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# The Parametric Representation of an Open Quantum System

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# *Abstract*

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## **The Parametric Representation of an Open Quantum System**

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In this thesis work, we developed an exact approach, dubbed parametric representation, to describe any open quantum system. The description associates to the couple “open system-environment” a set of pure states, parametrized by a variable representing the environmental degrees of freedom, whose occurrence is ruled by a probability distribution defined over the space containing such variable. The parametric representation acquires a surplus value when the environmental degrees of freedom are mapped into a continuous variable, in particular when univocally obtained through an algorithm that starts from the identification of the relevant dynamical group for the environment to produce the set of generalized coherent states, therefore implying that such variable is a point in an accordingly defined environmental phase space. As a first outcome, the usage of coherent states yields the possibility to straightforwardly obtain the classical limit of the environment; this in turn means to define such a limit without affecting the quantum character of the open system: the formalism yields, from a composite system, a closed but not isolated one, where the parameters appearing in the local Hamiltonian are related to the environmental and original global system configuration. Moreover, the state of the open system assumes in parametric representation a natural interpretation in terms of vector fiber bundles, so that a relevant part of the work has been devoted to the presentation of various aspects of differential geometry necessary to understand the construction. Thanks to such premises, the parametric representation eventually establishes a strict relationship between the entanglement pertaining to the original composite state and the geometric phase proper to the derived semiclassical description, as extensively presented in the application of the formalism to the physical situation of the spin-star with frustration.



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# Physical Constants

Planck's constant  $\hbar = 1$



# Symbols

|                                       |                                                                        |
|---------------------------------------|------------------------------------------------------------------------|
| $\mathcal{H}$                         | Hilbert spaces                                                         |
| $ \Psi\rangle$                        | state of a tensor product Hilbert space                                |
| $\rho$                                | density matrix                                                         |
| $\mathcal{D}(\mathcal{H})$            | space of density matrices defined over the Hilbert space $\mathcal{H}$ |
| $ \phi\rangle$                        | pure state of the principal system                                     |
| $H$                                   | Hamiltonian operators and functions                                    |
| $U(t; t_0)$                           | Unitary evolution operators                                            |
| $[, ]$                                | commutator (or Lie Brackets)                                           |
| $\mathcal{T}$                         | time-ordered product                                                   |
| $\Phi(t; t_0)$                        | dynamical map                                                          |
| $M, N$                                | differentiable manifolds                                               |
| $U_i$                                 | open subsets of a differentiable manifold                              |
| $\phi_i$                              | coordinate functions and local trivializations                         |
| $\psi_{ij}$                           | transition functions                                                   |
| $C^\infty$                            | set of infinitely differentiable functions                             |
| $S^2$                                 | two dimensional sphere                                                 |
| $(\theta, \varphi)$                   | $S^2$ polar angles                                                     |
| $T_p M$                               | tangent space at a point $p$ of a differentiable manifold $M$          |
| $\mathfrak{F}(M)$                     | set of functions over $M$                                              |
| $\mathfrak{X}(M)$                     | set of vector fields over $M$                                          |
| $f_*$                                 | differential map                                                       |
| $T_p^* M$                             | cotangent space at a point $p$ of a differentiable manifold $M$        |
| $\langle, \rangle, \langle   \rangle$ | inner products                                                         |
| $d$                                   | exterior derivative                                                    |
| $f^*$                                 | pullback map                                                           |
| $\mathfrak{T}(M)$                     | set of tensors over $M$                                                |
| $\Omega(M)$                           | set of differential forms over $M$                                     |
| $\iota_X$                             | interior product along the vector field $X$                            |
| $G$                                   | (Lie) Group                                                            |

|                                                |                                                                                            |
|------------------------------------------------|--------------------------------------------------------------------------------------------|
| $L_a, R_a$                                     | left and right action of a Lie group                                                       |
| $e$                                            | identity element of a group                                                                |
| $\mathfrak{g}$                                 | Lie algebra                                                                                |
| $E \xrightarrow{\pi} M$ or $(E, \pi, M, F, G)$ | fiber bundles                                                                              |
| $\pi$                                          | projection in a fiber bundle                                                               |
| $t_{ij}(p)$                                    | transiion functions in a fiber bundle                                                      |
| $g_i(p)$                                       | gauge transformations                                                                      |
| $s_i(p)$                                       | section over $U_i$                                                                         |
| $V_u P, H_u P$                                 | horizontal and vertical subspaces at a point $u$                                           |
| $\mathcal{A}_i$                                | local connection forms                                                                     |
| $\mathfrak{P}$                                 | path ordering operator                                                                     |
| $\nabla$                                       | covariant derivative                                                                       |
| $\varepsilon$                                  | dimensionless parameter such that $0 \leq \varepsilon < 1$                                 |
| $\sigma_*(t)$                                  | part of the spectrum of a $t$ -dependent Hamiltonian                                       |
| $P_*(t)$                                       | projection operator over $\sigma_*(t)$                                                     |
| $C_b^2(\mathbb{R}, \mathcal{L}_{sa})$          | set of two times continuously differentiable and bounded functions from $\mathbb{R}$ to th |
| $\mathbb{1}_{\mathcal{H}}$                     | identity operator on $\mathcal{H}$                                                         |
| $\Re, \Im$                                     | real and imaginary parts of a complex number                                               |
| $\sigma$                                       | set of the three Pauli matrices                                                            |
| $\mathbf{B}$                                   | magnetic field                                                                             |
| $\Delta_x$                                     | Laplacian operator in the coordinate $x$                                                   |
| $\mathcal{L}$                                  | Lesbegue spaces                                                                            |
| $\nabla_x$                                     | gradient operator in the coordinate $x$                                                    |
| $(q, p)$                                       | canonical coordinates                                                                      |
| $(\mathbf{r}, \mathbf{R})$                     | electronic and nuclear coordinates                                                         |
| $\chi(\mathbf{R})$                             | nuclear wavefunctions                                                                      |
| $\Pi$                                          | parametric representation projection onto the variable                                     |
| $\chi$                                         | parametric representation amplitudes                                                       |
| $ \Phi_0\rangle$                               | reference state                                                                            |
| $H_i, E_\alpha$                                | Cartan basis                                                                               |
| $\hat{T}(g), \hat{g}$                          | representations of an element $g$                                                          |
| $\Omega$                                       | point in the quotient space $G/F$ generating generalized coherent states                   |
| $D(\Omega), \hat{\Omega}$                      | generalized displacement operator                                                          |
| $ \Omega\rangle$                               | generalized coherent state                                                                 |
| $d\mu(\Omega)$                                 | measure on the space $\{ \Omega \}$                                                        |
| $\{ , \}_{PB}$                                 | Poisson brackets                                                                           |
| $g_n(\Omega)$                                  | holomorphic section in the coherent state line bundle                                      |
| $O_Q(\Omega)$                                  | $Q$ -representation of an observable $O$ onto the space $\{ \Omega \}$                     |
| $\mathbf{S}$                                   | environmental total spin operator                                                          |

---

|                                        |                                                                           |
|----------------------------------------|---------------------------------------------------------------------------|
| $\mathbf{J}, J$                        | total angular momentum operator and relative eigenvalue                   |
| $\tilde{S}$                            | $= S + \frac{1}{2}$ , $S$ being the eigenvalue relative to $\mathbf{S}^2$ |
| $M$                                    | total angular momentum component along the quantization axis              |
| $\theta_M$                             | defined by $\cos \theta_M = \frac{M}{\tilde{S}}$                          |
| $ \uparrow\rangle,  \downarrow\rangle$ | qubit eigenstates of the spin operator along the quantization axis        |
| $\mathcal{E}$                          | Von Neumann entropy                                                       |
| $p(\theta)$                            | latitude probability distribution                                         |
| $(\Theta, \Phi)$                       | Bloch sphere variables                                                    |
| $\hat{\mathbf{n}}$                     | unit vector in real space                                                 |
| $\gamma_i$                             | Berry's phase relative to the $i$ -th energy level                        |





*A mio padre*



# Chapter 1

## Introduction: Open Quantum Systems

Since its early development in the Twenties of the past century, Quantum Mechanics (QM) has been raising a large amount of problems about its interpretation as a physical theory of *reality*, the latter point being still subject of intense debate among scientific community members. Indeed, QM postulates imply a sharp conceptual separation between what is to be considered as a physical *state* and, on the other hand, what the *observables* are; in particular, the possibility that an observation abruptly perturbs the otherwise unitary dynamics of the state of the system (the so called wavefunction collapse) is still not explainable within the very structure of the theory but nevertheless is at the hearth of its predictive power. Though conceptually difficult to accept, it is therefore necessary to postulate this behaviour. Since this in turn implies the existence of an observer, any quantum system has to be embedded in some sort of (at least conceptual) environment in order to refine the view of reality that emerges from QM. Moreover, if the fundamental description of microscopic objects through QM is to be trusted, the passage from a quantum and *coherent* world to the classical non-coherent one which people experience in everyday life remains obscure, though great efforts have been done in this sense, see *e.g.* the famous paper by Zurek[1].

Besides these logical difficulties, any system apart from the whole universe is *not isolated* and *does* have a physical environment, which in most cases cannot be ignored in order to capture the essential phenomenology, and consequently has to be somehow characterized in the overall analysis: *open quantum systems* (OQS) are purely quantum physical systems whose behaviour is described taking into account their relationship with a suitably chosen (and accordingly described) environment. The interest towards the behaviour of OQS has recently acquired new stimulus in the context of quantum

information theory and quantum computation[2], where the same quantum mechanical features that make quantum computation so appealing, such as the quantum *coherence*, are extremely fragile and tend to be nullified by the influence of the environment, so that understanding the possible correlations between the principal system and its environment, especially in terms of *entanglement* if the environment is quantum too, is a crucial issue for these kind of studies. In order to introduce some basic terminology, we remark that the adjective “open” is usually devoted to the case where both the open system (also referred to as *principal*) and the environment are described in a quantum mechanical fashion[3]: in such cases, the description of the open system is commonly obtained by the *reduced density matrix* approach[2, 3], and is axiomatically exact. Nevertheless, there exist another, intermediate situation, where the principal system is under the effect of a local Hamiltonian depending on external and possibly time-dependent parameters, whose presence testifies the existence of a surrounding environment. At the heart of this approach stands the approximation that the environment be classical, so that the operators acting on its Hilbert space are replaced by c-number parameters; in this way, the interaction Hamiltonian is reduced to an effectively local one for the sole principal system: in such description the quantum system is usually referred to as *closed*.

This thesis work provides a framework, dubbed *parametric representation* and alternative to the reduced density matrix one, capable of exactly describing an open quantum system under the general assumption that the latter is actually a subsystem of a larger, fully quantum one, the remainder being its environment and, at the same time, of yielding an interpolating scheme between the two descriptions above denoted as “open” and “closed”. The thesis is structured as follows: the first, introductory chapter is devoted to a brief recall of the main features of the reduced density matrix approach, both from the state structure (paragraph 1.1) and dynamical perspective (paragraph 1.2); in chapter 2 we gather all the formal aspects and mathematical tools pertaining to the development of our formalisms: indeed, the parametric representation, and in particular its continuous version, is heavily characterized by the geometry underlying its very construction. The central chapters 3 and 4 are those containing the original part of the work and deal with, respectively, the abstract formulation of the parametric representation and a first, prototypical usage of it; finally, in chapter 5 we draw the conclusions and propose some further applications and extensions of our work.

## 1.1 Composite and Open systems

Quantum Mechanics postulates that when two quantum systems have to be considered as parts of a larger quantum systems, the possible states describing the latter belong

to the tensor product of the Hilbert spaces of the former ones. In order to fix the notation, let us denote the Hilbert spaces of the systems to be composed by  $\mathcal{H}_{\text{open}}$ , obviously intending that pertaining to the open system, and by  $\mathcal{H}_{\text{env}}$  the environmental one. Thus, a state  $|\Psi\rangle$  in the Hilbert space  $\mathcal{H} \equiv \mathcal{H}_{\text{open}} \otimes \mathcal{H}_{\text{env}}$  of the composite system “open  $\cup$  env” can be generally written as

$$\mathcal{H} \ni |\Psi\rangle = \sum_{\alpha n} c_{\alpha n} |\alpha\rangle \otimes |n\rangle , \quad (1.1)$$

where  $\{|\alpha\rangle\} \in \mathcal{H}_{\text{open}}$  and  $\{|n\rangle\} \in \mathcal{H}_{\text{env}}$  are local, orthonormal bases for the subsystem Hilbert spaces, and the coefficients  $c_{\alpha n}$  must satisfy  $\sum_{\alpha n} |c_{\alpha n}|^2 = 1$  in order to have a normalized global state  $|\Psi\rangle$ . From the tensor product structure of eq. (1.1) it is immediate to notice that there are states of  $\mathcal{H}$  which *cannot* be written as a tensor product of a vector in  $\mathcal{H}_{\text{open}}$  and a vector in  $\mathcal{H}_{\text{env}}$ . Those states are called *entangled*, and have no counterpart in classical physics; however, in such cases the notion of physical state of either subsystem can still be given in terms of a *reduced density operator*. In fact, to a given a pure state  $|\Psi\rangle \in \mathcal{H}$  it is always associated a projector  $\rho \equiv |\Psi\rangle\langle\Psi|$  in the space of density operators  $\mathcal{D}(\mathcal{H})$  on  $\mathcal{H}$ <sup>1</sup>; then, the reduced density operator  $\rho_{\text{open}}$  which expresses the “state” of the open system is defined as

$$\rho_{\text{open}} \equiv \text{Tr}_{\text{env}} \rho . \quad (1.2)$$

The symbol  $\text{Tr}_{\text{env}}$  means to perform the *partial trace* over the environmental degrees of freedom, *i.e.*, for example choosing the basis  $\{|n\rangle\} \in \mathcal{H}_{\text{env}}$ ,

$$\text{Tr}_{\text{env}}[\cdot] \equiv \sum_n \langle n | \cdot | n \rangle . \quad (1.3)$$

It is immediate to see, however, that the result of the partial trace operation does not depend on the basis chosen to perform it. In this language, if the original state  $|\Psi\rangle$  is entangled, the reduced density operator  $\rho_{\text{open}}$  is not a projector in the sense that  $\rho_{\text{open}} \neq |\phi\rangle\langle\phi|$  for any  $|\phi\rangle \in \mathcal{H}_{\text{open}}$ : in general,  $\rho_{\text{open}}$  defines a *mixed state*. Notice that  $\rho_{\text{open}}$  is a density operator on  $\mathcal{H}_{\text{open}}$ ,  $\rho_{\text{open}} \in \mathcal{D}(\mathcal{H}_{\text{open}})$ , meaning that it is positive definite, and has trace equal to one.

The reason why  $\rho_{\text{open}}$  defined as in eq. (1.2) represents the physical state of the open system is that it can be used to reproduce the correct expectation values for local observables. In fact, given a measure of a local observable  $A_{\text{open}}$  for the principal system, it is natural to require that the possible outcomes for this measure must be the same

---

<sup>1</sup>The following line of argument is correct starting from a generic density operator, *i.e.* not necessarily associated to a pure state (but still positive and with trace equal to one), but for the remainder this straightforward generalization would never be actually used.

as those relative to the *trivial* extension onto the total system of the same observable, which is defined as

$$A \equiv A_{\text{open}} \otimes \mathbb{1}_{\text{env}} , \quad (1.4)$$

$\mathbb{1}_{\text{env}}$  being the identity on  $\mathcal{H}_{\text{env}}$ . This means, in turn, to require that expectation values of  $A$  calculated on  $\rho$  and of  $A_{\text{open}}$  on  $\rho_{\text{open}}$  must be the same, or

$$\text{Tr}(\rho A) \equiv \langle A \rangle = \langle A_{\text{open}} \rangle_{\text{open}} \equiv \text{Tr}_{\text{open}}(\rho_{\text{open}} A_{\text{open}}) ; \quad (1.5)$$

it is immediate to notice that the definition of the reduced state  $\rho_{\text{open}}$ , eq. (1.2), ensures that this equality holds.

If, as we assumed, the composite system  $\mathcal{H}$  is bipartite and described by a pure state  $|\Psi\rangle$ , plenty of equivalent entanglement measures are available (see, *e.g.*, [4] for a nice review about the subject); at the hearth of this equivalence stands the existence of a very simple as well as very powerful algebraic property that pertains to the tensor product structure (1.1). Namely, the following famous theorem[5] holds.

**Theorem 1.1** (Schmidt's theorem). *For any pure state  $|\Psi\rangle \in \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ , there exist two local orthonormal bases  $\{|1_i\rangle\} \in \mathcal{H}_1, \{|2_i\rangle\} \in \mathcal{H}_2$  such that<sup>2</sup>:*

$$|\Psi\rangle = \sum_{i=1}^N \sqrt{\lambda_i} |1_i\rangle \otimes |2_i\rangle , \quad (1.6)$$

where  $N \equiv \min(\dim(\mathcal{H}_1), \dim(\mathcal{H}_2))$ .

Schmidt's theorem ensures that, given a *particular* state  $|\Psi\rangle$ , there exists a “canonical” local basis in each subsystem Hilbert space thanks to which the double sum in (1.1) is replaced by a single sum that, moreover, only involves, at most, a number of elements equal to the dimension of the smallest Hilbert space in the tensor product. The coefficients  $\lambda_i$ , called *Schmidt's coefficients*, are nonnegative, immediately satisfy  $\sum_i \lambda_i = 1$  and are the eigenvalues of the reduced density operator of *both* subsystems: they form the so-called *Schmidt simplex*[6], which is the “skeleton” of all entanglement measures for such  $|\Psi\rangle$ . In particular, the number  $r$  of non-zero Schmidt coefficients is called *Schmidt rank*,  $r \leq N$ , and a state  $|\Psi\rangle$  is separable if and only if  $r = 1$  since  $r$  is also the rank of the reduced density operator, and  $r = 1$  implies for the reduced density operator to be a projector. Notice that in the above line of reasoning we have not to specify which subsystem is considered.

Among all the entanglement measures of the composite state  $|\Psi\rangle \in \mathcal{H}$  (again, with respect to the bipartition  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ ), we mention a very useful one, namely the *Von*

---

<sup>2</sup>switching to a more abstract notation 1,2 to denote the subsystems in order to emphasize the complete generality of the statement

Neumann entropy (see [7] or [8] for a general reference textbook)

$$\mathcal{E}_{12}(\rho) \equiv -\text{Tr}_1 \rho_1 \log \rho_1 = -\text{Tr}_2 \rho_2 \log \rho_2 = -\sum_{i=1}^r \lambda_i \log \lambda_i , \quad (1.7)$$

where  $r$  is again the Schmidt rank, and where the basis of the log function only affects the upper limit of the entropy:  $\mathcal{E}$  ranges from zero for separable states to  $\log r$  for *maximally mixed states*  $\rho_* \equiv \frac{\mathbb{1}}{r}$  and for whatever basis of the log, so that if  $\log = \log_r$  the maximal Von Neumann entropy is normalized to one.

## 1.2 Open Quantum System dynamics

In the previous section we saw that the states of an open quantum system with Hilbert space  $\mathcal{H}_{\text{open}}$  cannot in general be written as pure states  $|\phi\rangle \in \mathcal{H}_{\text{open}}$  due to the tensor product postulate, and we briefly presented the “usual” reduced density operator formalism adopted to overcome such impossibility. An even more dramatic modification occurs when the dynamics of the open quantum system is considered: in this section, we recall some basic aspects concerning such issue.

Let us start by recalling that isolated and closed quantum systems dynamics is *unitary* and is completely specified by the Hamiltonian of the system  $H(t)$  though the Schrödinger equation

$$i \frac{dU(t; t_0)}{dt} = H(t)U(t; t_0), \quad U(t_0; t_0) = \mathbb{1}_{\mathcal{H}} , \quad (1.8)$$

where the evolution operator  $U(t; t_0)$ , that acts on elements of  $\mathcal{H}$ , satisfies  $UU^\dagger = U^\dagger U = \mathbb{1}$ . Notice that eq.(1.8) is a first order differential equation that admits a unique solution, which can be written in the general form

$$U(t; t_0) = \mathcal{T} \exp \left( -i \int_{t_0}^t d\tau H(\tau) \right) , \quad (1.9)$$

where the symbol  $\mathcal{T}$  denotes the time-ordering; given the evolution operator  $U(t; t_0)$ , a pure state  $|\phi(t_0)\rangle \in \mathcal{H}$  evolves to  $\mathcal{H} \ni |\phi(t)\rangle = U(t; t_0) |\phi(t_0)\rangle$ . The evolution is also linear; this implies that, if for some reason the state of the system at the initial time  $t_0$  has to be considered as a mixed state  $\rho(t_0)$ <sup>3</sup>, the unitary evolution also yields

$$\rho(t) = U(t; t_0) \rho(t_0) U^\dagger(t; t_0) \equiv \mathcal{U}(t; t_0)(\rho(t_0)) = \mathcal{T} \exp \left( \int_{t_0}^t d\tau \mathcal{L}(\tau) \right) \rho(t_0) , \quad (1.10)$$

---

<sup>3</sup>for instance, it has been coupled in the past to another system, the latter having been discarded before the evolution initial time  $t_0$

where the operator  $\mathcal{U}(t; t_0)$ , defined by the first equality, acts on the space  $\mathcal{D}(\mathcal{H})$  of the density matrices on  $\mathcal{H}$ , while in the second equality the operator  $\mathcal{L}(\tau)$  is called *Liouville operator* and is defined by

$$\mathcal{L}(\tau)(\cdot) \equiv -i[H(\tau), \cdot] , \quad (1.11)$$

again acting on elements of  $\mathcal{D}(\mathcal{H})$ . We remark that, at this level, eq. (1.10) is simply a different way of writing eq. (1.9), still describing a unitary dynamics.

The dynamics of an open quantum system is radically different from that of a closed one. Indeed, let us suppose that the composite system is isolated, undergoing unitary dynamics; if at the initial time  $t_0$  the global state is  $|\Psi(t_0)\rangle$ , the initial state for the open system is given by

$$\rho(t_0) \equiv \text{Tr}_{\text{env}} |\Psi(t_0)\rangle \langle \Psi(t_0)| . \quad (1.12)$$

The unitary evolution for  $|\Psi\rangle$  implies that, at any later time  $t$ , the global state is given by  $|\Psi(t)\rangle = U(t; t_0) |\Psi(t_0)\rangle$ ; in turn, this means that the reduced density matrix of the open system has evolved to

$$\rho(t) = \text{Tr}_{\text{env}} (|\Psi(t)\rangle \langle \Psi(t)|) = \text{Tr}_{\text{env}} \left( U(t; t_0) |\Psi(t_0)\rangle \langle \Psi(t_0)| U^\dagger(t; t_0) \right) . \quad (1.13)$$

Implicitly, eqs. (1.12)-(1.13) defines the so-called *dynamical map*  $\Phi(t; t_0)$  that maps the initial open system state  $\rho(t_0)$  into  $\rho(t)$  as

$$\rho(t) \equiv \Phi(t; t_0)(\rho(t_0)) , \quad (1.14)$$

and is the analogue of  $\mathcal{U}(t; t_0)$  in (1.10); the deep difference now occurring is that, in general,  $\Phi(t; t_0)$  does also depend on the initial state  $\rho(t_0)$  on which it acts. Indeed, let us write the initial global state projector  $|\Psi(t_0)\rangle \langle \Psi(t_0)|$  as

$$|\Psi(t_0)\rangle \langle \Psi(t_0)| \equiv \rho(t_0) \otimes |\text{env}\rangle \langle \text{env}| + \rho_{\text{corr}}(t_0) , \quad (1.15)$$

where in the first addend a separable term is singled out from the remainder. It is immediate to show that the *ansatz* (1.15) implies for the evolved principal system state the interesting characterization

$$\rho(t) = \sum_n K_n(t; t_0) \rho(t_0) K_n^\dagger(t; t_0) + \Delta\rho(t; t_0) , \quad (1.16)$$

where  $K_n(t; t_0) \equiv \langle n | U(t; t_0) | \text{env} \rangle$ , and  $\Delta\rho(t; t_0) \equiv \text{Tr}_{\text{env}} (U(t; t_0) \rho_{\text{corr}}(t_0) U^\dagger(t; t_0))$ . Thus, the open system evolved state is a sum of a term  $\sum_n K_n(t; t_0) \rho(t_0) K_n^\dagger(t; t_0)$ , originating from the separated part of the initial state (1.15), where the operators  $\{ K_n(t; t_0) \}$  describing the dynamics are independent of  $\rho(t_0)$ , and a correlated evolution  $\Delta\rho(t; t_0)$ .



As a result, for initial uncorrelated states of the form

$$|\Psi(t_0)\rangle \langle \Psi(t_0)| \equiv \rho(t_0) \otimes |\text{env}\rangle \langle \text{env}| , \quad (1.17)$$

the open system dynamics is generally characterized by<sup>4</sup>:

$$\rho(t) = \sum_n K_n(t; t_0) \rho(t_0) K_n^\dagger(t; t_0), \quad \sum_n K_n^\dagger(t; t_0) K_n(t; t_0) = \mathbb{1} , \quad (1.18)$$

where the last condition means that the trace of the evolved reduced density operator remains equal to one. We are thus naturally led to the notion of *universal dynamical map* (UDM), namely an evolution map  $\Phi(t; t_0) : \rho(t_0) \mapsto \rho(t) \equiv \Phi(t; t_0)\rho(t_0)$  for the open system that does *not* depend on the state on which it acts (see, *e.g.*, [6, 9]); as we see in eq. (1.18), the most general form of a universal dynamical map is given by eq. (1.18). Actually, also the converse statement is true, in the sense that if a dynamical map is universal, it must have been induced from a separable initial form.

The importance for a dynamical map of being universal is essentially given by the fact that universal dynamical maps evolve any physical state into another physical state; the latter statement is mathematically expressed as follows.

1.3 (UDM properties). For each  $(t; t_0)$ , an universal dynamical map  $\Phi$  such that  $\rho(t) = \Phi(t; t_0)(\rho(t_0))$  satisfies

- $\text{Tr}\Phi(\rho) = 1$ , namely it is trace preserving, ensuring the probability interpretation for the evolved  $\Phi(\rho)$ .
- $\Phi$  is a *convex linear map* so that  $\Phi(\sum_i p_i \rho_i) = \sum_i p_i \Phi(\rho_i)$  for any probability distribution  $p_i$ . This property ensures that if the initial density operator is defined as  $\rho = \sum_i p_i \rho_i$ , so that the “actual” initial state is randomly selected from an ensemble  $\{ p_i, \rho_i \}$ , the quantum operation  $\Phi$  allows a correct implementation of Bayes rule of conditioned probability on the final state.
- The map is *completely positive*, *i.e.*  $\Phi(\rho)$  is positive for any  $\rho \in \mathcal{D}(\mathcal{H}_{\text{open}})$  and, moreover, if one appends to  $\rho$  any state  $\sigma$  belonging to another system  $\mathcal{D}(\mathcal{H}_{\text{env}})$  of arbitrary dimensionality, the image of the extended map  $(\Phi \otimes \mathbb{1}_{\text{env}})(\rho \otimes \sigma)$  remains positive.

The last property of complete positivity deserves a little further comment: obviously, a physical state must be described by a positive definite density matrix; complete positivity is a stronger statement than simple positivity, but actually a very welcome one since

<sup>4</sup>actually, the general form 1.18 also holds for the wider class of initial states of the form  $\rho_{\text{TOT}}(t_0) = \rho(t_0) \otimes \sigma_{\text{env}}(t_0)$ ,  $\rho(t_0)$  and  $\sigma_{\text{env}}(t_0)$  being generic mixed states of the respective subsystems.

we should expect a physical evolution for both the open system and its trivial global extension irrespective to the environment dimensionality. From the above discussions, it should be clear that the form (1.18) implies the just stated properties. Again, also the converse is true, a result embodied in the famous *Kraus* theorem[10].

**Theorem 1.2** (Kraus Theorem). *A map  $\Phi$  satisfies the properties 1.3 if and only if it can be written in the form*

$$\Phi(\rho) = \sum_n K_n \rho K_n^\dagger, \quad \sum_n K_n^\dagger K_n = \mathbb{1} \quad (1.19)$$

where the set of operators  $\{ K_n \}$  are called *Kraus operator*.

Summing up, for a generic composite system evolution, the reduced dynamics is universal (in the sense that the operator that makes evolve the initial state to any other later times does not depend on the state itself) if and only if it can be written in the Kraus form or, equivalently, if the initial composite state is in a tensor product form. By the same line of arguments, however, a problem immediately arises when dealing with the compositions of the reduced evolutions. Let us suppose, indeed, that the dynamical map  $\Phi(t; t_0)$  rules the evolution starting from the initial time  $t_0$ , thus mapping  $\rho(t_0)$  into a physical  $\rho(t)$ ; if one considers instead of  $t$  an intermediate time  $s$ ,  $t_0 < s < t$ , then the state  $\Phi(s; t_0)(\rho(t_0)) \equiv \rho(s)$  is again a physical state, but is in general correlated, as in eq. (1.15). In turn, this means that the evolution from  $s$  to  $t$  is *not* ruled by a universal dynamical map, namely, that the composition rule

$$\Phi(t; t_0) = \Phi(t; s)\Phi(s; t_0) \quad (1.20)$$

cannot hold for a generic UDM  $\Phi(a; b)$ . This behaviour reflects itself in the impossibility to write a differential equation for the open system evolution, which is *reversible* and local in time, unlike the closed case (see the Schrödinger eq. (1.8)); put in a different way, the state of an open system at a certain time  $t$  depends on the whole history of its past evolution, not only on the previous configuration at  $t - \delta t$ . On the other hand, the property (1.20), called *Markovianity* or *divisibility*, can be assumed for the sake of simplification: clearly, the resulting dynamics is always only an approximation of the true one, but with the advantage that the reduced dynamics evolution turns out to be written as a “simple” differential equation for the density operator.

Without entering much in detail, we recall without proof that the most general form of the equation governing the reduced dynamic if the Markovianity condition (1.20) holds is given by a first-order differential equation, the so-called *Markovian master equation*,

which can be written in the canonical form (see, *e.g.*, [9] and references therein)

$$\frac{d\rho(t)}{dt} = -i[H(t), \rho(t)] + \sum_k \gamma_k(t) \left( L_k(t)\rho(t)L_k^\dagger(t) - \frac{1}{2}\{L_k^\dagger(t)L_k(t), \rho(t)\} \right), \quad (1.21)$$

with  $H(t)$  self-adjoint,  $\{L_k(t)\}$  generic time-dependent operators and  $\{\gamma_k(t) \geq 0\}$  positive time-dependent coefficients. The result (1.21) is an extension of the famous Gorini-Kossakowsky-Sudarshan-Lindblad master equation (GKSL)[11, 12], derived with the assumption that the dynamical map satisfy, in addition to (1.20),  $\Phi(t; t_0) = \Phi(t - t_0 = \tau)$ , so that (1.20) becomes

$$\Phi(\sigma + \tau) = \Phi(\sigma)\Phi(\tau). \quad (1.22)$$

Condition (1.22) is the so-called *quantum dynamical semigroup* property (indeed, it is not a group since the inverse of  $\Phi$  is not generally a UDM), and provides for the reduced dynamics the same form of (1.21), with the only difference that all the operators and the coefficients become time-independent:

$$\frac{d\rho(t)}{dt} = -i[H, \rho(t)] + \sum_k \gamma_k \left( L_k\rho(t)L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho(t)\} \right). \quad (1.23)$$

To conclude, from a physical perspective, the formal condition of Markovianity (also in the homogeneous case (1.22)) can be assumed in order to give a simplified version of the reduced dynamics as in (1.21), but obviously the validity of such an assumption strongly depends on the considered specific model. We refer to [3, 9] for a detailed discussion of the physical assumptions that ensure that conditions (1.20)-(1.22) hold within a good degree of approximation, and simply mention that, besides the strength of the interaction between the open system and its environment, the typical time scales over which the latter correlation functions decay play a fundamental role in this sense.



