle interacting with an external field represented by 4.2.7 varies slowly, we obtained in 4.2.17 that the Berry's phase depends explicitly on the transition frequency. If we consider the evolution of particle a, we will have that at the end of a cyclic evolution, the particle acquires a phase

$$\gamma = \pm\gamma_+ = \pm\pi(\cos\theta_+ - 1), \tag{4.2.23}$$

if the particle b is in the state $|0\rangle$ and

$$\gamma = \pm\gamma_- = \pm\pi(\cos\theta_- - 1) \tag{4.2.24}$$

if the particle b is in the state $|1\rangle$. The sign of the phase depends on the state of the particle a, being positive if a is in the state $|0\rangle$ and negative otherwise. As in 4.2.15 the angles θ_- and θ_- are given by

$$\cos\theta_+ = \frac{\omega_+ - \omega}{[(\omega_+ - \omega)^2 + \omega_1^2]^{\frac{1}{2}}}, \tag{4.2.25}$$

$$\cos\theta_- = \frac{\omega_- - \omega}{[(\omega_- - \omega)^2 + \omega_1^2]^{\frac{1}{2}}}. \tag{4.2.26}$$

The expression for the geometric phase in 4.2.23 and 4.2.24 will be used in the next chapter to implement a controlled phase shift gate between two qubits, that are essentially two two-level quantum systems.

4.3 Perturbative solution for a two-level system driven by periodic fields

Let us consider a system with evolution given by the Schrödinger equation

$$i\frac{d}{dt}\psi(t) = H(t)\psi(t), \tag{4.3.1}$$

where $\psi(t)$ is the state vector and $H(t)$ is the Hamiltonian of the system. In the previous section, we treated the case of a periodic driven two-level quantum system through the rotating wave approximation. The approximation allows us to solve the Schrödinger equation. However, for a general Hamiltonian, the evolution of the system is given by

$$\psi(t) = U(t)\psi(0), \tag{4.3.2}$$

where $\psi(t)$ is the state vector in an instant of time t, $U(t)$ is the time evolution operator, sometimes referred to as propagator, and $\psi(0)$ is the initial state of the system. The time evolution operator $U(t)$ can be obtained via the Dyson expansion

$$U(t) = \mathbb{1} + \sum_{n=1}^{\infty} (-i)^n \int_0^t H(t_1)dt_1 \dots \int_0^{t_{n-1}} H(t_n)dt_n. \tag{4.3.3}$$

The expression in 4.3.3 gives a straightforward method to compute $U(t)$. Unfortunately, the expansion is not guaranteed to be uniformly convergent in time.

In this section, we will use the method developed in [9] and [10] to compute $U(t)$ for a periodic driven two-level system. First, we will give a brief overview of the method (its particularities, validity and results), then we will use the results to obtain the phase factors for the two-level system.

A brief review

In [9] and [10] the Hamiltonian studied was of the form

$$H_1(t) = \epsilon\sigma_3 - f(t)\sigma_1, \tag{4.3.4}$$

where ϵ is a real constant and $f(t)$ is a periodic function of time. Let us consider a rotation of $\pi/2$ around the y-axis, denoted by $R_y(\pi/2)$, and the Schrödinger equation on this new rotated frame is given by

$$i\frac{d}{dt}\psi_2(t) = H_2(t)\psi_2(t), \tag{4.3.5}$$

where

$$\begin{aligned} \psi_2(t) &= R_y(\pi/2)\psi(t) \\ &= \exp(-i\pi\sigma_2/4)\psi(t) \end{aligned} \tag{4.3.6}$$

and

$$H_2(t) = \epsilon\sigma_1 + f(t)\sigma_3. \tag{4.3.7}$$

The Hamiltonian 4.3.4 can be interpreted as describing a system with a Hamiltonian independent of time $\epsilon\sigma_3$ subjected to a time-dependent perturbation $-f(t)\sigma_1$. The later is responsible for transitions between the two states of the system.

The method developed in [9] and [10] is valid for small ϵ and periodic and quasi-periodic functions of time. It consists in writing a perturbative expansion in ϵ for the time evolution operator. This method has proven to have the following advantages: the series expansion are uniformly convergent in time, the expression obtained for the time evolution operator is given in terms of series and so are easily implementable in numerical calculations and they can be employed for any periodic function. The uniform convergence is of great importance, since it means the results lead to stable numerical calculations and therefore it allows the study of long-time behavior of the observable quantities of the system.

It was shown in [9] that the time evolution operator $U(t)$ for the system described by 4.3.7 can be written as

$$U(t) = \begin{pmatrix} R(t)(1+ig_0S(t)) & -i\epsilon R(t)S(t) \\ -i\epsilon\overline{R(t)S(t)} & \overline{R(t)}(1-i\overline{g_0}\overline{S(t)}) \end{pmatrix}. \tag{4.3.8}$$

where $R(t)$ and $S(t)$ are given by

$$R(t) = e^{-i\Omega t}\sum_{m\in\mathbb{Z}} R_m e^{im\omega t} \tag{4.3.9}$$

and

$$S(t) = \sigma_0 + e^{2i\Omega t}\sum_{m\in\mathbb{Z}} S_m e^{im\omega t}. \tag{4.3.10}$$

R_m and S_m are coefficients of the expansion of $R(t)$ and $S(t)$, respectively. The Rabi frequency Ω is also obtained through an expansion, but it is fixed for each Hamiltonian and σ_0 is not related to the Pauli matrices, but it represents a complex constant relevant to the problem and its explicit expression can be found in [10]. Sometimes we will refer to the matrix elements of $U(t)$, for example, $U_{11}(t) = R(t)(1+ig_0S(t))$ and $U_{12}(t) = -i\epsilon R(t)S(t)$.

As done in [10], we implemented numerically the method developed there for a perturbation of the form

$$f(t) = F_0 + A\cos(\omega t), \tag{4.3.11}$$

where F_0 is a real number, A and ω is the amplitude and the frequency of the periodic perturbation, respectively. All the numerical calculations were done using

the C programming language and the necessary and appropriate libraries. Some specific details about this implementation are presented in Appendix A, such as the range taken on the sums in 4.3.9 and 4.3.10 and other numerical specifications.

Following the steps in [10], we considered the two eigenstates of the Hamiltonian 4.3.7, denoted by ψ_2^+ and ψ_2^-. The probability of transition $P(t)$ between them is a function of time and is given by

$$P(t) := |\langle \psi_2^+, U(t)\psi_2^- \rangle|^2 = |U_{12}(t)|^2. \tag{4.3.12}$$

We also considered the quantity $N(t)$ defined as

$$N(t) := |U_{11}(t)|^2 + |U_{12}(t)|^2 - 1. \tag{4.3.13}$$

Since $U(t)$ is unitary, that is, $U^*(t)U(t) = \mathbb{1}$, $N(t)$ should be 0. But, although the method presents an exact expression for $U(t)$, its numerical implementation involves a limited range of terms in the expansions present in $U(t)$. Thus, the quantity $N(t)$ estimates the accuracy of the numerical calculations. We adopted $F_0 = 0$ and $A = 1$ for all our calculations. In Figure 4.3 we present the graphical representations of $P(t)$ and $N(t)$ with $\omega = 2.0$ and $\epsilon = 0.01$ and $\epsilon = 0.1$.

As we can see from Figure 4.3, each system has a different period for different values of ϵ. We can associate this period with the Rabi frequency of each system. For example, for the cases considered in Figure 4.3, the Rabi frequencies are $T_\Omega \cong 261 t_\omega$ and $T_\Omega \cong 26 t_\omega$, for $\epsilon = 0.01$ and $\epsilon = 0.10$, respectively. We can also affirm that the Rabi frequency is a natural frequency of the system in the sense that the graph of $P(t)$ is similar to the graph of Rabi oscillations, $P(t) = \sin^2(\Omega t)$.

The method was applied to several values of ω and ϵ, the former ranging from 1.0 to 10.0 and the later from 0.01 to 0.40. But for all these values, the unitarity test were sufficiently satisfactory, since the error is bounded by 3×10^{-3} in one specific case (for $\omega = 1.0$ and $\epsilon = 0.40$), but and for most cases, is bounded by 10^{-5} or even 10^{-10}.

As said before, we implemented the directions in [9] and [10] and obtained almost the same results. There were some differences in the unitarity accuracy test. Our results presented smaller errors, probably due to the evolution of computational capacity since the publication of the method and our implementation. Our aim was to guarantee that this implementation was working so that we could use it to obtain the phase factors for the systems described by 4.3.4 and 4.3.7.

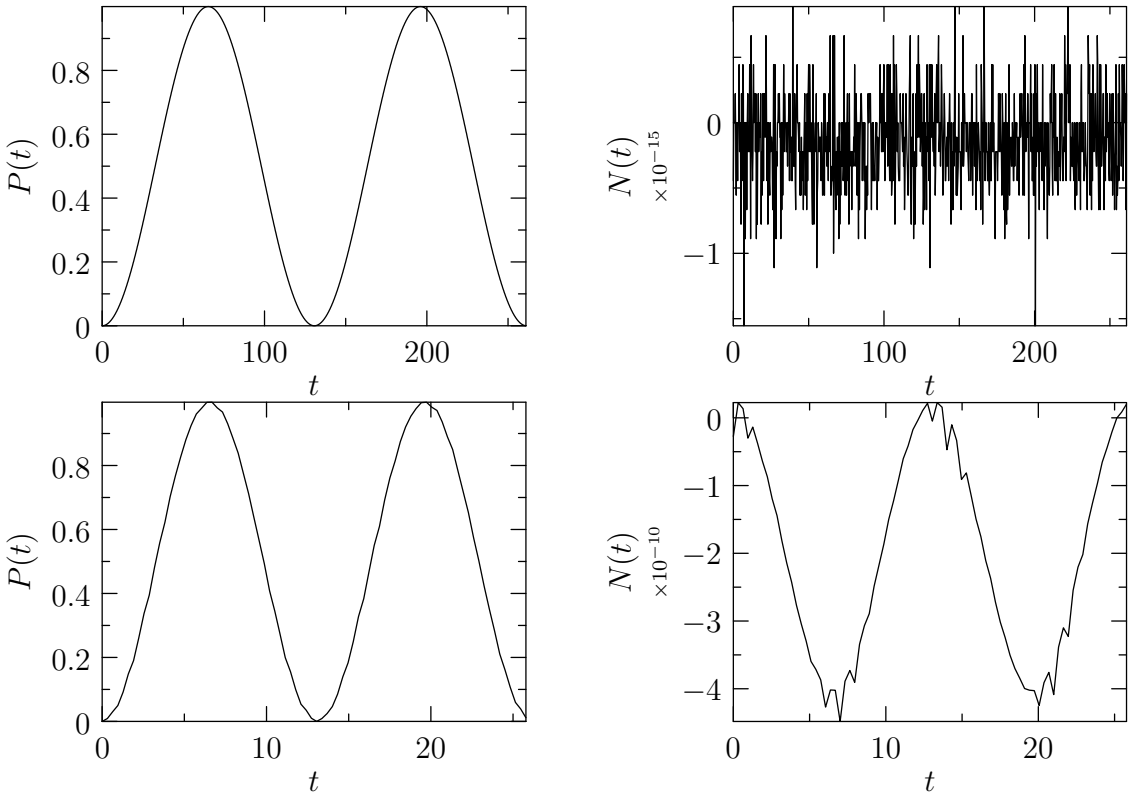


Figure 4.3: Transition probability $P(t)$ (left column) and the test for unitarity $N(t)$ (right column) as a function of time given by 4.3.12 and 4.3.13, respectively. The time is measured in units of $T_w = 2\pi/\omega$. The top row corresponds to the case in which $\epsilon = 0.01$ and the bottom row, $\epsilon = 0.10$. For both rows the chosen value for ω is the same, $\omega = 2.0$.

Phase factors for a two-level quantum system

Let us consider the system described by 4.3.7 with no interactions with the environment, i.e., a closed two-level quantum system. For this case, the total phase ϕ_{tot} can be obtained through

$$\phi_{tot}(t) = \arg\langle\psi(0), \psi(t)\rangle, \tag{4.3.14}$$

and the dynamical phase α_{dyn} is given by

$$\alpha_{dyn}(t) = i\int_0^t \langle\psi(t'), \dot{\psi}(t')\rangle \mathrm{d}t' \tag{4.3.15}$$

where $\psi(0)$ and $\psi(t)$ are the state vectors of the system at the initial instant of time and for an instant of time t, respectively. The dot indicates derivation relative to

time. The geometric phase γ_{geo} is given simply by

$$\gamma_{geo}(t) = \phi_{tot}(t) - \alpha_{dyn}(t). \tag{4.3.16}$$

We can note that the phase factors are functions of time, since they are defined by the evolution of the state vector $\psi(t)$. We saw that for a system with Hamiltonian given by equation 4.3.7

$$H_2(t) = \epsilon\sigma_1 + f(t)\sigma_3.$$

the time evolution operator $U(t)$ is given by equation 4.3.8

$$\begin{aligned} U(t) &= \begin{pmatrix} R(t)(1+ig_0S(t)) & -i\epsilon R(t)S(t) \\ -i\epsilon\overline{R(t)S(t)} & \overline{R(t)}(1-i\overline{g_0}\overline{S(t)}) \end{pmatrix} \\ &= \begin{pmatrix} U_{11}(t) & U_{12}(t) \\ -\overline{U}_{12}(t) & \overline{U}_{11}(t) \end{pmatrix} \end{aligned} \tag{4.3.17}$$

where $U_{11}(t) = R(t)(1+ig_0S(t))$ and $U_{12}(t) = -i\epsilon R(t)S(t)$ are the components of the matrix $U(t)$.

We must also remember that this system is a rotation of $\pi/2$ around the y-axis of the system described by the Hamiltonian 4.3.4. So, in order to use the previous expressions for the phase factors (equations 4.3.14, 4.3.15 and 4.3.16) for a state vector in the basis of the eigenvectors of σ_3, as is usually done, we must consider the rotated state vector ψ_2 given by 4.3.21. The expressions become

$$\phi_{tot} = \arg\langle\psi_2(0), U(t)\psi_2(0)\rangle, \tag{4.3.18}$$

for the total phase and

$$\alpha_{dyn}(t) = i\int_0^t \langle\psi_2(0), U^*(t)\dot{U}(t)\psi_2(0)\rangle \mathrm{dt} \tag{4.3.19}$$

for the dynamical phase. We can interpret equation 4.3.19 as the integration over time of the expectation value of $iU^*(t)\dot{U}(t)$. Considering the unitarity of $U(t)$, we have that

$$\begin{aligned} (iU^*(t)\dot{U}(t))^* &= -i\dot{U}^*(t)U(t) \\ &= -i(-U^*(t)\dot{U}(t)) \\ &= iU^*(t)\dot{U}(t), \end{aligned}$$

that is, the integration in 4.3.19 is the integration of the expectation value of a self-adjoint operator, so the result is necessarily a real number.