## Chapter 2

# Mathematical background: Differential Geometry and Adiabatic theory

Since its very beginning, the study of QM has always been intimately related to the development and subsequent usage of mathematical tools capable of structuring the physical theory in a rather simple and elegant fashion: indeed, Hilbert space theory was formulated *ad hoc* and provides together with the representation theory of symmetry groups a solid setting for the whole Copenhagen formulation of QM. On the other hand, OQS study does not need to be founded on a completely different (nor substantially more involved) mathematical language than closed QM; nonetheless even when challenging quite simple problems concerning the classification of states, maps, correlation measures and so on, it is quite natural to resort to geometric techniques to clarify the relationship among these objects. In this sense, geometry is regarded as a powerful tool to “visualize” the OQS structure [6]. In addition, as we shall see in chapters 3 and 4, the original part of this thesis work is greatly concerned with some geometrical and physical-mathematical topics which deserve a little more detailed exposition.

We therefore dedicate this chapter to a self-contained description of most of the formal aspects we will refer to in the development of our work. The chapter is divided into two main parts: the first one recalls some results due to the mathematical field of *differential geometry* (mainly referring to [13] and [14]), while in the second part we move to a more “physical” setting and briefly present a quite recent formulation of the *adiabatic theory* (see, *e.g.*, [15] and [16]). In doing this, we exploit the tools being developed to introduce the concept of *geometric phase* which will play an important role in the original part of the thesis.

## 2.1 Differential Geometry

In this section we want to schematically present some basic aspects of differential geometry. First of all, we should define what differential geometry *is*; loosely speaking, differential geometry is the study of *manifolds*, which are the generalization of curves and surfaces to arbitrary dimension  $m$ , and how the usual calculus on  $\mathbb{R}^m$  can be implemented on them. Then we present probably the most important class of manifold adopted in physics, that is *Lie groups*. At the end of the section we employ the whole machinery presented in these paragraphs to define a more sophisticated mathematical object, the *fiber bundle*, which, besides being the key concept to rigorously formulate *gauge theories*, is the proper tool to describe geometric phases.

### 2.1.1 Differentiable Manifolds: basic concepts

As we anticipated in the introduction, differentiable manifolds are the generalization of curves ( $\dim = 1$ ) and surfaces ( $\dim=2$ ) to arbitrary dimension  $m$ . Since the goal of differential geometry is to implement the standard calculus on  $\mathbb{R}^m$  on them, it is natural to require *by definition* that manifolds should *locally* “look like”  $\mathbb{R}^m$ . To make this intuition more precise, let’s proceed with the definition.

**Definition 2.1** (Differentiable manifold). A topological space  $M$  of dimension  $m$  is said to be a **differentiable manifold** if the following requirements are satisfied:

1.  $\exists \{ U_i \}$  that covers  $M$ , *i.e.*  $\bigcup_i U_i = M$ , and a corresponding set of homeomorphisms<sup>1</sup>  $\{ \phi_i \} : U_i \rightarrow U'_i \subset \mathbb{R}^m$ ;
2. given the intersection  $U_i \cap U_j$ , the map  $\psi_{ij} \equiv \phi_i \circ \phi_j^{-1} : \phi_j(U_i \cap U_j) \rightarrow \phi_i(U_i \cap U_j)$  is  $C^\infty$  (infinitely differentiable).

The pair  $(U_i, \phi_i)$  is called **chart** while the whole set  $\{ (U_i, \phi_i) \}$  is an **atlas**; the map  $\phi_i$  is the **coordinate** of a point  $p \in U_i \subset M$  and takes value in an open subset of  $\mathbb{R}^m$  (we shall usually write its image as  $\phi_i(p) = (x^1(p), \dots, x^m(p)) = \{ x^\mu(p), \mu = 1 \dots m \} \in \mathbb{R}^m$ ): they specify in what sense the manifold  $M$  is locally equivalent to  $\mathbb{R}^m$ . The second requirement in definition 2.1 ensures that the transition from one system of coordinates to another is *smooth*, and the maps  $\psi_{ij}$  ruling such transition are consequently called *transition functions*; notice that the differentiability is defined in the usual sense of calculus on  $\mathbb{R}^m$  (see also Fig. 2.1). In order to clarify this simple but very important

<sup>1</sup>a homeomorphism is a bijective map  $f : X \rightarrow Y$  between two topological spaces  $X$  and  $Y$ , which is moreover continuous with inverse  $f^{-1} : Y \rightarrow X$  continuous, too.

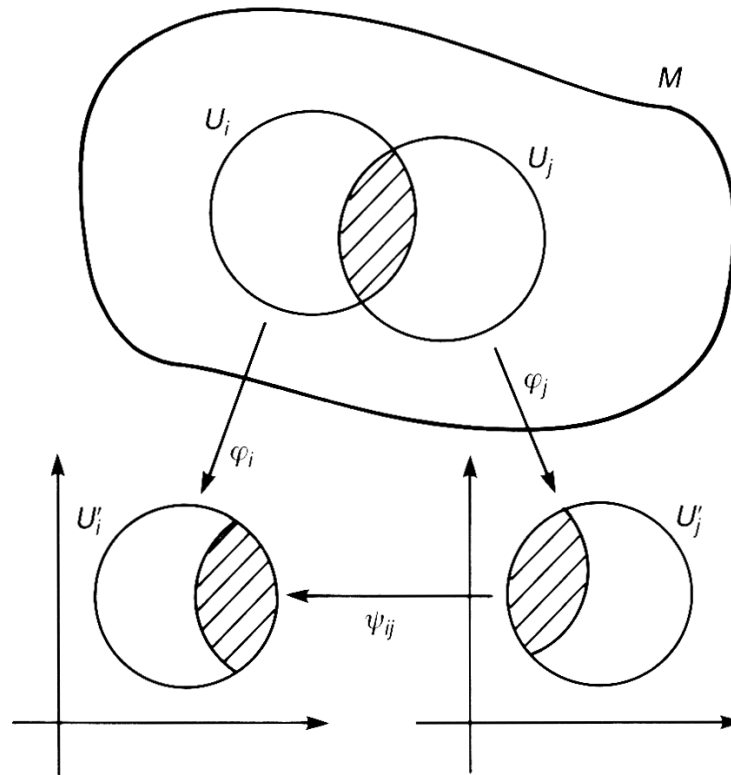


FIGURE 2.1: Differentiable manifold

An illustration of the definition 2.1 of a differentiable manifold, which schematically depicts the coordinate  $\phi_i$  and transition  $\psi_{ij}$  functions. - *Original Figure in [13]*

definition, we present in quite a detail an example which will be of central interest for our whole work.

**Example 2.1** (The  $S^2$  spherical surface). *The spherical surface of unit radius in real space (or, 2-sphere) is a prototypical example of differentiable manifold. As everyone knows, it is defined as*

$$S^2 = \{ (x, y, z) \in \mathbb{R}^3 \mid x^2 + y^2 + z^2 = 1 \} ; \quad (2.1)$$

*a common way to give a coordinate system on it is by specifying the two polar angles  $(\theta, \varphi)$  as*

$$x = \sin \theta \cos \varphi, \quad y = \sin \theta \sin \varphi, \quad z = \cos \theta \quad (2.2)$$

*with  $\theta$  running from 0 to  $\pi$  and  $\varphi$  from 0 to  $2\pi$ . As it is well known, the coordinate  $(\theta, \varphi) \subset \mathbb{R}^2$  is not well defined everywhere (recall, for example, that at the “North Pole”  $(0, 0, 1)$  the longitude  $\varphi$  is not defined at all), in this sense the homeomorphism between the spherical surface and  $\mathbb{R}^2$  breaks down; in other words, the sphere looks like  $\mathbb{R}^2$  only locally.*

Another way to define coordinates on  $S^2$  is given by the so-called stereographic projection, obtained by taking the intersection between the equatorial plane and a line connecting one of the poles (say, the North Pole) and a given point  $P = (x, y, z)$  on the 2-sphere. The resulting point  $(X, Y) = \phi_N(P)$  on the equatorial plane is ( $X$  and  $Y$  are Cartesian components parallel to the original  $x$  and  $y$  axes):

$$X = \frac{x}{1-z}, \quad Y = \frac{y}{1-z} \quad (2.3)$$

This coordinate system is well defined except at the North Pole; we can cover the entire sphere by taking another coordinate system as the stereographic projection from the South Pole  $(U, V) = \phi_S(P)$ , which reads (we take the  $V$  axis opposite to the  $Y$  axis as in Fig. 2.2):

$$U = \frac{x}{1+z}, \quad V = \frac{-y}{1+z} \quad (2.4)$$

It is not difficult to compute the transition functions  $\psi_{NS}$  from the South patch  $(U, V)$

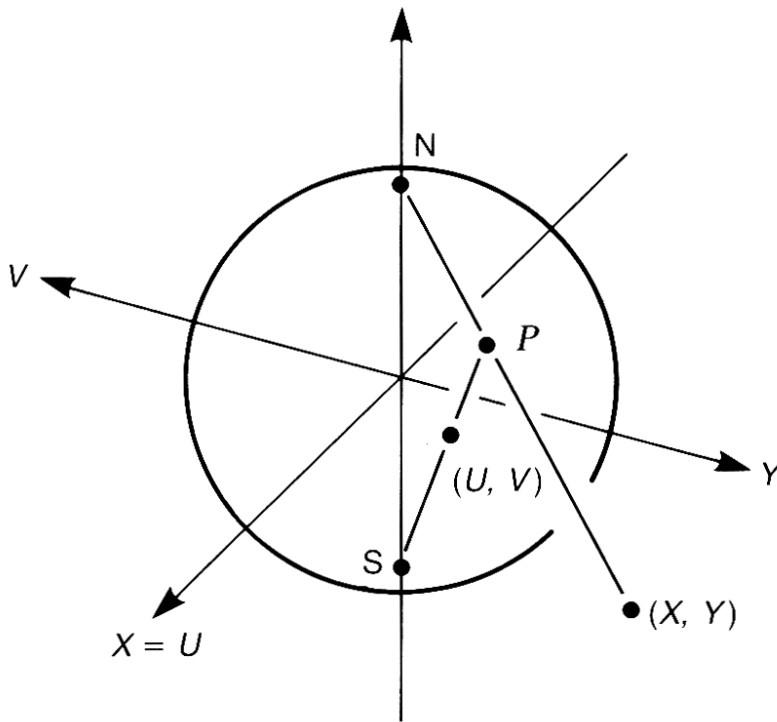


FIGURE 2.2: Stereographic projection

Stereographic projections of a point on  $S^2$  from both the Poles. - Original Figure in [13]

to the North patch  $(X, Y)$ , with the result:

$$X = \frac{U}{U^2 + V^2}, \quad Y = \frac{-V}{U^2 + V^2}, \quad (2.5)$$



which are obviously  $C^\infty$ <sup>2</sup>.

We end this paragraph by providing a natural definition regarding the properties that maps between manifolds should possess in order to preserve the differential structure given on the latters. The quite natural answer resides in the following

**Definition 2.2** (Diffeomorphism). Consider a map  $f : M \rightarrow N$  between two manifolds  $M$  and  $N$  (of dimension, respectively,  $m$  and  $n$ ), such that  $U \ni p \mapsto f(p) \in V$ , where  $(U, \phi)$  is a chart in  $M$  and  $(V, \psi)$  is a chart in  $N$ . In local coordinates the map reads  $f_c \equiv \psi \circ f \circ \phi^{-1} : \mathbb{R}^m \rightarrow \mathbb{R}^n$ . We say that  $f$  is **differentiable** or **smooth** at  $p$  if its coordinate presentation  $f_c$  is  $C^\infty$ .

If, moreover,  $f : M \rightarrow N$  is a homeomorphism,  $f_c$  is invertible and  $f_c^{-1}$  is  $C^\infty$ , too, then  $f$  is called **diffeomorphism**, and  $M$  and  $N$  are said to be **diffeomorphic**.

If two manifolds are diffeomorphic we shall write  $M \equiv N$ ; clearly the requirements on  $f_c^{-1}$  also imply  $\dim(M) = \dim(N)$ . By comparison with the definition 2.1, it is immediate to notice that a coordinate transformation (or reparametrization) is a diffeomorphism from  $M$  into itself; we shall denote the class of diffeomorphisms on  $M$  by  $\text{Diff}(M)$ .

### 2.1.2 Vectors, flows, and Lie derivatives

*Vectors* are central objects to implement the calculus on a manifold; in order to define what vectors are, we need a couple of preliminary notions:

**Definition 2.3.** A **curve**  $c$  on a manifold  $M$  is a injective map  $c : \mathbb{R} \supset (a, b) \rightarrow M$  from an open interval  $(a, b) \subset \mathbb{R}$  (including the 0 for convenience) to  $M$ . A **function**  $f$  on a manifold  $M$  is a smooth map  $f : M \rightarrow \mathbb{R}$ . We denote the set of functions on  $M$  by  $\mathfrak{F}(M)$ .

We immediately notice that these two definitions are in some sense complementary; the coordinate representation of a curve is just a map  $\{x^\mu(t)\} : \mathbb{R} \rightarrow \mathbb{R}^m$  (a curve in  $\mathbb{R}^m$ ), while that of a function is simply a real-valued function  $f(x^1, \dots, x^m)$  of  $m$  variables. Vectors are now defined as the directional derivative of a function  $f$  along a curve  $c$  at some point  $p$  on  $M$ . To be more explicit:

**Definition 2.4** (Tangent vector). With the previous notation, let  $p = c(0)$ . The **tangent vector** at  $p$  along  $c$  is a differential operator  $X_{p,c}$  that when applied to a function

<sup>2</sup>except on  $(0, 0)$  where the transition functions are not defined.

$f$  at the point  $p$  gives the directional derivative of the function itself along the curve  $c$ . In formulas, the directional derivative at  $p$  is:

$$\left. \frac{df(c(t))}{dt} \right|_{t=0} \xrightarrow{\text{coord.}} \left. \frac{\partial f}{\partial x^\mu} \frac{dx^\mu(c(t))}{dt} \right|_{t=0} \equiv \frac{\partial f}{\partial x^\mu} X^\mu, \quad (2.6)$$

where the last equality defines  $X^\mu \equiv dx^\mu(c(t))/dt|_{t=0}$ ; putting all together

$$\left. \frac{df(c(t))}{dt} \right|_{t=0} = X_{p,c}[f] \quad \text{with } X_{p,c} = X^\mu \frac{\partial}{\partial x^\mu}. \quad (2.7)$$

Thus, given a chart, a vector is specified by  $\{X^\mu\}$  which are the derivatives of the coordinate presentation of the curve  $c$  at  $p$ ; nevertheless, by definition it is clear that a vector does *not* depend on the choice of coordinates. It is immediate to show that, once another set of coordinate  $\{y^\mu\}$  is adopted, the vector components transform as

$$X = X^\mu \frac{\partial}{\partial x^\mu} = Y^\mu \frac{\partial}{\partial y^\mu}, \quad \text{with } Y^\mu = X^\nu \frac{\partial y^\mu}{\partial x^\nu} \quad (2.8)$$

The set of all distinct vectors at  $p$  forms a vector space, called **tangent space** at  $p$  and denoted by  $T_p M$ ; clearly,  $\dim(T_p M) = \dim M$ . A smooth assignment of a vector to each point  $p \in M$  is called **vector field**; it can be characterized, as well, in the following way: given a generic function  $f \in \mathfrak{F}(M)$ ,  $X$  is a vector field if  $X[f] \in \mathfrak{F}(M)$ . Conversely, given a vector field  $X$  on  $M$  (whose set will be denoted by  $\mathfrak{X}(M)$ ), its restriction to a point  $p$ , namely  $X|_p$ , is a tangent vector belonging to  $T_p M$ .

As known from the theory of ordinary differential equations (ODE) on  $\mathbb{R}^m$ , a vector field generates a *flow* in the space  $M$  where the vector field is defined.

**Definition 2.5** (Flow). Let's denote by  $x(t) \in M$  the (coordinate presentation of) a curve whose tangent vector at  $x(t)$  is  $X|_{x(t)}$ . This implies the following ODE:

$$\frac{dx^\mu}{dt} = X^\mu(x(t)) \quad (2.9)$$

Given an initial condition  $x(0) = x_0 \in M$ , ODE theory ensures that there always exists for some time  $t > 0$  a solution to (2.9), which we denote by  $\sigma(t, x_0)$ <sup>3</sup>, so that

$$\frac{d\sigma^\mu(t, x_0)}{dt} = X^\mu(\sigma(t, x_0)), \quad \text{with } \sigma^\mu(0, x_0) = x_0^\mu; \quad (2.10)$$

the map  $\sigma : \mathbb{R} \times M \rightarrow M$  is called **flow** generated by  $X$ .

<sup>3</sup>we introduce the new symbol  $\sigma$  to distinguish it from the curve  $x(t)$ , which is a map *only from*  $\mathbb{R}$  to  $M$  and in this sense *does not* depend on the initial condition  $x_0$ .

We now anticipate some group-theoretic arguments that we'll deal with in more detail in paragraph 2.1.4. Again recurring to the theory of ODE, it is simple to show that a flow satisfies  $\sigma(t, \sigma(s, x)) = \sigma(t + s, x)$ ; this in turn enables us to think at the flow as a *one-parameter group of transformations*. Indeed, fixing  $t$ , the map  $\sigma_t : M \rightarrow M$  is a diffeomorphism satisfying the group-like properties

1. composition:  $\sigma_t(\sigma_s(x)) = \sigma_{t+s}(x)$ , or  $\sigma_t \circ \sigma_s = \sigma_{t+s}$ ;
2. identity:  $\sigma_0(x) = x$ ;
3. inverse  $\sigma_{-t}(x) = (\sigma_t(x))^{-1}$ .

By solving the differential equation (2.10) in the neighborhood of  $x_0$ , we can write for small  $t \equiv \varepsilon$

$$\sigma_\varepsilon^\mu(x) = x^\mu + \varepsilon X^\mu, \quad (2.11)$$

so that  $X^\mu$  is regarded as the *infinitesimal generator* of the group transformation  $\sigma_t$ .

Finally, we conclude the paragraph by introducing the notion of *Lie derivative*. Lie derivative is an operation that allows us to compute the infinitesimal change of a generic vector  $Y$  at some point  $x$  along a flow  $\sigma(\varepsilon, x)$  associated to another vector  $X$  (again for small  $\varepsilon$ ). The difference between  $Y|_x$  and  $Y|_{x' \equiv \sigma_\varepsilon(x)}$  is ill defined since they belong to different tangent spaces, resp.  $T_x M$  and  $T_{x'} M$ . To avoid this inconvenience, let's first notice that any map  $f : M \rightarrow N$  induces a natural mapping, called **differential map**, between the tangent spaces, which we denote by  $f_* : T_p M \rightarrow T_{f(p)} N$ . Indeed, taking  $g \in \mathfrak{F}(N)$ ,  $g \circ f \in \mathfrak{F}(M)$  and hence a vector  $V \in T_p M$  can act on  $g \circ f$  to give its directional derivative. Then, the differential map  $f_*$  is just defined as

$$(f_* V)[g] \equiv V[g \circ f] \quad (2.12)$$

It is simple to show that, choosing coordinates in  $M$  and  $N$  in such a way that  $V = V^\mu \frac{\partial}{\partial x^\mu}$  and  $(f_* V) = W^\alpha \frac{\partial}{\partial y^\alpha}$ , the relationship between the components is just

$$W^\alpha = V^\mu \frac{\partial y^\alpha}{\partial x^\mu}, \quad (2.13)$$

the factor  $\frac{\partial y^\alpha}{\partial x^\mu}$  being the Jacobian of the map  $f$ .

Using the differential map, we are now able to “transport back”  $Y|_{x'}$  to  $T_x M$  by  $(\sigma_{-\varepsilon})_* : T_{x'} M \rightarrow T_x M$  and then compute the Lie derivative.

**Definition 2.6** (Lie derivative). The **Lie derivative** of a vector  $Y$  along the flow generated by  $X$  at some point  $x \in M$  is given by

$$\mathcal{L}_X Y \equiv \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} [(\sigma_{-\varepsilon})_* Y|_{\sigma_\varepsilon(x)} - Y_x] \quad (2.14)$$

A straightforward calculation shows that in local coordinates eq. (2.14) becomes (from now on we adopt the convention  $\frac{\partial}{\partial x^\mu} = \partial_\mu$ )

$$\mathcal{L}_X Y = (X^\mu \partial_\mu Y^\nu - Y^\mu \partial_\mu X^\nu) \partial_\nu . \quad (2.15)$$

Another way to express the Lie derivative is by means of the so called **Lie bracket**. Given two vector fields  $X$  and  $Y$ , the Lie bracket is a binary operation  $[\cdot, \cdot] : \mathfrak{X}(M) \times \mathfrak{X}(M) \rightarrow \mathfrak{X}(M)$  defined by

$$[X, Y][f] = X[Y[f]] - Y[X[f]] \quad \forall f \in \mathfrak{F}(M) ; \quad (2.16)$$

it is possible to prove that  $[X, Y]$  is itself a vector field on  $M$ , given exactly by

$$[X, Y] = \mathcal{L}_X Y . \quad (2.17)$$

From its definition *via* eq. (2.16), three important properties immediately follow:

1. Lie bracket is linear in both the arguments:  $[X, aY + bZ] = a[X, Y] + b[Y, Z]$  and  $[aX + bY, Z] = a[X, Z] + b[Y, Z]$ ;
2. it is skew-symmetric:  $[X, Y] = -[Y, X]$ ;
3. it satisfies the *Jacobi* identity:  $[[X, Y], Z] + [[Y, Z], X] + [[Z, X], Y] = 0$ .

As a last remark, we point out that Lie bracket has a simple geometrical interpretation: it indeed measures the *non commutativity* of the flows generated by the vectors it applies to. Let  $\sigma^\mu(t, x)$  and  $\tau^\mu(t, x)$  be the flows generated, respectively, by  $X$  and  $Y$ . Starting from  $x$  and moving first along  $\sigma$  for a small time interval  $\varepsilon$  and then along  $\tau$  for an interval  $\delta$  one arrives at a point  $x_1$  whose coordinates are computed by the composite flow  $\tau^\mu(\delta, \sigma(\varepsilon, x))$ ; if the flows are followed in the opposite order but for the same infinitesimal times, the arrival point  $x_2$  has coordinates  $\sigma^\mu(\varepsilon, \tau(\delta, x))$ . The infinitesimal expression for the flows, eq. (2.11), makes easy to see that

$$\tau^\mu(\delta, \sigma(\varepsilon, x)) - \sigma^\mu(\varepsilon, \tau(\delta, x)) = \varepsilon \delta [X, Y] \quad (2.18)$$

and that the arrival points coincide, that is  $x_1 = x_2$ , if and only if  $[X, Y] = 0$ .

### 2.1.3 Differential forms and (a bit of) integration

Differential forms play a fundamental role in developing the calculus on differentiable manifolds since, loosely speaking, they are the proper objects one can “integrate”. Unlike vector fields, one can define forms of any degree  $r = 1, \dots, m = \dim(M)$ , but for  $r = 1$  forms are in one-to-one correspondence with vectors as they are defined starting from the usual *dual* construction of the vector space  $T_p M$ .

**Definition 2.7** (One-form). Let  $T_p M$  be the tangent space at  $p \in M$  and consider its dual space  $T_p^* M$ , that is the space of linear operators  $T_p^* M \ni \omega : T_p M \rightarrow \mathbb{R}$ .  $T_p^* M$  is for obvious reasons called **cotangent space**, and  $\omega$  is a dual vector, or **one-form**.

The adjective “differential” can be easily understood as the simplest example of one-forms is just the differential of a function  $f \in \mathfrak{F}(M)$ . Denoting by the symbol  $\langle \cdot, \cdot \rangle : T_p^* M \times T_p M \rightarrow \mathbb{R}$  the action of a one form on a vector, which is called **inner product**, one can simply define for each vector  $V \in \mathfrak{X}(M)$

$$\langle df, V \rangle \equiv V[f] = V^\mu \frac{\partial f}{\partial x^\mu} \in \mathbb{R} \quad (2.19)$$

Since in local coordinates  $df = \partial_\mu f dx^\mu$ ,  $\{ dx^\mu \}$  is the coordinate local basis for  $T_p^* M$  with the obvious property

$$\left\langle dx^\mu, \frac{\partial}{\partial x^\nu} \right\rangle = \frac{\partial x^\mu}{\partial x^\nu} = \delta_\nu^\mu, \quad (2.20)$$

and a generic one-form  $\omega$  can be expressed as  $\omega = \omega_\mu dx^\mu$ . Its action on a vector  $V = V^\nu \partial_\nu$  therefore reads

$$\langle \omega, V \rangle = \omega_\mu V^\mu. \quad (2.21)$$

Analogously to the vector case, the one-form components must obey a consistency transformation equation which can be easily proven to be

$$\tilde{\omega}_\nu = \omega_\mu \frac{\partial x^\mu}{\partial x^\nu} \quad (2.22)$$

for each set of coordinates  $\{ x^\mu \}, \{ y^\nu \}$  such that  $\omega = \omega_\mu dx^\mu = \tilde{\omega}_\nu dy^\nu$ . Similarly to what happens for vectors, a function  $f : M \rightarrow N$  induces a natural mapping between the cotangent spaces at  $p \in M$  and  $f(p) \in N$ ; in this case, however, this natural mapping goes “backward”, namely  $f^* : T_{f(p)}^* N \rightarrow T_p^* M$ , hence the name **pullback**, and is defined as

$$\langle f^* \omega, V \rangle \equiv \langle \omega, f_* V \rangle, \quad (2.23)$$

where  $V \in T_p M, \omega \in T_{f(p)}^* N$ , the pairing  $\langle \cdot, \cdot \rangle$  between a form and a vector is given by eqs. (2.19) and (2.21), and the differential map  $f_*$  is given by eqs. (2.12) and (2.13).

In order to define higher order-forms, it is useful to introduce a generalization of the pairing operation (2.21) just presented between vectors and forms, that is the notion of *tensor*.

**Definition 2.8** (Tensor). A **tensor**  $T \in (\mathfrak{T}_r^q)_p(M)$  at  $p$  of order  $(q, r)$  is a multilinear object that maps  $q$  elements of  $T_p M$  and  $r$  elements of  $T_p^* M$  to  $\mathbb{R}$ :

$$(\mathfrak{T}_r^q)_p(M) \ni T : \otimes^q T_p M \otimes^r T_p^* M \rightarrow \mathbb{R} \quad (2.24)$$

As one can easily imagine, the coordinate presentation of a tensor is obtained by the coordinate presentation of one-forms and vectors:

$$T = T_{\nu_1, \dots, \nu_r}^{\mu_1, \dots, \mu_q} \frac{\partial}{\partial x^{\mu_1}} \cdots \frac{\partial}{\partial x^{\mu_q}} dx^{\nu_1} \cdots dx^{\nu_r} . \quad (2.25)$$

We shall denote the action of a tensor on one-forms and vectors with  $T(V_1, \dots, V_q; \omega_1, \dots, \omega_r)$ . Just alike vector fields were a smooth assignment of a vector  $X$  at each point  $p \in M$ , **tensor fields** are a smooth assignment of a tensor to each point of the manifold, its set being denoted by  $\mathfrak{T}_r^q(M)$  consistently with the previous notation.

Differential forms of order  $r > 1$  can now immediately defined.

**Definition 2.9** (Differential form). A **differential form** of order  $r$ , or  **$r$ -form**, is a *totally antisymmetric* tensor of type  $(0, r)$ .

By total asymmetry we mean the following: given a permutation  $P_r$  (of order  $r$ ), its action over a tensor  $\omega$  of type  $(0, r)$  is defined by  $P_r \omega(V_1, \dots, V_r) \equiv \omega(V_{P_r(1)}, \dots, V_{P_r(r)})$ ; a totally anti-symmetric permutation is then given by  $\mathcal{A}\omega = \frac{1}{r!} \sum_{P_r} \text{sgn}(P_r) P_r \omega$ :  $\mathcal{A}\omega$  is now a  $r$ -form.

Put in a different fashion, one can construct  $r$ -forms by composing lower dimensional forms with the help of the so called **wedge** or **exterior** product “ $\wedge$ ”; in the coordinate basis, it is simply defined as a totally anti-symmetrized tensor product of one-forms

$$dx^{\mu_1} \wedge \cdots \wedge dx^{\mu_r} \equiv \sum_{P_r} \text{sgn}(P_r) dx^{P_r(1)} \otimes \cdots \otimes dx^{P_r(r)} , \quad (2.26)$$

so that the left-hand side of eq. (2.26) is the coordinate basis on which a generic  $r$ -form  $\omega$  is expressed:

$$\mathfrak{Q}_p^r(M) \ni \omega = \frac{1}{r!} \omega_{\mu_1, \dots, \mu_r} dx^{\mu_1} \wedge \cdots \wedge dx^{\mu_r} . \quad (2.27)$$

We denoted by  $\mathfrak{Q}_p^r(M)$  the vector space of  $r$ -forms at  $p$ ; its dimension is equal to the number of ways  $r$  elements can be picked up from  $m$  ones, that is  $\dim(\mathfrak{Q}_p^r(M)) = \binom{m}{r}$ . It is worth to point out that the coefficients  $\omega_{\mu_1, \dots, \mu_r}$  are automatically anti-symmetrized

in all the indexes by the contraction with the wedge coordinate basis, in the sense that the symmetric components are suppressed in the sum. From the definition of binomial coefficient, it is immediate to notice that  $\dim(\Omega_p^m(M)) = 1$ , while for  $r > m$  the symmetry property of the wedge product basis immediately yields that  $\Omega_p^{r>m}(M) = \emptyset$ . The wedge product between forms of generic order  $q$  and  $s$  is a straightforward extension of that just defined in eq. (2.26): for  $\omega \in \Omega_p^q(M)$  and  $\xi \in \Omega_p^s(M)$ , define

$$\Omega_p^{r=q+s}(M) \ni (\omega \wedge \xi)(V_1, \dots, V_{q+s}) \equiv \frac{1}{q!s!} \sum_{P_{q+s}} \text{sgn}(P_{q+s}) P_{q+s} \omega(V_1, \dots, V_q) \xi(V_{q+1}, \dots, V_{q+s}), \quad (2.28)$$

where the permutation  $P_{s+q}$  separately permutes the indexes of the vectors  $\{V_1, \dots, V_q\}$  and  $\{V_{q+1}, \dots, V_{q+s}\}$  paired to each form. Clearly, if  $r = q + s$  turns out to be greater than  $m$ , then  $\omega \wedge \xi = 0$ .

Differential forms are a particular subclass of tensors; we can smoothly assign them to each point  $p \in M$ , obtaining the set  $\Omega^r(M) \subset \mathfrak{T}_r^0(M)$ ; it is customary not to distinguish with a specific term the local form  $\omega|_p \in \Omega_p^r(M)$  and the global assignment  $\omega \in \Omega^r(M)$ , they are both called “ $r$ -forms”.

There exists two particularly useful operations mapping forms whose degree differ exactly by one, called *exterior derivative* and *interior product*. Their action are complementary in the sense we are going to present.

**Definition 2.10** (Exterior derivative). Let  $\omega \in \Omega^r(M)$  be a  $r$ -form whose coordinate presentation is given by eq. (2.27). The exterior derivative  $d : \Omega^r(M) \rightarrow \Omega^{r+1}(M)$  acts on  $\omega$  as

$$d\omega \equiv \frac{1}{r!} \partial_\nu \omega_{\mu_1, \dots, \mu_r} dx^\nu \wedge dx^{\mu_1} \wedge \dots \wedge dx^{\mu_r}. \quad (2.29)$$

Notice that the smooth assignment of  $\omega$  at each  $p$  ensures that this local expression can be extended to the whole  $M$ , hence truly obtaining an element of  $\Omega^{r+1}(M)$ . A  $r$ -form  $\omega$  annihilated by  $d$ , that is  $d\omega = 0$  are called **closed**, while if  $\exists \theta$  s.t.  $d\theta = \omega$ ,  $\omega$  is said to be **exact**.

It is worth to provide a simple example to clarify the definitions 2.9 and 2.10 by applying it to the case of a three-dimensional manifold, where we will be able to recognize some objects already known from the usual calculus on  $\mathbb{R}^3$ .

**Example 2.2.** In a three dimensional manifold  $M$ , let  $(x, y, z)$  be the coordinates of  $p$ ; differential forms have the following local expression<sup>4</sup>:

$$\Omega_p^0(M) \ni \omega_0 = f(x, y, z) \quad (2.30a)$$

$$\Omega_p^1(M) \ni \omega_1 = \omega_x(x, y, z)dx + \omega_y(x, y, z)dy + \omega_z(x, y, z)dz \quad (2.30b)$$

$$\Omega_p^2(M) \ni \omega_2 = \omega_{xy}(x, y, z)dx \wedge dy + \omega_{yz}(x, y, z)dy \wedge dz + \omega_{zx}(x, y, z)dz \wedge dx \quad (2.30c)$$

$$\Omega_p^3(M) \ni \omega_3 = \omega_{xyz}(x, y, z)dx \wedge dy \wedge dz \quad (2.30d)$$

Notice that with eq. (2.30a) we have also considered functions as 0-forms and that we have included the  $1/3!$  factor in the definition of the coefficients. By acting with the differential operator  $d$  on each of the (2.30) via definition 2.10, we obtain

$$\Omega_p^1(M) \ni d\omega_0 = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy + \frac{\partial f}{\partial z}dz \quad (2.31a)$$

$$\Omega_p^2(M) \ni d\omega_1 = \left( \frac{\partial \omega_y}{\partial x} - \frac{\partial \omega_x}{\partial y} \right) dx \wedge dy + \left( \frac{\partial \omega_z}{\partial y} - \frac{\partial \omega_y}{\partial z} \right) dy \wedge dz + \left( \frac{\partial \omega_x}{\partial z} - \frac{\partial \omega_z}{\partial x} \right) dz \wedge dx \quad (2.31b)$$

$$\Omega_p^3(M) \ni d\omega_2 = \left( \frac{\partial \omega_{yz}}{\partial x} + \frac{\partial \omega_{zx}}{\partial y} + \frac{\partial \omega_{xy}}{\partial z} \right) dx \wedge dy \wedge dz \quad (2.31c)$$

$$d\omega_3 = 0 \quad (2.31d)$$

Since in this 3-d situation we can view a two-form as a vector by contracting with the **Levi-Civita** symbol, that is  $V^\mu \equiv \epsilon^{\mu\nu\lambda}\omega_{\nu\lambda}$  with  $\epsilon^{P(1)P(2)P(3)} = \text{sgn}(P)$ , we immediately recognize that the action of the differential operator on functions, one-forms and two-forms is, respectively, that of gradient, rotor and divergence.

**Definition 2.11** (interior product). Let  $X \in \mathfrak{X}(M)$ ; we define the **interior product**  $\iota_X : \Omega^r(M) \rightarrow \Omega^{r-1}(M)$  of a  $r$ -form with a vector field  $X$  as the contraction:

$$(\iota_X \omega)(X_1, \dots, X_{r-1}) \equiv \omega(X, X_1, \dots, X_{r-1}), \quad (2.32)$$

or, in local coordinates with  $X = x^\nu \partial_\nu$  and  $\omega$  given by eq. (2.27),

$$\iota_X \omega = \frac{1}{(r-1)!} X^\nu \omega_{\nu\mu_2 \dots \mu_r} dx^{\mu_2} \wedge \dots \wedge dx^{\mu_r} \quad (2.33)$$

It is in general possible to define Lie derivatives even for tensor fields (and hence for  $r$ -forms) in a fashion similar to that used for vectors in paragraph 2.1.2. Without entering much in detail, we present an elegant result which we can take as an operative definition of Lie derivative over forms.

<sup>4</sup>notice that here repeated indexes are *not* summed



**Proposition 2.12.** *Let  $X \in \mathfrak{X}(M)$  be a vector field over  $M$ , and  $\omega \in \Omega^r(M)$  a  $r$ -form. The Lie derivative of  $\omega$  along  $X$  can be written as*

$$\mathcal{L}_X \omega = (d\iota_X + \iota_X d)\omega . \quad (2.34)$$

For example, in the case of a one-form  $\omega = \omega_\mu dx^\mu$ , the Lie derivative along  $X$  reads

$$(d\iota_X + \iota_X d)\omega = (X^\nu \partial_\nu \omega_\mu + \partial_\mu X^\nu \omega_\nu) dx^\mu . \quad (2.35)$$

We end this paragraph by providing some hints about the way the theory of integration of forms is developed on differentiable manifolds. First of all, not every manifold admits a canonical recipe to define what integration means, only the *orientable manifolds*.

**Definition 2.13** (Orientable Manifold). A connected manifold  $M$  covered by the set  $\{U_i\}$  is said to be **orientable** if for every overlapping charts  $U_i \cap U_j$  there exist coordinates  $\{x^\mu\}$  and  $\{y^\alpha\}$  such that the **Jacobian**  $J \equiv \det(\partial x^\mu / \partial y^\alpha)$  of the transformation between them is strictly positive.

If a manifold is orientable, it makes sense to define on it a **volume form**  $\omega_{\text{Vol}} \equiv h(p) dx^{\mu_1} \wedge \dots \wedge dx^{\mu_m} \in \Omega^m(M)$ , that is a form of maximal degree  $m$  with a positive function  $h(p)$  as its coefficient. In fact, orientability ensures that when passing from a chart to another the coefficient of the form remains positive (and in particular it does not vanish) for each  $p \in M$ ; in this sense,  $\omega_{\text{Vol}}$  provides a “measure” on  $M$ .

Now, the integration of a function  $f \in \mathfrak{F}(M)$  with respect to the measure provided by  $\omega_{\text{Vol}}$  is readily defined on a chart  $U_i$  by<sup>5</sup>

$$\int_{U_i} f \omega_{\text{Vol}} \equiv \int_{\phi_i(U_i)} f(\phi_i^{-1}(x)) h(\phi_i^{-1}(x)) dx^1 \dots dx^m , \quad (2.36)$$

where the r.h.s. of (2.36) is indeed a well-defined quantity since it is simply the integral of a  $\mathbb{R}$ -valued function on a subspace of  $\mathbb{R}^m$ . The integral over the whole manifold  $M$  is then obtained by “pasting” together the “pieces” (2.36) in a consistent way. To this end, it is necessary to introduce the so-called **partition of unity**, which is a family of differentiable functions  $\{\rho_i(p)\}$  on  $M$  such that

$$0 \leq \rho_i(p) \leq 1 \quad \forall p \in M, \quad (2.37a)$$

$$\rho_i(p) = 0 \quad \text{if } p \notin U_i, \quad (2.37b)$$

$$\sum_i \rho_i(p) = 1 \quad \forall p \in M . \quad (2.37c)$$

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<sup>5</sup>we restore for a while the initial full notation that distinguishes points in  $U_i$  and their representation in local coordinates  $\{x^\mu\} = \phi_i(p) \in \mathbb{R}^m$  for the sake of clarity

Moreover, the manifold is assumed to be **paracompact**, which means that the set  $\{U_i\}$  is constituted by a finite number of elements, therefore ensuring that the sum in eq. (2.37c) is, in turn, a sum of finite terms. Eventually, we are able to define the integration of a function on  $M$  as the following.

**Definition 2.14** (Integration). Let  $f \in \mathfrak{F}(M)$ ,  $\omega_{\text{Vol}}$  be a volume form on a paracompact, orientable manifold  $M$  and the set  $\{\rho_i\}$  be a partition of unity on  $M$  relative to the finite covering  $\{U_i\}$ . Then, the integral of  $f$  w.r.t.  $\omega_{\text{Vol}}$  over  $M$  is given by

$$\int_M f \omega_{\text{Vol}} \equiv \sum_i \int_{U_i} f_i \omega_{\text{Vol}} , \quad (2.38)$$

where  $f_i(p) \equiv f(p)\rho_i(p)$  in the sense of eqs. (2.37) and the r.h.s. of eq. (2.38) is provided by eq. (2.36).

We have to remark that the definition 2.14 of the integral is invariant under a change of coordinates but the function  $h(p)$  appearing in  $\omega_{\text{Vol}}$  transforms as the Jacobian once such change of coordinates is performed, so that in general there is no canonical way to fix the positive function  $h(p)$  (for example by putting  $h(p) = 1$  everywhere). However, this inconvenience can be avoided when the manifold  $M$  is endowed with a *metric* structure that ensures the existence of a canonical volume form.

#### 2.1.4 Lie Groups and their action over Differentiable Manifolds

As anticipated, Lie Groups provide what is probably the most important example of differentiable manifolds: they are, indeed, differentiable manifolds which consistently support a group structure, as precisely stated by the following definition.

**Definition 2.15** (Lie Group). A **Lie Group**  $G$  is a differentiable manifold where the group operations

1. multiplication:  $\cdot : G \times G \rightarrow G$ , that is  $(g_1, g_2) \mapsto g_1 \cdot g_2$ , and
2. inverse:  $^{-1} : G \rightarrow G$ , that is  $g \mapsto g^{-1}$ ,

are differentiable. The dimension of  $G$  is defined as its dimension as a manifold.

Since Lie groups are well-known to physicists, we will not indulge in detailed examples; rather we just point out that matrix groups like  $GL(n, \mathbb{R})$  or  $GL(n, \mathbb{C})$  and their subgroups are the Lie Groups we are dealing with throughout this work<sup>6</sup>. Before proceeding

<sup>6</sup>a not at all trivial theorem ensures that a subgroup of a Lie Group is a Lie Group by itself

in the presentation of the interesting features pertaining Lie groups (and related algebras, see later) in the context of differential geometry, we recall the basic concept of *quotient* of (Lie) groups since it is at the hearth of a huge part of the results we are going to present in the next chapters. Given a Lie group  $G$  and a Lie subgroup  $H$ , it is possible to define an equivalence relation  $\sim$  between elements of  $G$  by identifying  $g' \sim g$  if  $g' = gh$  for some element  $h \in H$ . Then the **quotient** group  $G/H$  is defined as the set of equivalence classes  $[g] = \{ gh \mid h \in H \}$  with respect to  $\sim$ . This resulting set is in turn a Lie group if  $H$  is a **normal** subgroup of  $G$ , that is  $ghg^{-1} \in H$  for all  $g$  and  $h$  (otherwise it is simply a manifold).

On a Lie Group  $G$  vector fields and forms can inherit from the group structure of the manifold some relevant and useful properties; in order to proceed with this additional construction proper of the interplay between the group structure and the manifold, let's start by defining the concept of *left (right) translation* and invariant vector fields.

**Definition 2.16.** The **left** (resp. **right**) **translation** of an element  $g \in G$  by another element  $a \in G$  is a diffeomorphism  $L_a : G \rightarrow G$  (resp.  $R_a : G \rightarrow G$ ) defined by

$$L_a g = ag \quad (\text{resp.} \quad R_a g = ga) \quad (2.39)$$

These mappings, as explained in paragraph 2.1.2, induce differential maps on the corresponding tangent spaces  $T_g M$ , that is  $L_{a*} : T_g G \rightarrow T_{ag} G$  (resp.  $R_{a*} : T_g G \rightarrow T_{ga} G$ )<sup>7</sup>. A vector field  $X \in \mathfrak{X}(G)$  is said to be **left-invariant** if

$$L_{a*} X|_g = X_{ag} \quad \forall a, g \in G. \quad (2.40)$$

On a Lie Group there exists a “preferential” point, namely the unit element  $e \in G$  with respect to which the following constructions will result a little more apparent; for example, a vector  $V \in T_e G$  defines a *unique* left-invariant vector field  $X_V$  by  $X_V|_g \equiv L_{g*} V$  and, conversely, a left invariant vector field  $X$  defines a unique vector  $V \equiv X|_e \in T_e G$ . If we denote by  $\mathfrak{g}$  the set of left-invariant vector fields on  $G$ , the previous mappings  $V \mapsto X_V$  and  $X_V \mapsto V$  allow us to consider  $\mathfrak{g}$  isomorphic to  $T_e G$ . Moreover, on vector fields the binary operation of Lie bracket is defined (cfr. definition 2.6 and eq. (2.16)), therefore this is true in particular for  $X, Y \in \mathfrak{g}$ ; it immediate to prove that  $\mathfrak{g}$  is closed under Lie bracket, that is the Lie bracket  $Z = [X, Y]$  is an element of  $\mathfrak{g}$  for all  $X, Y \in \mathfrak{g}$ . Eventually, we are naturally led to the definition of *Lie algebra*.

**Definition 2.17** (Lie algebra). The set  $\mathfrak{g}$  of left-invariant vector fields on a Lie Group  $G$ , once equipped with the Lie bracket  $[\cdot, \cdot] : \mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$ , is the **Lie algebra** of  $G$ .

<sup>7</sup>unless otherwise specified, from now on we will only be concerned with the left translation-based construction, since the right one is completely equivalent.

As explained in paragraph 2.1.2, a vector field on a differentiable manifold induces a flow; let's see how this concepts are specified in the context of Lie Groups and hence of left-invariant vector fields. It turns out that a left-invariant vector field  $X$  induces a flow  $\sigma(t, g)$  which is also a **one-parameter subgroup** of  $G$ , the latter being a curve  $\phi : \mathbb{R} \rightarrow G$  that satisfies the composition rule  $\phi(s+t) = \phi(s)\phi(t)$ , with the identifications

$$X \equiv \frac{d\sigma(t, g)}{dt}, \quad \sigma(e, t) \equiv \phi(t) \quad (2.41)$$

Conversely, given a one-parameter subgroup  $\phi(t)$  of  $G$  there always exists a left-invariant vector field that generates it. Thanks to the previous considerations, It should be clear that an element  $X$  of the algebra  $\mathfrak{g}$  has a one-to-one correspondence with a flow in the original Lie group  $G$ , this correspondence being clearly embodied in the definition of *exponential map*.

**Definition 2.18** (Exponential map). Let  $G$  be a Lie Group and  $X \in T_e G$  an element of its algebra (in the sense of the isomorphism explained above). The **exponential map** is a map  $\exp : T_e G \rightarrow G$  given by

$$\exp(X) \equiv \phi_X(1) \quad (2.42)$$

where  $\phi_X(t)$  is the one-parameter subgroup generated by  $X$ .

Given the definition 2.18, it is immediate to prove that the whole subgroup can be obtained by the exponential map (2.42) as

$$\exp(tX) \equiv \phi_X(t) \quad (2.43)$$

As all physicists know very well from quantum mechanics, the exponential map is indeed the “usual” exponential function (its definition in terms of power series) in the case of matrix Lie groups.

It is natural to ask ourselves how the concept of left-invariant vector fields in translated in terms of differential one-forms *via* the duality relation between  $T_e G$  and  $T_e^* G$ . To this end, define a basis  $\{X_\mu\} \in T_e G$ ; this basis corresponds via the isomorphism between  $T_e G$  and  $\mathfrak{g}$  to a set of linearly independent left-invariant vector fields (which are defined on the whole  $G$  even if we start from vectors defined only in  $T_e G$ ). We can expand any element of  $\mathfrak{g}$  on this basis, and in particular we can write the Lie bracket between any two elements as

$$[X_\mu, X_\nu] = c_{\mu\nu}^\lambda X^\lambda \quad (2.44)$$

The coefficients  $c_{\mu\nu}^\lambda$  are the **structure constants** of the Lie Group  $G$ , and by construction they do not depend on the point  $g$  relative to tangent space  $T_g G$  from which the

starting basis vectors are taken (so that we can safely take a basis in  $T_eG$ ). Now, thanks the duality relation introduced together with the definition 2.7 of one forms, we can take a basis  $\{\theta^\mu\} \in T_e^*G$  dual to  $\{X_\nu\} \in T_eG$ , that is  $\langle \theta^\mu, X_\nu \rangle = \delta_\nu^\mu$ ; it can be easily seen (by applying the definition of exterior derivative 2.10) that the structure equation (2.44) translates to the so-called **Maurer-Cartan** structure equation

$$d\theta^\mu = -\frac{1}{2}c_{\nu\lambda}^\mu \theta^\nu \wedge \theta^\lambda . \quad (2.45)$$

The above properties are made frame-independent with the help of the left-invariant **Maurer-Cartan one-form**  $\theta : T_gG \rightarrow T_eG$ <sup>8</sup>, defined by

$$X \mapsto L_{g^{-1}*}X \quad \forall g \in G, \forall X \in \mathfrak{X}(G) \quad (2.46)$$

In other terms, the action of  $\theta$  on a vector  $X \in T_gG$  is to “push forward” it from a point  $g$  to  $e$ . The Maurer-Cartan form satisfies the following properties:

$$\theta = V_\mu \otimes \theta^\mu, \quad \{V_\mu\} \in T_eG \quad \text{and} \quad \{\theta^\mu\} \in T_e^*G , \quad (2.47a)$$

$$d\theta = -\frac{1}{2}[\theta, \theta] \equiv -\frac{1}{2}[V_\mu, V_\nu]\theta^\mu \wedge \theta^\nu . \quad (2.47b)$$

Eq. (2.47b) is a consequence of the Maurer-Cartan structure equation (2.45), while the (2.47a) just provides a canonical way to represent it in terms of a basis in  $T_eG$  and its dual in  $T_e^*G$ .

We presented so far how the group structure allows Lie Groups to act on themselves (from a differential geometry point of view); however, Lie groups can also act on a different, generic manifold  $M$ .

**Definition 2.19** (Action of a Lie group). Let  $G$  be a Lie group and  $M$  be a differentiable manifold. A smooth map  $\Phi : G \times M \rightarrow M$  defines a **(left) group action** on  $M$  if it fulfills the group-like properties

$$\Phi_e(p) = p \quad \forall p \in M , \quad (2.48a)$$

$$(\Phi_g \circ \Phi_h)(p) = \Phi_{gh}(p) \quad \forall g, h \in G \text{ and } p \in M . \quad (2.48b)$$

Moreover a group action can manifest these further following characterizations:

1.  $\Phi$  is **transitive** if for every two points  $p_1, p_2 \in M$  there exists an element  $g \in G$  such that  $\Phi_g(p_1) = p_2$  ;
2.  $\Phi$  is **effective** if  $\Phi_g = \mathbb{1}_M$  implies  $g = e$ , that is the unit element  $e$  is the only one that defines a trivial action on the whole  $M$ ;

---

<sup>8</sup>notice that  $\theta$  takes value in the Lie algebra and not in  $\mathbb{R}$

3.  $\Phi$  is **free** if it has no fixed points, namely  $\Phi_g(p) = p$  implies  $g = e$  for any  $p \in M$ <sup>9</sup>.

Starting from  $p \in M$ , the group action defines an **orbit** by varying  $g$ , namely  $\mathcal{O}_p \equiv \{ \Phi_g(p) \mid g \in G \}$ ; if the action is transitive, it is clear that any orbit coincides with  $M$ . The set  $H(p)$  of elements  $g \in G$  whose action on a given point  $p$  is trivial is called, on the other hand, **isotropy subgroup**<sup>10</sup> of  $G$  at  $p$ , namely  $H(p) \equiv \{ g \in G \mid \Phi_g(p) = p \}$ ; if the action is free, the isotropy group  $H(p)$  just consists of the unit element for any  $p \in M$ . An important construction arises if a group  $G$  act transitively on  $M$ ; in this case  $M$  is called **homogeneous space** of  $G$ , and all the isotropy groups  $H(p)$  are isomorphic. This allows to canonically construct the quotient space  $G/H$  as the set of classes with respect to the equivalence  $g_1 \sim g_2 \leftrightarrow \exists h \text{ s.t. } g_1 = hg_2$ , and  $G/H \simeq M$  itself. In order to clarify these last concepts, let's deal with a prototypical example which will prove to be very useful in the following.

**Example 2.3** (Spheres and rotations). *As our intuition confirms, the group of orthogonal matrices in  $\mathbb{R}^{n+1}$ , which we denote by  $O(n+1)$  acts transitively on the unit sphere  $S^n \subset \mathbb{R}^{n+1}$ . Therefore there is a common isotropy subgroup  $H \subset O(n+1)$  when acting on  $S^n$ . If one consider the point  $p = (1, 0, \dots, 0) \in S^n$ , it is immediate to understand that the class of orthogonal matrices that leave this point fixed is of the form*

$$A = \begin{pmatrix} 1 & 0 \\ 0 & B \end{pmatrix} \quad (2.49)$$

where  $B$  is a generic  $n \times n$  matrix but, since  $A$  must be orthogonal,  $B$  itself must belong to  $O(n)$ . Therefore, we have proved that any sphere  $S^n$  can be obtained as the quotient space:

$$S^n \simeq \frac{O(n+1)}{O(n)} \quad (2.50)$$

It is not difficult to prove that a similar relation also holds in the case of unitary groups, this time reading  $S^{2n+1} \simeq U(n+1)/U(n)$ , and in the case of the restrictions  $SO(n)$  and  $SU(n)$ . We want to stress, however, that  $S^n$  in general does not have a group structure, since  $SO(n)$  is not necessarily a normal subgroup of  $SO(n+1)$  (cfr. the considerations made about the definition 2.15).

We now end this paragraph by inquiring the behavior of left invariants vector fields of a group  $G$  when it acts on a manifold  $M$ . To fix the ideas, let  $G$  be a matrix group of the “right dimension” acting on some manifold as  $\Phi_g(p) = gx$  where  $x$  are as usual local coordinates on  $M$  (as in the previous example). A left invariant vector field  $V$  in

<sup>9</sup>notice that this is a stronger condition than 2, since if the map is effective, it could happen that for some  $g \neq e$  there exist some points  $p \in M$  left unchanged by  $\Phi_g$ , that is  $\Phi_g(p) = p$ .

<sup>10</sup>indeed, it's a Lie subgroup

$G$  produces, by means of the exponential map 2.18 an element of  $g$  which can hence act on  $M$  producing, in turn. a flow in  $M$ :

$$V \mapsto \exp(tV) \xrightarrow{\text{action on } M} \exp(tV)x \equiv \sigma(t, x) \quad (2.51)$$

where the latter is a one-parameter group of transformations that defines a vector field in  $M$  by

$$V^\#|_x \equiv \left. \frac{d\sigma}{dt} \right|_{t=0} = \left. \frac{d \exp(tV)x}{dt} \right|_{t=0}, \quad (2.52)$$

and in the last equality we have made use of eq. (2.51). Therefore, we have established an isomorphism  $\# : T_e G \rightarrow \mathfrak{X}(M)$ .

The action of a Lie group  $G$  onto itself is obviously of particular interest, and deserve a special terminology; a homomorphism  $\text{ad}_a : G \rightarrow G$  defined by

$$\text{ad}_a(g) \equiv aga^{-1} \quad (2.53)$$

is called **adjoint representation** of  $G$ . Clearly, this action induces a natural mapping between the tangent spaces *via* the differential map, see eq. (2.12), and the isomorphisms between  $T_e G$  and the Lie algebra  $\mathfrak{g}$  of  $G$  allows one to canonically extend this action to the latter. Explicitly, take the differential map  $\text{ad}_{a*} : T_g G \rightarrow T_{\text{ad}_a(g)} G$  and define:

$$\text{Ad}_a \equiv \text{ad}_{a*}|_{T_e G} : T_e G \rightarrow T_e G \quad \Rightarrow \quad \text{Ad}_a : \mathfrak{g} \rightarrow \mathfrak{g} \quad (2.54)$$

where the target space of  $\text{Ad}_a$  is again  $T_e G$  since by definition (2.53) it is  $\text{ad}_a(e) = e$

## 2.1.5 Fiber Bundles

### 2.1.5.1 Preliminary definitions

Fiber bundles provide the natural geometrical setting to describe the most part of physical concepts we are going to discuss in the next chapters, so that a quite detailed presentation of their properties is now in order. The explanation of what a fiber bundle is requires the usage of almost every concept of differential geometry we have presented so far, thus in the following we will heavily rely on the basic definitions and properties discussed in the previous paragraphs. From a physical point of view, a fiber bundle is a unified geometric framework to discuss the action of a symmetry group on some theory which possesses a natural hierarchy in its degrees of freedom that, in turn, generally intertwines in a nontrivial way. We dedicate this paragraph to the whole abstract construction and subsequently present some prototypical examples of its application in physics in the next section.

**Definition 2.20** (Fiber bundle). A **fiber bundle** is a differentiable manifold that *locally* looks like a cartesian product of two manifolds but globally may not. More precisely, a fiber bundle (which in the following we will denote with the shorthand  $E \xrightarrow{\pi} M$  or  $(E, \pi, M, F, G)$ ) is made up of the following ingredients:

1. a **total space**  $E$  (differentiable manifold);
2. a **base space**  $M$  (differentiable manifold);
3. a **typical fiber**  $F$  (differentiable manifold);
4. a **structure group**  $G$  (Lie group) acting transitively on  $F$  on the left (cfr. def. given in paragraph 2.1.4);
5. a **projection**  $\pi : E \rightarrow M$  (surjection), such that for  $p \in M$  the counterimage  $\pi^{-1}(p) \equiv F_p$  is called **fiber** at  $p$  and  $F_p \simeq F$  (it is isomorphic to the typical fiber);
6. **local trivializations**  $\phi_i : U_i \times F \rightarrow \pi^{-1}(U_i)$  where  $\{U_i\}$  is a finite open covering of  $M$ , and  $\{\phi_i\}$  are diffeomorphisms such that  $\pi \circ \phi_i(p, f) = p \quad \forall p \in U_i, f \in F$ ;
7.  $G$ -valued **transition functions** when passing from a chart to another, that is fixing  $p \in U_i \cap U_j$  define  $G \ni t_{ij,p} \equiv \phi_{i,p}^{-1} \circ \phi_{j,p} : F \rightarrow F$ . As maps  $t_{ij}(p) : U_i \cap U_j \rightarrow G$  they are required to be smooth.

These last two points 6 and 7 deserve a little further explanation. Local trivializations embody the meaning of the statement: “fiber bundles locally look like the cartesian product of two manifolds”, since they map a point in the total space  $u$  (with the restriction that it has to be projected at some point  $p$  in the base manifold) to a couple  $(p, f) \in U_i \times F$ . Then, transition functions define the rule to translate this diffeomorphism from one chart to another; in order to convince ourselves that they belong indeed to the structure group, we may write the definition in 7 as

$$\phi_j(p, f_j) = \phi_i(p, t_{ij}(p)f_j) \equiv \phi_i(p, f_i) , \quad (2.55)$$

*i.e.* in the overlap of the two charts two different local trivializations map the same point  $u \in E$  to two different couples  $(p, f_i)$  and  $(p, f_j)$ , where  $f_i$  and  $f_j$  are points of the fiber and hence are connected by a group transformation (recall that  $G$  acts transitively on  $F$ ) (cfr. figure 2.3). Moreover, in order to consistently “glue” together the local trivializations, transition functions must obey the following conditions:

$$t_{ii}(p) = \mathbb{1}_{U_i} \quad \forall p \in U_i ; \quad (2.56a)$$

$$t_{ji}(p) = t_{ij}^{-1}(p) \quad \forall p \in U_i \cap U_j ; \quad (2.56b)$$

$$t_{ij}(p)t_{jk}(p) = t_{ik}(p) \quad \forall p \in U_i \cap U_j \cap U_k . \quad (2.56c)$$



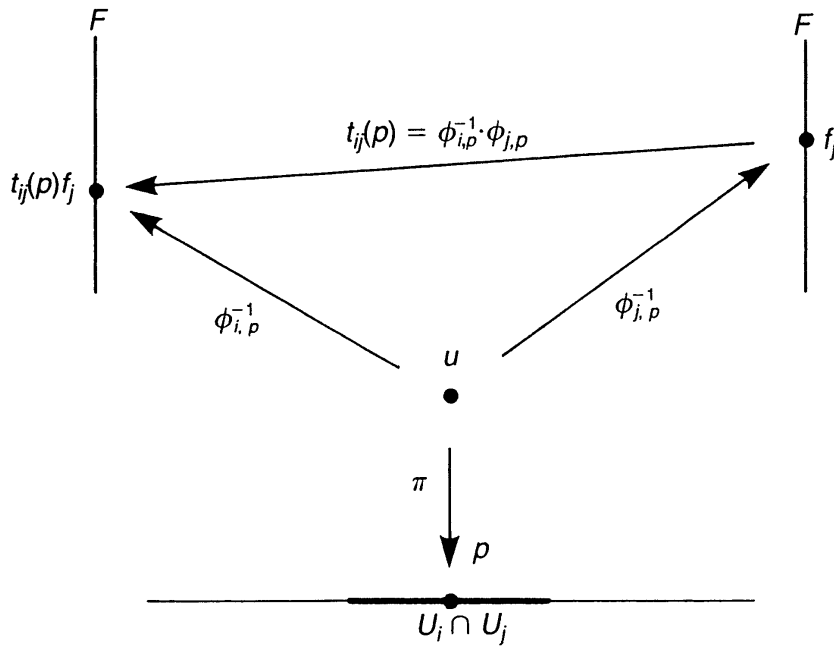


FIGURE 2.3: Local trivializations

Local trivializations referring to a point  $u$  whose image on  $M$  is  $p \in U_i \cap U_j$ . - *Original Figure in [13]*

A bundle is said to be **trivial** once it is  $M \times F$  globally or, in other words, when all the transition functions can be taken as the identity map.

Given a covering  $\{U_i\}$  on  $M$ , there are many choices of local trivializations that give rise to the same fiber bundle. Denote by  $\{\phi_i\}$  and  $\{\psi_i\}$  two sets of them; then, the corresponding transition functions  $t^\phi$  and  $t^\psi$  are related by the homeomorphisms  $G \ni g(p) : F \rightarrow F$ :

$$t_{ij}^\psi(p) = g_i^{-1}(p) \circ t_{ij}^\phi(p) \circ g_j(p), \quad g_i(p) \equiv \phi_{i,p}^{-1} \circ \psi_{i,p} \quad (2.57)$$

Eq. (2.57) defines the so-called **gauge transformations**  $g(p)$ ; moreover, putting  $t_{ij}^\phi(p) = \mathbb{1}_{U_i \cap U_j}$ , one obtains the most general form transition functions can take in a given fiber bundle, *i.e.*  $t_{ij}(p) = g_i^{-1}(p)g_j(p)$ . As should be clear from this discussion, transition functions play a prominent role in the theory of fiber bundles: indeed, they are more “fundamental” than local trivializations in the sense of the *reconstruction* theorem we are going to state.

**Theorem 2.21** (Reconstruction theorem for a fiber bundle). *Given a set  $(M, U_i, t_{ij}(p), F, G)$ , there exists a unique fiber bundle  $(E, \pi, M, F, G)$  with the notation conventions used so far, that is: the minimum information required to construct a fiber bundle is contained in the choice of a base manifold  $M$ , a covering  $\{U_i\}$ , the transition functions  $\{t_{ij}\}$  (instead of the set of local trivializations!), the fiber  $F$  and the structure group  $G$ .*

On a fiber bundle there exists a natural concept of which the physics we are going to develop in this work will make an extensive use, that is the notion of *section*.

**Definition 2.22.** A **section** (or **global section**) of a fiber bundle is a smooth map  $s : M \rightarrow E$  such that  $\pi \circ s = \mathbb{1}_M$ ; when this map is defined only from a patch  $U_i \subset M$ , which we will denote by  $s_i : U_i \rightarrow E$ , the section is called **local**. The set of sections on  $M$  (resp.,  $U_i$ ) is denoted by  $\Gamma(M, E)$ . Notice that  $s|_p \equiv s(p) \in F_p \simeq F$ .

Sections are therefore maps that allow one to express an element of the total space as a function of the base space coordinates, at least locally. In general, fiber bundles may not admit global sections. In the following we will be concerned with two particular types of fiber bundles, namely *vector* and *principal* bundles, where sections will manifest different behaviors.

**Definition 2.23** (Vector bundle). A **vector bundle**  $E \xrightarrow{\pi} M$  is a fiber bundle whose typical fiber  $F$  is a vector space  $\simeq \mathbb{R}^k$  (or  $\mathbb{C}^k$ ) and the structure group is given by the corresponding matrix group  $GL(k, \mathbb{R})$  (or  $GL(k, \mathbb{C})$ ).

A typical example of vector bundle is that given by the so-called *tangent bundle*, known from Lagrangian formulation of classical mechanics.