The geometric phase is still obtained through 4.3.16. Let us consider an initial state vector

$$\psi(0) = \alpha|0\rangle + \beta|1\rangle, \tag{4.3.20}$$

where α and β are complex constants and $|0\rangle$ and $|1\rangle$ are the eigenvectors of the Pauli matrix σ_3. Applying the rotation $R_y(\pi/2)$ on this state vector, it becomes

$$\psi_2(0) = \frac{1}{\sqrt{2}}\left[(\alpha-\beta)|0\rangle + (\alpha+\beta)|1\rangle\right]. \tag{4.3.21}$$

Using 4.3.17 and the expression 4.3.21 for a general initial state vector, the expression for the total phase then becomes

$$\begin{aligned}\phi_{tot}(t) = \arg\{&\operatorname{Re} U_{11}(t) + i(-2\operatorname{Re}(\overline{\alpha}\beta)\operatorname{Im} U_{11}(t) \\ &+ 2\operatorname{Im}(\overline{\alpha}\beta)\operatorname{Re} U_{12}(t) + (2|\alpha|^2-1)\operatorname{Im} U_{12}(t))\}.\end{aligned} \tag{4.3.22}$$

The expression above is easily calculated by our code, since the components $U_{11}(t)$ and $U_{12}(t)$ are, as we shall remember, given in terms of the functions $R(t)$ and $S(t)$ (equations 4.3.9 and 4.3.10). $R(t)$ and $S(t)$, in turn, are expansions involving the Rabi frequency Ω, the expansion coefficients (R_m and S_m, respectively) and the complex constant σ_0. These terms are calculated in our code and are different for different values of ϵ and ω.

In terms of the initial state vector 4.3.20 and the matrix components of the time evolution operator $U(t)$, the expression for the dynamical phase takes the form

$$\begin{aligned}\alpha_{dyn}(t) = |\alpha|^2 &\left(-\operatorname{Im}\int_0^t a_{11}(t')dt' + i\operatorname{Re}\int_0^t a_{12}(t')dt'\right) \\ &- 2i\operatorname{Re}(\overline{\alpha}\beta)\operatorname{Re}\int_0^t a_{11}(t')dt' - 2i\operatorname{Im}(\overline{\alpha}\beta)\operatorname{Im}\int_0^t a_{12}(t')dt' \\ &+ |\beta|^2\left(-\operatorname{Im}\int_0^t a_{11}(t')dt' - i\operatorname{Re}\int_0^t a_{12}(t')dt'\right),\end{aligned} \tag{4.3.23}$$

where $a_{11}(t)$ and $a_{12}(t)$ are matrix elements of the product of $U^*(t)$ and $\dot{U}(t)$:

$$U^*(t)\dot{U}(t) = \begin{pmatrix} a_{11}(t) & a_{12}(t) \\ -\overline{a}_{12}(t) & \overline{a}_{11}(t)\end{pmatrix}. \tag{4.3.24}$$

The explicit form of the terms $a_{11}(t)$ and $a_{12}(t)$ are

$$a_{11}(t) = \overline{R(t)}(1 - i\overline{g_0}\,\overline{S(t)})[\dot{R}(t) + ig_0(\dot{R}(t)S(t) + R(t)\dot{S}(t))] + \epsilon^2 R(t)S(t)(\dot{\overline{R(t)S(t)}} + \overline{R(t)\dot{S(t)}}) \tag{4.3.25}$$

and

$$a_{12}(t) = -i\epsilon\{\overline{R(t)}(1 - i\overline{g_0}\,\overline{S(t)})(\dot{R}(t)S(t) + R(t)\dot{S}(t)) - R(t)S(t)[\dot{\overline{R(t)}} - i\overline{g_0}(\dot{\overline{R(t)S(t)}} + \overline{R(t)\dot{S(t)}})]\}. \tag{4.3.26}$$

As we can see, the expression for the dynamical phase involves integrations over time of long expressions containing various expansions. These expansions are highly oscillatory (equations 4.3.9 and 4.3.10). There are several integration routines for highly oscillatory functions, but we chose not to calculate the integrations in the expression 4.3.23 for the dynamical phase through an integration routine, since we would have to test each one for our specific functions and then we would have to estimate the error inherent to the routine and add it to the machine built-in errors. Thus, to obtain the numerical value of the dynamical phase, the integrations in 4.3.23 were carried out analytically and then explicitly written as code.

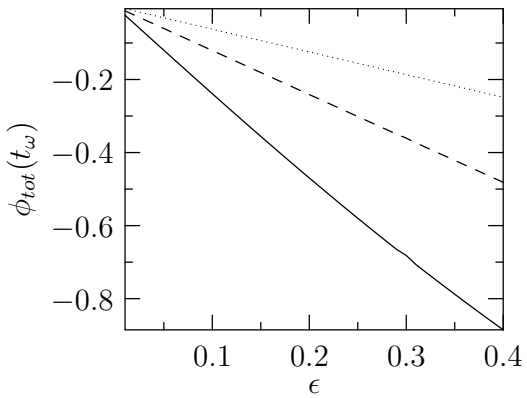
The code, overviewed in Appendix A, has functions that calculates the total and dynamical phase for any instant of time. The next inquiry is what instant of time is physically meaningful to the calculations of the geometric phase given by 4.3.16. One could argue that the appropriate instant of time would be the "natural" frequency of the system, characterized by the Rabi frequency Ω. But we must recollect the nature of the geometric phase, that is, the phase acquired over the course of the evolution of the system resulted from the geometrical properties of the parameter space of the Hamiltonian. In our case, the parameter space is two-dimensional, with each dimension associated to the parameters A and ω in 4.3.11. So, if we consider a cyclic evolution on the parameter space and a fixed amplitude A of the external field, the relevant instant of time is precisely

$$t_\omega = 2\pi/\omega. \tag{4.3.27}$$

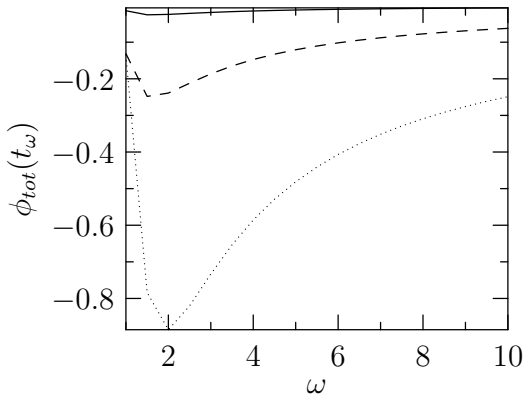
Therefore, the expressions 4.3.22, 4.3.23 and 4.3.16 for the respective total phase, dynamical phase and geometric phase of the system are taken at t_ω. Next, we present some results of our calculations for the phase factors of the system as graphical representations. Without loss of generality, we considered the initial state

vector to be $\psi(0) = |0\rangle$, that is, the state vector is initially aligned with the z-axis. The calculations were performed for values of ϵ ranging from 0.01 to 0.40 with steps of 0.01; and values of ω ranging from 1.0 to 10.0 with steps of 0.5.

As previously stated, the numerical implementation of the total phase was easily accomplished. We note that since the total phase is defined as an argument, there was no need to test if the numerical function had relevant imaginary parts due to built-in machine errors. Figure 4.4a shows the relation between the values of the total phase and the parameter ϵ. We can see that the absolute value of the total phase is proportional to the value of ϵ. According to the interpretation of 4.3.4 in which ϵ is the energy gap between the two eigenstates of σ_3, we can say that the total phase is proportional to this gap. Moreover, we note that as the value of ω increases, the rate in which the total phase increases with ϵ decreases, in other words, the value of ω modulates the curve $\phi_{tot} \times \epsilon$. Figure 4.4b shows graphs of the total phase as a function of ω with fixed values of ϵ. The same behavior observed in Figure 4.4a is present in Figure 4.4b, but in this case, the value of ϵ modulates the curve $\phi_{tot} \times \omega$ in the following way: as ϵ increases, the curve gets more accentuated. It is also notable that for ω around 2.0, the absolute value of the total phase is maximized. Figure 4.5 presents a three-dimensional representation of the total phase as a function of ω and ϵ.



(a) Total phase $\phi_{tot}(t_\omega)$ as a function of ϵ for fixed $\omega = 2.0$ (full line), 5.0 (dashed line) and 10.0 (dotted line).



(b) Total phase $\phi_{tot}(t_\omega)$ as a function of ω for fixed $\epsilon = 0.01$ (full line), 0.10 (dashed line) and 0.40 (dotted line).

Figure 4.4: Total phase plotted as a function of ϵ and ω.

The numerical implementation of the dynamical phase is not as straightforward as that of the total phase, since it involves several integrations over time (equation

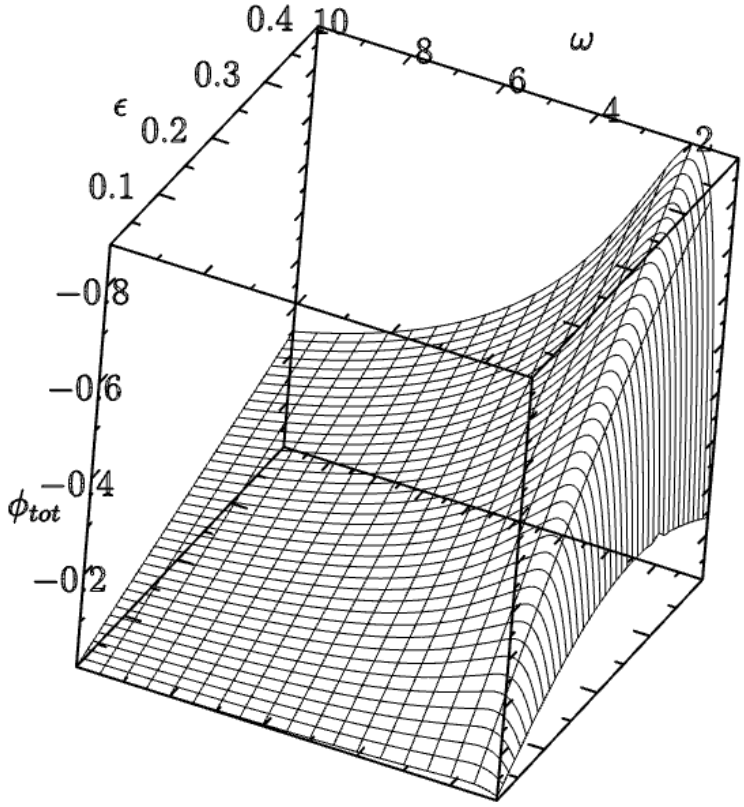
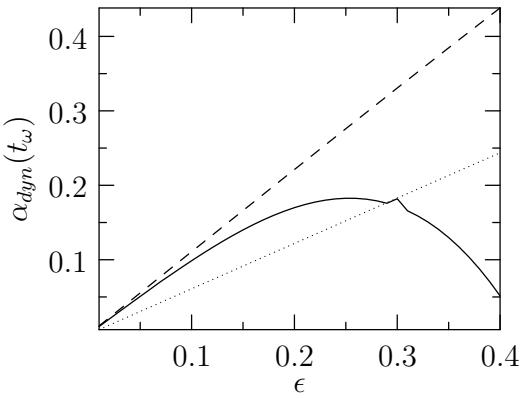
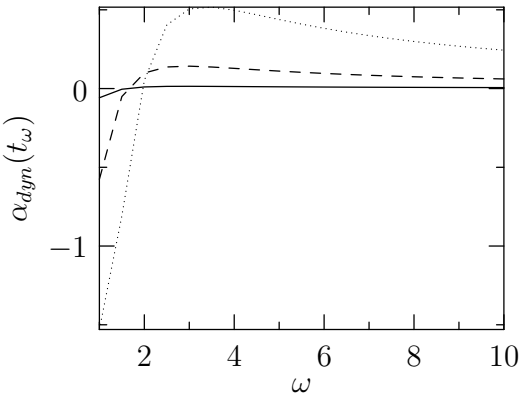


Figure 4.5: Graphical representation of the total phase ϕ_{tot} as a function of ω and ϵ.

4.3.23). These integrations, as we said before, were done analytically and then implemented in the code. The dynamical phase is expected to be real, but the expansions in our implementation are truncated, so we tested if the imaginary part of the dynamical phase had relevant contributions. The imaginary parts are not identically zero, but are within the machine accuracy. The relation between the dynamical phase and the values of ω has a particular behavior: for $\omega = 1.0, 1.5, 2.0, 2.5$ the curve $\alpha_{dyn} \times \epsilon$ resembles a parabola a for higher values the curve resembles a linear function. Figure 4.6a shows the dynamical phase as a function of ϵ for some fixed values of ω. Figure 4.6b shows the curve $\alpha_{dyn} \times \omega$ for some values of ϵ. We can see that, similar to Figure 4.4b, ϵ seems to modulate the curve and there is a value of ω that maximizes α_{dyn}, but this value shifts according to the value of ϵ. Figure 4.7 shows a three-dimensional representation of the dynamical phase as a function of ω and ϵ.



(a) Dynamical phase $\alpha_{dyn}(t_\omega)$ as a function of ϵ for fixed $\omega = 2.0$ (full line), 5.0 (dashed line) and 10.0 (dotted line).



(b) Dynamical phase $\alpha_{dyn}(t_\omega)$ as a function of ω for fixed $\epsilon = 0.01$ (full line), 0.10 (dashed line) and 0.40 (dotted line).

Figure 4.6: Dynamical phase plotted as a function of ϵ and ω.