**Example 2.4** (Tangent bundle). *Given some manifold  $M$  (with  $\dim(M) = m$ ), we dub the collection of all tangent spaces as the **tangent bundle**  $TM$ , and write:*

$$TM \equiv \bigcup_{p \in M} T_p M \quad (2.58)$$

*It is indeed a fiber bundle: locally (in a patch  $U_i$  with coordinates  $\{x^\mu\}$ ), any element of  $u \in TM$  can be decomposed in the couple  $(p, V^\mu(p))$  with  $p \in M$ , and  $V^\mu(p) \in \mathbb{R}^m$  are the coordinates in the tangent space at  $p$ , that is  $T_p M \ni V|_p = V^\mu \partial_\mu$ . Therefore,  $T_p M$  serves as fiber at  $p$ , and  $TM$  is locally diffeomorphic to the cartesian product  $\mathbb{R}^m \times \mathbb{R}^m$ . The projection  $\pi : TM \rightarrow M$  simply associates to a point  $u \in TM$  the point  $p \in M$  at which the tangent space is taken. As for the structure group, we notice that a vector  $V|_p \in T_p M$  is expressed through its coordinates  $V^\mu$  which change via equation (2.8) as  $\tilde{V}^\nu = \partial_\mu y^\nu V^\mu$ , where  $\partial_\mu y^\nu = \partial_\mu y^\nu(p) \in GL(m, \mathbb{R})$  is the transformation matrix (and, therefore, must be non-singular), so that the structure group acting on the fiber is just  $GL(m, \mathbb{R})$ . Finally, a vector field  $X \in \mathfrak{X}(M)$  is a smooth assignment of a vector in a tangent space  $X_p \in T_p$  for each point  $p \in M$ ; now, we can think that this assignment is trivially extended to the whole  $TM$  by simply requiring that  $p \mapsto u_p \in TM$  with  $\pi^{-1}(p) = X_p \in T_p M$ . In other words, vector fields on  $M$  are just sections of  $TM$ .*

The last consideration in the previous example suggests that a notable property holds for vector bundles, namely in a vector bundle sections can be pointwisely added and multiplied by a scalar function as:

$$(s + s')(p) \equiv s(p) + s'(p), \quad s, s' \in \Gamma(M, E) \quad (2.59a)$$

$$(fs)(p) \equiv f(p)s(p), \quad f \in \mathfrak{F}(M), s \in \Gamma(M, E), \quad (2.59b)$$

where the right-hand sides of eq. (2.59) make sense since are combinations of vectors and numbers. In this context, the null vector in each  $T_pM$  plays a prominent role and allows to define the **null section** as  $\phi_i(p, 0) \equiv s_0(p)$  for *all* the local trivializations  $\{\phi_i\}$ , meaning in turn that a vector bundle always admits a global section (notice that the null vector is left invariant by the action of the structure group at each fiber  $T_pM$ ).

This behavior substantially changes if one is concerned with *principal bundles*.

**Definition 2.24** (Principal bundle). A **principal bundle**  $P \xrightarrow{\pi} M$  (or, more commonly,  $P(M, G)$  in order to emphasize the structure group  $G$ ) is a fiber bundle whose fiber is the structure group  $G$  itself.

A fundamental feature deriving from the principal bundle structure is that it is possible to define, together with the left action of  $G$  onto itself *via* the transition functions, a “canonical” *right* action on  $\pi^{-1}(U_i)$  *via*

$$ua \equiv \phi_i(p, g_i a) \quad (2.60)$$

where  $u \in \pi^{-1}(U_i)$  is a point in the total space trivialized in the patch  $U_i$  by  $\phi_i(p, g_i) = u$ , with  $\pi(u) = p$ , and where  $a \in G$ . The notable property of the right action is that it can be defined independently of the choice of local trivializations since right and left action obviously commute. We shall therefore define  $R_a : P \times G \rightarrow P \leftrightarrow (u, a) \equiv ua$  globally. It is easy to see that the right action on the fiber at  $p$ ,  $G_p \simeq G$ , is both transitive (any two points on the fiber are connected by a right transformation, and  $G_p$  is just the orbit passing through  $p$ , cfr. paragraph 2.1.4) and free, as  $ua = u$  implies  $a = e$ , the identity element  $\in G$ . The existence of a trivialization-independent right action for a principal bundle implies the possibility to define a preferred, or **canonical**, local trivialization, namely, given a section  $s_i(p) : M \rightarrow P$ , put

$$\phi_i(p, e) \equiv s_i(p). \quad (2.61)$$

Now,  $s_i(p)$  associates to  $p$  a certain point  $u^*$  belonging to  $\pi^{-1}(p)$ ; by the right action, this point can be connected to any other point on the same fiber, say  $u = u^* g_u$  with an appropriate choice of  $g_u$ . This in turn implies that  $u$  is again canonically trivialized

making use of eq. (2.61), that is  $u = s_i(p)g_u = \phi_i(p, g_u)$  where in the last equality we employed the definition of right action, eq. (2.60).

There exists an important relationship between principal and vector bundles, namely it is possible to associate a vector bundle (in fact, a generic fiber bundle) to a given principal bundle, and *vice versa*. Indeed, a principal bundle  $P \xrightarrow{\pi_P} M$  induces an associated vector bundle *via* the following construction. Let  $V$  be a  $k$ -dimensional vector space; the group  $G$  can act on  $V$  from the left with its  $k$ -dimensional representation, say  $\rho(g)$ ; then the associated vector bundle  $E \equiv P \times_{\rho} V$  is given by identifying the points  $P \times V \ni (u, v) \sim (ug, \rho(g^{-1})v)$ , that is the total space of the resulting bundle is made up of the set of equivalence classes of the previously defined equivalence relation, and the base manifold  $M$  is the original one. The projection in  $E$ ,  $\pi_E : E \rightarrow M$  is defined starting from the projection  $\pi_P$  in  $P$  by ignoring the  $V$  component of the cartesian product, that is  $\pi_E(u, v) = \pi(u) \quad \forall v \in V$ . Notice that in this way the projection is well-defined since  $\pi_P(u) = \pi_P(ug)$  (right action on  $P$ ) and  $\pi_E(u, v) = \pi_E(ug, \rho(g^{-1})v) \equiv \pi_P(ug)$  (definition of the associated bundle and its projection). Local trivializations are simply maps  $\phi_i : U_i \times V \rightarrow \pi_E^{-1}(U_i)$  and the transition functions are just the representation of those of the principal bundle,  $t_{E,ij}(p) = \rho(t_{P,ij}(p))$ . For instance, associated to a principal bundle  $P(M, GL(k, \mathbb{R}))$  there is the vector bundle with fiber  $\mathbb{R}^k$  over  $M$ . As anticipated, also the “backward” construction is possible: obviously the structure group of the vector bundle is used as fiber for the principal one, and the transition functions are taken to be the same; therefore a single principal bundle is associated to a given vector bundle, whereas the converse statement is not true, as should be clear from the previous explanation.

We end this preliminary part on fiber bundles with an important theorem concerning the existence of a global section in a principal bundle<sup>11</sup>.

**Theorem 2.25** (Triviality of a principal bundle). *A principal bundle  $P(M, G)$  is trivial if and only if it admits a global section. As a corollary, a vector bundle is trivial if and only if its associated principal bundle is.*

### 2.1.5.2 Connections, parallel transport and holonomy in fiber bundles

The definitions and properties we have presented so far concern the “static” (but still quite involved) structure of a fiber bundle. In the following we will introduce the concepts necessary to define the “dynamical” picture of a fiber bundle, especially aiming at answering the natural question: “how can I compare objects defined at different fibers

<sup>11</sup>we have already seen that for a vector bundle it is always possible to globally define the null section, so that the existence of a global section cannot be a condition of triviality.

and transport them from one to another?”. It turns out that in order to give a response to this problem it is sufficient to endow the fiber bundle with a *connection*<sup>12</sup>. Let’s then proceed with its definition on a principal bundle: we want to stress that the restriction to principal bundles on one hand provides a more concrete approach, on the other it is still a quite general construction thanks to the association procedure we have dealt with at the end of the previous paragraph.

**Definition 2.26** (Connection on a principal bundle). A **connection** on a principal bundle  $P(M, G)$  is a *unique* decomposition of the tangent spaces  $T_u P \quad \forall u \in P$  into *vertical* and *horizontal* subspaces  $V_u P$  and  $H_u P$  (see later) such that the following axioms are satisfied:

1.  $T_u P = V_u P \oplus H_u P \quad \forall u \in P$  ;
2. a generic vector field  $X \in \mathfrak{X}(P)$  is separated into vector fields  $X^V, X^H \in \mathfrak{X}(P)$  such that  $X^V|_u \in V_u P$ ,  $X^H|_u \in H_u P$  and  $X|_u = X^V|_u + X^H|_u$ . In other words, the decomposition is smooth ;
3. the right action is compatible with this assignment, meaning that  $R_{g*} H_u P = H_{ug} P$  for any  $u \in P$  and  $g \in G$  .

The crucial feature of this definition is the fact that the principal bundle structure *completely determines* the vertical subspaces  $V_u P$ , whereas the *choice* of the connection is equivalent to the *choice* of the horizontal subspaces  $H_u P$ : this assignment is free, provided the properties 1-3 of 2.26 are satisfied. Namely, given a certain fiber  $G_p$  which contains the point  $u$  in the sense  $\pi(u) = p$ , the vertical subspace  $V_u P$  is the subspace of  $T_u P$  which is also tangent to the fiber. Therefore, a generic vector belonging to the vertical subspace at  $u$  can be completely characterized as follows, without making reference to the connection: by the right action, it is possible to define a curve lying in  $G_p$  passing through  $u$  as

$$c_u^A(t) \equiv u \exp(tA), \quad A \in \mathfrak{g} \quad (2.62)$$

since  $\pi(c_u^A(t)) = \pi(u)$ , where we made use of the exponential map 2.18. Then, for a generic function  $f : P \rightarrow \mathbb{R}$ , define the **fundamental vector field**  $A^\sharp$  generated by  $A$  as

$$(A^\sharp f)(u) \equiv \frac{d}{dt} f(c_u^A(t))|_{t=0} . \quad (2.63)$$

Clearly,  $A^\sharp|_u$  is a vertical vector  $\in V_u P$  being tangent to the fiber at  $u$  by construction, and the related vector field  $A^\sharp$  defines an isomorphism between the algebra  $\mathfrak{g}$  and  $V_u P$

<sup>12</sup>if the fiber bundle has already a metric structure, there is a canonical way to provide a connection. We shall return to this point in the following, when dealing with the physical situations we are interested in.

through  $\sharp : \mathfrak{g} \ni A \mapsto A^\sharp|_u \in V_u P$ . Therefore, we have also demonstrated that the vertical subspace have dimension equal to that of the fiber and hence  $\dim(H_u P) = \dim(P) - \dim(G)$ . Moreover it is immediate to prove that  $\pi_* X = 0$ ,  $X \in V_u P$ , that is a vertical vector is projected (*via* the differential map) to the null vector on the base manifold, and that the isomorphism  $\sharp$  preserves the Lie bracket, namely  $[A, B] = C$  implies  $[A^\sharp, B^\sharp] = C^\sharp$ .

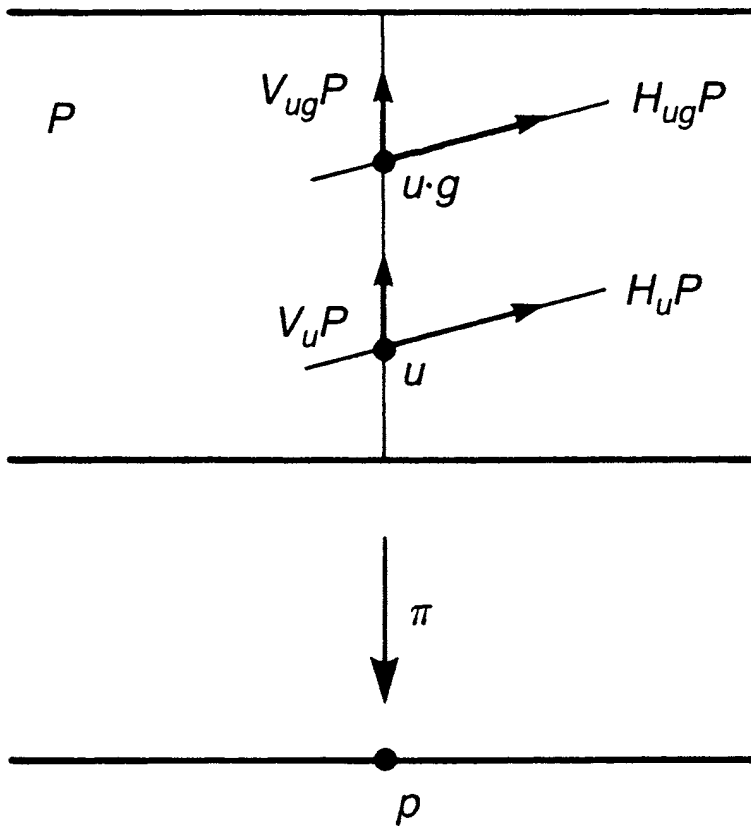


FIGURE 2.4: Tangent space decomposition

The tangent space at a point  $u$ , resp.  $ug$  (both projecting onto  $p$ ), decomposed into vertical and horizontal subspace, compatibly with the right action  $u \mapsto ug$ . - *Original Figure in [13]*

The definition 2.26 has a clear geometrical interpretation, see fig. 2.4, but it would be convenient to find a more practical and computable way to describe a connection. Not surprisingly, the solution to this inconvenience is provided by the language of differential forms, and in particular of one-forms (cfr. paragraph 2.1.3), now taking values in the Lie algebra  $\mathfrak{g}$  of  $G$ .

**Definition 2.27** (Connection one-form). A **connection one-form**  $\omega$  taking values in the Lie algebra of the structure group, that is  $\omega \in \Omega^1(P) \otimes \mathfrak{g}$ , is defined by the two requirements:

1.  $\omega(A^\sharp) = A$ ,  $A \in \mathfrak{g}$ ;

$$2. R_g^* \omega = \text{Ad}_{g^{-1}} \omega ,$$

where  $R_g^*$  is the pullback of the right action on one-forms, cfr. eq. (2.23) and the adjoint map  $\text{Ad}$  on a Lie algebra is given by eq. (2.54). Given  $\omega$ , the relationship with the previous definition of connection is established by assigning the horizontal subspaces  $H_u P$  as the kernel of  $\omega$ , that is

$$H_u P \equiv \{ X_u \in T_u P \mid \omega(X)|_u = 0 \} . \quad (2.64)$$

The statement that the two definitions 2.26 and 2.27 is embodied in the following proposition (very simple to demonstrate).

**Proposition 2.28.** *The horizontal subspace defined as in eq. (2.64) satisfies axiom 3 of definition 2.26. The uniqueness and smoothness of the assignment of  $H_u P$  through  $\omega$  is guaranteed by the basic properties of differential forms (linearity of the pairing with vectors and smoothness).*

Essentially, the connection one-form projects any element of  $T_u P$  onto its vertical component  $V_u P \simeq \mathfrak{g}$ , so that the kernel of  $\omega$  is constituted by vectors which does not have a vertical component and hence are defined to be “horizontal”.

As anticipated, when a physics problem relies on the geometry of a fiber bundle, sections play a prominent role in the whole description, since they provide, in general only locally, a mapping between the base manifold degrees of freedom and the the information stored in a point of the total space: the connection one-form previously defined in 2.27 assumes an immediate physical meaning when it is made local, too, by the choice of a local section.

**Definition 2.29** (Local connection form - gauge potential). Given a local section  $s_i : U_i \rightarrow P$  of a principal bundle  $P(M, G)$  and the connection form  $\omega$  as in 2.27, the pullback of  $\omega$  through  $s_i$

$$s_i^* \omega \equiv \mathcal{A}_i \in \Omega^1(U_i) \otimes \mathfrak{g} \quad (2.65)$$

is called **local connection form**. It is again a Lie algebra valued one-form, now defined on a chart  $U_i \subset M$  of the base manifold. In a principal bundle a section is canonically associated to a local trivialization  $\phi_i$  on  $U_i$  through eq. (2.61) so that, given another patch  $U_j$  with canonical local trivialization  $\phi_j(e) = s_j$ , the local connection form (2.65) on  $U_j$  is

$$\mathcal{A}_j \equiv s_j^* \omega = \phi_j^*(e) \omega . \quad (2.66)$$

Obviously, in the overlap  $U_i \cap U_j$  the local forms  $\mathcal{A}_j$  and  $\mathcal{A}_i$  must be related by the transition functions  $t_{ij}$ ; explicitly, for  $p \in U_i \cap U_j$ , it is

$$\mathcal{A}_j(p) = t_{ij}^{-1}(p)\mathcal{A}_i(p)t_{ij}(p) + t_{ij}^{-1}(p)dt_{ij}(p) . \quad (2.67)$$

Eq. (2.67) should be regarded as a consistency condition for the set  $\{\mathcal{A}_i\}$  to give rise to a single and globally defined connection  $\omega$ .

On the other hand, since we are dealing with a principal bundle, a different interpretation is available: suppose that another section  $s'_i$  is chosen on the *same* patch  $U_i$  so that, again, a different local connection form  $\mathcal{A}'_i$  is defined as  $\mathcal{A}'_i \equiv (s'_i)^*\omega$ , cfr. eq. (2.65). The images of a point by two sections  $s_i$  and  $s'_i$  are in turn related by the right action, namely  $s'_i(p) = s_i(p)g_i(p)$  with  $p \in U_i$  and  $g_i(p) \in G$ . Now,  $g_i(p) : U_i \rightarrow G$  (hence as a function mapping  $p \mapsto g(p)$ ) is just a **gauge transformation**, introduced in eq. (2.57), and  $\mathcal{A}'_i$  is consequently related to  $\mathcal{A}_i$  by

$$\mathcal{A}'_i = g_i^{-1}\mathcal{A}_i g_i + g_i^{-1}dg_i . \quad (2.68)$$

Eqs. (2.67) and (2.68) are formally identical but, as we pointed out, have slightly different meanings which “overlap” for principal bundles; physicists prefer to adopt this second point of view, that is “changing a section by means of a gauge transformation”, and in this context the local connection form  $\mathcal{A}_i$  is called **local gauge potential**.

Having defined the connection, we are now able to move back to the original question about the notion of “transport” on principal bundles, and in particular of *parallel transport*.

**Definition 2.30** (Horizontal lift). A curve  $\gamma : [0, 1] \rightarrow M$  in the base manifold  $M$  of a principal bundle  $P(M, G)$  endowed with a connection  $\omega$  is said to be **horizontally lifted** to a curve  $\tilde{\gamma} : [0, 1] \rightarrow P$  if  $\pi \circ \tilde{\gamma} = \gamma$  and its tangent vector is always horizontal, namely

$$\omega(X)|_{\tilde{\gamma}(t)} = 0 \quad \forall t \in [0, 1] \quad (2.69)$$

where  $X$  is the vector field such that  $X|_{\tilde{\gamma}(t)} = d\tilde{\gamma}/dt$ .

The definition of horizontal lift clearly depends on the connection  $\omega$ : another choice  $\omega'$  implies a different set of horizontal lifts  $\{\tilde{\gamma}'\}$ ; in other words, a connection selects a horizontal vector field (defined from  $t = 0$  to  $t = 1$  in this conventions) and hence a “horizontal flow”. Again, the theory of ODEs guarantees the uniqueness of this flow once a initial condition is selected, which exactly provides the being looked for condition of **parallel transport** (of a point  $u_0 \in P$  along  $\gamma \in M$ ), as precisely stated in the following theorem.



**Theorem 2.31** (Parallel transport). *Let  $P(M, G)$  be a principal bundle with connection  $\omega$ ,  $\gamma : [0, 1] \rightarrow M$  be a curve in  $M$ , and let  $u_0 \in \pi^{-1}(\gamma(0))$ , that is  $u_0$  belongs to the fiber at  $\gamma(0)$ . Then, there exists a unique horizontal lift  $\tilde{\gamma} \in P$  of  $\gamma$  such that  $\tilde{\gamma}(0) = u_0$ ;  $u_0$  is said to be parallel transported along  $\gamma$  to the “endpoint”  $u_1 \equiv \tilde{\gamma}(1) \in \pi^{-1}(\gamma(1))$ . Moreover, parallel transport commutes with the right action, that is if  $u_0$  is transported to  $u_1$  along the horizontal lift  $\tilde{\gamma}(t)$ , then  $u_0 g$  is transported to  $u_1 g$  along  $\tilde{\gamma}(t)g$  which is again horizontal (see fig. 2.5).*

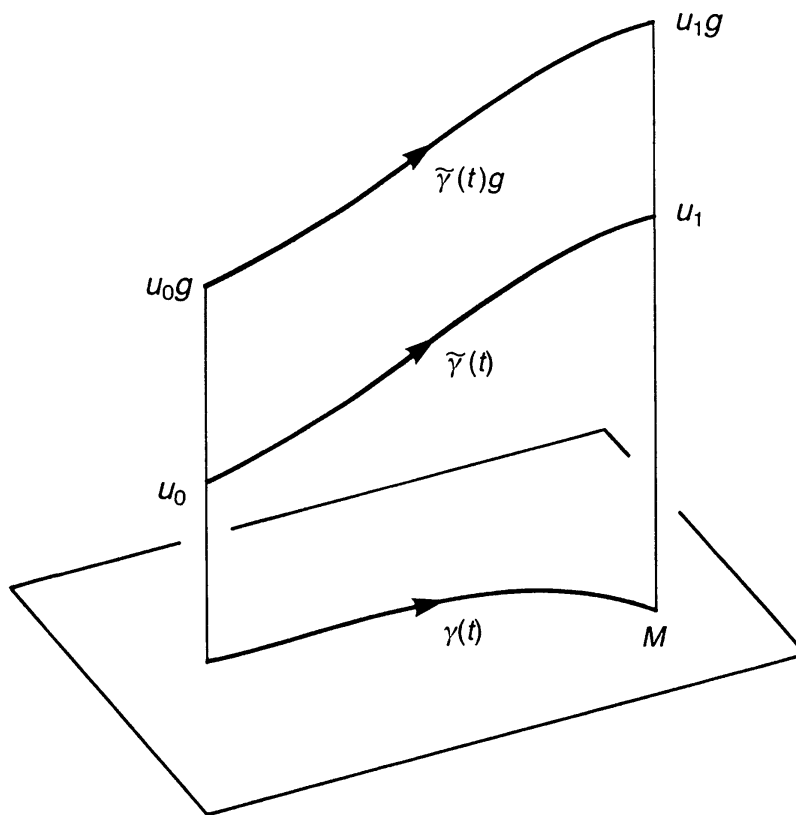


FIGURE 2.5: Parallel transport

An illustration of the parallel transport of a point  $u_0$  to  $u_1$  along  $\gamma$ , also showing that parallel transport commutes with the right action. - *Original Figure in [13]*

Let us now consider the situation where the curve  $\gamma \in M$  is closed, namely  $\gamma(0) = \gamma(1)$ . From theorem 2.31, it is evident that a point  $u_0$  is parallel transported to  $u_1 \in \pi^{-1}(\gamma(1)) = \pi^{-1}(\gamma(0))$ , that is  $u_0$  and  $u_1$  lie on the same fiber, in turn implying that there exists a right transformation  $g_{\gamma, u_0}$  connecting the two points, say  $u_1 = u_0 g_{\gamma, u_0}$ . The group element  $g_{\gamma, u_0}$  is called **holonomy element** of the curve  $\gamma$  in the point  $u_0$  with respect to the connection  $\omega$ .

**Definition 2.32** (Holonomy group). The **holonomy group** based at  $u_0$  is the set of holonomy elements at  $u_0$  with varying closed  $\gamma$ :

$$\text{Hol}_{u_0} \equiv \{ g_{\gamma, u_0} \mid \gamma \in M, \gamma(0) = \gamma(1), \tilde{\gamma}(0) = u_0 \} . \quad (2.70)$$

A few final remarks are now in order. Firstly, different curves in  $M$  may give rise to the same holonomy element, whereas the holonomy group is indeed a subgroup of  $G$ , hence deserving its name. Secondly, the fact that the right action commutes with parallel transport suggests that holonomy groups based at different points on the same fiber cannot be independent. Indeed the relation

$$\text{Hol}_{u_0 h} = h^{-1} \text{Hol}_{u_0} h \quad (2.71)$$

holds for any  $h \in G$  in the sense that one can obtain any given element  $g_{\gamma, u_0 h} \in \text{Hol}_{u_0 h}$  by conjugation of the corresponding element  $g_{\gamma, u_0} \in \text{Hol}_{u_0}$  with  $h$ , proving that the holonomy groups based at different points of the same fiber are isomorphic. Finally, it is obviously possible to give a characterization of an holonomy element as a proper solution of the condition of parallel transport, see theorem 2.31 and the definition of horizontal lift 2.30 in terms of global and local connection. From an operative point of view, giving the latter amounts to solve the differential equation the lift  $\tilde{\gamma}$  of  $\gamma$  (such that the initial condition  $\tilde{\gamma}(0) = u_0$  holds) has to obey in terms of the local quantities in order to be horizontal. Namely, taking a section  $s_i$  over  $U_i$  with  $s_i(\gamma(0)) = u_0$ , it is always possible to express the horizontal lift of  $\gamma$  by a suitable gauge transformation  $g_i(\gamma(t))$  (we are assuming the curve  $\gamma \in U_i \subset M$ ):

$$\tilde{\gamma}(t) \equiv s_i(\gamma(t)) g_i(t) \quad t \in [0, 1] \quad (2.72)$$

Hence, from the horizontality condition induced by the connection  $\omega \xrightarrow{s_i} \mathcal{A}_i$ , it is easily seen that the gauge  $g_i(t)$  has to fulfill

$$\frac{dg_i}{dt} = -\mathcal{A}_i(X) g_i(t) , \quad (2.73)$$

where  $X$  is the tangent vector to  $\gamma$  in  $t = 0$ . The formal solution for a subsequent  $t$  of eq. (2.73) (with  $g_i(0) = e$  by eq. (2.72)) is given by

$$g_i(t) = \mathfrak{P} \exp \left( - \int_{\gamma(0)}^{\gamma(t)} \mathcal{A}_{i, \mu}(\gamma(t)) dx^\mu \right) \quad (2.74)$$

where the symbol  $\mathfrak{P}$  denotes the path ordering<sup>13</sup>, and  $x^\mu$  are the local coordinates in

<sup>13</sup>Recall that  $\mathcal{A}_{i, \mu}$  are the coefficients of a  $\mathfrak{g}$ -valued one-form and, therefore, at different times  $t_1$  and  $t_2$ , corresponding to different points in the base space, the  $\mathfrak{g}$ -elements  $\mathcal{A}_{i, \mu}(\gamma(t_1))$  and  $\mathcal{A}_{i, \nu}(\gamma(t_2))$  in

$U_i$ . Eventually, when  $t = 1$  (that is, once the loop in the base space is completed), the holonomy element of  $\gamma$  at  $u_0$  is computable as the integral of the connection over the base curve  $\gamma$ :

$$g_{\gamma, u_0} = \mathfrak{P} \exp \left( - \oint_{\gamma} \mathcal{A} \right) \quad (2.76)$$

Notice that the integral is expressed only in terms of local objects on  $U_i \subset M$ . If the curve  $\gamma$  in the base manifold had extended to more than a single chart  $U_i$ , the integral should have been cut-and-pasted accordingly to the construction yielding eq. (2.38). Eq. (2.76) is an intrinsically gauge-dependent expression since changing the initial point  $u_0 = s_i(\gamma(0)) \rightarrow u'_0 = s'_i(\gamma(0)) \equiv u_0 h$  for an appropriate element  $h \in G$  implies, as embodied in eq. (2.71), that

$$g_{\gamma, u_0 h} = h^{-1} g_{\gamma, u_0} h . \quad (2.77)$$

However, taking the trace of (2.77) a gauge-invariant quantity is clearly obtained: the so called **Wilson Loop** [17].

### 2.1.5.3 The covariant derivative in associated vector bundles

As we sketched above, a principal bundle can be taken as the minimal ingredient starting from which it is possible to construct any fiber bundle; in particular, we are interested in the mechanism through which a connection of a principal bundle allows one to implement the parallel transport on an associated vector bundle; to this end, we introduce the notion of *covariant derivative* of sections.

Let  $E = P \times_{\rho} V$  be a vector bundle associated with  $P(M, G)$ , and denote a point in  $E$  by the equivalence class  $[(u, v)] = \{ (ug, \rho(g^{-1})v \mid u \in P, g \in G, v \in V \}$ ; a section  $s \in \Gamma(M, E)$  is then described by the representative

$$E \ni s(p) = [(\sigma(p), \xi(p))] \quad (2.78)$$

where  $p \in U \subset M$  is a point in a given chart  $U$  of  $M$ ,  $\sigma$  is a section in  $P$  and  $\xi$  a section in  $V$ . Changing the gauge in  $P$ , that is  $\sigma(p) \rightarrow \sigma(p)g(p)$ , amounts to re-define the section in  $V$ , namely  $s(p) \rightarrow s'(p) = [(\sigma(p), g(p)\xi(p))] \equiv [(\sigma(p), \xi'(p))]$ . Now, a section in  $E$  is parallel transported along  $\gamma \in M$  if the section in  $P$  is a horizontal lift  $\tilde{\gamma}(t)$  of  $\gamma$  and the section in  $V$  is constant: indeed, it is always possible to change the gauge in order

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general *do not* commute. In turn, this implies that the exponential power series is ill-defined, unless some specification is provided. The path ordering just accomplish the job since, given any two non commuting quantities  $A(t)$  and  $B(s)$ , it is defined as:

$$\mathfrak{P}(A(t)B(s)) \equiv \begin{cases} A(t)B(s) & t > s \\ B(s)A(t) & s < t \end{cases} \quad (2.75)$$

to make the section in  $P$  horizontal ( $\equiv \tilde{\gamma}(t)$ ), therefore we can generically characterize a horizontal section in  $E$  by

$$s(\gamma(t)) = [(\tilde{\gamma}(t), \eta(\gamma(t)))], \quad \gamma(t) \in U \subset M \forall t \in [0, 1] . \quad (2.79)$$

and  $\eta(\gamma(t))$  constant, namely  $d\eta/dt = 0$ . We remark that this condition apparently depends on the choice of the particular horizontal lift  $\tilde{\gamma}$  but, again, by the definition of the vector bundle it is clear that, given another horizontal lift  $\tilde{\gamma}'(t) = \tilde{\gamma}(t)h$ , with  $h \in G$  forced to be *constant* by the commutativity of the right action with parallel transport, the vector part only changes as  $\eta(t) \rightarrow h\eta(t)$  and therefore remains constant if it was constant with respect to  $\tilde{\gamma}$ .

We are eventually led to the definition of covariant derivative of a generic section in the associated vector bundle  $E$ .

**Definition 2.33** (Covariant derivative in an associated vector bundle). Let  $s \in \Gamma(M, E)$  be an arbitrary section of  $E$  (vector bundle associated to  $P(M, G)$ ), and denote its parametrization along the curve  $\gamma(t) : [0, 1] \rightarrow M$  as  $s(t) = [(\tilde{\gamma}(t), \eta(\gamma(t)))]$ , with  $\tilde{\gamma}$  arbitrary horizontal lift of  $\gamma$  w.r.t. the connection defined on  $P$ . Let  $X_p$  be the tangent vector of  $\gamma(t)$  in  $p \equiv \gamma(0)$ . The covariant derivative of  $s$  along  $\gamma$  in  $p$  is given by

$$\nabla_X s|_p \equiv \nabla_{X_p} s \equiv \left[ \left( \tilde{\gamma}(0), \left. \frac{d}{dt} \eta(\gamma(t)) \right|_{t=0} \right) \right] . \quad (2.80)$$

It is possible to *globally* extend the definition given by expression (2.80) by resorting again to the theory of differential forms. Namely, instead of taking the vector  $X_p \in T_p$ , take the whole vector field  $X \in \mathfrak{X}(M)$  (tangent to  $\gamma$  when restricted to  $p$  in order to make the link with the previous definition), and consider the map  $\nabla_X : \Gamma(M, E) \rightarrow \Gamma(M, E)$ ; in turn, the latter can be thought as a map

$$\nabla : \Gamma(M, E) \rightarrow \Gamma(M, E) \otimes \Omega^1(M) , \quad (2.81)$$

therefore the image of  $\nabla$  is a section-valued one-form over  $M$ .

## 2.2 Adiabatic Theory

The geometric construction we presented in the previous section is general and rich, therefore a vast part of theoretical physics is naturally led to adopt differential geometry as its underlying skeleton; for example, the fiber bundle approach provides the mathematical toolbox to rigorously formulate gauge field theories on curved backgrounds, but many and various other physical descriptions get advantaged from such a general

scheme. Among these, some aspects of non-relativistic Quantum Mechanics acquire both an elegant formulation and a surplus value when treated by means of differential geometry. In particular, our thesis work is greatly concerned with the notions of adiabaticity and geometric phases; as we shall see in this section, these two concepts are deeply related and provide the formal framework from which the original part of this thesis work takes origin. For the sake of concreteness, we first pose the prototypical problem, proper to quantum mechanics, of a “slowly” varying time-dependent or, in other words, *adiabatic* Hamiltonian in the usual approach; subsequently, we present the abstract formalism underlying this still quite general situation, namely the so-called *time-adiabatic* theory[15, 18]. Then, we are able to introduce the first example of geometric phase in quantum mechanics, the well-known *Berry’s phase*[19, 20], by heavily relying both on the adiabatic theory and the fiber bundle construction. Finally, we devote the last part of this section to sketch the extension of the time-adiabatic theory to a more general setting, called *space-adiabatic* theory[15, 16] which includes and systematically improves the Born-Oppenheimer approximation[21] widely adopted in molecular and solid-state physics.

### 2.2.1 Introduction: slowly varying time-dependent Hamiltonians

In quantum mechanics a system described by a time-dependent parametric Hamiltonian is considered *closed* but not *isolated* (see Chapter 1); as thoroughly discussed, the fact that time explicitly appears in the dynamical generator does not spoil the unitarity of the evolution, but in the general case the propagator has to be expressed as a time-ordered product of nested exponentials, and is indeed the fingerprint that the system under consideration is embedded in an environment whose description can be carried on classically (indeed, the time evolution of the parameters is usually known and under full control, having no dynamical origin). The formal treatment of such a situation greatly simplifies once the time variation of the external parameter is slow compared to the natural time scales of the system, namely that introduced by the spacing of the instantaneous energy levels: in this case, a system in an eigenstate at a certain time  $t$  evolves in time following the externally-induced evolution of the corresponding eigenspace, and the evolution is called *adiabatic*. To explicitly cope with this *quasi*-static picture, let us consider the instantaneous Schrödinger eigenvalue equation:

$$H(t) |n(t)\rangle = E_n(t) |n(t)\rangle \quad (2.82)$$

where we assume for the sake of clarity the instantaneous eigenstates  $|n(t)\rangle$  to be non-degenerate. At each time  $t$ , they form an orthonormal basis in the Hilbert space  $\mathcal{H}$ ,

$\langle n(t) | m(t) \rangle = \delta_{nm}$ , hence a generic state  $|\psi(t)\rangle \in \mathcal{H}$  can be expanded as

$$|\psi(t)\rangle = \sum_n c_n(t) \exp\left(-i \int_0^t E_n(\tau) d\tau\right) |n(t)\rangle \quad (2.83)$$

where  $\sum_n |c_n(t)|^2 = 1$ ; moreover, in eq. (2.83) we singled out the dynamical phase factors  $\exp\left(-i \int_0^t E_n(\tau) d\tau\right)$  for further convenience and we assumed the dynamics starting from the reference time  $t = 0$ . The coefficients evolution is generally ruled by the time-dependent Schrödinger equation, yielding the following coupled system of differential equations:

$$\dot{c}_n = -c_n \langle n | \dot{n} \rangle + \sum_{m \neq n} c_m \langle n | \dot{m} \rangle \exp\left(-i \int_0^t (E_m(\tau) - E_n(\tau)) d\tau\right) \quad (2.84)$$

where by  $\dot{f}$  we denote the time derivative of a function  $f$ , and we suppressed the explicit time dependence in order to lighten the notation. Now, by differentiating the instantaneous eigenvalue equation eq. (2.82), it is easy to see that the overlap  $\langle n | \dot{m} \rangle$  satisfies

$$\langle n | \dot{m} \rangle = \frac{1}{E_m(t) - E_n(t)} \langle n | \dot{H} | m \rangle, \quad n \neq m. \quad (2.85)$$

Heuristically, eq. (2.85) means that the off-diagonal terms in eq. (2.84) are sensitive to the ratio between the expectation value of the “velocity” at which the Hamiltonian  $H(t)$  changes compared to the gap  $E_n(t) - E_m(t)$  between the corresponding energies. Therefore, we anticipate that the time-adiabatic limit amounts to consider  $\frac{1}{E_n(t) - E_m(t)} \langle n | \dot{H} | m \rangle \rightarrow 0$ , or  $\langle n | \dot{m} \rangle \rightarrow 0$  for  $m \neq n$ , but we shall return to this point later and in a systematic way. Let us however consider the consequences of such an hypothesis: the evolution eq. (2.84) for each of the expansion coefficients immediately simplifies into:

$$\dot{c}_n = -c_n \langle n | \dot{n} \rangle, \quad (2.86)$$

implying that the transition between different eigenspaces is fully suppressed, and that, choosing an initial condition of the type  $c_n(0) = \delta_{nk}$  (namely, only the  $k$ -th level is initially populated),

$$c_k(t) = e^{i\phi_k(t)}, \quad \dot{\phi}_k = i \langle k | \dot{k} \rangle, \quad \phi_k(0) = 0, \quad (2.87)$$

that is  $c_k(t)$  is just a phase factor. Eventually, returning to the state expansion eq. (2.83), it is

$$|\psi(t)\rangle = e^{i\phi_k(t)} \left(-i \int_0^t E_k(\tau) d\tau\right) |k(t)\rangle \quad \text{for} \quad |\psi(0)\rangle = |k(0)\rangle \quad (2.88)$$

Eq. (2.88) clearly embodies the initial statement that, in the adiabatic limit, a state belonging at  $t = 0$  to a certain eigenspace, say  $\text{Ran}(|k(0)\rangle\langle k(0)|)$ <sup>14</sup> accordingly to the notation we used, at later times belongs to the “evolved” eigenspace  $\text{Ran}(|k(t)\rangle\langle k(t)|)$ , the latter instantaneously determined by the eigenvalue Schrödinger equation eq. (2.82). We called this picture *quasi-static* exactly meaning that it is only the explicit time-dependence of the Hamiltonian  $H(t)$  that “moves” the eigenspaces  $\text{Ran}(|k(t)\rangle\langle k(t)|)$  and hence gives rise to an *assigned*, externally driven dynamics  $|k(0)\rangle \rightarrow |k(t)\rangle$  but the overall dynamics is automatically decoupled in each of the eigenspaces similarly to the time-independent case.

The additional phase factor  $e^{i\phi_k(t)}$  in eq. (2.88) has been neglected in the literature for over 50 years thanks to the following argument: the instantaneous eigenstates  $|k(t)\rangle$  are determined by the Schrödinger equation (2.82) up to a phase factor, and hence if one *chooses* at *each* time  $t$   $|\tilde{k}(t)\rangle \equiv e^{i\phi_k(t)}|k(t)\rangle$  instead of  $|k(t)\rangle$ , the phase factor itself is absorbed in the definition of the eigenstates  $|\tilde{k}(t)\rangle$ , therefore disappearing from eq. (2.88); since  $\phi_k(t)$  and  $|k(t)\rangle$  are in turn related by eq. (2.87), this amounts to state that in the *gauge*  $|\tilde{k}(t)\rangle$  it is<sup>15</sup>

$$0 = \langle \tilde{k} | \dot{\tilde{k}} \rangle, \quad (2.89)$$

this situation being denoted in literature by the term *Born-Fock gauge*. However, as we shall thoroughly discuss in the whole remaining of this thesis work starting from paragraph 2.2.3, this argument can fail from a formal point of view, this failure manifesting itself in the physical *observable* effect of Berry’s phase.

## 2.2.2 Time-adiabatic theory

Having introduced the heuristic notion of adiabatic approximation in a system governed by a slowly varying, time-dependent Hamiltonian and its consequences on the evolution of a physical state, we now address the same problem rigorously, starting from a systematic definition of “slow variation”: the subsequent formalism, eventually embodied by the *time-adiabatic theorem*, naturally reproduces and extends the results of the previous paragraph, with many further advantages. As an immediate consequence, the errors occurring while adopting such a simplified treatment can be quantified; moreover, the method we are now going to introduce on one hand can be naturally generalized to more complicated situations, on the other is also amenable of a direct and plain geometric

<sup>14</sup>where with the notation “Ran” we hereafter mean the image of the projector

<sup>15</sup>we will clarify in the subsequent paragraphs, obviously referring to the formal language introduced in the previous section 2.1, why we call this choice a *gauge* choice, yet the heuristic reason is well understood.

description (see the next paragraph 2.2.3), paving the way to a solid treatment of Berry's phase.

Let us start by considering the family of time-dependent Hamiltonians  $H(s)$ ,  $s \in \mathbb{R}$ , which by definition are self-adjoint operators acting on some Hilbert space  $\mathcal{H}$ ; we also assume them bounded to avoid unnecessary technicalities (we shall denote the set of self-adjoint operators on  $\mathcal{H}$  as  $\mathcal{L}_{\text{sa}}(\mathcal{H})$ ). Following the notation conventions of [15], here  $s$  denotes the *microscopic* time (or *fast* time scale), namely  $H(s)$  enters the Schrödinger equation as

$$i \frac{d}{ds} U^\varepsilon(s; s_0) = H(\varepsilon s) U^\varepsilon(s; s_0), \quad U^\varepsilon(s_0; s_0) = \mathbb{1}_{\mathcal{H}}, \quad (2.90)$$

where  $U^\varepsilon(s; s_0)$  is the unitary propagator. The dimensionless quantity  $\varepsilon$ , with  $0 \leq \varepsilon \ll 1$ , is here introduced as the adiabaticity parameter that rules the rate at which the Hamiltonian varies: the smaller  $\varepsilon$  is, the more microscopic time  $s$  is needed to appreciate an actual change in the Hamiltonian  $H(\varepsilon s)$ , hence the more the latter is “slowly changing”, adopting the language of the previous paragraph. It should then be clear that if one defines  $t \equiv \varepsilon s$ ,  $t$  is indeed the *slow* and *macroscopic* time scale at which the Hamiltonian actually varies; therefore it is convenient to write eq. (2.90) as

$$i \varepsilon \frac{d}{dt} U^\varepsilon(t; t_0) = H(t) U^\varepsilon(t; t_0), \quad U^\varepsilon(t_0; t_0) = \mathbb{1}_{\mathcal{H}} \quad (2.91)$$

where it is understood that we denote  $U^\varepsilon(t; t_0) \equiv U^\varepsilon(s; s_0)|_{s=t/\varepsilon}$ . Another way to state the adiabatic problem is now the following: how can I systematically find approximate solutions to eq. (2.91) exploiting the fact that  $\varepsilon$  is small? As we have seen in the previous paragraph, it is the competition between the time-scale variation of the Hamiltonian and the spacing between the energy levels that make the adiabatic machinery available; in the present context, the condition which substitutes the heuristic one relative to eq. (2.85) can be naturally formulated in terms of the spectrum of the slow Hamiltonian  $H(t)$ ; namely, let us denote the spectrum of  $H(t)$  as  $\sigma(t)$ , and consider a subset  $\sigma_*(t) \subset \sigma(t)$  (which typically will consist of a single, non-degenerate eigenvalue  $E_*(t)$  as in the introductory example).

**Definition 2.34** (Gap).  $\sigma_*(t)$  is separated by a **gap**  $g > 0$  from the remainder of the spectrum if there exist two bounded and continuous functions  $f_\pm(t)$  defining an interval  $I(t) = [f_-(t), f_+(t)]$  such that  $\sigma_*(t) \subset I(t)$  and

$$\inf_{t \in \mathbb{R}} \text{dist}(I(t), \sigma(t) - \sigma_*(t)) = g > 0, \quad (2.92)$$

where the symbol  $\sigma(t) - \sigma_*(t)$  stands for the set of elements of  $\sigma(t)$  that does not belong to  $\sigma_*(t)$ . This definition may look a little involved, but it simply states the fact that, uniformly in the *macroscopic* time  $t$ , the part of the spectrum  $\sigma_*(t)$  which is involved in



the dynamics (*via* the initial condition on the state  $\psi$ ) is far from the remainder of the spectrum at least of a finite distance  $g$ , as illustrated in fig. 2.6.

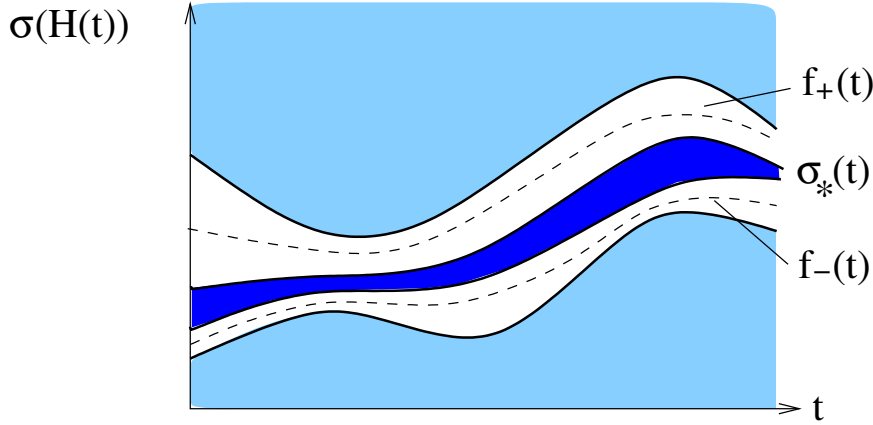


FIGURE 2.6: Gap condition

An illustration of the definition 2.34 concerning the separation from the remainder of a part of the spectrum  $\sigma_*(t)$ . *Original Figure in [15]*

Substantially, the definition 2.34 is useful to our purposes both for technical reasons (the condition therein stated ensures some regularity properties which are necessary in order to prove a rigorous version of the time-adiabatic theorem) and because  $g$  is finite compared to the adiabatic parameter  $\varepsilon$  which “tends to zero”. Let us now denote by  $P_*(t)$  the projector onto the eigenspaces relative to  $\sigma_*(t)$ : in the guideline treatment of the previous paragraph  $P_*(t)$  was the one-dimensional projector  $|k(t)\rangle\langle k(t)|$ . Before dealing with the theorem itself, a last (but not least) definition is in order.

**Definition 2.35** (Adiabatic Hamiltonian-propagator). Let  $H(t)$  be the Hamiltonian (again, self-adjoint and uniformly bounded) acting on some Hilbert space  $\mathcal{H}$ , and denote by  $\sigma_*(t)$  a part of its spectrum isolated by a gap from the remainder in the sense of definition 2.34,  $P_*(t)$  being the corresponding projector. The **adiabatic Hamiltonian**  $H_a(t)$  relative to  $\sigma_*(t)$  is defined as

$$H_a(t) \equiv H(t) - i\varepsilon P_*(t)\dot{P}_*(t) - i\varepsilon P_*^\perp(t)\dot{P}_*^\perp(t) \quad (2.93)$$

where  $P_*^\perp(t) \equiv \mathbb{1}_{\mathcal{H}} - P_*(t)$  is the orthogonal complement of  $P_*(t)$ . The corresponding **adiabatic propagator** is defined by the Schrödinger equation

$$i\varepsilon \frac{d}{dt} U_a^\varepsilon(t; t_0) = H_a(t) U_a^\varepsilon(t; t_0), \quad U_a^\varepsilon(t_0; t_0) = \mathbb{1}_{\mathcal{H}}. \quad (2.94)$$

The adiabatic Hamiltonian (2.93), as to be soon proven, is the effective generator actually responsible for the time evolution of the spectral subspace  $P_*(t)$ ; its definition

immediately confirms the intuition that in the adiabatic setting, that is for small  $\varepsilon$ ,  $H_a(t)$  is, indeed, a good approximation of the original full Hamiltonian  $H(t)$ .

**Theorem 2.36** (Time-adiabatic theorem). *Let  $H(\cdot) \in C_b^2(\mathbb{R}, \mathcal{L}_{sa}(\mathcal{H}))$ , and be  $\sigma_*(\cdot)$  a part of its spectrum satisfying the gap condition 2.34. Then  $P_*(\cdot) \in C_b^2(\mathbb{R}, \mathcal{L}(\mathcal{H}))$  and there is a constant  $C < \infty$  such that  $\forall t, t_0 \in \mathbb{R}$*

$$\|U^\varepsilon(t; t_0) - U_a^\varepsilon(t; t_0)\|_{\mathcal{L}(\mathcal{H})} < C\varepsilon(1 + |t - t_0|) \quad (2.95)$$

in the norm of bounded operators  $\mathcal{L}(\mathcal{H})$ , and where  $U^\varepsilon(t; t_0)$  and  $U_a^\varepsilon(t; t_0)$  are, respectively, solutions of (2.91) and (2.94) with  $H_a(t)$  given by eq. (2.93). Moreover,  $U_a^\varepsilon(t; t_0)$  is constructed in such a way that it exactly evolves the spectral projector  $P_*(t_0)$  into  $P_*(t)$  as

$$P_*(t)U_a^\varepsilon(t; t_0) = U_a^\varepsilon(t; t_0)P_*(t_0) , \quad (2.96)$$

hence eq. (2.95) yields

$$\|(\mathbb{1}_{\mathcal{H}} - P_*(t))U^\varepsilon(t; t_0)P_*(t_0)\|_{\mathcal{L}(\mathcal{H})} < C\varepsilon(1 + |t - t_0|) . \quad (2.97)$$

*Comments and sketch of the proof.* Eq. (2.95) is a stronger result than (and imply by virtue of eq. (2.96)) eq. (2.97) since the latter “simply” states that the true dynamics adiabatically decouples the spectral subspaces, while eq. (2.95) can be used to define an *effective dynamics* inside each subspace (see later).

The idea of the proof is the following. Thanks to the gap condition 2.34 (which is also necessary to prove the regularity of  $P_*(t)$ ), a straightforward but tedious calculation shows that the difference of the exact and adiabatic propagators can be expressed as the integral of a rapidly oscillating function, ideally of the form

$$U^\varepsilon(t; t_0) - U_a^\varepsilon(t; t_0) \sim \int_{t_0}^t d\tau e^{i\tau/\varepsilon} = i\varepsilon \left( e^{it/\varepsilon} - e^{it_0/\varepsilon} \right) , \quad (2.98)$$

therefore  $\|U^\varepsilon(t; t_0) - U_a^\varepsilon(t; t_0)\| = \mathcal{O}(\varepsilon)$ , heuristically justifying the bound (2.95). On the other hand, as the geometry of the evolution of the spectral subspaces implies a nice geometric picture to be shown in the subsequent paragraph, we prefer to deal in a little more detail with the condition (2.96): in particular we want to show that it is exactly satisfied given the adiabatic Hamiltonian (2.93) as the generator occurring in the Schrödinger eq. (2.94). Let us now define the adiabatic Hamiltonian as a small correction to the true one, *via*

$$H_a = H(t) + \varepsilon K(t) , \quad (2.99)$$

where we will derive that

$$K(t) = -i(P_*(t)\dot{P}_*(t) + P_*^\perp(t)\dot{P}_*^\perp(t)) \quad (2.100)$$

as in eq. (2.93). The projectors evolution condition (2.96) forces the form of this correction since it implies

$$0 = \frac{d}{dt} (U_a^\varepsilon(t_0; t)P_*(t)U_a^\varepsilon(t; t_0)) = \frac{i}{\varepsilon} U_a^\varepsilon(t_0; t) \left( [H_a(t), P_*(t)] - i\varepsilon\dot{P}_*(t) \right) U_a^\varepsilon(t; t_0) \quad (2.101)$$

where we have made use of eq. (2.94). As the true Hamiltonian commutes with the spectral subspace by definition, that is  $[H(t), P_*(t)] = 0$ , eq. (2.101) reduces to

$$\dot{P}_*(t) = -i[K(t), P_*(t)] \quad (2.102)$$

where we have employed the definition (2.99). It remains to invert the Von Neumann-like equation (2.102); to this end, we exploit the projector property  $(P_*(t))^2 = P_*(t)$  to write<sup>16</sup>

$$\dot{P} = \dot{P}P + P\dot{P} \rightarrow P\dot{P}P = 0, \rightarrow \dot{P} = P^\perp\dot{P}P + P\dot{P}P^\perp. \quad (2.103)$$

The first property of eq. (2.103) allow us to compute  $\dot{P} = [[\dot{P}, P], P]$ , so that by a direct confrontation with eq. (2.102) we are led to

$$K(t) = i[\dot{P}_*(t), P_*(t)], \quad (2.104)$$

which, thanks to the second property derived in eq. (2.103), yields exactly the desired (2.100).  $\square$

Substantially, the above theorem states that the dynamics of a given spectral subspace, relative to a part of the spectrum separated by a gap from the remainder, is approximately decoupled from that of the others; making use of the same assumptions necessary to prove this theorem, it is possible to simply characterize the dynamics *inside* the subspace itself. To this end, let us now consider a single eigenvalue  $\sigma_*(t) \equiv E(t)$  with multiplicity  $d$ ; by the time adiabatic theorem, it is clear that if the initial state of the system  $\psi(t_0)$  lies in  $P_*(t_0)\mathcal{H}$ , at any later time  $t > t_0$   $\psi(t)$  *approximately* lies in  $P_*(t)\mathcal{H}$  in the sense of eq. (2.97). Moreover, the  $d$ -dimensional subspaces  $P_*(t)\mathcal{H}$  admit, instant by instant, orthonormal bases  $\{|\eta_\alpha(t)\rangle, \alpha = 1 \dots d\}$ , through which it is possible to map the dynamics inside  $P_*(t)\mathcal{H}$  to the **reference subspace**  $\mathbb{C}^d$  *via* the family of unitary operators:

$$\mathcal{U}(t) \equiv \sum_{\alpha=1}^d |\chi_\alpha\rangle \langle \eta_\alpha(t)|, \quad \mathcal{U}(t) : P_*(t)\mathcal{H} \rightarrow \mathbb{C}^d, \quad (2.105)$$

<sup>16</sup>omitting the understood time dependence and pedices “\*” referring to the chosen subspace

where  $\{|\chi_\alpha\rangle\}$  is a given basis in  $\mathbb{C}^d$ . Indeed, let us define the unitary propagator in the reference space as

$$U_{\text{eff}}^\varepsilon(t; t_0) \equiv \mathcal{U}(t)U_a^\varepsilon(t; t_0)\mathcal{U}^*(t_0) \quad (2.106)$$

It is easy to show that  $U_{\text{eff}}^\varepsilon(t; t_0)$  satisfies the effective Schrödinger equation

$$i\varepsilon \frac{d}{dt} U_{\text{eff}}^\varepsilon(t; t_0) = H_{\text{eff}}(t)U_{\text{eff}}^\varepsilon(t; t_0), \quad U_{\text{eff}}^\varepsilon(t_0; t_0) = \mathbb{1}_{\mathbb{C}^d} . \quad (2.107)$$

where the **effective Hamiltonian**  $H_{\text{eff}}(t)$  takes the simple form:

$$(H_{\text{eff}}(t))_{\alpha\beta} = E(t)\delta_{\alpha\beta} - i\varepsilon \langle \eta_\alpha(t) | \dot{\eta}_\beta(t) \rangle , \quad (2.108)$$

where the matrix indexes  $\alpha\beta$  refers to the choice of the basis in  $\mathbb{C}^d$ . Evidently, eq. (2.108) provides for the dynamics of interest a much simpler expression than the original  $H(t)$  or its adiabatic version  $H_a(t)$  as, on one hand, it acts on the smaller and time-independent reference subspace  $\mathbb{C}^d$ , on the other takes an almost diagonal form, with a non-diagonal correction  $-i\varepsilon \langle \eta_\alpha(t) | \dot{\eta}_\beta(t) \rangle$  proportional to the adiabatic parameter  $\varepsilon$ <sup>17</sup>. In the example of the previous paragraph, the situation was almost trivial in the sense that each spectral subspace was one-dimensional, so that the effective Hamiltonian (2.108) in that case would have just been the *function*

$$H_{\text{eff}}^{(k)}(t) = E_k(t) - i\varepsilon \langle k(t) | \dot{k}(t) \rangle , \quad (2.109)$$

where the index  $k$  labels the subspace of interest, namely that including the initial state  $|\psi(t_0)\rangle = |k(t_0)\rangle$ . Consistently, the time-dependent Schrödinger equation relative to the effective Hamiltonian (2.109) reproduces eq. (2.88), with the only difference that here the adiabaticity parameter  $\varepsilon$  is explicitly singled out. Moreover, we want to stress that the effective Hamiltonian (2.108) is gauge dependent, and indeed, for example, choosing the Born-Fock gauge (see. eq (2.89)) the second term of (2.109) is locally wiped away. However we have to still remark that this is not always possible, as thoroughly discussed in the subsequent part of this section.

### 2.2.3 Adiabaticity, Geometry and Berry's Phase

In physical applications, the time-dependence usually enters the Hamiltonian  $H(t)$  through a set of external parameters describing some differentiable manifold  $M$  (recall the construction depicted in section 2.1). We are now going to present the way the formal machinery there presented enters the adiabatic treatment of such class of dynamics, and

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<sup>17</sup>the “i” factor here present is actually a consequence of the fact that the diagonal terms  $\langle \eta_\alpha(t) | \dot{\eta}_\alpha(t) \rangle$  are purely imaginary, while the off-diagonal elements are skew-symmetric, consistently yielding a Hermitian Hamiltonian.

in particular we are going to show that an adiabatic evolution can be nicely characterized as the parallel transport of a canonically defined connection (cfr. paragraph 2.1.5.2) in the fiber bundle construction which naturally emerges in these physical settings; the eventual reach of such a geometric treatment is to characterize the to be defined *Berry's phase* as the relative holonomy element.

From the discussion in the above paragraph 2.2.2, it should be clear that the generator  $K(t)$ , given by eq. (2.100) or equivalently by eq. (2.104), is the responsible for the completely adiabatic evolution (namely, for the evolution of the projection  $P_*(t)$  onto the desired spectral subspaces, see the Von-Neumann eq. (2.102)). Clearly, a physical state  $|\psi(t)\rangle$  lying in such a subspace, which is characterized as in eq. (2.88) if the subspace is one-dimensional, satisfies at each time  $t$

$$P_*(t) |\psi(t)\rangle = |\psi(t)\rangle \quad \text{if} \quad |\psi(t_0)\rangle \in \text{Ran}(P_*(t_0)) . \quad (2.110)$$

Taking the time derivative of both members and exploiting again the relation  $P\dot{P}P = 0$ , it is easy to prove that the state  $|\psi(t)\rangle$  satisfies, in this case,

$$Pd |\psi\rangle = 0 , \quad (2.111)$$

where  $d$  here is the differential operator on  $M$ , replacing the time derivative as  $d = \partial_t dt = \sum_\mu \partial_\mu dx^\mu$ , and  $x^\mu$  are the local coordinates on  $M$ . Actually, eq. (2.111) states that an adiabatically evolving vector  $|\psi\rangle$  satisfies a relation of the form:

$$\nabla |\psi\rangle = 0, \quad \nabla \equiv Pd , \quad (2.112)$$

where  $\nabla$  has to be seen as a *covariant derivative* in the vector bundle associated to the spectral projector  $P_*(t)$ , which is easily constructed as follows. Let us denote by  $p$  a point in  $M$  and, as above, be  $\{x^\mu\}$  its coordinates. The Hamiltonian of the system is a function of the parameters associated to the point  $p$ , namely  $H = H(p)$ , with  $p$  (slowly) varying in time as  $p = p(t) = (x^1(t), \dots, x^m(t))$ : in other words, the time variation of the parameters entering the Hamiltonian defines a curve in  $M$ . Then, a set of spectral projections  $\{P_{(n)}(p)\}$  is associated to  $H(p)$ , the index  $(n)$  labelling the different spectral subspaces. Let us suppose now to choose among them a spectral projection  $P_*(p)$  satisfying the gap condition 2.34 in order to have the adiabatic machinery available. At each point  $p$ ,  $\text{Ran}(P_*(p))$  defines a vector subspace of the full Hilbert space  $\mathcal{H}$ , whose elements are hence defined up to a unitary transformation leaving invariant the subspace: for example, If  $\text{Ran}(P_*(p))$  is one-dimensional, the normalized vector belonging to it, say  $|\psi_*(p)\rangle$ , is defined up to  $p$ -dependent phase factor. Eventually, it should be clear that

$\text{Ran}(P_*(p)) \equiv F_*(p)$  is a vector *fiber* at  $p$ , so that

$$\mathcal{H}_* \equiv \bigcup_{p \in M} F_*(p) \quad (2.113)$$

is a vector bundle (which is a sub-bundle of the trivial bundle given by the cartesian product  $M \times \mathcal{H}$ ) with base manifold  $M$ , fiber  $F(p)$ , structure group given by the unitary transformations inside the spectral subspace considered, and a projection  $\pi$  that associates to a given vector  $\in \mathcal{H}_*$  the point  $p$  at which it is defined; such a vector, once expressed as a function of the base manifold coordinates, is actually a *section* of this vector bundle, called for obvious reasons **spectral bundle**. The adiabatic setting plays a two-fold fundamental role in such a construction: on one hand, the adiabatic hypothesis ensures that the fiber bundle structure is preserved during the evolution, otherwise it would have been completely useless from a physical point of view. On the other, eq. (2.111) provides a rule to parallel transport sections (vectors) from a fiber to another: parallel transported sections are those annihilated by  $\nabla \equiv Pd$ , so that the bundle is naturally endowed with a connection (in this case, a covariant derivative) simply by the requirement of adiabatic evolution.

We are now in the position to develop the formal treatment of Berry's phase. We present it in the case considered in the introductory paragraph 2.2.1, namely that of one-dimensional spectral subspaces, hence of one-dimensional fibers<sup>18</sup>. Let, as before,  $M$  be the external parameters manifold, and consider the one-dimensional fiber at  $p$ , or the set of vectors belonging to a given spectral subspace  $\text{Ran}(P_{(k)}(p))$ <sup>19</sup>:

$$F_p = \{ q |k(p)\rangle \mid q \in \mathbb{C} - \{0\} \} . \quad (2.114)$$

Restricting the treatment to normalized vectors for physical reasons, the number  $q$  must be a phase factor, so that

$$F_p = \{ e^{i\alpha} |k(p)\rangle \mid \alpha \in \mathbb{R} \} , \quad (2.115)$$

that is, the fiber is isomorphic to  $U(1)$ . Therefore, we can also look at the one-dimensional (normalized) spectral bundle as a *principal*  $U(1)$ -bundle over  $M$ , and denote it by  $P(M, U(1))$ ; a different choice in the representative  $|k(p)\rangle$  amounts to redefine its phase, namely to perform a local gauge transformation. The connection, expressed

<sup>18</sup>It is, indeed, the case considered by Berry, although the generalization to multi-dimensional fibers has also been straightforwardly considered, and in literature is referred to as *Wilczek-Zee* non-Abelian phase[22].