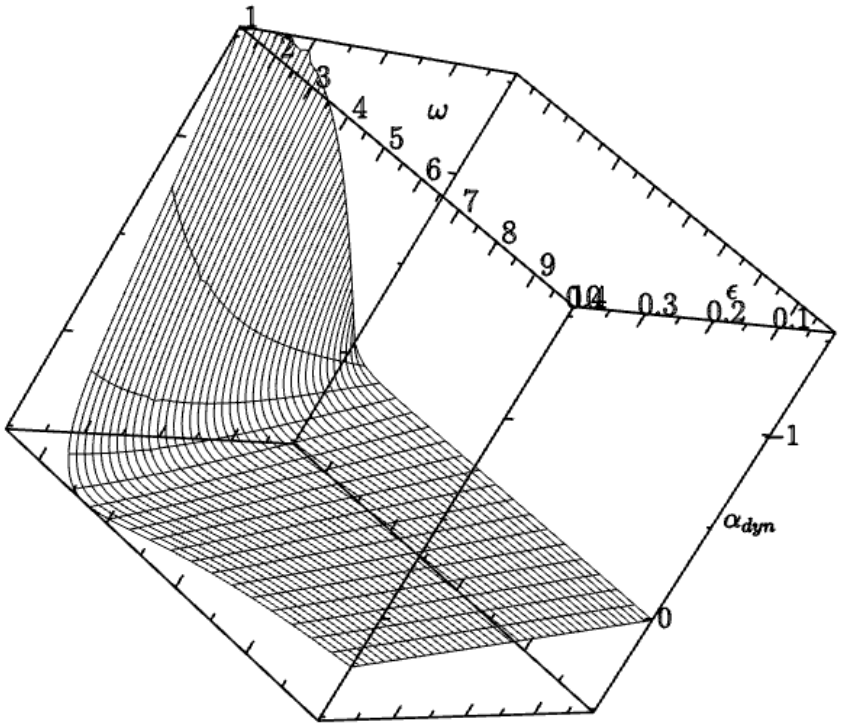
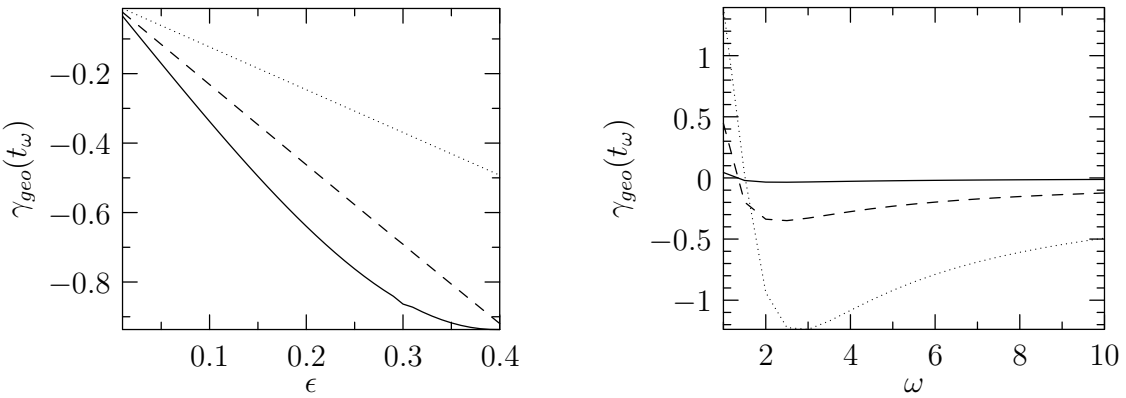


Figure 4.7: Graphical representation of the dynamical phase α_{dyn} as a function of ω and ϵ.

Figures 4.8a and 4.8b show the same behavior observed for the total and dynamical phase obtained through 4.3.16: the absolute value of the geometric phase increases as ϵ increases, the curve $\gamma_{geo} \times \omega$ is modulated by ϵ and it presents a value of ω that maximizes the absolute value of the geometric phase. Figure 4.9 shows the graphical representation of the geometric phase as a function of ω and ϵ.



(a) Geometric phase $\gamma_{geo}(t_\omega)$ as a function of ϵ for fixed $\omega = 2.0$ (full line), 5.0 (dashed line) and 10.0 (dotted line).

(b) Geometric phase $\gamma_{geo}(t_\omega)$ as a function of ω for fixed $\epsilon = 0.01$ (full line), 0.10 (dashed line) and 0.40 (dotted line).

Figure 4.8: Geometric phase plotted as a function of ϵ and ω.

Two two-level quantum systems and phase factors

We now consider two two-level quantum systems with individual Hamiltonians given by 4.3.4. First, we consider that the two systems do not interact with each other. In this case, the Hamiltonian $H_0^{(1)}$ of the composite system is given by

$$H_1^{(0)} = H_1^{(a)} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes H_1^{(b)}, \tag{4.3.28}$$

where $H_1^{(a)}$ and $H_1^{(b)}$ are the Hamiltonians of the first and second systems acting on their respective Hilbert space $\mathcal{H}_a$ and $\mathcal{H}_b$. The subscript in $H_1^{(0)}$ indicates that the two systems do not interact with each other. The matrix form of 4.3.28 written

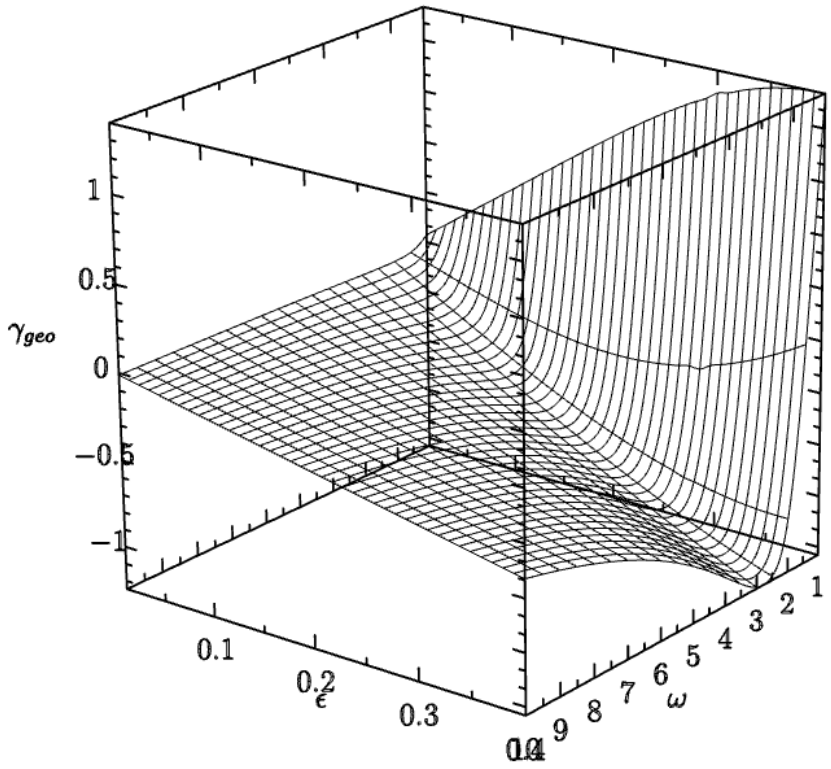


Figure 4.9: Graphical representation of the geometric phase γ_{geo} as a function of ω and ϵ.

in the computational basis is

$$H_1^{(0)} = \begin{pmatrix} \epsilon_a + \epsilon_b & -f_b(t) & -f_a(t) & 0 \\ -f_b(t) & \epsilon_a - \epsilon_b & 0 & -f_a(t) \\ -f_a(t) & 0 & -\epsilon_a + \epsilon_b & -f_b(t) \\ 0 & -f_a(t) & -f_b(t) & -\epsilon_a - \epsilon_b \end{pmatrix}, \tag{4.3.29}$$

where the subscripts a and b indicate the relevant constants of each individual system.

In the same way, the Hamiltonian of the equivalent composite system described by $H_2(t)$ in 4.3.7 has the matrix form

$$H_2^{(0)} = \begin{pmatrix} f_a(t)+f_b(t) & \epsilon_b & \epsilon_a & 0 \\ \epsilon_b & f_a(t)-f_b(t) & 0 & \epsilon_a \\ \epsilon_a & 0 & -f_a(t)+f_b(t) & \epsilon_b \\ 0 & \epsilon_a & \epsilon_b & -f_a(t)-f_b(t) \end{pmatrix} \tag{4.3.30}$$

We note again that working with the Hamiltonian $H_1(t)$ (equation 4.3.4) or $H_2(t)$ (equation 4.3.7) is equivalent, they describe the same physical system. The

former is the usual Hamiltonian for a system with a time-independent Hamiltonian aligned with the z-axis and a periodic time-dependent perturbation that induces transitions between the eigenstates of the unperturbed Hamiltonian. The later is just a rotation of $\pi/2$ around the y-axis of the former. We will indicate the terms in the first system with a subscript 1 and the terms associated with the "rotated" system with a subscript 2, for example, $\psi_2(t) = R_y(\pi/2)\psi_1(t)$. Except for the time evolution operator, which is always assumed to be associated with the "rotated" system, hence, for the sake of light notation, we will not write $U_2(t)$, but simply $U(t)$. The majority of our calculations in this section will be carried out in the "rotated" system, unless mentioned otherwise.

Next, we derive some necessary results for the calculations of the geometric phase for two non-interacting two-level systems. In this case, the time evolution operator of the composite system $U(t)$ is given by

$$U(t) = U_a(t) \otimes U_b(t) \tag{4.3.31}$$

and acts on the Hilbert space of the composite system $\mathcal{H} = \mathcal{H}_a \otimes \mathcal{H}_b$. The time evolution operators on the right hand side of 4.3.31 are given by 4.3.8 and generally have different constants ϵ and ω for each subsystem.

The composite system is closed. Therefore, the phase factors can be obtained through 4.3.14, 4.3.15 and 4.3.16. Let us first consider the total phase as defined by 4.3.14

$$\phi_{tot}(t) = \arg\langle\psi(0), \psi(t)\rangle,$$

where $\psi(t) = \psi_a(t) \otimes \psi_b(t)$ is the state vector of the composite system, and $U(t)$ is the time evolution of the composite system (equation 4.3.31. Hence, the total phase is

$$\begin{aligned}
\phi_{tot}(t) &= \arg\langle\psi(0), \psi(t)\rangle \\
&= \arg\langle\psi(0), U(t)\psi(0)\rangle \\
&= \arg\langle\psi_a(0) \otimes \psi_b(0), (U_a(t) \otimes U_b(t))(\psi_a(0) \otimes \psi_b(0)\rangle \\
&= \arg\langle\psi_a(0) \otimes \psi_b(0), (U_a(t)\psi_a(0) \otimes U_b(t)\psi_b(0)\rangle \\
&= \arg\langle\psi_a(0), U_a(t)\psi_a(0)\rangle\langle\psi_b(0), U_b(t)\psi_b(0)\rangle \\
&= \arg\langle\psi_a(0), U_a(t)\psi_a(0)\rangle + \arg\langle\psi_b(0), U_b(t)\psi_b(0)\rangle \\
&= \phi_{tot}^{(a)}(t) + \phi_{tot}^{(b)}(t).
\end{aligned} \tag{4.3.32}$$

As expected, the total phase of two non-interacting systems is simply the sum of the individual total phases $\phi_{tot}^{(a)}$ and $\phi_{tot}^{(b)}$. The same occurs with the dynamical phase given by 4.3.15:

$$\begin{aligned}
\alpha_{dyn}(t) &= i\int_0^t \langle \psi(0), U^*(t')\dot{U}(t')\psi(0)\rangle dt' \\
&= i\int_0^t \langle \psi_a(0)\otimes\psi_b(0), (U_a^*(t')\otimes U_b^*(t')) \\
&\qquad \times (\dot{U}_a(t')\otimes U_b(t') + U_a(t')\otimes \dot{U}_b(t'))(\psi_a(0)\otimes\psi_b(0))\rangle dt' \\
&= i\int_0^t \langle \psi_a(0), U_a^*(t')\dot{U}_a(t')\psi_a(0)\rangle dt' \\
&\qquad + i\int_0^t \langle \psi_b(0), U_b^*(t')\dot{U}_b(t')\psi_b(0)\rangle dt' \\
&= \alpha_{dyn}^{(a)}(t) + \alpha_{dyn}^{(b)}(t).
\end{aligned} \tag{4.3.33}$$

Hence, the geometric phase of the composite system (equation 4.3.16) is also the sum of the individual phases:

$$\gamma_{geo}(t) = \gamma_{geo}^{(a)}(t) + \gamma_{geo}^{(b)}(t). \tag{4.3.34}$$

For a two-level quantum system, we already determined the instant of time relevant to the calculations of the phase factors (equation 4.3.27). For a system composed of two two-level quantum systems, we must again determine what instant of time is relevant to the composite system. The trivial case is the one in which the two subsystems have the same ω, then the time entering the calculations of the phase factors is simply t_ω. In this work, we consider commensurable systems, that is, systems with ω_a/ω_b given by a rational number.