<sup>19</sup>slightly changing the notation in order to make an explicit link with the expressions appearing in 2.2.1

before as a covariant derivative, can now be immediately interpreted as the natural connection provided by the Hilbert space itself[20]: the Hilbert space, indeed, is endowed with a scalar product, so that if an element of the fiber is the vector  $|k(p)\rangle$ , a vector  $|h\rangle$  orthogonal to it has the natural meaning of being horizontal:

$$\langle k(p) | h \rangle = 0 \quad \leftrightarrow \quad h \text{ "horizontal"} . \quad (2.116)$$

Consider now the curve  $p(t)$  in the parameters space: a horizontal lift of such a curve w.r.t. the connection (2.116) is, thanks to the definition 2.30 and the explicit fiber bundle construction here adopted, a section  $|\psi(p)\rangle$  such that:

$$\left\langle k(p) \left| \dot{\psi}(p) \right. \right\rangle = 0 \quad (2.117)$$

holds for each  $t$  parametrizing the curve  $p \in M$ . Equivalently, as the projector  $P_{(k)}(p)$  can be unambiguously written as  $|k(p)\rangle \langle k(p)|$ , eq. (2.117) becomes:

$$P_{(k)} d\psi = 0 , \quad (2.118)$$

which is exactly the expression (2.111) for transport of spectral subspaces derived from the adiabatic setting. Let us note that a vector in the Born-Fock gauge is the horizontal lift of the corresponding curve in the parameter space. The fundamental point is now the following: if the curve  $p(t)$  in the parameters space is closed, namely  $p(0) = p(T)$ , for some  $T > 0$ , a parallel transported vector  $|\psi(p(0))\rangle \rightarrow |\psi(p(T))\rangle$  comes back to the original fiber, but may have acquired an holonomy phase factor just as explained in paragraph 2.1.5.2. The explicit form of this phase factor is readily found: indeed, eq. (2.87) and eq. (2.88) give (apart from the dynamical phase factor which can be always gauged away)

$$|\psi(T)\rangle = e^{i\phi_k(T)} |k(0)\rangle , \quad (2.119)$$

with

$$\phi_k(T) = i \int_0^T d\tau \left\langle k \left| \dot{k} \right. \right\rangle = i \oint_{p(t) \in M} \langle k | dk \rangle , \quad (2.120)$$

that is, the phase factor  $\phi_k(T)$  becomes a circuit integral along the closed curve  $p(t) \in M$  of the quantity  $\langle k(p) | dk(p) \rangle$ : since the curve is closed, a point-by-point redefinition of the vectors  $|k(p)\rangle$  such that the term  $\langle k(p) | dk(p) \rangle$  is gauged away is not possible everywhere, since it would imply a multi-valued definition at  $p(0) = p(T)$ ; in other words, the Born-Fock gauge can be chosen only locally. Such an impossibility is embodied by the last equality of the expression (2.120), as the closed loop is indeed gauge invariant (while  $\langle k | dk \rangle$  was not, of course, as it was possible to locally put it as zero). Moreover, it should be clear that

$$\mathcal{A}_{(k)}(p) \equiv i \langle k(p) | dk(p) \rangle \in \mathbb{R} \quad (2.121)$$

is precisely the definition of the *local* connection form relative to the abstract connection (2.116) given by the Hilbert space structure; such a connection (form) is usually referred to as **Berry-Simon connection** (form); it is easy to see that it takes value in  $\mathbb{R}$ , which is just the algebra of the structure group  $U(1)$ <sup>20</sup>, as required by the fiber bundle theory, cfr. paragraph 2.1.5.2. We want to remark, again, that  $A_{(k)}(p)$  is gauge dependent in the sense that a different choice of the representative  $|k(p)\rangle \rightarrow |\tilde{k}(p)\rangle$  makes the local connection form vary accordingly to eq. (2.68); it is important not to be confused by the fact that the index ( $k$ ) here also refers to the ( $k$ )-th spectral bundle, which is the “name” of the overall bundle and does not change unless another spectral projection, and hence another bundle, is considered. Putting together eqs. (2.120) and (2.121), we end up in the being looked for definition of **Berry’s phase**:

$$\phi_k(C) = \oint_C A_{(k)} , \quad (2.122)$$

where  $C$  stands for the closed curve spanned by the parameters in  $M$ . The phase factor  $\exp(i\phi_k(C))$  is thus recognized as the holonomy element of  $C$  based at  $|\psi(0)\rangle = |k(0)\rangle$ ; as the structure group is abelian, the holonomy element is gauge invariant in the sense that it does not even depend on the point at which it is based, but just on the curve  $C$  and the connection  $\mathcal{A}_{(k)}$ , cfr. expression (2.77). The gauge invariance of (2.122) can be also stressed by making use of *Stoke’s theorem*<sup>21</sup>: for our purposes, this means that the line integral in (2.122) can be replaced by a surface integral of the Berry’s **curvature two-form**  $\mathcal{F}_{(k)}$

$$\phi_k(C) = \iint_{\Sigma} \mathcal{F}_{(k)}, \quad \mathcal{F}_{(k)} \equiv d\mathcal{A}_{(k)} , \quad (2.123)$$

where  $\Sigma$  is any two-dimensional sub-manifold of  $M$  such that its boundary is given by  $C$ , and it is immediate to find  $\mathcal{F}_{(k)} = -\Im \langle dk | \wedge | dk \rangle$ . As  $\mathcal{F}_{(k)}$  itself is gauge invariant, its surface integral is, as well. Usually, Berry’s phase is actually computed exploiting the relation (2.123), and given that a straightforward calculation yields for the curvature two-form

$$\mathcal{F}_{(k)} = -\Im \sum_{n \neq k} \frac{\langle k | dH | n \rangle \wedge \langle n | dH | k \rangle}{(E_n - E_k)^2} . \quad (2.124)$$

Summing up, Berry’s phase factor is recognized as the holonomy element of the curve  $C$  w.r.t. the natural connection  $\mathcal{A}_{(k)}$ , inherited by the overall Hilbert space structure, in the spectral bundle arising when considering the adiabatic evolution of a state belonging to a certain spectral subspace  $P_{(k)}(p)$  of a parametric dependent Hamiltonian  $H(p)$ ;

<sup>20</sup>apart from an  $i$  factor which is just a matter of conventions.

<sup>21</sup>Since the complete and rigorous formulation of Stoke’s theorem goes beyond the scope of this work, we address the interested reader to specific references, such as[13]; we want to point out, however, that Berry’s himself in his seminal paper[19] already adopts this point of view in order to stress the gauge invariance of his to be celebrated phase.



the adiabatic hypothesis both guarantees to dynamically preserve such a geometric construction and to define a natural rule of parallel transport along the evolution, which is compatible with the Hilbert space inner product.

In order to clarify the above discussion, let's deal with the specific but still prototypical example of the simplest quantum system, a spin- $\frac{1}{2}$  or *qubit*, embedded into an external, adiabatically precessing magnetic field  $\mathbf{B}(t)$ .

**Example 2.5** (Qubit in external field). *Let  $H(t) = \frac{\mu}{2}\boldsymbol{\sigma} \cdot \mathbf{B}(t)$  be the Hamiltonian acting on a spin- $\frac{1}{2}$  Hilbert space  $\mathcal{H}$ , where  $\boldsymbol{\sigma}$  is the vector of Pauli matrices and  $\mathbf{B}(t)$  is an external magnetic field with fixed modulus  $B$ , describing in time a curve in the manifold  $M \simeq BS^2$  (that is, a two-sphere of radius  $B$ ). The energy levels of the system, as the Hamiltonian is rotationally invariant, just depend on the physical coupling  $\mu$  and on the modulus of the field, reading*

$$E_{\pm} = \pm \frac{\mu}{2} B . \quad (2.125)$$

*The corresponding eigenspaces are the range of the spectral projectors*

$$P_{\pm}(\mathbf{B}) = \frac{1}{2}(\mathbb{1}_{\mathcal{H}} \pm \boldsymbol{\sigma} \cdot \frac{\mathbf{B}}{B}) . \quad (2.126)$$

*Notice that the spectral projectors are regular functions, everywhere defined, of the magnetic field  $\mathbf{B}$ , as they do not depend on the specific choice of local coordinates. In order to characterize a vector in either of the two subspaces, it is convenient to notice that if  $\mathbf{B} = (0, 0, B)$ , i.e. the magnetic field is directed along the positive  $z$ -axis in real space, the Hamiltonian is  $H(B_z) = \frac{\mu}{2}\sigma_z B$ , hence the positive and negative energy eigenvectors are just those of  $\sigma_z$ , which we denote by  $|\pm\rangle$ . The eigenvectors for an arbitrary  $\mathbf{B}$ -direction are obtained by appropriately rotating the latter, yielding*

$$\text{Ran}(P_+(\mathbf{B})) \ni |+(\mathbf{B})\rangle = \cos \frac{\theta}{2} |+\rangle + \sin \frac{\theta}{2} e^{i\varphi} |-\rangle , \quad (2.127a)$$

$$\text{Ran}(P_-(\mathbf{B})) \ni |-(\mathbf{B})\rangle = -\sin \frac{\theta}{2} |+\rangle + \cos \frac{\theta}{2} e^{i\varphi} |-\rangle , \quad (2.127b)$$

*where  $(\theta, \varphi)$  are the usual spherical coordinates denoting the point  $\mathbf{B}$ . As discussed above, the  $\mathbf{B}$ -dependent eigenvectors are defined up to a phase factor, so that their explicit expression must be recognized as that of sections in the principal  $U(1)$  bundle over  $M$ ; moreover, the base manifold itself, being the two-dimensional sphere, is non-trivial, meaning that at least two charts are required to cover the entire sphere  $BS^2$  (cfr. example 2.1). Indeed, for  $\theta = 0, \pi$ , respectively, the sections  $|-(\mathbf{B})\rangle$  and  $|+(\mathbf{B})\rangle$  are ill-defined: this situation is an explicit example of the fact that in a non-trivial principal bundle no global sections are admitted. In order to avoid confusion, let us restrict ourselves to the spectral bundle relative to the positive energy eigenvalue, namely in the following  $P_*(p)$*

will be  $P_+(\mathbf{B})$ . Adopting the conventions of paragraph 2.1.5, the canonical local trivialization associated to the local section (2.127a) reads  $\phi_N(\mathbf{B}, \mathbf{e}) = |+(\mathbf{B})\rangle \equiv |+(\mathbf{B})\rangle_N$ , where the index  $N$  refers to the fact that it is defined on a patch  $U_N$  containing the North Pole; a different section is required at the south Pole  $(0, 0, -B)$ , for instance

$$|+(\mathbf{B})\rangle_S \equiv \cos \frac{\theta}{2} e^{-i\varphi} |+\rangle + \sin \frac{\theta}{2} |-\rangle . \quad (2.128)$$

Clearly, it is  $|+(\mathbf{B})\rangle_S = e^{-i\varphi} |+(\mathbf{B})\rangle_N$ , so that the corresponding canonical local trivialization is  $\phi_S(\mathbf{B}, \mathbf{e}) = |+(\mathbf{B})\rangle_S = \phi_N(\mathbf{B}, \mathbf{e}) e^{-i\varphi}$ . Therefore, we can immediately compute the unique transition function using the definition 7 of the fiber bundle construction or the property (2.55):

$$t_{NS}(\mathbf{B}) \equiv \phi_N^{-1} \circ \phi_S(\mathbf{B}) = e^{-i\varphi} : U_N \cap U_S \rightarrow U(1) , \quad (2.129)$$

where  $U_S$  is the patch containing the south Pole at which the section  $|+(\mathbf{B})\rangle_S$  is defined. The local connection form in the north patch reads, according to eq. (2.121)

$$\mathcal{A}_{(+)}^N = i \langle +(\mathbf{B}) | d | +(\mathbf{B})\rangle_N = -\frac{1}{2} (1 - \cos \theta) d\varphi , \quad (2.130)$$

and, consistently with the compatibility condition (2.67) (recall the “ $i$ ” factor in the definition of the Berry-Simon connection),  $\mathcal{A}_{(+)}^S = \mathcal{A}_{(+)}^N + d\varphi = \frac{1}{2} (1 + \cos \theta) d\varphi$ . Finally, according to the definition (2.122), Berry’s phase for the positive energy spectral subspace reads (we will hereafter use the symbol  $\gamma$  instead of  $\phi$  in order to avoid confusion with the local trivialization):

$$\gamma_+(C) = \oint_C \mathcal{A}_{(+)}^N \quad (2.131)$$

where  $C$  is a closed curve on  $BS^2$ . For a path of the type  $\theta = \text{const}$ , the integral in eq. (2.131) is readily computed as

$$\gamma_+(C_\theta) = -\pi(1 - \cos \theta) \quad (2.132)$$

For generic paths, one can always resort to Stoke’s theorem and apply the formula (2.123), with  $\mathcal{F}_{(+)} = -\frac{1}{2} \sin \theta d\theta \wedge d\varphi$ , therefore yielding

$$\gamma_+(C) = -\frac{1}{2} \Omega(C) , \quad (2.133)$$

where  $\Omega(C)$  is the solid angle subtended at the origin by the curve  $C$ .

### 2.2.4 First order Born-Oppenheimer theory

A more general and refined treatment than that presented in paragraph 2.2.2 is provided by the so-called **space-adiabatic theory**[15, 16]; although we shall present the theory restricting ourselves to the first order (see below) and adopt it in the specific case of molecular Hamiltonians, we remark that the space adiabatic theory provides a systematic way to improve the accuracy at any given order in the parameter ruling the approximation and can be applied to a wide class of systems. In the subsequent treatment the similarities with the time-adiabatic theory before presented will be apparent; moreover, we shall introduce an important approach, namely the semiclassical one, we will be concerned with in the next chapters 3-4.

Let us prepare the physical setup by recalling that the Hamiltonian of a molecule, once the spin degrees of freedom are neglected, can be in general written in the following form:

$$H_{\text{mol}} = -\frac{1}{2m_{\text{n}}}\Delta_x - \frac{1}{2m_{\text{e}}}\Delta_y + V_{\text{e}}(y) + V_{\text{n}}(x) + V_{\text{en}}(x, y), \quad (2.134)$$

where  $x = (x^1, \dots, x^l)$  is the vector of positions of all the  $l$  nuclei and  $y = (y^1, \dots, y^k)$  that of the  $k$  electrons (each of the coordinates is the point denoting a single nucleus or electrons, so that the latter are, respectively, vectors in  $\mathbb{R}^{3l}$  and  $\mathbb{R}^{3k}$ ); the constants  $m_{\text{n}}$  (resp.,  $m_{\text{e}}$ ) represents the masses of the nuclei (resp., the electrons), all taken equal for simplicity of notation, while  $\Delta_{x,y}$  are the Laplacian operators and pertain to the kinetic energy terms of the nuclei and the electrons. The remaining terms, denoted by  $V$ , only depend on the positions of the particles and represent the Coulomb interactions; summing up, the Hamiltonian (2.134) is a Hermitian operator acting on the Lebesgue Hilbert space  $\mathcal{H}_{\text{mol}} \equiv \mathcal{L}^2(\mathbb{R}^{3(l+k)})$ , and displays an intertwined structure as there is the term  $V_{\text{en}}(x, y)$  explicitly coupling the different coordinates  $x$  and  $y$ . The “standard” way to tackle this kind of Hamiltonians dates back to the very birth of Quantum Mechanics[21], and indeed consists in an adiabatic-approximation scheme that resides on the heuristic separation of the typical energy scales over which the nuclei and the electrons “move”: as the mass  $m_{\text{n}}$  is much larger than that of the electrons, it is expected that, even for comparable kinetic energies<sup>22</sup>, nuclei change their configuration much more slowly than the electrons, so that the nuclear coordinate  $x$  is effectively seen from the electrons as an “external”, slowly varying parameter. Moreover, the slow motion of the nuclei would suggest that a quasi-classical treatment of their evolution can be applied. These intuitions, which are strictly related but actually well-separated concepts, can be made rigorous and precise in the context of the space-adiabatic theory, whose application to such a physical setting (2.134) can be substantially summarized as follows.

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<sup>22</sup>the fact that the kinetic energy of the nuclei remains bounded at any macroscopic time is indeed a crucial assumption in the development of the theorem, see below

Let us put the electronic mass  $m_e = 1$ , so that  $m_n \gg 1$ , and introduce the dimensionless parameter  $\varepsilon = \sqrt{1/m_n}$ , therefore  $0 < \varepsilon \ll 1$  as in the previous time-adiabatic setting. The molecular Hamiltonian (2.134) then becomes

$$H_{\text{mol}}^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x + H_e(y; x), \quad (2.135)$$

where we defined the “electronic” Hamiltonian

$$H_e(y; x) \equiv -\frac{1}{2}\Delta_y + V_e(y) + V_n(x) + V_{\text{en}}(x, y) \quad (2.136)$$

as it contains all the electronic degrees of freedom and the *positions* of the nuclei only. Therefore, the electronic Hamiltonian can be seen as an operator  $H_e(x)$  acting on the Hilbert space  $\mathcal{H}_e \equiv \mathcal{L}^2(\mathbb{R}^{3k})$  of the electrons alone, each of the  $H_e(x)$  parametrically depending on the positions  $x$  of the nuclei. Similarly to the time-adiabatic setting, the properties of the spectrum of the parametrically-dependent Hamiltonian is crucial in order to obtain physical results when applying such an approximation scheme; let us then denote the discrete spectrum of  $H_e(x)$ <sup>23</sup> by  $\sigma(x) = \{E_j(x)\}$ , and assume that there is a part of the spectrum, say  $\sigma_*(x)$ , isolated by a gap from the remainder:

**Definition 2.37** (Gap on  $\Lambda$ ). Let  $\sigma_*(x) \subset \sigma(x)$ ,  $x \in \Lambda \subset \mathbb{R}^{3l}$  be a part of the spectrum, and be  $f_\pm$  two continuous and bounded functions defining the interval  $I(x) = [f_-(x), f_+(x)]$ , such that

$$\sigma_*(x) \subset I(x), \quad \inf_{x \in \Lambda} \text{dist}(I(x), \sigma(x) - \sigma_*(x)) \equiv g > 0. \quad (2.137)$$

Then,  $\sigma_*(x)$  is said to be isolated by a gap  $g$  from the remainder over  $\Lambda$ .

Clearly, definition 2.37 is the perfect analogue of 2.34 of the time-adiabatic setting, where here the time dependence is replaced by the space-dependence and the dominion  $\Lambda$  over which it holds is specified. In practical situations,  $\Lambda$  does not extend to the whole  $\mathbb{R}^{3l}$  as the electronic energy surfaces  $E_j(x)$ , hereafter also referred to as **bands**, do in generally cross. Again, to each spectral subspace is uniquely associated a projector  $P_j(x)$ , which in the case of non-degenerate eigenvalue is associated to an electronic eigenstate  $|\phi_j(x)\rangle$ , apart from an  $x$ -dependent phase factor. Given the spatial-gap condition 2.37, and the form of the molecular Hamiltonian as in (2.135), we want to find approximate solutions of the time-dependent Schrödinger equation

$$i\varepsilon \frac{d\psi}{dt} = H_{\text{mol}}^\varepsilon \psi, \quad \psi(t_0) = \psi(0) \in \mathcal{L}^2(\mathbb{R}^{3(l+k)}) \quad (2.138)$$

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<sup>23</sup>we hereafter omit the electronic dependence

where the small parameter  $\varepsilon$  also enters the l.h.s. of eq. (2.138) as we are interested in the evolution over the macroscopic time scale  $t$ , at which the nuclei actually change their configuration (cfr. the discussion in paragraph 2.2.2). At the zeroth order, the molecular Hamiltonian reduces to the electronic one (2.136), so that if the dynamics is restricted by the initial conditions to the electronic subspace  $\text{Ran}(P_*(x))$ , it will remain there for all later times. Namely, assuming that  $P_*$  is  $d$ -dimensional and denoting by  $\{|\phi_n(x)\rangle, n = 1, \dots, d\}$  the corresponding electronic eigenfunctions (parametrically dependent on the nuclear position  $x$ ), a state of the form

$$\sum_n \chi_n(x) |\phi_n(x)\rangle \quad (2.139)$$

is an exact eigenfunction of the total system for each nuclear wavefunction  $\chi_n(x)$ <sup>24</sup>. However, since  $\varepsilon$  is small but differs from zero, the restriction to  $P_*\mathcal{H}_{\text{mol}}$  (that is, to states of the form (2.139)) only yields approximate solutions of eq. (2.138), as the nuclear Laplacian  $\Delta_x$  weakly couples different spectral subspaces thanks to the  $x$ -dependence. In other words, the commutator

$$[P_*, H_{\text{mol}}^\varepsilon] \neq 0. \quad (2.140)$$

The key observation in order to state a space-adiabatic theorem is that, provided some regularity conditions on the nuclear wavefunction are embraced (the most important being the request that their kinetic energy be uniformly bounded), the commutator  $[P_*, H_{\text{mol}}^\varepsilon] = \mathcal{O}(\varepsilon)$  so that the spectral subspace  $P_*\mathcal{H}_{\text{mol}}$  is approximately left invariant during the evolution. Equivalently, it is convenient to define the “diagonal” Hamiltonian

$$H_{\text{diag}}^\varepsilon \equiv P_* H_{\text{mol}}^\varepsilon P_* + P_*^\perp H_{\text{mol}}^\varepsilon P_*^\perp \quad (2.141)$$

which is an approximate generator of the true dynamics, in the sense of the

**Theorem 2.38** (Space-Adiabatic theorem). *Assuming that the gap condition 2.37 is satisfied for  $\Lambda = \mathbb{R}^{3l}$ , then there exists a constant  $C$  such that*

$$\left\| \left( e^{-iH_{\text{mol}}^\varepsilon t/\varepsilon} - e^{-iH_{\text{diag}}^\varepsilon t/\varepsilon} \right) P_* \right\| \leq C\varepsilon(1 + |t|)(1 + |\mathcal{E}|) \quad (2.142)$$

when acting on wavefunctions  $\psi \in \mathcal{L}^2(\mathbb{R}^{3(l+k)})$  with bounded kinetic energy  $\mathcal{E} < \infty$  uniformly in  $\varepsilon$ .

The content of the above theorem is the perfect analogue of that of 2.36, where in this case, however, the adiabatically-varying parameters are true quantum mechanical

<sup>24</sup>On the other hand, if  $\varepsilon = 0$  exactly, it would make no sense to consider the time-dependent Schrödinger eq. (2.138) over finite macroscopic times.

degrees of freedom (the nuclear positions), so that further requirements on the initial state are needed in order to uniformly control their behaviour during the macroscopic evolution; moreover, it is usually impossible in a true physical system that the gap condition 2.37 is satisfied over the whole configuration space, so that the theorem can be applied only locally.

However, from a practical perspective, the diagonal Hamiltonian (2.141) still provides the initial useful tool to study the dynamics inside the relevant spectral subspace  $P_*\mathcal{H}_{\text{mol}}$ ; at variance with the time-adiabatic case (cfr. the discussion following theorem 2.36), the reference space is now given by  $\mathbb{C}^d \otimes \mathcal{L}^2(\Lambda)$ , where  $d$  represents the multiplicity of the considered eigenvalue as before, but a tensor product with the nuclear Hilbert space is present due to the fact that the nuclear degrees of freedom are left undetermined by the choice of the electronic eigenstates  $\{|\phi_n(x)\rangle\}$ . In other words, the relevant part of the “diagonal” Hamiltonian (2.141), is diagonal only in the electronic sector and the Laplacian term  $\Delta_x$  pertaining to the nuclear sector has not so far been considered. In particular, an effective Hamiltonian on the reference subspace can be defined as

$$\begin{aligned}
H_{\text{eff}}^\varepsilon &\equiv P_* H_{\text{mol}}^\varepsilon P_* = \\
&= \sum_{m,n=1}^d |\phi_m(x)\rangle \left( E(x)\delta_{mn} + \frac{1}{2} \sum_{l=1}^d (p\delta_{ml} - \varepsilon\mathcal{A}_{ml}(x)) \cdot (p\delta_{ln} - \varepsilon\mathcal{A}_{ln}(x)) \right) \langle\phi_n(x)| = \\
&\equiv \sum_{m,n=1}^d |\phi_m(x)\rangle (H_{\text{BO}}^\varepsilon)_{mn} \langle\phi_n(x)|
\end{aligned} \tag{2.143}$$

where

$$\mathcal{A}_{nl}(x) = \text{i} \langle\phi_n(x)| \nabla_x |\phi_l(x)\rangle \tag{2.144}$$

and  $p = -\text{i}\varepsilon\nabla_x$  is the momentum of the nuclei. In the last equality of eq. (2.143), we defined in round brackets the **Born-Oppenheimer** effective Hamiltonian for the nuclei; in the here considered case of a single eigenvalue  $E$  with finite multiplicity  $d$ , the Hamiltonian is matrix valued, and a similar formal treatment occurs whenever more than one band, each of multiplicity one, is involved in the projector  $P_*$  (it is sufficient to replace  $E(x) \rightarrow E_m(x)$ ). Besides the already diagonal part  $E(x)\delta_{mn}$ , in eq. (2.143) the terms originating from the nuclear Laplacian  $\sim \varepsilon^2\Delta_x$  do appear; in particular, the nuclear momentum  $p$  results corrected by the terms  $\mathcal{A}_{nl}(x)$  of eq. (2.144) which arise as the  $x$ -derivatives also act onto the electronic parametric eigenfunctions  $|\phi_n(x)\rangle$ . These quantities are the analogue of that present in eq. (2.108) and have a geometrical origin, as they are the components of a matrix-valued connection form in the spectral bundle constructed over the nuclear coordinates support  $\mathbb{R}^{3l}$ : in analogy with the time-adiabatic case, they are called **Berry’s (vector) potential**. Generally speaking, the geometric

properties of such a bundle is affected by the possibility that, at some point  $\tilde{x}$ , the energy levels involved in the restricted dynamics intersect among them or, analogously, that the domain  $\Lambda$  for which the gap condition 2.37 holds cannot be extended to the whole  $\mathbb{R}^{3l}$  when a single energy band somewhere crosses another one. In any case, energy level intersections of co-dimension two makes impossible to gauge away the Berry's potential term by appropriately choosing the representative electronic eigenfunctions, giving in turn rise to Berry's phases for cyclic nuclear motion.

As a last step, without entering much in detail, we address the question about the classical behaviour of the nuclei. As it should be clear from the above discussion, the adiabatic decoupling procedure in molecular systems does not rely on classical-like approximations. On the other hand, if the initial nuclear wavepacket is sufficiently localized in the configuration space about some point  $q(0)$ , one would expect that a semiclassical treatment of the time-dependent Schrödinger equation relative to the Born-Oppenheimer Hamiltonian becomes available, and it is indeed the case even for a much broader class of initial states. To be a little more explicit, let us assume, for simplicity, a real-valued (*i.e.*, one dimensional) Born-Oppenheimer effective Hamiltonian, whose semiclassical symbol (*i.e.*, the phase-space function whose Weyl quantization  $q \rightarrow \hat{x}$  and  $p \rightarrow -i\varepsilon\nabla_x$  gives back the quantum  $H_{\text{BO}}^\varepsilon$ ) reads

$$H_{\text{BO}}^{\text{cl}} = \frac{1}{2}p^2 + E(q) . \quad (2.145)$$

Notice that in such a case the geometric term is omitted as it can be suitably made vanish. Then, the  $x$ -support of the solution of

$$i\varepsilon \frac{d\chi^\varepsilon}{dt} = H_{\text{BO}}^\varepsilon \chi^\varepsilon, \quad \chi^\varepsilon(0) = \chi_0^\varepsilon \in \mathcal{L}^2(\mathbb{R}^{3l}) \quad (2.146)$$

can be approximately evaluated by the classical evolution (*i.e.*, with a uniform error of order  $\varepsilon$ ):

$$\dot{q} = p, \quad \dot{p} = -\nabla_q E(q) . \quad (2.147)$$

as long that this classical evolution, for the considered duration  $T$  of the dynamics, does not make  $q(T)$  exceed the border of the domain  $\Lambda$  inside which the space-adiabatic machinery works. The other important condition that enables the usage of such a semiclassical treatment<sup>25</sup> is the existence, not always guaranteed, of a classical distribution  $\rho^{\text{cl}}$  over the phase space to which the initial nuclear wavefunction  $\chi_0$  weakly converge. This means, in formulas, to require

$$\lim_{\varepsilon \rightarrow 0} \left| \left\langle \chi_0^\varepsilon \left| \hat{O} \right| \chi_0^\varepsilon \right\rangle_{\mathcal{H}_n} - \int dq dp O(q, p) \rho^{\text{cl}}(q, p) \right| = 0 \quad (2.148)$$

<sup>25</sup>we leave the details to [15] and references therein

for any semiclassical symbol  $O(q, p)$ , where  $\hat{O}$  stands for its Weyl quantization. As anticipated, such semiclassical treatment provides a *further* controlled approximation and a consequent practical simplification than that adopted in the space-adiabatic framework. However, we remark that in the formalism we shall develop in the subsequent chapters, and especially in paragraph 4.2, the semiclassical approach will play a prominent role, while a neat distinction between the latter and the adiabatic framework will be no more available due to the structure of the formalism itself.



## Chapter 3

# The Parametric Representation

In the introductory chapter 1 we briefly presented the traditional analysis methods adopted whenever a quantum system is in contact with some surrounding environment, classifying the possible situations of interests into two main categories: *closed* systems, where the environment is classically treated and consequently formalized as a set of external, usually time-dependent parameters, and *open* ones, where the environment is ideally quantum, too, but its presence in the overall description actually manifests itself only as its “coarse-grained” effects onto the open system, whose non-unitarity character of the dynamics, together with the non-pureness of the state, are indeed the defining features of “openness”. By contrast, closed systems are those evolving unitarily and described by pure states.

In this chapter we are going to present the generalities of the original part of this thesis work, which provides an alternative but, at the same time, interpolating scheme between the two approaches summarized above: the *parametric representation* of an open quantum system. Loosely speaking, the parametric representation is an exact formalism which allows to simultaneously treat a composite, bipartite quantum system in such a way that the principal (open) system, instead of being represented by a density operator, becomes a collection of pure states with an additional dependence on a “label” that specifies a possible environmental “configuration”, their occurrence (pure parametrized state + corresponding environmental configuration) ruled by a certain probability distribution<sup>1</sup>. The possibility of such a representation relies on two crucial assumptions, both conceptual and technical, which we now want to introduce due to their importance, but that, obviously, we shall widely discuss throughout the whole chapter:

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<sup>1</sup>We here emphasize with the usage of quotation marks that the terms we are adopting are intentionally vague, as their specification will be formally and conceptually different in the two main cases we are going to discuss

1. the composite, global system (open system + its environment) is actually global, in the sense that it *isolated* (cfr. chapter 1) and hence is described by a pure state with no further “external” dependences; pushing forward the idea of such a physical set-up, this pure state should also be an *eigenstate* (actually, the ground state) of the underlying Hamiltonian operator but, as the parametric representation does not need such a specification, we will develop the general formalism forgetting about this additional, physical requirement, postponing its discussion to the application of the formalism itself in the subsequent chapter 4.
2. On the environment it is possible to define a partition (or, equivalently, resolution) of the identity operator in terms of projectors onto normalized states; in the case of separable Hilbert spaces<sup>2</sup>, this condition is automatically satisfied since a countable orthonormal basis exists by definition, ensuring in turn the possibility of such a partition through the basis states themselves; whichever way the identity resolution is defined, the resulting description will be strongly affected by the “structure” that the chosen partition induces on the description of the environment . As we shall see, a different choice from that ensured by the existence of a countable basis actually provides the interpolating scheme mentioned above, as it is achieved through a continuous of states rather than a countable set; nevertheless, separability will play an important role, as well, even in the continuous case.

We divide the chapter in two sections: in the first one we present in detail the whole formalism of the parametric representation. The parametric representation by itself is a tool to describe a pure state without implying the existence of an underlying dynamics, and the description is exact as in the case of the reduced density operator. On the other hand, starting from paragraph 3.1.2, we present a general recipe to develop such a method employing *generalized coherent states* which provide the requested resolution of the identity on the environment and whose construction is actually suggested by the form of the Hamiltonian of the system: we remark again that, although this construction takes origin from the dynamics, its implementation for the parametric representation has nothing to do with the dynamics itself. In the second section 3.2 of this chapter we will take into account the Hamiltonian of the system and investigate some dynamical aspects in the context of the parametric representation in general, and some more specific related to the choice of generalized coherent states, in particular.

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<sup>2</sup>on the other hand, almost every Hilbert space adopted in quantum mechanics is actually separable; in any case, we emphasize that the necessary condition in order to proceed with the parametric representation construction is the possibility to define the identity resolution on the environment, the separability just being a sufficient one.

### 3.1 An alternative approach to Open Quantum Systems: the Parametric Representation

In this section we describe in detail all the formal aspects concerning the parametric representation; as we provide both a *discrete* and a *continuous* version of such a description, we hope, on one hand, to highlight the complete generality and feasibility of the approach, on the other to emphasize the deep differences between these two main cases, and in particular the advantages obtained when adopting the latter.

As mentioned in the chapter introduction, the parametric representation is a formalism to exactly describe the state of a *composite* bipartite system, but its actual implementation is devised in such a way that the *physical* distinction between the two subsystems as “principal (open) system+its environment” is apparent; by our definition, the parametric representation pertains to the *open* system, but the information that it provides is sufficient to reconstruct the whole, composite, state; consistently, the construction starting from the global state can be in principle reversed if the role of open system and environment are for some reasons reversed. Indeed, we conceived the idea to implement such a representation to describe an open quantum system being inspired by the long-standing adiabatic representation of a molecule (which is by all means a composite system) that we sketched in the context of the space-adiabatic theory of paragraph 2.2.4. In the more recent framework of OQS theory, the nuclei (resp., the electrons) can be viewed as the environment of the open system constituted by the electrons (resp., the nuclei) and the adiabatic representation of the global wavefunction (cfr., *e.g.*, eq. (2.139) with only one addend) *is* a parametric representation. In order to explain our motivations more precisely, let us focus on such inspiring example in a little more detail, resorting to a change of notation which is (hopefully) more natural in this context. Denoting now the collective vectors of electronic and nuclear coordinates by  $\mathbf{r}$  and  $\mathbf{R}$ , respectively, the adiabatic representation of the molecular wavefunction (2.139) reads

$$\Psi(\mathbf{r}, \mathbf{R}) = \sum_n \chi_n(\mathbf{R}) \phi_n(\mathbf{r}, \mathbf{R}), \quad H_e(\mathbf{R}) \phi_n(\mathbf{r}, \mathbf{R}) = E_n(\mathbf{R}) \phi_n(\mathbf{r}, \mathbf{R}), \quad (3.1)$$

where we have recalled that the electronic states  $\phi_n(\mathbf{r}, \mathbf{R})$  are obtained as the set of eigenfunctions of the electronic Hamiltonian  $H_e(\mathbf{R})$  (cfr. eq. (2.136)). Those states can be both seen as functions of the Hilbert space of the composite system  $\mathcal{L}^2(\mathbb{R}^{3(l+k)})$  and states of the electronic Hilbert space, parametrically dependent on  $\mathbf{R}$ . The infinite, countable set  $\{ \phi_n(\mathbf{r}, \mathbf{R}) \}$ , moreover, provides a basis for  $\mathcal{L}^2(\mathbb{R}^{3(l+k)})$ , hence the description (3.1) is indeed exact when the sum involves the whole electronic basis, and the further  $\mathbf{R}$ -dependence of the nuclear wavefunction is dictated by physical reasons but is in principle unnecessary at this level. However, this adiabatic representation is mainly

adopted only taking a finite, small number of adiabatic states, while the nuclear wavefunction has to be explicitly singled out in order to pursue such a decoupling scheme at the first order in the adiabatic parameter  $\varepsilon$ , the resulting total wavefunction being only a (controlled) approximation of the true one (cfr. the discussion in paragraph 2.2.4). In the case of a single, non-degenerate electronic state<sup>3</sup>, the expansion (3.1) reads

$$\Psi(\mathbf{r}, \mathbf{R}) \simeq \chi(\mathbf{R})\phi(\mathbf{r}, \mathbf{R}) . \quad (3.2)$$

In order to highlight the analogies with the subsequent construction, we restore the Dirac “bra-ket” notation by ignoring the fact that the Hilbert spaces involved are indeed functional Hilbert spaces, so that an “abstract” state  $|\psi\rangle \in \mathcal{H}$  (either electronic, nuclear or molecular) is related to its wavefunction  $\psi(x)$  by the expansion

$$|\psi\rangle = \int d\mathbf{x} \psi(\mathbf{x}) |\mathbf{x}\rangle , \quad (3.3)$$

where  $\psi(\mathbf{x}) \equiv \langle \mathbf{x} | \psi \rangle$ ,  $\mathbf{x}$  is the appropriate coordinate (either  $\mathbf{r}$ ,  $\mathbf{R}$  or  $(\mathbf{r}; \mathbf{R})$ ), and  $|\mathbf{x}\rangle$  is the related generalized basis state (which in this coordinate case, actually, does not belong to the Hilbert space as it is only a distribution): in other words, the wavefunction  $\psi(\mathbf{x})$  is the set of the Fourier coefficients of an element  $|\psi\rangle \in \mathcal{H}$  with respect to the position eigenstates  $|\mathbf{x}\rangle$  and contains the whole information about  $|\psi\rangle$ . By applying the expansion (3.3) on the molecular state  $|\Psi(\text{e,n})\rangle$ , the relationship with its total wavefunction  $\Psi(\mathbf{r}, \mathbf{R})$  is given by

$$|\Psi(\text{e,n})\rangle = \int d\mathbf{r}d\mathbf{R} \Psi(\mathbf{r}, \mathbf{R}) |\mathbf{r}\rangle |\mathbf{R}\rangle , \quad (3.4)$$

Ignoring the actual choice of the electronic basis, one may equivalently write eq. (3.4) as

$$|\Psi(\text{e,n})\rangle \equiv \int d\mathbf{R} \langle \mathbf{R} | \Psi(\text{e,n}) \rangle |\mathbf{R}\rangle , \quad (3.5)$$

where we have defined the “partial” overlap

$$\langle \mathbf{R} | \Psi(\text{e,n}) \rangle \equiv \int d\mathbf{r} \Psi(\mathbf{r}, \mathbf{R}) |\mathbf{r}\rangle ; \quad (3.6)$$

for any given  $\mathbf{R}$ , the latter is an element of the electronic Hilbert space and has to be seen as a projection  $\Pi_{\mathbf{R}} \equiv \langle \mathbf{R} | \cdot \rangle : \mathcal{H}_{\text{mol}} \rightarrow \mathcal{H}_{\text{e}}$ . We remark that eq. (3.5) is an *exact* representation of the composite, molecular state  $|\Psi(\text{e,n})\rangle$ , as the set  $\{ \langle \mathbf{R} | \Psi(\text{e,n}) \rangle, \mathbf{R} \in \mathbb{R}^l \}$  is sufficient to reconstruct  $|\Psi(\text{e,n})\rangle$  through the integral over the nuclear coordinate basis, in the same way eq. (3.3) is just an expansion of a generic state  $|\psi\rangle$  of the Hilbert space onto the coordinate basis  $\{ |\mathbf{x}\rangle \}$ ; indeed, and in sharp contrast to the reduced density matrix formalism, cfr. section 1.1, the integral over the environmental degrees

<sup>3</sup>which is, indeed, the situation usually referred to as Born-Oppenheimer approximation

of freedom (the nuclear coordinates) reproduces through (3.5) the composite state (the molecule), instead of yielding the reduced density operator for the principal system (the electrons). We shall return to the connection between the two approaches when dealing with the general construction presented in paragraphs 3.1.1-3.1.2.2.

In the adiabatic setting, see eq. (3.2) the expansion (3.5) has to fulfill

$$\langle \mathbf{R} | \Psi(e,n) \rangle \equiv \chi(\mathbf{R}) |\phi_e(\mathbf{R})\rangle , \quad (3.7)$$

where the “abstract” electronic state is immediately given by

$$|\phi_e(\mathbf{R})\rangle = \int d\mathbf{r} |\mathbf{r}\rangle \phi(\mathbf{r}, \mathbf{R}) . \quad (3.8)$$

Eq. (3.7), together with the expansion (3.5), naturally displays the very structure we have been inspired by when developing the parametric representation for a generic quantum composite system. Some remarks are therefore in order both to clarify its meaning in this particular situation and to notice, in the subsequent, the relevant differences with respect to the general construction. Firstly, as we mentioned in the introduction, the formal passage from a generic representation of the molecular state to a parametric one is achieved by introducing a resolution of the identity operator in the Hilbert space of the nuclei  $\mathcal{H}_n$ , which in this case relies on the generalized position basis

$$\mathbb{1}_{\mathcal{H}_n} = \int d\mathbf{R} |\mathbf{R}\rangle \langle \mathbf{R}| \quad (3.9)$$

and realizes the mapping, for each  $\mathbf{R}$

$$\Pi_{\mathbf{R}} : \mathcal{H}_{\text{mol}} \rightarrow \mathcal{H}_e, \quad |\Psi(e,n)\rangle \mapsto \langle \mathbf{R} | \Psi(e,n) \rangle . \quad (3.10)$$

Notice that the parametrized states  $\langle \mathbf{R} | \Psi(e,n) \rangle$  have to be seen, in this context, as *unnormalized* states of the electronic (open) subsystem. Their decomposition, as in eq. (3.7) or eq. (3.2), besides being an essential *ansatz* in order to pursue the adiabatic decoupling scheme, is dictated by requiring the correct quantum mechanical interpretation of probabilities, both for the electrons and the nuclei. Indeed, the electronic parametrized states  $\langle \mathbf{R} | \Psi(e,n) \rangle$  can be in principle normalized for each  $\mathbf{R}$ , by dividing by the appropriate  $\mathbf{R}$ -dependent normalization factor:

$$\langle \mathbf{R} | \Psi(e,n) \rangle \xrightarrow{\text{norm.}} \frac{\langle \mathbf{R} | \Psi(e,n) \rangle}{\| \langle \mathbf{R} | \Psi(e,n) \rangle \|_{\mathcal{H}_e}} , \quad (3.11)$$

where we have here explicitly stressed in the subscripts that the scalar product is taken

over the *electronic* Hilbert space<sup>4</sup>. It is immediate now to notice that the decomposition (3.7) can in general perform the electronic state normalization, by identifying:

$$|\phi_e(\mathbf{R})\rangle \equiv e^{i\lambda(\mathbf{R})} \frac{\langle \mathbf{R} | \Psi(e,n) \rangle}{\| \langle \mathbf{R} | \Psi(e,n) \rangle \|_{\mathcal{H}_e}}, \quad (3.12a)$$

$$\chi(\mathbf{R}) \equiv e^{-i\lambda(\mathbf{R})} \| \langle \mathbf{R} | \Psi(e,n) \rangle \|_{\mathcal{H}_e}, \quad (3.12b)$$

in agreement with the normalizations implied in eq. (3.2). In the definitions (3.12), we had the freedom to single out two compensating  $\mathbf{R}$ -dependent phase factors, which embody, on one hand, the *gauge* freedom in choosing the representative electronic eigenfunctions (sections in the spectral bundle over  $\mathbf{R}$ , see paragraph 2.2.3) and, thus, reflect themselves in the definition of the Berry's potential (cfr. eq. (2.144)) and the related possible emergence of Berry's phase; on the other hand, they allow one to truly treat  $\chi(\mathbf{R})$  as a nuclear wavefunction, making it a probability *amplitude*. As for this last point, it is immediate to calculate from (3.12b) and the overall normalization  $\langle \Psi(n,e) | \Psi(n,e) \rangle_{\mathcal{H}_{\text{mol}}} = 1$  that

$$\int d\mathbf{R} |\chi(\mathbf{R})|^2 = 1, \quad (3.13)$$

meaning that the electronic state (local) normalization automatically implies that of the nuclear wavefunction.

The starting point in the presentation of the above paradigmatic example was the total wavefunction decoupling induced by the first order Born-Oppenheimer theory, eq. (3.2); however, the parametric representation of a molecule is *not* a specific feature of such an approximation scheme: indeed, it is immediate to notice that the abstract construction from eq.(3.5) to eqs. (3.12) does *not* rely on any approximation, as the initial composite molecular state  $|\Psi(e,n)\rangle$  can be in principle completely generic and, consequently, the decomposition in a parametrized and normalized electronic state  $|\phi_e(\mathbf{R})\rangle$  and its  $\mathbf{R}$ -dependent normalization  $\chi(\mathbf{R})$  does *not* force the former to be an adiabatic eigenfunction, nor the latter to be the adiabatic nuclear wavefunction. In this sense, the adiabatic form of eq. (3.2) is a particular case of parametric representation, obtained through the resolution of the identity over the nuclear coordinates when applied to a specific class of molecular states. The same line of reasoning can be adopted to conclude that the decomposition (3.2) can be made *exact* by an appropriate choice of the parametrized electronic and nuclear wavefunction, as extensively explained in [23, 24] in the context of probability amplitudes in quantum chemistry. In particular, in [24] a minimization procedure in order to systematically express in the form (3.2) the exact

<sup>4</sup>It is clear that, since the latter is the functional Hilbert space  $\mathcal{L}^2(\mathbb{R}^{3k})$ , the scalar product is calculated as an integral over the electronic coordinates, but we still prefer to avoid any formal reference to the Hilbert space structure of the electrons since it is both in general unnecessary and in particular may rise confusion.

ground state of a molecular Hamiltonian (see, *e.g.*, eq. (2.134)) is devised: not surprisingly, such minimization has to be carried over by involving Lagrange multipliers that take into account, firstly, the normalization of the electronic parametrized state for each nuclear position, secondly, that of the nuclear wavefunction, in perfect analogy with the above presented construction.

### 3.1.1 The parametric representation with a discrete resolution of the identity

We are now in the position to present the general construction yielding the parametric representation of an open quantum system *obtained starting from a composite system*. The only assumption we make, as anticipated in the chapter introduction, is the separability of the environmental Hilbert space, which we shall denote by  $\mathcal{H}_{\text{env}}$  in the following; the reason for such a requirement is two-fold: as for the current paragraph, it guarantees the existence of countable bases  $\in \mathcal{H}_{\text{env}}$  providing an identity resolution, but it will be also necessary in the generalized coherent states construction we will extensively discuss in the remainder of this work.

Let us then consider a pure state  $|\Psi\rangle$  belonging to the tensor product Hilbert space  $\mathcal{H} \equiv \mathcal{H}_{\text{open}} \otimes \mathcal{H}_{\text{env}}$ ,  $\mathcal{H}_{\text{open}}$  denoting the Hilbert space of the open (principal) system. In order to avoid unnecessary complications and, at the same time, still comprising a huge class of physical systems usually treated as OQS (cfr. chapter 1), we restrict the discussion to the case where  $\mathcal{H}_{\text{open}}$  is finite-dimensional. Choosing two orthonormal bases  $\{|\alpha\rangle \in \mathcal{H}_{\text{open}}, \alpha = 1, \dots, \dim(\mathcal{H}_{\text{open}}) \equiv d < \infty\}$  and  $\{|n\rangle \in \mathcal{H}_{\text{env}}\}$ <sup>5</sup>, any global state  $|\Psi\rangle$  can be written as

$$|\Psi\rangle = \sum_{\alpha n} c_{\alpha n} |\alpha\rangle \otimes |n\rangle , \quad (3.14)$$

with  $\sum_{\alpha n} |c_{\alpha n}|^2 = 1$  as we assume  $|\Psi\rangle$  normalized to unity. The basis  $|n\rangle$  actually provides the most immediate parametric representation: indeed, defining  $\Pi_n \equiv \langle n | \cdot \rangle : \mathcal{H} \rightarrow \mathcal{H}_{\text{open}}$ , eq. (3.14) becomes

$$|\Psi\rangle = \sum_n |n\rangle \Pi_n(\Psi) , \quad (3.15)$$

where

$$\Pi_n(\Psi) = \sum_{\alpha=1}^d c_{\alpha n} |\alpha\rangle \quad (3.16)$$

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<sup>5</sup>from now on we shall distinct the labels pertaining the open system and the environment using, respectively, greek and latin letters

is the resulting unnormalized and  $n$ -dependent state of the open system, and is an explicit version of the l.h.s. of eq. (3.7) thanks to the local bases expansion of (3.14). In the same way the r.h.s. of eq. (3.7) provides the parametrized state normalization, we define

$$\Pi_n(\Psi) \equiv \chi_n |\phi_n\rangle, \quad (3.17)$$

where, again in perfect analogy with eqs. (3.12), the separation reads

$$|\phi_n\rangle \equiv e^{i\lambda_n} \frac{\Pi_n(\Psi)}{\|\Pi_n(\Psi)\|_{\mathcal{H}_{\text{open}}}} = e^{i\lambda_n} \frac{\sum_{\alpha=1}^d c_{\alpha n} |\alpha\rangle}{\sqrt{\sum_{\alpha=1}^d |c_{\alpha n}|^2}}, \quad (3.18a)$$

$$\chi_n \equiv e^{-i\lambda_n} \sqrt{\sum_{\alpha=1}^d |c_{\alpha n}|^2}, \quad (3.18b)$$

with a generic  $\lambda_n \in \mathbb{R}$ . It is trivial to verify that the choices (3.18) ensure

$$\| |\phi_n\rangle \|_{\mathcal{H}_{\text{open}}} = 1 \quad \forall n, \quad (3.19a)$$

$$\sum_n |\chi_n|^2 = 1. \quad (3.19b)$$

Summing up, we have the following

**Definition 3.1.** (Parametric Representation - discrete version) We define **parametric representation** of an open system (belonging to an isolated bipartite system described by the pure state  $|\Psi\rangle \in \mathcal{H}$ ), induced by the set

$$\left\{ \Pi_n \equiv \langle n | \cdot \rangle : \mathcal{H} \rightarrow \mathcal{H}_{\text{open}}, \sum_n |n\rangle \langle n| = \mathbb{1}_{\mathcal{H}_{\text{env}}} \right\}, \quad (3.20)$$

the set of couples

$$\{ (|\phi_n\rangle, \chi_n), |\phi_n\rangle \in \mathcal{H}_{\text{open}}, \| |\phi_n\rangle \|_{\mathcal{H}_{\text{open}}} = 1, \chi_n \in \mathbb{C} \}, \quad (3.21)$$

where  $|\Psi\rangle$  is given by eq. (3.14) and  $|\phi_n\rangle, \chi_n$  are defined by (3.18).

Several comments and clarifications are now in order. The most important one concerns the definition of the set of maps  $\{ \Pi_n \}$  that, when applied to a global state  $|\Psi\rangle \in \mathcal{H}$ , produces a countable set  $\{ \Pi_n(\Psi) \}$  belonging to the open system Hilbert space. Such a definition relies on the fact that the state  $|\Psi\rangle$  is understood as a composite state whose generic expansion is cast into the form of eq. (3.14), so that the overlap  $\langle n | \Psi \rangle$  has to be interpreted in the same sense of the partial trace over the environmental degrees of freedom (cfr. section 1.1), and hence can be calculated by evaluating the scalar products with the environmental basis states appearing in (3.14), without affecting the



principal system. On the other hand, eq. (3.16) do provide the resulting definition of the action of this set of maps on a generic  $|\Psi\rangle$ , so that the passage through the overlap  $\langle n|\Psi\rangle$  may seem unnecessary. However, this complication is due to the fact that we want to associate the parametric representation to a given partition of the unity in the environmental Hilbert space without making any assumption on the environmental basis the global state is written in; in fact, if the latter has a different expansion,

$$|\Psi\rangle = \sum_{\alpha,i} c'_{\alpha i} |\alpha\rangle \otimes |u_i\rangle, \quad (3.22)$$

the “new” basis  $\{|u_i\rangle\}$  is related to  $\{|n\rangle\}$  by a unitary transformation and, consistently, the coefficients  $c'_{\alpha i}$  oppositely change, so that the result of the action of any  $\Pi_n$  on  $|\Psi\rangle$  is the same, the only dependence being that inherited from the choice of the resolution of the identity on  $\mathcal{H}_{\text{env}}$ . Moreover, the fact that the set  $\{\Pi_n\}$  is associated to an identity resolution  $\sum_n |n\rangle\langle n| = \mathbb{1}_{\mathcal{H}_{\text{env}}}$  ensures that the global state becomes exactly written as in eq. (3.15) and can be in principle reconstructed from the set defining the parametric representation, eq. (3.21). As for this subject, we point out that the resolution of the identity leaves the possibility to redefine the phases of the states  $|n\rangle$  since the composite state  $|\Psi\rangle$  is obviously unaffected by a transformation of the type  $|n\rangle \rightarrow \exp(i\mu_n)|n\rangle$ ; however, such a freedom manifests itself in  $\Pi_n(\Psi) = \chi_n |\phi_n\rangle$ , yielding an additional overall phase ambiguity which can be eventually appended to the phases of  $\chi_n$  or  $|\phi_n\rangle$ . Many conventions can be adopted in this sense, but we prefer to postpone their discussion to the paragraph 3.1.2.2 which deals with a continuous parametric representation, where such freedoms assume their more natural interpretation as *gauge* freedoms.

The property stated in eq. (3.19b) has been derived from the physical assumption that the starting composite state is normalized, and must be seen as a consistency condition the parametric representation 3.1 has to fulfill when adopted in the converse sense, namely when the sets (3.20) and (3.21) are *assumed* and used to reconstruct the full state  $|\Psi\rangle$ . Moreover, a nice physical picture eventually emerge from such property: a parametric representation of an open quantum system derived from a composite pure state is a collection of pure parametrized (and normalized) states  $\{|\phi_n\rangle \in \mathcal{H}_{\text{open}}\}$  whose occurrence is ruled by the set of **probability amplitudes**  $\{\chi_n\}$  concerning the corresponding environmental state  $|n\rangle$ . It is now natural to wonder about the relationship between such a representation and the reduced density matrix formalism, and the simple answer is given by the immediate calculation:

$$\rho_{\text{open}} \equiv \text{Tr}_{\text{env}}(|\Psi\rangle\langle\Psi|) = \sum_n |\chi_n|^2 |\phi_n\rangle\langle\phi_n| \quad (3.23)$$

so that, for any open system local observable  $O_{\text{open}}$ , it is

$$\langle O \rangle = \text{Tr}_{\text{open}} (\rho_{\text{open}} O_{\text{open}}) = \sum_n |\chi_n|^2 \langle \phi_n | O_{\text{open}} | \phi_n \rangle . \quad (3.24)$$

Eqs. (3.23)-(3.24) state that the parametric representation does provide all the information needed to calculate the expectation values of any local observable for the principal system, and indeed provide much more than simply that, as it actually contains the information stored in the whole composite system, where the reduced density matrix is in this context its “summed” version. Moreover, it is immediate to see that

$$|\chi_n|^2 = (\rho_{\text{env}})_n \equiv \langle n | \rho_{\text{env}} | n \rangle \quad (3.25)$$

where  $\rho_{\text{env}} \equiv \text{Tr}_{\text{open}} (|\Psi\rangle \langle \Psi|)$  is the reduced density matrix of the environment, meaning, in turn, that the probabilities  $|\chi_n|^2$  are the *populations* of the environment in the basis  $|n\rangle$ , irrespective to the configuration of the principal system.

For the sake of concreteness, we now move to the simplest example of two qubits forming a composite system in an entangled Bell state[2].

**Example 3.1** (Bell state). *Let us consider a quantum system made up by two qubits, and denote the composite Hilbert space as  $\mathcal{H} \equiv \mathcal{H}_A \otimes \mathcal{H}_B$ , where the labels  $A$  and  $B$  refer to each single qubit subsystem. We assume such a system to be described by the Bell state*

$$|\Phi^+\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B) , \quad (3.26)$$

where the local orthonormal bases  $(|0\rangle_i, |1\rangle_i)$ ,  $i = A, B$  are expressed as computational bases, and physically we think of them as referring to the two eigenvalues of the spin operator along a given direction, say  $z$ , implying that the logical qubit is actually realized by a spin- $\frac{1}{2}$  particle: the states  $|0\rangle_i$  correspond, in each subsystem  $A$  and  $B$ , to a local measurement of  $(\sigma_z)_i = +\frac{1}{2}$ , and  $|1\rangle_i$  to  $(\sigma_z)_i = -\frac{1}{2}$ . The role of the two subsystems is perfectly interchangeable as the state (3.26) is invariant as  $A \leftrightarrow B$ ; in order to avoid confusion, however, we think of the qubit  $A$  as the open system so that  $B$  is its environment, and we firstly consider the parametric representation induced by the resolution of the identity relative to the same computational basis, that is  $\mathbb{1}_B = \sum_{n=0,1} |n\rangle_B \langle n|_B$ . The resulting parametrized states for  $A$  immediately read:

$$\Pi_0(\Phi^+) \equiv \langle 0_B | \Phi^+ \rangle = \frac{1}{\sqrt{2}} |0\rangle_A \quad (3.27a)$$

$$\Pi_1(\Phi^+) \equiv \langle 1_B | \Phi^+ \rangle = \frac{1}{\sqrt{2}} |1\rangle_A \quad (3.27b)$$

Therefore (putting the phases  $\lambda_n = 0$ ) the normalized and parametrized states together with their amplitudes (cfr. eq. (3.18)) can be simultaneously written as

$$|\phi_n\rangle = |n\rangle_A, \quad \chi_n = \frac{1}{\sqrt{2}}, \quad n = 0, 1 \quad (3.28)$$

The initial total state is then trivially reconstructed as in eq. (3.15) using the above expression, eq. (3.28):

$$|\Phi^+\rangle = \sum_n |n\rangle_B \chi_n |\phi_n\rangle . \quad (3.29)$$

In other words, the initial state was already in the parametric representation induced by the computational basis on the environment. This fact is obviously not a mere coincidence, as the Bell state (3.26) (alike the other Bell states) is written in the Schmidt decomposed form (cfr. section 1.1), and the Schmidt decomposition is a particular kind of parametric representation. In fact, in general, a bipartite state in Schmidt form has the following structure:

$$|\Psi_{Schmidt}\rangle = \sum_j \sqrt{p_j} |j\rangle_A \otimes |j\rangle_B , \quad (3.30)$$

where the sum runs over the lower dimensionality between the two subsystems, and  $|j\rangle_A, |j\rangle_B$  are local orthonormal bases elements. The natural identifications with the parametric representation formalism are, considering the system  $A$  as the principal one,  $\sqrt{p_j} \leftrightarrow \chi_j$  and  $|j\rangle_A \leftrightarrow |\phi_j\rangle$ , remembering that the phases of  $\chi_j$  can always be adjusted to make them positive real numbers; the only apparent difference resides in the fact that, if the dimensionality of the environment  $d_B$  is strictly greater than that of the open system (unlike the previous explicit case), the environmental states  $|j\rangle_B$  appearing in (3.30) are fewer than  $d_B$ , thus not forming an identity resolution in  $\mathcal{H}_B$ . However, it is not an actual problem to exactly make (3.30) a parametric representation in the sense of the definition 3.1, since one may trivially complete the resolution of the identity with the basis remainder  $|k\rangle_B, k = 1, \dots, d_B - d_A$  and extend the sum to the whole basis while putting to zero the amplitudes of the previously missing states,  $\chi_k = 0$  for  $k = 1, \dots, d_B - d_A$ . More importantly, it is clear that the converse is not true: not every discrete parametric representations is a Schmidt decomposition. Indeed (besides the identity resolution issue) whichever of the two subsystems you choose as being the open one, the corresponding basis states are automatically orthonormal in (3.30), while for a general parametric representation it is not:  $\langle \phi_n | \phi_{n'} \rangle \neq \delta_{nn'}$ , as immediately verifiable from the definition (3.18a).

Let us now suppose to parametrize the same Bell state (3.26) using a different resolution of the identity, namely that given by the orthonormal basis:

$$|\pm\rangle_B \equiv \frac{1}{\sqrt{2}} (|0\rangle_B \pm |1\rangle_B) , \quad (3.31)$$

hence corresponding to the  $\sigma_x$  eigenvectors. It is readily seen that, using the same basis also for  $A$ , one can write  $|\Phi^+\rangle$  as

$$|\Phi^+\rangle \equiv \frac{1}{\sqrt{2}} (|+\rangle_A \otimes |+\rangle_B + |-\rangle_A \otimes |-\rangle_B) , \quad (3.32)$$

thus immediately yielding the parametric representation:

$$|\phi_n\rangle = |n\rangle_A, \quad \chi_n = \frac{1}{\sqrt{2}}, \quad n = +, -. \quad (3.33)$$

Notice that, although the form of the parametric representation is the same as before, the parametrized states are different consistently with the change of the environmental identity resolution, as previously they were  $\{|\phi_n\rangle\} = |0\rangle_A, |1\rangle_A$ , now they are  $\{|\phi_n\rangle\} = |+\rangle_A, |-\rangle_A$ , while the amplitudes do coincide due to the special choice of a Bell state for the to be parametrized composite state.

### 3.1.2 The parametric representation with generalized coherent states

In the previous paragraph we introduced the formal aspects that concern the parametric representation using a countable identity resolution on the environmental Hilbert space. Although we consider such a construction interesting *per se* thanks to both its novelty and generality, we saw in the example 3.1 that the Schmidt decomposition is indeed a prototypical form of parametric representation, thus suggesting that, at least in the “direct way” (namely, that starting from the composite state and arriving to the parametrized couples  $\{(|\phi_n\rangle, \chi_n)\}$ ), there is no *a priori* reason to prefer the generalized construction (the parametric representation) to the “canonical” Schmidt decomposition. However, rather than exploring in detail the “converse way” in the discrete case, which would surely involve a non-trivial extension of the Schmidt formalism and would result to be an interesting issue both from a mathematical (algebraic) and from a physical (information-theoretic) point of view, we prefer to adopt the approach mentioned in the chapter introduction, and resort to a continuous variable formalism.

The motivations for such a choice are various, both conceptual and practical: besides the intention to radically distinguish the parametric representation formalism to that induced by the Schmidt decomposition, the most important reason to adopt a continuous version of the parametric representation is the pursuit of a natural scheme to relate the

fully quantum treatment of an open quantum system to closed systems, since, from our point of view, the latter approach has to be derived from the former in a systematic way; in particular, the intuition suggests that when a quantum system surrounded by an environment is effectively treated as closed, the parameters characterizing its environment are classical objects that should be, in principle, derived as “classical limits” of some *a priori* exactly quantum description. A detailed discussion of the crossover from a quantum to a classical “world” does really go beyond the scope of this thesis work, as such a topic is deeply connected to the subtlest conceptual aspects concerning the very interpretation of quantum mechanics as a physical theory of reality. In the following, we will just limit our discussion to the crossover from a quantum to a classical environment as obtained from our construction using generalized coherent states, which provides such a being looked for interpolating scheme in a rather natural way, and referring to the literature for all the other approaches to this huge problem (see, *e.g.*, [1] or [25]).

Moreover, the parametric representation formalism suggests a completely different approach to the dynamics of an open quantum system, since, in principle, the environment quantum character remains entirely retained rather than traced out: as we will briefly present in the next section 3.2, one might exploit the peculiar properties characterizing the dynamics of generalized coherent states, in order to relate a possible dynamical evolution of the global system to that of the principal one. Indeed, the formal scheme here presented opens the possibility of using established approaches for dealing with quantum dynamics in phase space, such as the the path-integral formalism [26, 27], the adiabatic perturbation theory and the Born-Oppenheimer approximation previously presented, and generalizations to curved phase spaces of multi-configurational Eherenfest methods [28, 29], as tools for taking into account the effects of the environment on the principal system and *vice versa*.

Finally, as we shall see in an explicit physical application of the whole formalism in chapter 4, the continuous implementation of the parametric representation, thanks to its interpolating behaviour between a fully quantum and an effectively closed and local approach, provides a natural way to display a deep relationship between two different manifestations of *non-locality* in quantum mechanics: on one hand, the entanglement characterizing a state of a composite system, on the other the Berry’s phase possibly arising in parametrically dependent closed ones (recall paragraph 2.2.3).

### 3.1.2.1 The construction of generalized coherent states

As suggested by the name itself, generalized coherent states are an extension of the “usual” coherent states introduced in 1963 by Glauber and Sudarshan[30–32] to describe the quantized radiation field: we will hereafter refer to this kind of coherent states, which therefore concern the properties of the harmonic oscillator algebra, as *field coherent states* in order to emphasize that they are indeed a particular implementation of the general construction, independently developed about ten years later by Gilmore[33] and Perelomov[34]. For the subsequent, we will mainly adopt Gilmore’s construction, following the nice review on this subject made by Gilmore himself and some co-authors[35] (see also the book[36] for further details).