We next consider two two-level quantum systems interacting with each other. We assume that this interaction is given by $H'(t)$:

$$H'(t) = \kappa v(t)\ \sigma_3^{(a)}\otimes\sigma_3^{(b)}, \tag{4.3.35}$$

where κ is a real constant and $v(t)$ is a real function of time. The Hamiltonian of the composite system is given by

$$H_1(t) = H_1^{(a)}\otimes\mathbb{1}_2 + \mathbb{1}_2\otimes H_1^{(b)} + \kappa v(t)\ \sigma_3^{(a)}\otimes\sigma_3^{(b)}, \tag{4.3.36}$$

or, in matrix form

$$H_1(t) = \begin{pmatrix}
\epsilon_a+\epsilon_b+\kappa v(t) & -f_b(t) & -f_a(t) & 0 \\
-f_b(t) & \epsilon_a-\epsilon_b-\kappa v(t) & 0 & -f_a(t) \\
-f_a(t) & 0 & -\epsilon_a+\epsilon_b-\kappa v(t) & -f_b(t) \\
0 & -f_a(t) & -f_b(t) & -\epsilon_a-\epsilon_b+\kappa v(t)
\end{pmatrix} \tag{4.3.37}$$

where ϵ_a and ϵ_b are the respective constants of the individual systems and $f_a(t)$ and $f_b(t)$ are the external fields applied to each subsystem. The subscript 1 indicates that the Hamiltonian of the subsystems are given by 4.3.4. We note that the external fields are not necessarily the same, since the constants A and ω in equation 4.3.11 are determined by the individual characteristics of the system. The same Hamiltonian can be written in the "rotated" equivalent system, with the individual Hamiltonians given by 4.3.7. The interaction Hamiltonian in this system is given by

$$\begin{aligned} H_2'(t) &= R_y(\pi/2)\kappa v(t)\ \sigma_3^{(a)} \otimes \sigma_3^{(b)} R_y^*(\pi/2) \\ &= \kappa v(t)\ \sigma_1^{(a)} \otimes \sigma_1^{(b)}, \end{aligned} \tag{4.3.38}$$

and the Hamiltonian , in the equivalent system, is given by

$$H_2(t) = \begin{pmatrix} f_a(t)+f_b(t) & \epsilon_b & \epsilon_a & \kappa v(t) \\ \epsilon_b & f_a(t)-f_b(t) & \kappa v(t) & \epsilon_a \\ \epsilon_a & \kappa v(t) & -f_a(t)+f_b(t) & \epsilon_b \\ \kappa v(t) & \epsilon_a(t) & \epsilon_b & -f_a(t)-f_b(t) \end{pmatrix} \tag{4.3.39}$$

In order to obtain the phase factors for the composite system, we consider the interaction picture. We will denote the state vector in this picture by $\psi_I(t)$ and it relates to the state vector in the Schrödinger picture by the unitary transformation

$$\psi_I(t) = U^*(t)\psi(t), \tag{4.3.40}$$

where $U(t)$ is the time evolution operator (equation 4.3.31) for the system evolving according to $H_0(t)$ without interaction (in our case, $H_0(t)$ is given by the Hamiltonians in 4.3.28 or 4.3.30). In the interaction picture, the time evolution operator $U_I(t)$ is given by the Dyson series

$$U_I(t) = \mathbb{1} + \sum_{n=1}^{\infty} (-i)^n \int_0^t V_I(t_1)\,\mathrm{d}t_1 \ldots \int_0^{t_{n-1}} V_I(t_n)\,\mathrm{d}t_n. \tag{4.3.41}$$

where $V_I(t)$ is the interaction Hamiltonian in the interaction picture given by

$$V_I(t) = U^*(t)H'(t)U(t), \tag{4.3.42}$$

We can choose to calculate the phase factors and the respective relevant operators in the system with dynamics determined by the Hamiltonian $H_1(t)$ (equation 4.3.4) or in the equivalent rotated system with Hamiltonian $H_2(t)$ (equation 4.3.7). Once again, we choose the rotated system, since the time evolution operator in 4.3.17

corresponds to the time evolution of this system. In this case, the interaction Hamiltonian in 4.3.42 is given by 4.3.38. Hence, $V_I(t)$ is obtained using the time evolution operator in 4.3.31 and the interaction Hamiltonian in the interaction picture in 4.3.38:

$$\begin{aligned} V_I(t) &= (U_a^*(t) \otimes U_b^*(t))(\kappa v(t)\, \sigma_1^{(a)} \otimes \sigma_1^{(b)})(U_a(t) \otimes U_b(t)) \\ &= \kappa v(t)(U_a^*(t)\sigma_1^{(a)}U_a(t)) \otimes ((U_b^*(t)\sigma_1^{(b)}U_b(t)) \\ &= \kappa v(t) \begin{pmatrix} V_{11}(t) & V_{12}(t) \\ \overline{V}_{12}(t) & -V_{11}(t) \end{pmatrix}^{(a)} \otimes \begin{pmatrix} V_{11}(t) & V_{12}(t) \\ \overline{V}_{12}(t) & -V_{11}(t) \end{pmatrix}^{(b)}, \end{aligned} \tag{4.3.43}$$

with

$$V_{11}(t) = -\overline{U}_{11}(t)\overline{U}_{12}(t) - U_{11}(t)U_{12}(t) \tag{4.3.44}$$

$$V_{12}(t) = \overline{U}_{11}(t)^2 - U_{12}(t)^2, \tag{4.3.45}$$

where $U_{11}(t)$ and $U_{12}(t)$ are matrix components of the time evolution operator in 4.3.17.

The time evolution operator in the interaction picture given by the Dyson expansion in 4.3.41, considering the expression for the operator $V_I(t)$ in 4.3.43, is

$$U_I(t) = \mathbb{1} - i\kappa \int_0^t (U_a^*(t')\sigma_1^{(a)}U_a(t')) \otimes ((U_b^*(t')\sigma_1^{(b)}U_b(t'))\, \mathrm{d}t' + \mathcal{O}(\kappa^2).$$

In this work, we will only consider the Dyson expansion up to first order. Our aim is to explore the possibility of using the expressions for the time evolution operator to determine the phase factors for two two-level quantum systems and study how these phase factors depend on the parameters of the interaction. The matrix form of the time evolution operator in the interaction picture, in first order, is given by

$$U_I(t) = \mathbb{1}_4 - i\kappa \int_0^t v(t') \begin{pmatrix} V_{11}^{(a)}V_{11}^{(b)} & V_{11}^{(a)}V_{12}^{(b)} & V_{12}^{(a)}V_{11}^{(b)} & V_{12}^{(a)}V_{12}^{(b)} \\ V_{11}^{(a)}\overline{V}_{12}^{(b)} & -V_{11}^{(a)}V_{11}^{(b)} & V_{12}^{(a)}\overline{V}_{12}^{(b)} & -V_{12}^{(a)}V_{11}^{(b)} \\ \overline{V}_{12}^{(a)}V_{11}^{(b)} & \overline{V}_{12}^{(a)}V_{12}^{(b)} & -V_{11}^{(a)}V_{11}^{(b)} & -V_{11}^{(a)}V_{12}^{(b)} \\ \overline{V}_{12}^{(a)}\overline{V}_{12}^{(b)} & -\overline{V}_{12}^{(a)}V_{11}^{(b)} & -V_{11}^{(a)}\overline{V}_{12}^{(b)} & V_{11}^{(a)}V_{11}^{(b)} \end{pmatrix} \mathrm{d}t', \tag{4.3.46}$$

$$= \mathbb{1}_4 - i\kappa V^{(1)}(t) \tag{4.3.47}$$

where $\mathbb{1}_4$ is the identity operator acting on a four-dimensional Hilbert space and we omitted the time-dependency of the expressions for $V_{11}(t)$ and $V_{12}(t)$ given by equations 4.3.44 and 4.3.45, respectively. The operator $V^{(1)}(t)$ stands for the integral

on the right hand side of 4.3.46 and will be useful for evaluating the expressions for the phase factors of the composite system. Also, we must note that $V^{(1)}(t)$ is a self-adjoint operator, since $v(t)$ is a real function of t and the matrix operator in the integrand on the right hand side of 4.3.46 is self-adjoint, thus, $V^{(1)}(t)$ is the result of the integration of a self-adjoint operator.

Equation 4.3.40 establishes the relation between the state vector in the interaction picture and the state vector in the Schrödinger picture. From this relation, we can write the state vector of the composite system as

$$\begin{aligned}\psi_2(t) &= U(t)\psi_I(t)\\ &= U(t)U_I(t)\psi_I(0)\\ &= U(t)U_I(t)\psi_2(0)\\ &= U(t)U_I(t)(\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0))\end{aligned} \tag{4.3.48}$$

where we used that $\psi_I(t) = U_I(t)\psi_I(0)$ and that $\psi_I(0) = \psi_2(0)$. Also, the subscript in $\psi_2(t)$ indicates that we are considering the system with dynamics given by $H_2(t)$ (equation 4.3.7), the time evolution operator $U(t)$ for the composite system has the explicit form

$$\begin{aligned}U(t) &= U_a(t)\otimes U_b(t)\\ &= \begin{pmatrix} u_{11}^{(a)}u_{11}^{(b)} & u_{11}^{(a)}u_{12}^{(b)} & u_{12}^{(a)}u_{11}^{(b)} & u_{12}^{(a)}u_{12}^{(b)}\\ -u_{11}^{(a)}\overline{u}_{12}^{(b)} & u_{11}^{(a)}\overline{u}_{11}^{(b)} & -u_{12}^{(a)}\overline{u}_{12}^{(b)} & u_{12}^{(a)}\overline{u}_{11}^{(b)}\\ -\overline{u}_{12}^{(a)}u_{11}^{(b)} & -\overline{u}_{12}^{(a)}u_{12}^{(b)} & \overline{u}_{11}^{(a)}u_{11}^{(b)} & \overline{u}_{11}^{(a)}u_{12}^{(b)}\\ \overline{u}_{12}^{(a)}\overline{u}_{12}^{(b)} & -\overline{u}_{12}^{(a)}\overline{u}_{11}^{(b)} & -\overline{u}_{11}^{(a)}\overline{u}_{12}^{(b)} & \overline{u}_{11}^{(a)}\overline{u}_{11}^{(b)}\end{pmatrix}\end{aligned} \tag{4.3.49}$$

The total phase for the composite system can be obtained through 4.3.14:

$$\begin{aligned}\phi_{tot}(t) &= \arg\langle\psi_2(0),\psi_2(t)\rangle\\ &= \arg\langle\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0), U(t)U_I(t)(\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0))\rangle\\ &= \arg\langle\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0), U(t)(\mathbb{1}_4 - i\kappa V^{(1)}(t))(\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0))\rangle\\ &= \arg\Big\{\langle\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0), (U_a(t)\otimes U_b(t))(\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0))\rangle\\ &\qquad - i\kappa\langle\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0)), U(t)V^{(1)}(t)(\psi_2^{(a)}(0)\otimes\psi_2^{(b)}(0))\rangle\Big\}\\ &= \arg\Big\{\langle\psi_2^{(a)}(0), U_a(t)\psi_2^{(a)}(0)\rangle\langle\psi_2^{(b)}(0), U_b(t)\psi_2^{(b)}(0)\rangle\\ &\qquad - i\kappa\langle\psi_2(0), U(t)V^{(1)}(t)\psi_2(0)\rangle.\Big\}\end{aligned} \tag{4.3.50}$$

We note that an expansion of the expression above for a sufficiently small κ reduces itself to the total phase of two non-interacting systems given by 4.3.32.

Using the expression 4.3.15 for the dynamical phase and the expansion in κ for the time evolution operator in the interaction picture, we have

$$\begin{aligned}
\alpha_{dyn}(t) &= i\int_0^t \langle \psi_2(t'), \dot{\psi}_2(t')\rangle \,\mathrm{d}t' \\
&= i\int_0^t \langle U(t')U_I(t')\psi_2(0), (\dot{U}(t')U_I(t') + U(t')\dot{U}_I(t'))\psi_2(0)\rangle \,\mathrm{d}t' \\
&= i\int_0^t \langle \psi_2(0), U_I^*(t')U^*(t')(\dot{U}(t')U_I(t') + U(t')\dot{U}_I(t'))\psi_2(0)\rangle \,\mathrm{d}t' \\
&= i\int_0^t \langle \psi_2(0), \, (\mathbb{1}_4 + i\kappa V^{(1)}(t')^*)U^*(t')(\dot{U}(t') \\
&\qquad \times (\mathbb{1}_4 - i\kappa V^{(1)}(t')) - i\kappa U(t)\dot{V}^{(1)}(t'))\psi_2(0)\rangle \,\mathrm{d}t' \\
&= i\int_0^t \langle \psi_2(0), U^*(t')\dot{U}(t')\psi_2(0)\rangle \,\mathrm{d}t' \\
&\quad + \kappa\int_0^t \langle \psi_2(0), U^*(t')U(t')V^{(1)}(t')\psi_2(0)\rangle \,\mathrm{d}t' \\
&\quad + \kappa\int_0^t \langle \psi_2(0), U^*(t')\dot{U}(t')\dot{V}^{(1)}(t')\psi_2(0)\rangle \,\mathrm{d}t' \\
&\quad - \kappa\int_0^t \langle \psi_2(0), V^{(1)}(t')^*U^*(t')\dot{U}(t')\rangle \,\mathrm{d}t' + \mathcal{O}(\kappa^2),
\end{aligned}$$

since $U(t)$ is unitary, the identity $U^*(t)\dot{U}(t) = -\dot{U}^*(t)U(t)$ holds and the third term on the right hand side of the expression above can be rewritten as the complex conjugate of the second term. Hence, the dynamical phase up to first order in κ is given by

$$\begin{aligned}
\alpha_{dyn}(t) = \alpha_{dyn}^{(0)}(t) &+ 2\kappa\,\mathrm{Re}\int_0^t \langle \psi_2(0), U^*(t')\dot{U}(t')V^{(1)}(t')\psi_2(0)\rangle \,\mathrm{d}t' \\
&+ \kappa\int_0^t \langle \psi_2(0), \dot{V}^{(1)}(t')\psi_2(0)\rangle \,\mathrm{d}t' + \mathcal{O}(\kappa^2),
\end{aligned} \tag{4.3.51}$$

where the $\alpha_{dyn}^{(0)}(t)$ is exactly the expression for the dynamical phase for two non-interacting two-level systems in equation 4.3.33. Also, the third term on the right hand side of 4.3.51 is the integral over time of the expectation value of the self-adjoint operator $V^{(1)}(t)$. Therefore, this term is also real and so is the expression for the dynamical phase. The geometric phase for the composite system is still given

by the difference between the total phase and the dynamical phase, as in equation 4.3.34.

Now, let us consider the case in which the interaction is given by

$$v(t) = \delta(t - t_0), \tag{4.3.52}$$

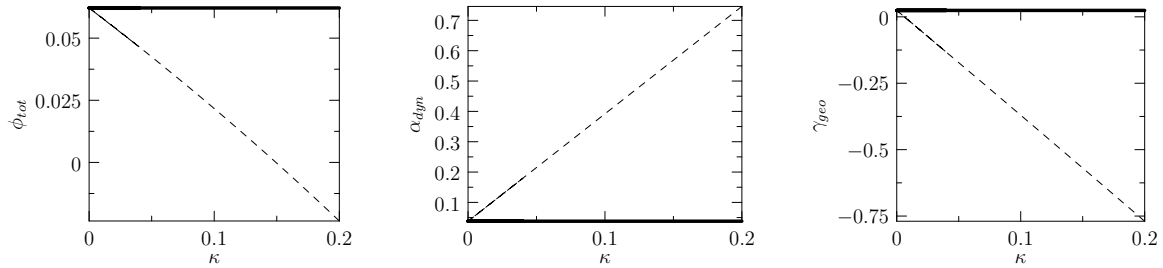
where t_0 is any instant of time. The time evolution operator in the interaction picture, according to 4.3.46, is

$$U_I(t) = \mathbb{1}_4 - i\kappa \begin{pmatrix} V_{11}^{(a)} V_{11}^{(b)} & V_{11}^{(a)} V_{12}^{(b)} & V_{12}^{(a)} V_{11}^{(b)} & V_{12}^{(a)} V_{12}^{(b)} \\ V_{11}^{(a)} \overline{V}_{12}^{(b)} & -V_{11}^{(a)} V_{11}^{(b)} & V_{12}^{(a)} \overline{V}_{12}^{(b)} & -V_{12}^{(a)} V_{11}^{(b)} \\ \overline{V}_{12}^{(a)} V_{11}^{(b)} & \overline{V}_{12}^{(a)} V_{12}^{(b)} & -V_{11}^{(a)} V_{11}^{(b)} & -V_{11}^{(a)} V_{12}^{(b)} \\ \overline{V}_{12}^{(a)} \overline{V}_{12}^{(b)} & -\overline{V}_{12}^{(a)} V_{11}^{(b)} & -V_{11}^{(a)} \overline{V}_{12}^{(b)} & V_{11}^{(a)} V_{11}^{(b)} \end{pmatrix}_{t=t_0} , \tag{4.3.53}$$

where the time dependency of $V_{11}(t)$ and $V_{12}(t)$ are respectively given by 4.3.44 and 4.3.45. The time dependency in the second term on the right hand side was omitted, but we assume that $0 < t_0 < t$ and so, both $V_{11}(t)$ and $V_{12}(t)$ are calculated for t_0, as is indicated by the subscript on the matrix on the right hand side of 4.3.53.

Up to first order in κ, the time evolution operator in 4.3.53 is constant in time. Thus, the third term of the expression for the dynamical phase in 4.3.51, that involves the time derivative of $V^{(1)}(t)$, is null. We implemented in our code functions that calculate the phase factors for the interaction given by 4.3.52. To investigate the relation between the phase factors and the constant κ, we considered a system composed of two commensurable subsystems with fixed ω_a, ω_b, ϵ_a and ϵ_b, a fixed t_0 that characterizes the delta interaction and we varied κ from 0 to 0.2, with steps of 0.01. Considering this set of parameters, the code calculates the phase factors for each of the computational basis states ($|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$). Figure 4.10 shows the results for the initial state $|00\rangle$ and $\omega_q = 1.0$, $\omega_b = 2.0$, $\epsilon_a = \epsilon_b = 0.01$ and $t_0 = 0.5$. The results are similar for others sets of parameters. We note that the main contribution to the geometric phase comes from the dynamical phase. Also, since our approximation of the Dyson expansion (equation 4.3.41) is only up to first order, the dependency of the phase factors on κ is linear. The parameter κ is not, as one could imagine, a parameter of the control space of the system. It simply modulates the interaction between the subsystems and can be thought of as an structural constant.

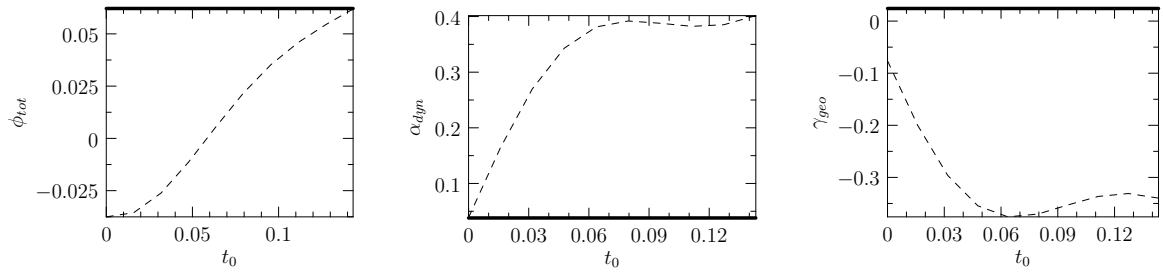
Figure 4.11 shows the dependency of the phase factors on the instant of time t_0 of the interaction for the initial state $|00\rangle$. The presented relation between the



(a) Total phase. (b) Dynamical phase. (c) Geometric phase.

Figure 4.10: Plots of the phase factors for the initial state $|00\rangle$ as functions of the parameter κ. The thick line represents the value of the phase factors for a system with non-interacting subsystems. The dashed line represents the interaction given by 4.3.52. We considered subsystems with $\omega_a = 1.0$, $\omega_b = 2.0$, $\epsilon_a = \epsilon_b = 0.01$ and $t_0 = 0.5$.

phase factors and t_0 is similar for the others states of the computational basis and for different sets of parameters. We note that there is a value of t_0 that maximizes the absolute value of the geometric phase, but we cannot state that this is a global maximum.



(a) Total phase. (b) Dynamical phase. (c) Geometric phase.

Figure 4.11: Plots of the phase factors for the initial state $|00\rangle$ as functions of the instant of time of the interaction t_0. The thick line represents the value of the phase factors for a system with non-interacting subsystems. The dashed line represents the interaction given by 4.3.52. We considered subsystems with $\omega_a = 1.0$, $\omega_b = 2.0$, $\epsilon_a = \epsilon_b = 0.01$ and $\kappa = 0.1$. The time is measured in unites of $2\pi/\omega$.

Chapter 5

Geometric phases and quantum computation

The study of information processing (storage, manipulation, transmission) passes through our understanding of physical systems, since information is something that is encoded in the state of a physical system and its processing is related to actions on such systems. Therefore, information theory is intimately connected to the theory used to describe physical systems. Considering that the advent of quantum theory changed drastically our understanding of nature, it consequently changed the way we perceive information.

In 1982, R. Feynman [31], facing the question about the simulation of quantum physical systems, posed the question about the efficiency of a classical computer to simulate quantum systems [1], he then suggested the possibility of building a computer out of quantum systems. In 1985, Deutsch [27] established the conceptual basis for a universal quantum computer by suggesting that quantum a computer might have computational powers exceeding those of its classical counterpart. This suggestion was finally carried out by P. Shor [61] with his quantum algorithm for prime factorization of integers, in which he showed that this problem could be solved in an efficient time, contrary to what is expected from a classical computer. Shor's algorithm is a powerful indication that quantum computers are, at least in principle, more efficient than classical ones. In the same direction, L. Grover [36]

[1] "*...and therefore these [quantum] phenomena have to be understood very well in analyzing the situation. And I'm not happy with all the analyses that go with just the classical theory, because 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.*" [31]

showed that a quantum algorithm for searching an element on an unstructured search space would be faster than its classical analogue.

Although quantum computation is a promising field, it faces two main difficulties: finding new algorithms besides Shor's and Grover's and performing quantum computation that is resilient to errors. Nielsen and Chuang argument in their accomplished book [49] that algorithm design for quantum computers is hard because our human intuition is rooted in the classical world and because it does not suffice a quantum algorithm to be merely quantum, it has to be better than its existing classical equivalents. The second difficulty is related to the physical realization of quantum computers. To perform quantum computation, it is necessary a reliable preparation and manipulation of the quantum systems that compose the quantum computer, but a perfect isolation of these systems is not possible and the subsequently interaction between them and the environment might cause errors that degrade the quantum information encoded on such systems. Besides decoherence, that is a source of error exclusive to quantum computation, there is the usual source of errors that arises from the inaccuracies of performing operations in physical systems. To overcome this problem, P. Shor [60] and Steane [69] developed quantum error correcting codes and showed that, theoretically, it is possible to correct errors and perform meaningful quantum information processing. After that, many works on quantum error correcting have been published ([50], [45], [28], [20]).

The many aspects of Quantum Mechanics yields several quantum computing schemes: adiabatic quantum computation (Farhi et al. [30]) based on adiabatic evolution, geometric quantum computation ([79], [29]) based on the concept of geometric phases, topological quantum computation ([43]) based on topological phases and many other schemes. For a thorough survey on quantum computation and quantum information, we refer to the by Nielsen and Chuang [49] and the lecture notes by J. Preskill [55].

In this chapter we will present the basics of geometric quantum computation. In Section 5.1 we introduce the fundamentals of quantum computation (qubits, quantum gates and source of errors). Section 5.2 is devoted to geometric quantum computation and the implementation of a quantum gate through geometric phases.

5.1 Quantum computation

Qubits

The basic unit of quantum information is the quantum bit, or qubit. A qubit is a two-level quantum system. In order to make reference to its classical counterpart, we write the two-dimensional Hilbert space associated to the qubit as $\mathcal{H} = \{|0\rangle, |1\rangle\}$. An arbitrary state $|\psi\rangle$ of the qubit can be expressed as

$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle, \tag{5.1.1}$$

where a_0 and a_1 are complex numbers that satisfy $|a_0|^2 + |a_1|^1 = 1$. The geometric representation of a qubit is the Bloch sphere (Definition 2.4.1). The possibility of representing a qubit as a superposition between two states is one of the main differences between quantum and classical computation and is one of the reasons that makes the qubit a more powerful computational resource. Another difference is the way qubits form a composed state. The general state of N qubits is given by

$$|\psi\rangle = \sum_{i_1,i_2,\ldots,i_N=\{0,1\}^N} a_{i_1,i_2,\ldots,i_N}|i_1\rangle \otimes |i_2\rangle \otimes \ldots \otimes |i_N\rangle, \tag{5.1.2}$$

where $a_{i_1,i_2,\ldots,i_N}$ are complex coefficients with $\sum_{i_1,i_2,\ldots,i_N=\{0,1\}^N} |a_{i_1,i_2,\ldots,i_N}|^2 = 1$. To store the information encoded in the state 5.1.2 on a classical computer, it would be necessary the storage of 2^N complex coefficients. For a not very large N, the task of storing these coefficients would not be feasible in any possible classical computer. Therefore, the possibility of superposition and entanglement presented by the qubit is what indicates it as a more powerful computational resource.

Quantum gates and universality

In order to process information, classical computers use wires and logic gates responsible for transporting and manipulating information, respectively. Analogously, the processing of quantum information is made through a quantum circuit made of wires and quantum logic gates. Quantum logic gates are unitary operations performed on one, two or more qubits, simultaneously. We associate the size of the circuit to the numbers of gates it contains.

It is known in classical computation that a small set of gates can be used to compute any arbitrary function. Such a set is said to be universal for classical

computation. A natural question is if there is a universal set of quantum gates. Fortunately, the answer is positive: any unitary operation can be approximated to arbitrary accuracy using any two-qubit gate. Therefore, the implementation of two-qubit gates is of crucial importance for the development of quantum computation. A choice of universal set of gates is, by no means, unique. We will consider the set formed by the Hadamard gate and the controlled phase shift gate.

The Hadarmard gate is a single qubit gate $\boldsymbol{H}$ that performs the unitary transformation that transforms the states $|0\rangle$ and $|1\rangle$ into superpositions:

$$|0\rangle \to \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$
$$|1\rangle \to \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle),$$

its matrix representation in the computational basis $\{|0\rangle, |1\rangle\}$ is

$$\boldsymbol{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5.1.3}$$

The controlled phase shift gate is a two-qubit gate that leaves the first qubit unchanged (it serves as a control qubit) and acts on the second one by adding a phase such that

$$|0\rangle \otimes |0\rangle \to |0\rangle \otimes |0\rangle$$
$$|0\rangle \otimes |1\rangle \to |0\rangle \otimes |1\rangle$$
$$|1\rangle \otimes |0\rangle \to |1\rangle \otimes |0\rangle$$
$$|1\rangle \otimes |1\rangle \to e^{i\phi}|1\rangle \otimes |1\rangle,$$

written in the computational basis $\{|0\rangle \otimes |0, \rangle |0\rangle \otimes |1\rangle, |1\rangle \otimes |0\rangle, |1\rangle \otimes |1\rangle\}$, the controlled shift gate $B(\phi)$ is given by

$$B(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}. \tag{5.1.4}$$

Hence, the two main features of quantum computation – superposition and entanglement – might be represented by the two quantum gates previously described. The implementation of quantum gates is already possible for some physical systems (nuclear magnetic resonance, ion traps, photonic systems and cavity quantum electrodynamics), [14] presents a survey on the experimental realizations in quantum computation and information.

Source of errors

In quantum information processing, the information is encoded in a superposition of states and its manipulation we carried out through operations in these states. To achieve reliable quantum computation, it is necessary to guarantee that the information is not lost in this process. Source of errors in quantum computation comes from the intrinsic inaccuracies of experimental procedures and from the interaction between the systems that compose the quantum circuit and the environment. Following Preskill [55] we can classify some errors that may occur in quantum information processing:

Phase errors In classical computation, a source of error is the bit-flip error:

$$|0\rangle \to |1\rangle$$
$$|1\rangle \to |0\rangle.$$

In quantum computation that may also occur and is represented by the action of the operator σ_1. In addition to bit-flip errors, phase-flip errors may also occur:

$$|0\rangle \to |0\rangle$$
$$|1\rangle \to -|1\rangle,$$

and is associated to the action of the operator σ_3. There is no classical code to protect information from this kind of error, since it arises from a fundamentally quantum property: superposition.

Small errors The manipulation of qubits is made through unitary transformations. A protocol for applying an operation represented by the unitary transformation U_0 may (and will not) be ideal, so the actual transformation

$$U = U_0(1 + \mathcal{O}(\epsilon)),$$

will be changed by an amount of order ϵ. There are classical error-correcting methods for this kind of source of error, but always considering only bit-flip errors.

Measurement The process of measuring qubits to retrieve the encoded information changes the evolution of the system (as we saw in Section 3.1).

5.2 Geometric quantum computation

In 1999, Zanardi and Rasetti [79] proposed that the concept of geometric phase could be used for enabling quantum computation. They considered a system with a degenerate Hamiltonian with an associated control space and they showed that adiabatic cyclic evolutions in the control space induced non-trivial unitary transformations on the system. They used these transformations to implement quantum gates. In the following year, Jones et al. [40] demonstrated experimentally a quantum gate based on geometric phase. The grounds for geometric quantum computation were established.

The difference between the implementation of quantum gates by the geometric approach is that geometric phases are global properties of quantum evolutions, therefore, are robust against local errors (fluctuations on the Hamiltonian's parameters). Nevertheless, parameter fluctuations are not the only source of error, the effect of decoherence must also be studied. There are already some works on how to protect the system (thus, the information) from errors induced by the environment ([77], [50]), but it is still a challenge reaching models for fault-tolerant geometric quantum computation.

A central element of geometric quantum computation is the implementation of quantum gates through purely geometric phases. In Chapter 4 we studied two-level systems and obtained the phase factors for the case in which the rotating wave approximation is valid (Section 4.2) and for a system driven by periodic fields with dynamics given by a perturbative solution (Section 4.3). For these systems, we calculated all the phase factors (total, dynamical and geometric phases). However, for achieving geometric quantum computation, the dynamical phase accumulated by the system must be removed. We will briefly present some of the methods used to remove/avoid the dynamical phase.

Also, we follow the work of A. Ekert et al. [29] in which an implementation of a controlled phase shift gate was obtained through geometric phase. The geometric

phase obtained by Ekert et al. considers the rotating wave approximation, therefore is subjected to the limitations of this approximation. We extend the implementation of the controlled phase shift gate to systems driven by periodic fields with solutions given by the perturbative method described in Section 4.3.

Elimination of the dynamical phase

In order achieve geometric quantum computation, it is necessary to eliminate or avoid the dynamical phases accumulated by the system, so that the phase gates implemented are purely geometric and possess the interesting features of the geometric phase, mainly inherent fault-tolerance against local errors. This can be achieved in various ways. We will delineate the basic ideas of some of the schemes to remove the dynamical phase. It is not the intention of this work to make a detailed derivation of each method or to explain in detail the physical systems in which they are feasible.

Parallel Transport Equation 4.3.15 defines the dynamical phase for a quantum system. We note that if

$$\langle \psi(0), U^*(t)\dot{U}(t)\psi(0)\rangle = 0, \tag{5.2.1}$$

then the dynamical phase is null and the geometric phase is the total phase. When 5.2.1 is satisfied, $\psi(t)$ is said to be parallel transported. This notion was previously presented for the Uhlmann's phase (equation 3.2.3) and also for non-unitary evolution in the context of interferometry in equation 3.3.17. This approach to eliminating the dynamical phase was already successfully implemented for NMR (nuclear magnetic resonance) experiments ([72], [51], [67]).

Parameter tuning A simple method to remove the dynamical phase is to choose specific external parameters of the Hamiltonian such that the dynamical phase in the evolution of the system vanishes or satisfies $\alpha_{dyn} = \text{integer} \times 2\pi$. This method was proposed and analyzed in [81] and [83]. In the context of geometric quantum computation, the authors present a scheme to achieve a set of universal quantum gates based on cyclic geometric operations that can be experimentally tested in existing quantum computer prototypes.

Refocusing technique The basic idea of this method, also known as spin-echo or multi-loop, is to apply the cyclic evolution twice in a way that effectively the dynamical phases accumulated in the second cycle cancels out the dynamical phase accumulated in the first cycle, or add up to a global phase. In more detail, let us consider a two-level quantum system with two eigenstates $|0\rangle$ and $|1\rangle$, their respective curves C_0 and C_1 in the parameter space during a cyclic evolution and their respective dynamical phases α_0 and α_1, and geometric phases γ_0 and γ_1. Considering a spin-half particle in a magnetic field, Berry's phase in 2.4.9 gives $\gamma_1 = -\gamma_0$. Now we denote a loop $\bar{C}_0$ in the parameter space corresponding to a cyclic evolution with the same period as C_0 and opposite geometric phase. The sequence of operations performed is

$$C \quad \rightarrow \quad \pi \quad \rightarrow \quad \bar{C} \quad \rightarrow \quad \pi\,. \tag{5.2.2}$$

In our example, this can be achieved by inverting the direction of the external magnetic field. In summary, we start with the system in the initial state $|0\rangle$, then it evolves along the curve C_0, afterwards the spin is flipped through fast π transformations, also called 180° pulses that swaps the eigenvectors $|0\rangle$ and $|1\rangle$. Then, the system evolves along the curve $\bar{C}_1$. Lastly another 180° pulse is applied. The same series of curves and π transformations can be used for a system with initial state $|1\rangle$. The total evolution can be viewed as follows:

$$|0\rangle \xrightarrow{C_0} e^{i(\alpha_0+\gamma_0)}|0\rangle \xrightarrow{\pi} e^{i(\alpha_0+\gamma_0)}|1\rangle \xrightarrow{\bar{C}_1} e^{i(\alpha_0+\alpha_1-\gamma_1+\gamma_0)}|1\rangle \xrightarrow{\pi} e^{i(\alpha_0+\alpha_1+2\gamma_0)}|0\rangle$$
$$|1\rangle \xrightarrow{C_1} e^{i(\alpha_1+\gamma_1)}|1\rangle \xrightarrow{\pi} e^{i(\alpha_1+\gamma_1)}|0\rangle \xrightarrow{\bar{C}_0} e^{i(\alpha_0+\alpha_1+\gamma_1-\gamma_0)}|0\rangle \xrightarrow{\pi} e^{i(\alpha_0+\alpha_1-2\gamma_0)}|1\rangle$$

The phase factor $\alpha_0 + \alpha_1$ is a global phase factor and has no physical significance. The relevant phase factor is double the geometric phase γ_0.. This method was used for the theoretical implementation of geometric gates ([29] and [82]) and was also done experimentally in nuclear magnetic resonance techniques ([40]).

Unconventional geometric quantum computation A new class of quantum phase gates were proposed by Zhu and Wang ([80]) and present a total phase with dynamical component non-zero, thus the name unconventional. Despite the non-vanishing dynamical phase, they proved that, for some systems, the dynamical phase is proportional to the geometric phase, i.e.,

$$\alpha_{dyn} = \eta\gamma_{geo}, \quad \eta \neq 0, -1.$$

This feature results in a phase gate that possess the same advantages of purely geometric quantum gates with the additional advantage of simplifying experimental operations, since it is not necessary to use the previous methods to eliminate the dynamical phase. The phase gate proposed in [80] was experimentally demonstrated by Liebfried et al. ([46]);

A controlled phase shift gate through geometric phase

The aim of the following part is to implement a controlled phase shift gate using the concept of geometric phase. As previously explained, a controlled phase shift gate is a two-qubit gate where one qubit is the target and the other one is the control qubit. Here, we consider the second qubit, or qubit b, as the control qubit, and the first one, qubit a, as the target qubit. The idea is that the state of the control qubit influences the phase acquired by the target qubit. In general lines, a quantum gate is represented by a unitary operation on the system. In the specific context of geometric quantum computation, a gate is implemented by an unitary operator U acting on the system such that

$$U : |\psi\rangle \mapsto e^{i\phi}|\psi\rangle$$

where ψ is the state vector of the system and ϕ is a phase factor. To The gate will be implemented using the rotating wave approximation ([29]) and the method described in Section 4.3 ([9], [10]).

Rotating wave approximation

Following the directions in [29], Section 4.2 described a system of two two-level quantum systems subjected to an external field, where the rotating wave approximation was considered, and interacting with each other. The Hamiltonian of the system is given by equation 4.2.21:

$$H = \frac{1}{2}\omega_a \sigma_3^{(a)} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \frac{1}{2}\omega_b \sigma_3^{(b)} + \frac{\pi}{2} J \sigma_3^{(a)} \otimes \sigma_3^{(b)}, \tag{5.2.3}$$

where ω_a and ω_b are the transition frequencies of each qubit and $\frac{\pi}{2} J \sigma_3^{(a)} \otimes \sigma_3^{(b)}$ models the interaction between the qubits. The setup is the following: the target qubit a acquires a geometric phase γ that depends on the transition probabilities

ω_+ and ω_- (equation 4.2.22) and the state of the control qubit b:

$$|11\rangle \xrightarrow{\omega_-} |01\rangle$$
$$|10\rangle \xrightarrow{\omega_+} |00\rangle.$$

Figure 4.2 shows the energy levels of the composite system. Now we consider that the qubit a is subjected to a rotating field that is slowly varied. The rotating field undergoes an adiabatic cyclic evolution. In Section 4.2 we obtained that the geometric phase acquired by the system depends on the transition probabilities and, for the case considered — a two two-level system with Hamiltonian given by 5.2.3 and a rotating field applied to the first system —, the geometric phase for the states of the computational basis is

$$|00\rangle : \gamma = \gamma_+ = \pi(cos(\theta_+ - 1)$$
$$|01\rangle : \gamma = \gamma_- = \pi(cos(\theta_- - 1)$$
$$|10\rangle : \gamma = -\gamma_+ = -\pi(cos(\theta_+ - 1)$$
$$|11\rangle : \gamma = -\gamma_- = -\pi(cos(\theta_- - 1)$$

where θ_+ and θ_- are given by equations 4.2.25 and 4.2.26, respectively. To eliminate the dynamical phase, the refocusing technique is used by applying a sequence similar to 5.2.2, but adapted for a system composed by two two-level systems:

$$C \rightarrow \pi_a \rightarrow \bar{C} \rightarrow \pi_b \rightarrow C \rightarrow \pi_a \rightarrow \bar{C} \rightarrow \pi_b\,, \tag{5.2.4}$$

where C is the cyclic evolution of the target qubit and π_a and π_b are 180° pulses applied to the target and control qubit, respectively. During the cyclic evolution $\bar{C}$ the state picks up a dynamical phase and the opposite geometric phase of C. The evolution of the state $|00\rangle$ upon the above sequence of operations is

$$|00\rangle \xrightarrow{C} e^{i(\alpha_{00}+\gamma_+)}|00\rangle \xrightarrow{\pi_a} e^{i(\alpha_{00}+\gamma_+)}|10\rangle \xrightarrow{\bar{C}} e^{i(\alpha_{00}+\gamma_+\alpha_{10}+\gamma_+)}|10\rangle \xrightarrow{\pi_b}$$
$$e^{i(\alpha_{00}+\alpha_{10}+2\gamma_+)}|11\rangle \xrightarrow{C} e^{i(\alpha_{00}+\alpha_{10}+\alpha_{11}+2\gamma_+-\gamma_-)}|11\rangle \xrightarrow{\pi_a} e^{i(\alpha_{00}+\alpha_{10}+\alpha_{11}+2\gamma_+-\gamma_-)}|01\rangle$$
$$\xrightarrow{\bar{C}} e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+2\gamma_+-\gamma_--\gamma_-)}|01\rangle \xrightarrow{\pi_b} e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+2\Delta\gamma)}|00\rangle$$

where α_{00}, α_{01}, α_{10} and α_{11} are the dynamical phases of the computational basis states $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$, respectively. From equations 4.2.25 and 4.2.26, the

phase shift $\Delta\gamma$ is defined as

$$\begin{aligned}\Delta\gamma &:= \gamma_+ - \gamma_- \\ &= \pi\left(\frac{\omega_+ - \omega}{[(\omega_+ - \omega)^2 + \omega_1^2]^{\frac{1}{2}}} - \frac{\omega_- - \omega}{[(\omega_- - \omega)^2 + \omega_1^2]^{\frac{1}{2}}}\right).\end{aligned} \tag{5.2.5}$$

Applying this same operations on each state of the computational basis, we get

$$\begin{aligned}|00\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+2\Delta\gamma)}|00\rangle \\ |01\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}-2\Delta\gamma)}|01\rangle \\ |10\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}-2\Delta\gamma)}|10\rangle \\ |11\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+2\Delta\gamma)}|11\rangle,\end{aligned}$$

and, since the contributions of the dynamical phases add up to a global phase, we can once again neglect it. This sequence of transformations and cyclic evolutions in 5.2.4 result on the operator

$$B(\Delta\gamma) = \begin{pmatrix} e^{21\Delta\gamma} & 0 & 0 & 0 \\ 0 & e^{-2i\Delta\gamma} & 0 & 0 \\ 0 & 0 & e^{-2i\Delta\gamma} & 0 \\ 0 & 0 & 0 & e^{2i\Delta\gamma} \end{pmatrix}, \tag{5.2.6}$$

that is essentially a purely geometric controlled phase shift gate, since the target qubit acquires a geometric phase depending on the state of the control qubit.

In [29], Ekert et al. obtained this controlled phase shift gate and also showed its fault-tolerance for determined choices of the amplitude of the oscillating field ω_1. Thus, a fault-tolerant geometric computation is possible and has already been implemented using nuclear magnetic resonance [40].

Perturbative solution for a two-level system driven by periodic fields

Now we apply the method developed in [9] and [10] and the results obtained in Section 4.3 to implement a geometric controlled phase shift gate. Analogously to the implementation accomplished by Ekert et al. ([29]), we consider a sequence of operations acting on the states of the computational basis. The sequence in question, based on the refocusing technique and described in 5.2.4, consists of cyclic evolutions C, $\bar{C}$ and pi transformations. The cyclic evolutions C and $\bar{C}$ have the

same period and the system acquires a dynamical phase.... After applying the sequence of operations described, the states of the computational basis acquires the following phase factors:

$$
\begin{aligned}
|00\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+\gamma_{00}+\bar{\gamma}_{01}+\bar{\gamma}_{10}+\gamma_{11})}|00\rangle \\
|01\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+\bar{\gamma}_{00}+\gamma_{01}+\gamma_{10}+\bar{\gamma}_{11})}|01\rangle \\
|10\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+\bar{\gamma}_{00}+\gamma_{01}+\gamma_{10}+\bar{\gamma}_{11})}|10\rangle \\
|11\rangle &\to e^{i(\alpha_{00}+\alpha_{01}+\alpha_{10}+\alpha_{11}+\gamma_{00}+\bar{\gamma}_{01}+\bar{\gamma}_{10}+\gamma_{11})}|11\rangle.
\end{aligned}
$$

The cyclic evolutions used in the refocusing technique must correspond to an initial and final state differing only by a phase factor. In Section 4.3 we studied the method developed in [9] and [10] to compute perturbative solutions for two-level quantum systems driven by periodic fields. Using this method, we also presented expressions for calculating the phase factors for a two-level quantum system and for a system composed of two two-level quantum systems. Since it is our goal to implement a controlled phase shift gate, we consider a two two-level system with dynamics given by 4.3.28 (non-interacting systems):

$$H_1^{(0)} = H_1^{(a)} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes H_1^{(b)},$$

where $H_1^{(a)}$ and $H_1^{(b)}$ are the Hamiltonians of the first and second systems acting on their respective Hilbert space $\mathcal{H}_a$ and $\mathcal{H}_b$. We also considered two systems with interaction given by 4.3.36

$$H_1(t) = H_1^{(a)} \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes H_1^{(b)} + \kappa v(t)\, \sigma_3^{(a)} \otimes \sigma_3^{(b)},$$

where κ is a real constant and $v(t)$ is a real function of time. For non-interacting systems, the time evolution operator is given by 4.3.49. For systems with interaction given by 4.3.52, the time evolution operator, up to first order of interaction, is obtained through 4.3.53. Using this time evolution operators, we calculated the probability $P(t)$

$$P(t) = |\langle \psi(0), U(t)\psi(0)\rangle|^2,$$

where $U(t)$ is the time evolution operator and $\psi(0)$ is the initial state of the system. We calculated $P(t)$ for each state of the computational basis. Figure 5.1 shows $P(t)$ as a function of time. We observe that the system returns to its initial state after a time $T_\Omega \cong 456 t_\omega$, where $t_\omega = 2\pi/\omega$. T_Ω is also obtained through $T_\Omega = 2\pi/\Omega$,

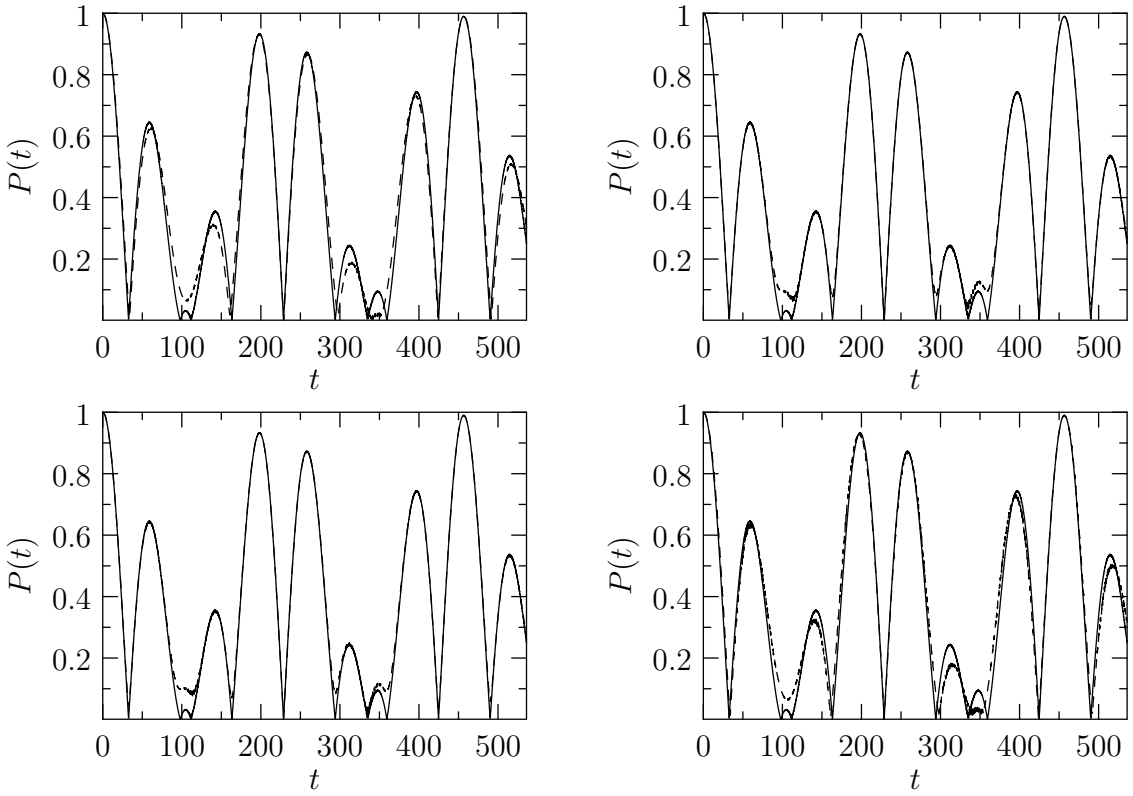


Figure 5.1: Probability of the system remaining in its initial state. Starting from the graph in the left column and first row, in clockwise order the graphs correspond to the initial states $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. The full line corresponds to non-interacting subsystems and the dashed line corresponds to an interaction of the form 4.3.52. The time is measured in units of $t_\omega = 2\pi/\omega$. The relevant constants of the systems are $\omega_a = 1.0$, $\omega_b = 2.0$, $\epsilon_a = \epsilon_b = 0.01$, $\kappa = 0.1$ and $t_0 = .16\, t_\omega$.

where Ω is the Rabi frequency and is calculated numerically. We considered a system with $\omega_a = 1.0$, $\omega_b = 2.0$, $\epsilon_a = \epsilon_b = 0.01$. The constants that determine the interaction are $\kappa = 0.1$ and $t_0 = 0.5 = 0.16\, t_\omega$. For this values, the correspondent Rabi frequency is $\Omega = 0.0022$, resulting in $T_\Omega \cong 456\, t_\omega$, as observed in Figure 5.1.

Once we determined the period that the system takes to return to its initial state (T_Ω), we can use the expressions for the phase factors in Section 4.3 (equations 4.3.32, 4.3.33, 4.3.50 and 4.3.51) to build a controlled phase shift gate. The considered system is composed of two subsystems subjected to periodic external fields, each characterized by ω_a and ω_b, respectively. Using equation 4.3.32 and 4.3.50, we can calculate the total phase factor of the composite system. Table 5.2 shows values of the total phase for a set of ω_a and ω_b values. Figure 5.2 shows the total phase

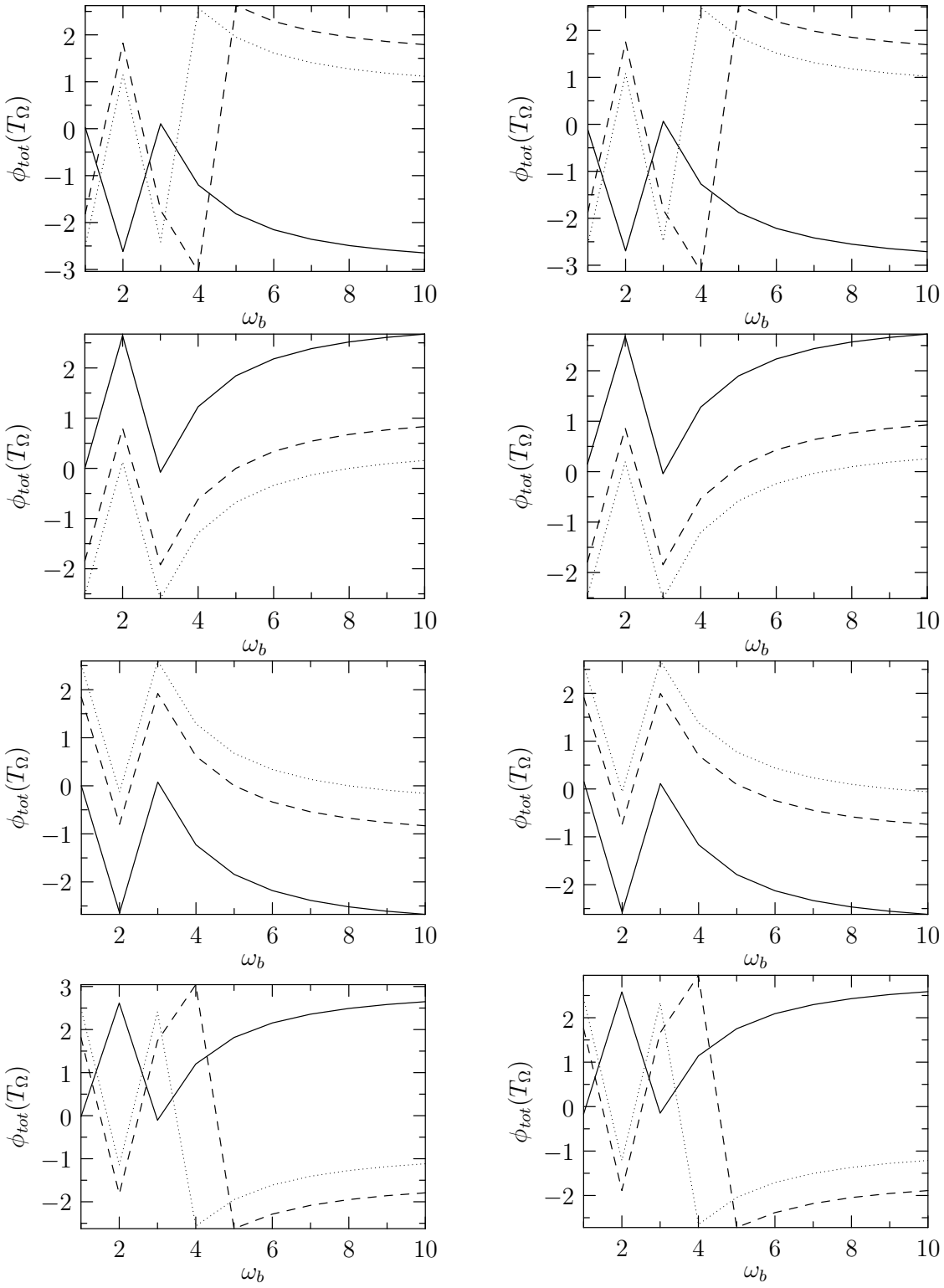


Figure 5.2: Total phase of the composite system as a function of ω_b for fixed values of ω_a. The parameters of the system are $\epsilon_a = \epsilon_b = 0.01$, $t_0 = 0.5$ and $\kappa = 0.1$. The full line corresponds to $\omega_a = 1.0$, the dashed line corresponds to $\omega_a = 5.0$ and the dotted line corresponds to $\omega_a = 8.0$. The left column corresponds to non-interacting systems, the right column corresponds to systems with an interaction modeled by a delta function. Each row corresponds to a state of the computational basis, from top to bottom: $|00\rangle$, $|01\rangle$, $|10\rangle$, $|11\rangle$.

	$\omega_b = 1.0$		$\omega_b = 5.0$		$\omega_b = 8.0$	
	$\phi_{tot}^{(0)}$	$\phi_{tot}^{(\delta)}$	$\phi_{tot}^{(0)}$	$\phi_{tot}^{(\delta)}$	$\phi_{tot}^{(0)}$	$\phi_{tot}^{(\delta)}$
$\|00\rangle$	0.027	-0.116	-1.816	-1.878	-2.491	-2.552
$\|01\rangle$	0.000	0.151	1.843	1.898	2.518	2.570
$\|01\rangle$	0.000	0.151	-1.843	1.790	-2.518	-2.466
$\|00\rangle$	-0.027	-0.116	1.816	1.752	2.491	2.429

Table 5.1: Values of the total phase ϕ_{tot} for each state of the computational basis, considering different values of ω_b and fixed $\omega_a = 1.0$. The subscript $\phi_{tot}^{(0)}$ and $\phi_{tot}^{(\delta)}$ indicate systems with no interaction and interaction given by a delta function, respectively. The values were obtained using equations 4.3.32 and 4.3.50. The other relevant constants of the system are: $\epsilon_a = \epsilon_b = 0.01$, $t_0 = 0.5$ and $\kappa = 0.1$.

as a function of ω_b for fixed values of ω_a, we see that the interaction preserves the behaviour of the total phase. We note that when $\omega_a = \omega_b$, we can write the following transformation:

$$B(\phi) = \begin{pmatrix} e^{i\phi} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{pmatrix}, \tag{5.2.7}$$

where ϕ is the total phase associated with the basis state $|00\rangle$. This transformation implements a conditional evolution of the basis states, we can say that 5.2.7 is a conditional phase gate in the sense that the state of one system influences the state of the other, although it does present the usual symmetric form of controlled phase shift gates. This gate is not purely geometrical, since the total phase factor involves both the dynamical and geometric phases. When $\omega_a \neq \omega_b$, the transformation on the basis state can no longer be represented by 5.2.7, as can be seen in Table 5.2.

Figure 5.3 shows the total phase as a function of ϵ_a and ϵ_b for fixed $\omega_a = \omega_b = 1.0$, $t_0 = 0.5$ and $\kappa = 0.1$. As was observed before, the behaviour of the total phase is not greatly affected by the interaction modeled by a delta function.

In the case considered by Ekert et al. ([29]), the dynamical phase is removed using the refocusing technique. This method not only relies on the approximation that the state vector evolves adiabatically, but the calculation of the dynamical phase for the state vector neglects the external field and only one of the systems is considered to be subjected to the external field. The system studied in Section 4.3

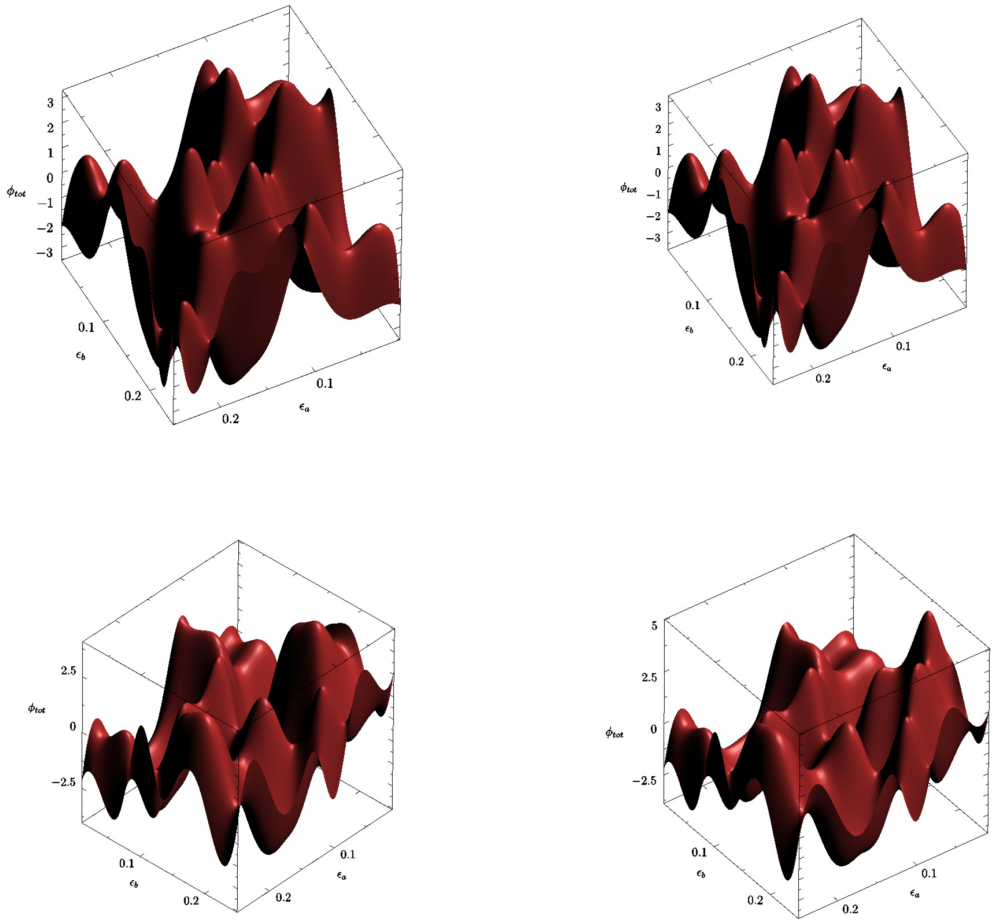


Figure 5.3: Total phase of the composite system as a function of ϵ_a and ϵ_b. The parameters of the system are $\omega_a = \omega_b = 1.0$, $t_0 = 0.5$ and $\kappa = 0.1$. The left column corresponds to two non-interacting system and the right column corresponds to systems with an interaction given by a delta function. The top row corresponds to the state $|00\rangle$ and the bottom row to the state $|01\rangle$.

does not consider the rotating wave approximation, nor the adiabatic evolution of the system along the cyclic trajectory, nor the systems must present different energy gaps. The resulting system presents stable solutions for the phase factors, but removing the dynamical contribution to the overall phase is not a straightforward task. When we consider two cyclic trajectories of the state vector for opposite field directions, as is considered in the refocusing technique, the dynamical phase does not cancel. This is due to the fact that the expressions 4.3.33 and 4.3.51 for the dynamical phase for non-interacting and for two systems with interaction modeled by a delta function were obtained already considering that both subsystems are subjected to a periodic external field. Among the several approaches to remove the dynamical phase, our next investigation will be finding a Hamiltonian that cancels the dynamical phase of the system along a cyclic trajectory.

Chapter 6

Conclusion

We presented various formulations of geometric phase in closed and open quantum systems and for most of them we illustrated the results in two-level quantum systems. This is motivated by the fact that qubits, the basic unit of quantum information, is a two-level quantum system. Hence, studying this simple system we can already obtain interesting results with a straightforward application. In particular, we used the results for a non-unitary evolution in the context of interferometry presented in [53] to obtain the phase factors for a two-level quantum system subjected to typical sources of decoherence (Section 3.3).

Our main contribution is using the method developed in [9] and [10] to obtain phase factors for a two-level quantum system and two two-level quantum systems interacting and non-interacting. This method presents a solution stable for long-time periods and the resulting phase factors also present this property. Our work can be extended in many ways. For example, using the method developed in [53] for non-unitary evolutions, it could be possible to obtain phase factors for a system subjected to a time-dependent perturbation; we could also use the time-evolution operator obtained in Section 4.3 in the Quantum Jump Approach. Also, further investigation of the result in Section 4.3 could be obtained by considering more terms on the Dyson expansion and considering other perturbation models, e. g., a constant perturbation.

The implementation of a quantum gate by Ekert et al. [29] invokes the rotating wave approximation (RWA) and is valid for an adiabatic evolution and, in the context of two two-level systems interacting, only one is subjected to an external time-dependent field. In our case, both systems are subjected to an external periodic field and neither the adiabatic approximation nor the rotating wave approximation

are necessary. Using the results for phase factors we were able to implement a controlled phase shift gate. The resulting gate is not purely geometrical. We are still investigating appropriate methods to remove the dynamical phase for the considered system. On the applicational side, more work is needed in the study of quantum error correction for the gates obtained and in the study of the possibility of physical realizations of the results obtained.

Appendix A

Details about the numerical implementation

In this appendix we review the numerical implementation of the method developed in [9] and [10] and explained in Section 4.3. The aim of the method is to obtain the time evolution operator given by 4.3.8:

$$U(t) = \begin{pmatrix} R(t)(1+ig_0S(t)) & -i\epsilon R(t)S(t) \\ -i\epsilon\overline{R(t)S(t)} & \overline{R(t)}(1-i\overline{g_0}\overline{S(t)}) \end{pmatrix}.$$

with

$$R(t) := \exp\left(-i\int_0^t (f(t')+g(t'))\,\mathrm{d}t'\right) \tag{A.0.1}$$

and

$$S(t) := \int_0^t R(t')^{-2}\,\mathrm{d}t'. \tag{A.0.2}$$

The function $g(t)$ is a particular solution of a differential equation (specifically the generalised Ricatti equation) and is obtained through the expansion

$$g(t) = \sum_{n=1}^{\infty} G^{(n)}(t)\epsilon^n, \tag{A.0.3}$$

where

$$G^{(n)}(t) := q(t)c_n(t)$$

with

$$q(t) := \exp\left(i\int_0^t f(t')\,\mathrm{d}t'\right) \tag{A.0.4}$$

and

$$c_n(t) = \sum_{m\in\mathbb{Z}} C_m^{(n)} e^{im\omega t}. \tag{A.0.5}$$

In order to compute $U(t)$, various Fourier expansions are made. The steps can be visualized in the "chain" reproduced from [10]:

$$\begin{array}{lllllll}
f(t) & \rightarrow & F_m & \rightarrow & Q_m, Q_m^{(2)} & \rightarrow & \alpha_n \\
 & & & & & & \downarrow \\
H_m & \leftarrow & \Omega & \leftarrow & G_m^{(n)}, g_0 & \leftarrow & C_m^{(n)} \\
\downarrow & & & & & & \\
W_m, W_m^{(-2)} & \rightarrow & R_m, S_m & \rightarrow & R(t), S(t) & \rightarrow & U(t).
\end{array}$$

Now, we proceed to explain each of the elements of the "chain" above. The first element is the time-dependent perturbation $f(t)$ that appears in the Hamiltonian of the system (equation 4.3.4). In our case, $f(t)$ is given by equation 4.3.11

$$f(t) = A\cos(\omega t),$$

where A and ω are real constants. Then, we decompose $f(t)$:

$$f(t) = \sum_{n=0}^{\infty} F_n e^{im\omega t} = \sum_{a=1}^{2J} f_a e^{in_a\omega t} \tag{A.0.6}$$

where F_n are the Fourier coefficients of $f(t)$, $J \geq 1$ is a natural number and $n_1, n_2, \ldots, n_{2J} \neq 0$ are integers. Considering our specific perturbation, we have

$$\begin{aligned}
f_1 = f_2 &= \frac{A}{2}, \\
n_1 &= -n_2 = -1.
\end{aligned}$$

The next elements are the Fourier coefficients Q_m and $Q_m^{(-2)}$ of the functions $q(t)$ and $q(t)^2$, respectively:

$$\begin{aligned}
q(t) &= \sum_{m\in\mathbb{Z}} Q_m e^{im\omega t}, & Q_m &= \mathcal{K}_m(1); \\
q(t)^2 &= \sum_{m\in\mathbb{Z}} Q_m^{(-2)} e^{im\omega t}, & Q_m^{(-2)} &= \mathcal{K}_m(2).
\end{aligned}$$

Both can be obtained through the function $\mathcal{K}_m(\kappa)$:

$$\mathcal{K}_m(\kappa) = e^{i\kappa\gamma_f} \sum_{p_1,\ldots,p_{2J}=0}^{\infty} \delta(P,m) \prod_{a=1}^{2J} \left[\frac{1}{p_a!} \left(\frac{\kappa f_a}{n_a \omega} \right)^{p_a} \right],$$

where $\gamma_f := i\sum_{a=1}^{2J}(f_a/n_a\omega)$, $P := \sum_{b=1}^{2J} p_b n_b$ and $\delta(P,m)$ is the usual Kronecker delta. In our case, we have $\gamma_f = 0$ amd $P = p_1 - p_2$. The above expression yields

$$\mathcal{K}_m(\kappa) = \sum_{p_1=0}^{\infty} \frac{(-1)^{p_1}}{p_1!(m+p_1)!} \left(\frac{\kappa A}{2\omega} \right)^{2p_1+m} = J_m\left(\frac{\kappa A}{2\omega} \right).$$

where J_m is the Bessel function of first kind and of order m. So, the coefficients are $Q_m = J_m(A/2\omega)$ and $Q_m^{(-2)} = J_m(A/\omega)$. Our code is initialized by defining these coefficients, since the previous steps are analytical.

The next element of the "chain" is α_n. Here, we refrain to say that these elements are constants that have closed forms and are a by-product of the expansion of $g(t)$ (equation A.0.3).

The coefficients $C_m^{(n)}$ of $c_n(t)$ (equation A.0.5) also have closed forms. We refer the reader to [10] in order to get the exact expressions for these coefficients, It suffices to say that we used those expressions to calculate numerically the coefficients and each $c_n(t)$ is calculated with coefficients $C_m^{(n)}$ with m ranging from -25 to 25.

We then proceed to calculate the coefficients of the expansion of $g(t)$. We can write equation A.0.3 as

$$\begin{aligned} g(t) &= \sum_{n=1}^{\infty} G^{(n)}(t)\epsilon^n \\ &= \sum_{n=1}^{\infty} q(t)c_n(t)\epsilon^n \\ &= \sum_{n=1}^{\infty} \left(\sum_{m\in\mathbb{Z}} Q_m e^{im\omega t} \right) \left(\sum_{p\in\mathbb{Z}} C_p^{(n)} e^{ip\omega t} \right) \epsilon^n \\ &= \sum_{n=1}^{\infty} \left(\sum_{m\in\mathbb{Z}} G_m^{(n)} e^{im\omega t} \right) \epsilon^n, \end{aligned}$$

where $G_m^{(n)} = \sum_{p\in\mathbb{Z}} Q_{m-p} C_p^{(n)}$ is obtained by the convolution of $q(t)$ and $c_n(t)$. This coefficient is the next fucntion to be calculated in our code. The constant g_0 is

obtained by simply setting $g_0 = g(0)$ in the expression above. The Rabi frequency is given by

$$\Omega = \sum_{n=1}^{\infty} G_0^{(n)} \epsilon^n. \tag{A.0.7}$$

It is useful to expand the function $W(t) := \exp(-i \int_0^t g(\tau)\, \mathrm{d}\tau)$:

$$W(t) = e^{-i\Omega T} \sum_{m\in\mathbb{Z}} W_m e^{im\omega t}, \tag{A.0.8}$$

since the functions $R(t)$ and $S(t)$ involve $W(t)$. To determine the coefficients of $W(t)$, we first define H_m:

$$H_m = \begin{cases} 0, & \text{if } x = 0; \\ \frac{G_m(\epsilon)}{m\omega}, & \text{if } x \neq 0. \end{cases} \tag{A.0.9}$$

Next, we define

$$\mathcal{W}_m(\kappa) = e^{i\kappa\gamma_f(\epsilon)} \left(w_m + \sum_{p=1}^{\infty} \frac{(-\kappa)^{p+1}}{(p+1)!} \sum_{n_1,\ldots,n_p\in\mathbb{Z}} H_{n_1} \ldots H_{n_p} H_{m-N_p} \right), \tag{A.0.10}$$

where $\gamma_f(\epsilon) := i\sum_{m\in\mathbb{Z}} H_m$, $w_m = -\kappa H_m$ for $m \neq 0$ and $w_0 = 1$, and $N_p := \sum_{a=1}^{p} n_a$. The sums involving p in A.0.10 ranged from 1 to 4 and the sums involving $n_1, \ldots, n_p$, as the other sums over integers, ranged from -25 to 25.

Using the fact that $R(t) = \overline{q}(t)W(t)$, we expand $R(t)$:

$$R(t) = e^{-i\Omega T} \sum_{m\in\mathbb{Z}} R_m e^{im\omega t}, \tag{A.0.11}$$

where the coefficients R_m are given by the convolution

$$R_m = \sum_{p\in\mathbb{Z}} \overline{Q_{p-m}} W_p, \tag{A.0.12}$$

with $W_m = \mathcal{W}_m(1)$. The same proceeding is followed to obtain the coefficients of the expansion of $S(t)$ (more details can be obtained in [10]):

$$S(t) = \sigma_0 + e^{2i\Omega t} \sum_{m\in\mathbb{Z}} S_m e^{im\omega t}, \tag{A.0.13}$$

with

$$S_m := -i \frac{R_m^{(-2)}}{m\omega + 2\Omega}, \tag{A.0.14}$$

and

$$\sigma_0 := -\sum_{m\in\mathbb{Z}} S_m. \tag{A.0.15}$$

The coefficient $R_m^{(-2)}$ comes from the expansion of $R(t)^{-2} = e^{2i\Omega t}\sum_{m\in\mathbb{Z}} R_m^{(-2)} e^{im\omega t}$, and is given by the convolution $R_m^{(-2)} = \sum_{p\in\mathbb{Z}} Q_{m-p}^{(2)} W_p^{(-2)}$, with $W_m^{(-2)} = \mathcal{W}_m(-2)$ for all $m \in \mathbb{Z}$.

Finally, we have all the elements of the chain and the time evolution operator $U(t)$ can be numerically calculated. So far, all steps were followed as indicated in [9] and [10]. We must again note that all the Fourier cofficients with sums over the integers were taken within the range $m = -25, \ldots, 25$. The sum involving p in A.0.10 ranges from 1 to 4. We initially considered $p = 1, \ldots, 5$, but the calculation time was long and the results for the unitarity test for $p = 1, \ldots, 4$ were considered accurate enough, as Figure 4.3 in Section 4.3 shows.

The calculation of the phase factors for one two-level system is simple: the total phase is given by 4.3.18 and its implementation is straightforward. The dynamical phase, given by 4.3.23, however, depends on a series of integrations of Fourier series. These integrations were analytically obtained and then implemented in the code, resulting in various summations. As explained in Section 4.3, we chose not to use an integration routine, since the functions to be integrated are highly oscillatory and we would have to test several routines and estimate respective errors. The analytical approach presents only the machine error. For two two-level systems, the phase factors were obtained analytically and implemented in the code using equations 4.3.32, 4.3.33 and 4.3.34 for non-interacting systems and equations 4.3.50 and 4.3.51 for systems with an interaction given by a delta function.

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