We recall that field coherent states can be defined in many equivalent ways; probably, the best known concerns the fact that a field coherent state  $|\alpha\rangle$  is an eigenstate of the annihilation operator describing a harmonic oscillator,  $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$ , with  $[\hat{a}, \hat{a}^\dagger] = \mathbb{1}$ ; it is worth mentioning that, as  $\hat{a}$  is *not* a Hermitian operator,  $\alpha$  is a complex number. A more interesting definition that paves the way to the generalization of coherent states to arbitrary dynamical systems is that one can define  $|\alpha\rangle$  as the state obtained by applying the *displacement operator*  $\hat{D}(\alpha)$  to the Fock vacuum:

$$|\alpha\rangle \equiv \hat{D}(\alpha)|0\rangle, \quad \hat{D}(\alpha) \equiv e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}. \quad (3.34)$$

The idea underlying the extension of the concept of coherent states, yielding the construction of the latter for whatever quantum dynamical system, consists in resorting to a group-theoretic framework, where the expression (3.34) enters as the last, defining step of a self-consistent algorithm. Such an algorithm only needs the specification of a dynamical system, in the sense that a Hamiltonian acting on some Hilbert space is given: in the above case of field coherent states, the underlying Hamiltonian has the form

$$H_{\text{field}} = \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k + \gamma_k(t) \hat{a}_k^\dagger + \gamma_k^*(t) \hat{a}_k, \quad (3.35)$$

representing the radiation field (described by the modes  $k$ ) interacting with some external, time dependent source embodied into the  $\gamma_k(t)$ s, where  $\omega_k \hat{a}_k^\dagger \hat{a}_k$  is the usual free term. For each mode  $k$ , the algebraic structure of the Hamiltonian is constituted by a term linear in the creation and annihilation operator, and the quadratic term  $\hat{a}_k^\dagger \hat{a}_k \equiv \hat{n}_k$  that represents the number of excitations in the chosen mode. Those operators<sup>6</sup>, together

<sup>6</sup>again, for any  $k$  which we hereafter omit

with the identity operator, span a Lie Algebra, which is denoted by  $\mathfrak{h}_4$ :

$$[\hat{n}, \hat{a}^\dagger] = \hat{a}^\dagger, \quad [\hat{n}, \hat{a}] = \hat{a}, \quad [\hat{a}, \hat{a}^\dagger] = \mathbb{1}, \quad (3.36a)$$

$$[\hat{n}, \mathbb{1}] = [\hat{a}, \mathbb{1}] = [\hat{a}^\dagger, \mathbb{1}] = 0. \quad (3.36b)$$

The corresponding Lie Group, that hereafter will be in general referred to as the **dynamical group** induced by the Hamiltonian of the system, is in this case the well-known Heisenberg-Weyl group  $\equiv H_4$ [37]. The Hilbert space where the Hamiltonian (3.35) acts is obviously the tensor product of the Fock spaces  $\bigotimes^k \mathcal{F}_k$ , with  $\mathcal{F}_k$  referring to a single mode of radiation, which are the natural carrier spaces of the infinite-dimensional representation of  $H_4$  spanned by the number operator  $\hat{n}_k$  eigenstates,  $\mathcal{F}_k = \text{Span}(|0\rangle, |1\rangle, \dots, |n\rangle, \dots)_k$ . In order to proceed in the definition of coherent states *via* the group-theoretic algorithm, it is necessary to set a last ingredient, namely a **reference state**  $|\Phi_0\rangle$ , that in principle is a free choice, but in practical situations becomes the ground state of a part of the Hamiltonian which for physical reasons has to be interpreted as the free part (the number operator term, in this case) and/or it is the maximal weight of the considered representation. Such a choice strongly influences the properties of the generated coherent states and, consequently, their practical usefulness; in the harmonic oscillator case, in order to cope with the previous definitions, the reference state is indeed the ground state of the number operator,  $|\Phi_0\rangle \equiv |0\rangle$ , that moreover is the maximal weight of the representation of the algebra  $\mathfrak{h}_4$  (3.36).

Field coherent states  $|\alpha\rangle$  are then generated, starting from the three ingredients above depicted, in three subsequent steps: firstly, one has to identify the **maximum stability subgroup** of the dynamical group  $H_4$ , that is the set of group members that leave the reference state  $|0\rangle$  invariant *up to a phase factor*; this last requirement has obvious physical reasons and slightly distinguishes the maximum stability subgroup from the isotropy subgroup defined in paragraph 2.1.4, but the consequences of such a specification on the subsequent construction will result to be non-trivial at all. In this guideline case, a generic element  $f$  of the maximum stability subgroup  $\equiv F \subset H_4$  acting on the Fock vacuum  $|0\rangle$  can be easily found to be of the form

$$f = e^{i(\delta\hat{n} + \phi\mathbb{1})} = e^{i\delta\hat{n}} e^{i\phi\mathbb{1}} \quad (3.37)$$

with  $\delta, \phi$  real parameters, hence  $F \simeq U(1) \times U(1)$  (two independent phase factors). The maximum stability subgroup is then used to construct the quotient space  $H_4/F$  (cfr. paragraph 2.1.4), so that a generic element  $g$  of the dynamical group can be decomposed as  $g = Df$ , where  $D \in H_4/F$  and  $f \in F$ . Finally, the element  $D$  of the quotient space inherits the representation  $T$  of the corresponding group element  $g$  when acting on the Fock space as  $\hat{T}(g) = \hat{T}(D)\hat{T}(f)$ : in particular, field coherent states are defined by the

following relation again involving the reference state  $|0\rangle$

$$\hat{T}(g)|0\rangle = \hat{T}(D)\hat{T}(f)|0\rangle = \hat{T}(D)|0\rangle e^{i\phi} \equiv \hat{D}(\alpha)|0\rangle e^{i\phi}, \quad (3.38)$$

where we have made explicit use of the form of the maximum stability subgroup representation (3.37) (identifying with a slight abuse of notation the abstract group element  $f$  with its representation  $\hat{T}(f)$ ), and where we denote by  $\hat{D}(\alpha)$  the representation of  $D$ . This last notation is not a mere coincidence, as it is straightforward to prove (see for more details[35]) that  $\hat{D}(\alpha)$  coincides with the displacement operator defined in eq. (3.34), and the parameter  $\alpha$  has to be seen as the coordinate of the point  $D \in H_4/F$ . In other words, coherent states are in one-to-one correspondence with the elements of the quotient space between the Heisenberg-Weyl dynamical group  $H_4$  and the maximum stability subgroup  $F \simeq U(1) \times U(1)$ :

$$|\alpha\rangle \equiv \hat{D}(\alpha)|0\rangle, \quad \hat{D}(\alpha) \equiv \hat{T}(D), \quad D \in H_4/F. \quad (3.39)$$

Once the group-theoretic argument above sketched in the case of the harmonic oscillator (Heisenberg-Weyl) algebra is generalized to an arbitrary dynamical group  $G$  induced by the generators appearing in the Hamiltonian (its algebra  $\mathfrak{g}$ ), one is naturally led to the notion of *generalized coherent states*. In order to both introduce the notation and clarify several details of such construction, let us start back from the beginning of the algorithm, and write the Hamiltonian of the physical system under investigation in the abstract form

$$H = H(\{X_i\}), \quad X_i \in \mathfrak{g}. \quad (3.40)$$

In practical applications,  $\mathfrak{g}$  is usually a Lie algebra (cfr. paragraph 2.1.4 and in particular the definition 2.17) so that  $G$  is a Lie Group (and in the following we will adopt such restriction), but in principle the construction can be carried over for a generic dynamical group. The Lie algebra  $\mathfrak{g}$  is characterized by the commutation relations:

$$[X_i, X_j] = \sum_k c_{ij}^k X_k, \quad \{X_i\} \in \mathfrak{g}, \quad (3.41)$$

where the coefficients  $c_{ij}^k$  are the structure constants (recall the structure equation (2.44) for the geometric construction of a Lie algebra associated to  $G$ ). If, moreover, the Lie algebra  $\mathfrak{g}$  is semisimple<sup>7</sup>, the generators and the commutation relations (3.41) are written

<sup>7</sup>A semisimple algebra is a direct sum of simple algebras; a simple algebra is an algebra that does not contain proper ideals, the latter being invariant subalgebras in the following sense: denoting by  $\mathfrak{g}$  a simple algebra and  $\mathfrak{h}$  any of its subalgebras,  $[\mathfrak{h}, \mathfrak{g}] = \mathfrak{h}$  implies that  $\mathfrak{h}$  is either zero or  $\mathfrak{g}$  itself. For a more detailed discussion, please refer to[38] or other group-theoretic textbooks; apart from the very definition, for our purposes the commutation relations (3.42) are those we are interested in.



in the so-called **Cartan basis**  $(\{H_i\}, \{E_\alpha, E_{-\alpha}\})$  as following:

$$[H_i, H_j] = 0, \quad [H_i, E_\alpha] = \alpha_i E_\alpha, \quad [E_\alpha, E_{-\alpha}] = \sum_i \alpha^i H_i, \quad [E_\alpha, E_\beta] = c_{\alpha;\beta} E_{\alpha+\beta}. \quad (3.42)$$

Therefore, if the Hamiltonian (3.40) is linear in the generators, in the case of semisimple Lie algebra it takes the “canonical” form

$$H = \sum_i \epsilon_i H_i + \sum_\alpha \gamma_\alpha E_\alpha + \gamma_\alpha^* E_{-\alpha}, \quad (3.43)$$

where we can recognize the form of (3.35)<sup>8</sup> by identifying  $H_i$  with  $\hat{n}, \mathbb{1}$  and  $E_\alpha \equiv E$  with  $\hat{a}^\dagger$ <sup>9</sup>: to this respect, it is worth to point out that the radiation Hamiltonian (3.35) is indeed *linear* in the generators of  $\mathfrak{h}_4$  as the quadratic term  $\hat{n} \equiv \hat{a}^\dagger \hat{a}$  is considered itself as an *elementary* object.

The Hilbert space of the system  $\mathcal{H}$  is, in such context, the carrier space of a unitary irreducible representation of the dynamical group  $G$ , which we denoted before by the symbol  $\hat{T}$ <sup>10</sup>. It is worth to point out that, although the choice of the representation is *a priori* not given by the Hamiltonian (3.40) itself, it is again the physical set up that determines it.

As anticipated, a last ingredient is needed in order to pursue the algorithm, namely the choice of a reference state  $|\Phi_0\rangle \in \mathcal{H}$  normalized to unity,  $\langle \Phi_0 | \Phi_0 \rangle = 1$ . In the case of the decomposition (3.42) and linear Hamiltonian (3.43), the part containing the generators  $H_i$  is usually associated to the “free” term, while the generators  $E_\alpha, E_{-\alpha}$  embody the “perturbation”, and from the theory of representation it is possible to choose the  $H_i$ s diagonal and Hermitian,  $\hat{H}_i^\dagger = \hat{H}_i$  in every irreducible representation, while the representative of the  $E_\alpha, E_{-\alpha}$  becomes shift-up and shift-down operators such that  $\hat{E}_\alpha^\dagger = \hat{E}_{-\alpha}$ <sup>11</sup>. In this case, the reference state  $|\Phi_0\rangle$  is usually chosen to be both an eigenstate of the free part,  $\hat{H}_i |\Phi_0\rangle = \Lambda_i |\Phi_0\rangle$ ,  $\Lambda_i$  depending on the particular representation, and a maximal weight state, in the sense that it is annihilated by all the shift-up operators,  $\hat{E}_\alpha |\Phi_0\rangle = 0 \forall \alpha$ .

To sum up, the algorithm to construct generalized coherent states needs the following three inputs:

<sup>8</sup>again, for *each* mode  $k$  that should not be confused with the index labeling the elements of the Cartan basis of  $\mathfrak{g}$

<sup>9</sup>namely, the structure of the Heisenberg-Weyl algebra  $\mathfrak{h}_4$  in the Cartan basis has only one non-trivial element of type “ $H_i$ ” and only one of type “ $E_\alpha$ ”

<sup>10</sup>The representation of a group is usually defined itself as the couple  $(\mathcal{H}, \{\hat{T}(g)\})$  of the carrier space together with the unitary operators representing the action of the group on it for each element  $g \in G$ .

<sup>11</sup>We drop the representation symbol by replacing it with a “ $\hat{\phantom{x}}$ ” to lighten the notation.

1. a Hamiltonian  $H(\{X_i\})$ , the generators  $\{X_i\}$  spanning a (Lie) algebra that specifies the dynamical group  $G$ ;
2. an unitary irreducible representation of  $G$  ( $\mathcal{H}, \hat{T}(g) \forall g \in G$ );
3. the choice of a normalized reference state  $|\Phi_0\rangle \in \mathcal{H}$ .

Once such ingredients are given, the algorithm firstly provides the **maximum stability subgroup** of  $G$ , namely the set  $F \subset G$  of all elements  $f$  that leave the reference state invariant up to a phase factor, namely

$$f \in F \leftrightarrow T(f)|\Phi_0\rangle = |\Phi_0\rangle e^{i\phi(f)} \quad (3.44)$$

where we made explicit the fact that in general the phase factor  $\phi(f)$  depends on  $f$ ; we remark that such a subgroup is strongly affected by the choice of the reference state. The maximum stability subgroup is then used in the second step to define the quotient space  $G/F$ , which is in general a differentiable manifold provided that  $G$  is a Lie group, as we assume for physical reasons. Any group element  $g \in G$  is then decomposed as  $g = \Omega f$ , with  $\Omega \in G/F$  and  $f \in F$ , where such a decomposition, according to the geometric properties of  $G$  and  $G/F$ , may or may not be given *globally* (see later). As a last step, **generalized coherent states** are defined by the action of the dynamical group on the reference state, *via* the representation of the above decomposition:

$$\hat{g}|\Phi_0\rangle = \hat{\Omega}\hat{f}|\Phi_0\rangle = \hat{\Omega}|\Phi_0\rangle e^{i\phi(f)} \equiv |\Omega\rangle e^{i\phi(f)}, \quad (3.45)$$

where we defined  $\hat{\Omega}|\Phi_0\rangle \equiv |\Omega\rangle \in \mathcal{H}$ . Generalized coherent states are therefore in one-to-one correspondence with the elements  $\Omega$  of the quotient space  $G/F$ , thus inheriting from the latter many useful differential properties, which we shall present shortly after. Resorting again to the useful (but not so restricting) hypothesis of a semisimple Lie algebra (3.42) and a linear Hamiltonian (3.43), the general expression of the representation  $\hat{\Omega}$  can be put in the “generalized displacement operator” form:

$$\hat{\Omega} = \exp\left(\sum_{\beta} \eta^{\beta} \hat{E}_{\beta} - \eta^{\beta*} \hat{E}_{-\beta}\right) \quad (3.46)$$

where the sum runs over those shift-down operators that do not annihilate the reference state<sup>12</sup>, and the complex parameters  $\eta^{\beta}$  are coordinates on  $G/F$ .

To sum up, the three ordered outputs of the generalized coherent states algorithm are:

1. the maximum stability subgroup  $F$ ;

<sup>12</sup>clearly, if  $\hat{E}_{\beta}$  is a shift-down operator,  $\hat{E}_{-\beta}$  acts as a shift-up.

2. the quotient space  $G/F$  (a differentiable manifold when dealing with Lie groups);
3. the coherent states  $|\Omega\rangle \equiv \hat{\Omega} |\Phi_0\rangle$ ,  $\Omega \in G/F$ .

The resulting geometry of  $G/F$  strongly influences the properties of the coherent states. It turns out that, in general,  $G/F$  is an even dimensional manifold, and if the algebra  $\mathfrak{g}$  is semisimple and satisfies the Cartan decomposition in the form  $\mathfrak{g} = \mathfrak{f} \oplus \mathfrak{p}$ , where  $\mathfrak{f}$  is the algebra of  $F$  and  $\mathfrak{p} = \eta^\beta E_\beta - \eta^{\beta*} E_{-\beta}$  is its orthogonal complement,  $G/F$  is also a symmetric space[39], and an element in  $G/F$  can be expressed in matrix form (of dimension  $\dim(G)$ ), according to the fact  $G$  is either compact (-) or non-compact (+):

$$\begin{pmatrix} \sqrt{\mathbb{1} \mp z z^\dagger} & z \\ \mp z^\dagger & \sqrt{\mathbb{1} \mp z^\dagger z} \end{pmatrix}, \quad (3.47)$$

where the new “coordinates”  $z$  are matrices of dimension  $\dim(f) \times \dim(p)$ , related to a  $\dim(f) \times \dim(p)$  matrix representation of the  $\eta$ s, *via*

$$z = \eta \frac{\sin \sqrt{\eta^\dagger \eta}}{\sqrt{\eta^\dagger \eta}} (-), \quad z = \eta \frac{\sinh \sqrt{\eta^\dagger \eta}}{\sqrt{\eta^\dagger \eta}} (+) \quad (3.48)$$

A last useful coordinate is that yielding a complex projective representation of  $G/F$ , related to  $z$  as

$$\tau = z(\mathbb{1} \mp z^\dagger z)^{-\frac{1}{2}}; \quad (3.49)$$

for our purposes (see later the application in paragraph 4.1.2), however,  $\eta, z, \tau$  will actually be  $c$ -numbers and we will be only interested in the explicit transformations relating them.

More interestingly, the quotient space  $G/F$  is endowed with a natural metric structure, inherited by the dynamical group  $G$ , which is useful to express in the  $\tau$  coordinates as

$$ds^2 = \sum_{\alpha\beta} g_{\alpha\beta} d\tau^\alpha d\tau^{\beta*}. \quad (3.50)$$

The metrics  $g_{\alpha\beta}$ , in turn, is related to the non-normalized form of the coherent states: namely, it is  $g_{\alpha\beta} = \partial_\alpha \bar{\partial}_\beta F(\tau, \tau^*)$ , where

$$F(\tau, \tau^*) \equiv \ln N(\tau, \tau^*), \quad (3.51)$$

and  $N(\tau, \tau^*)$  is a normalization factor that relates the normalized coherent state  $|\Omega\rangle = \hat{\Omega} |\Phi_0\rangle$  defined by eq. (3.46) and the  $\tau$  expression  $|\tau\rangle \equiv \exp(\sum_\beta \tau^\beta \hat{E}_\beta) |\Phi_0\rangle$  through

$$|\Omega\rangle = N(\tau, \tau^*)^{-\frac{1}{2}} |\tau\rangle. \quad (3.52)$$

Since the manifold  $G/F$  is endowed with a metric tensor  $g$ , it is possible to define on it a *canonical* volume form (see, *e.g.*, [13]), in the sense that such a form is invariant under reparametrization, and the corresponding volume element can be written as

$$d\mu(\Omega) = \text{const} \times \det(g) \prod_{\alpha} d\tau^{\alpha} d\tau^{\alpha*} \quad (3.53)$$

for whatever coordinate system.

Moreover, the quotient space  $G/F$  also admits a *symplectic* structure; such property has a relevant physical significance since the symplectic form allows one to consider  $G/F$  a *phase space* over which a Poisson bracket is defined; indeed, under rather general assumptions,  $G/F$  turns out to be *the* phase space the quantum dynamical system collapse into as a proper classical limit is performed. Since we will deal more precisely with this issue in the following chapter 4, for the moment we restrict ourselves to the statement of the abstract and geometrical aspects, but we still remark that coherent states are actually a well-known link between the quantum and the classical world as, for instance, they are a class of minimum uncertainty states[40]. The symplectic form is a closed, non-degenerate two-form defined on  $G/F$  which has the coordinate representation

$$\omega = i \sum_{\alpha\beta} g_{\alpha\beta} d\tau^{\alpha} \wedge d\tau^{\beta*}, \quad (3.54)$$

and is used to define the Poisson brackets

$$\{f, g\}_{\text{PB}} \equiv -i \sum_{\alpha\beta} g^{\alpha\beta} \left( \frac{\partial f}{\partial \tau^{\alpha}} \frac{\partial g}{\partial \tau^{\beta*}} - \frac{\partial g}{\partial \tau^{\alpha}} \frac{\partial f}{\partial \tau^{\beta*}} \right). \quad (3.55)$$

Switching to the  $z$  coordinates and putting

$$z^{\beta} \equiv \frac{1}{\sqrt{2}}(q^{\beta} + ip^{\beta}), \quad z^{\beta*} \equiv \frac{1}{\sqrt{2}}(q^{\beta} - ip^{\beta}), \quad (3.56)$$

the Poisson brackets (3.55) display the canonical form:

$$\{f, g\}_{\text{PB}} = \sum_{\alpha} \left( \frac{\partial f}{\partial q^{\alpha}} \frac{\partial g}{\partial p^{\alpha}} - \frac{\partial g}{\partial p^{\alpha}} \frac{\partial f}{\partial q^{\alpha}} \right). \quad (3.57)$$

It is worth to point out that, since the differential structure of the quotient space  $G/F$  is in general non-trivial, the coordinates are only locally defined, so as the classical phase space coordinates  $\{ (q^{\alpha}, p^{\alpha}) \}$ ; nevertheless, the Poisson structure is everywhere defined as it relies on the existence of an intrinsically given symplectic form  $\omega$  (even though in (3.54) we only report its coordinate presentation for the sake of clarity).

We now move to a more algebraic treatment of generalized coherent states, namely we

present their relevant properties as vectors in the Hilbert space  $\mathcal{H}$  they belong to; in particular, we shall see in what sense they provide a way to expand a generic state onto them and, most importantly, that they provide a continuous resolution of the identity in  $\mathcal{H}$  which, as we explained in the previous paragraph 3.1.1, is the key ingredient to define a parametric representation when a composite system is considered, see paragraph 3.1.2.2. From their very definition through the displacement operator (3.46), generalized coherent states naturally come *normalized* but *non-orthogonal*:

$$\langle \Omega | \Omega \rangle = \langle \Phi_0 | \hat{\Omega}^\dagger \hat{\Omega} | \Phi_0 \rangle = \langle \Phi_0 | \hat{T}(g^{-1}g) | \Phi_0 \rangle = 1 \quad (3.58)$$

since the representation  $\hat{T}$  is unitary, and, similarly

$$\langle \Omega | \Omega' \rangle = \langle \Phi_0 | \hat{T}(g'' = g^{-1}g') | \Phi_0 \rangle e^{i\phi} \equiv K(\Omega, \Omega') e^{i\phi} \neq 0 \quad (3.59)$$

in general, where we defined the overlap function  $K(\Omega, \Omega') \equiv \langle \Omega | \Omega' \rangle$ . Generalized coherent state are usually referred to as forming an **overcomplete** set of states, in the sense that, although they are not orthogonal, they provide, as an immediate consequence of Schur's lemma, a resolution of the identity by

$$1_{\mathcal{H}} = \int_{G/F} |\Omega\rangle d\mu(\Omega) \langle \Omega| , \quad (3.60)$$

where the group-invariant measure  $d\mu(\Omega)$  is defined as in eq. (3.53) by appropriately choosing the constant pre-factor. Overcompleteness is usually associated to the simultaneous properties (3.59) and (3.60), and becomes even more apparent where the considered representation is finite-dimensional. In fact, on a finite-dimensional Hilbert space  $\mathcal{H}$  a basis (that provides an identity resolution, too) has a finite number of elements, while generalized coherent states are an infinite, continuous set labeled by the point  $\Omega \in G/F$ ; this way, only a “zero measure” subset of them can indeed constitute a proper basis, whose elements be orthogonal to each other.

Belonging to  $\mathcal{H}$ , coherent states can be expanded on a proper basis  $\{|n\rangle\}$  for any  $\Omega$ :

$$|\Omega\rangle = \sum_n g_n^*(\Omega) |n\rangle , \quad (3.61)$$

where the expansion coefficients  $g_n^*(\Omega)$ <sup>13</sup> are the overlaps  $\langle n | \Omega \rangle$ , and are uniquely defined once a representative in the quotient space  $G/F$  is chosen, that is the decomposition  $\hat{T}(g) = \hat{\Omega} \hat{T}(f)$  is made explicit (see later the fiber bundle interpretation). On the other hand, as coherent states provide an identity resolution (3.60) in  $\mathcal{H}$ , a generic state  $|\psi\rangle$

<sup>13</sup>the complex conjugate is put for further convenience

can be expanded onto them as

$$|\psi\rangle = \int d\mu(\Omega) \psi(\Omega) |\Omega\rangle , \quad (3.62)$$

for appropriate coefficients  $\psi(\Omega)$ ; by the non-orthogonality property (3.59), however, the expansion (3.62) is not unique: if one chooses  $\phi(\Omega) \neq 0$  such that  $\int d\mu(\Omega') \langle \Omega | \Omega' \rangle \phi(\Omega') = 0$ , it is also

$$\int d\mu(\Omega) |\Omega\rangle (\psi(\Omega) + \phi(\Omega)) = \int d\mu(\Omega) \psi(\Omega) |\Omega\rangle = |\psi\rangle . \quad (3.63)$$

Notice that the choice of a nonzero  $\phi(\Omega)$  is possible only because the overlap  $\langle \Omega | \Omega' \rangle \neq \delta(\Omega - \Omega')$ , unlike a true basis. Nevertheless, this last consideration suggests that a condition on the coefficients  $\psi(\Omega)$  for providing a unique decomposition can still be given, namely by requiring that

$$\int d\mu(\Omega') \langle \Omega | \Omega' \rangle \psi(\Omega') = \psi(\Omega) , \quad (3.64)$$

as can be easily seen by inserting it into (3.62). A not surprising solution of (3.64) is obtained by expanding the state  $|\psi\rangle$  in the true basis  $|n\rangle$  of eq. (3.61) as  $|\psi\rangle = \sum_n \psi_n |n\rangle$ , and by defining in (3.62):

$$\psi(\Omega) \equiv \langle \Omega | \psi \rangle = \sum_n \langle \Omega | n \rangle \psi_n = \sum_n g_n(\Omega) \psi_n , \quad (3.65)$$

thus leaving no ambiguities in a generic state  $|\psi\rangle \in \mathcal{H}$  expansion, except from the above mentioned one that pertains the choice of the representative in the quotient space  $G/F$ . As for this last point, the fact that the output space of the algorithm is a quotient space between a group  $G$  and its maximum stability subgroup naturally paves the way to the interpretation of the interplay between  $G$ ,  $F$  and  $G/F$  in terms of a *principal bundle*, cfr. paragraph 2.1.5, where  $G$  is the total space,  $G/F$  the base manifold (there denoted by  $M$ ) and  $F$  the structure group-fiber. In other words, a point  $g$  in the total space is trivialized by the couple  $(\Omega, f)$  that is in one-to one correspondence to the choice of a section  $g(\Omega)$ : the bundle is in general non-trivial, and therefore the trivialization can be given only locally in  $G/F$ , as it will be apparent in the example given in 4.1.2. Different sections are related by gauge transformations  $\in F$ , which in the case where  $F$  is abelian (we remark that it should be “at least” a  $U(1)$  due to the definition of the maximum stability subgroup), such a transformation can be cast into the form  $\exp(i\lambda(\Omega))$ . Generalized coherent states are then constructed as representation of the action of the group  $G$  onto the carrier Hilbert space  $\mathcal{H}$  so that, to be precise, instead of the principal bundle structure just sketched one should resort to the procedure also depicted in paragraph 2.1.5 that associates to the former a vector bundle. Generalized coherent states are eventually interpreted in such framework as *holomorphic* sections in an associated line

bundle (one dimensional vector bundle) over (the complexification of)  $G/F$ [41]; without entering much in detail, for our purposes it is important to interpret the coherent state expansion coefficients  $g_n^*(\Omega)$  of eq. (3.61) as *sections* over  $G/F$  (instead of functions) and that, moreover, these sections are holomorphic, actually meaning that they are holomorphic functions of the complex coordinates that locally express the point  $\Omega$  in  $G/F$  (for example, the  $\tau$  above presented). Consequently, the coefficients  $\psi(\Omega)$  in the state expansion (3.62) inherit from the relation  $\psi(\Omega) = \langle \Omega | \psi \rangle$  (see (3.65)) the property of being holomorphic sections: this means, in turn, as the state  $|\psi\rangle \in \mathcal{H}$  is completely generic, that physical states are in one-to one correspondence with the holomorphic sections  $\psi(\Omega)$  of the complex line bundle over  $G/F$  associated to the principal bundle  $G \rightarrow G/F$ .

We end this paragraph by stating another important application of coherent states, that is intimately connected with the quantum-to-classical transition issue: being (quite generally) sections defined on  $G/F$ , coherent states provide a natural way to express operators in the Hilbert space  $\mathcal{H}$  as distributions on the corresponding classical phase space (see, *e.g.*, [42] for a nice review about the subject). Reversing the point of view, starting from a phase-space distribution, an operator on  $\mathcal{H}$  can be obtained by a generalized quantization procedure (for instance, the Weyl transform[37]): the usual replacement of the canonical coordinates on the phase space,  $\{q, p\}_{\text{PB}} = 1$ , by operators  $\hat{x}, \hat{p}$  satisfying  $[\hat{x}, \hat{p}] = i$  has to be regarded, in this sense, as a particular case (with flat phase space) of such a general framework. An even more general (geometrical) approach is provided by the so-called *geometrical quantization* (see, *e.g.*, [43]) that naturally copes with curved phase spaces. Let us then present the three kinds of such distributions, that correspond to the three possible orders of the operators obtained by the converse quantization procedure.

1. *P representation*: given an observable  $\hat{O}$ , its  $P$  representation  $O_P(\Omega)$  is defined by the relation

$$\hat{O} = \int d\mu(\Omega) |\Omega\rangle O_P(\Omega) \langle \Omega| . \quad (3.66)$$

In the case of field coherent states  $|\alpha\rangle$ , it corresponds to a normally ordered quantization, namely, the creation-annihilation operators obtained when canonically quantizing the phase space variables appearing in  $O_P(\alpha = (q, p))$ , once ordered as  $\prod_i a_i^\dagger \prod_k a_k$ , yield the original  $\hat{O}$ ; moreover,  $O_P(\alpha)$  is always defined for bounded operators. On the other hand, for generic coherent states  $|\Omega\rangle$ , the expansion (3.66) can correspond to unphysical phase space distributions.

2. *Q representation*; given an observable  $\hat{O}$ , its *Q* representation (or **Husimi Q-function**)  $O_Q(\Omega)$  is *uniquely* defined as

$$\hat{O} \rightarrow \langle \Omega | \hat{O} | \Omega \rangle \equiv O_Q(\Omega) , \quad (3.67)$$

and corresponds to an anti-normal ordering. Interestingly, the statistical average of an operator  $\hat{O}$  on the density matrix  $\rho$  can be expressed as a combination of *P* and *Q* distributions:

$$\text{Tr}(\rho \hat{O}) = \int d\mu(\Omega) \rho_Q(\Omega) O_P(\Omega) , \quad (3.68)$$

as can be immediately seen by the definitions (3.66)-(3.67).

3. *W representation*: the last phase space distribution is the *W* representation (the “*W*” standing for Wigner), that corresponds to a symmetric ordering, and is abstractly defined by requiring that  $\hat{O} \leftrightarrow O_W$  (it is a bijection) and that for any two operators  $\hat{A}, \hat{B}$  on  $\mathcal{H}$  it is:

$$\text{Tr}(A^\dagger B) = \int d\mu(\Omega) A_W^*(\Omega) B_W(\Omega) , \quad (3.69)$$

so that  $\langle \rho \hat{O} \rangle = \int d\mu(\Omega) \rho_W(\Omega) O_W(\Omega)$ .

In general, the *P*, *Q* and *W* representations are only *quasi*-probability distributions over the phase space, in the sense that they may not be globally positive-definite; however, in the practical situation we shall thoroughly discuss in the subsequent, we will encounter the *Q* representation of the environmental density matrix, that will result to be a true probability distribution (see later and paragraph 4.1.2).

### 3.1.2.2 Using generalized coherent states for a parametric representation

We are now in the position to present the continuous parametric representation of a state  $|\Psi\rangle$  of a composite system  $\mathcal{H} \equiv \mathcal{H}_{\text{open}} \otimes \mathcal{H}_{\text{env}}$ , mimicking step by step the formal construction of paragraph 3.1.1 by only replacing the discrete identity resolution in  $\mathcal{H}_{\text{env}}$  with the continuous one provided by generalized coherent states, eq. (3.60); due to the importance of such a construction for the following, we prefer to repeat the essential steps, using the same notation as before unless otherwise stated.

Let us suppose that on the system  $\mathcal{H}$  a Hamiltonian  $H$  is defined, the latter being a sum of a local part  $H_{\text{env}}$  in the sense that it only contains operators acting on  $\mathcal{H}_{\text{env}}$ , and an interaction part  $H_{\text{int}}$  containing operators acting on both Hilbert spaces; ignoring the



operators acting on  $\mathcal{H}_{\text{open}}$ , the Hamiltonian is usually linear in the generators  $X_i$ , or can be taken to be linear as in the field coherent state example (it was made so by appending the number operator to the algebra of the dynamical group), but we remark that the construction does not rely on any assumption of this kind. Anyway, let us suppose that the dynamical group  $G$  of the *environment* is given together with its representation  $(\mathcal{H}_{\text{env}}, \hat{T})$ , and that a highest weight state  $|\Phi_0\rangle \in \mathcal{H}_{\text{env}}$  is chosen as reference state, so that generalized environmental coherent states  $|\Omega\rangle$  are defined according to the algorithm summed up in 3.1.2.1.

The identity resolution (3.60) provides a continuous set of maps  $\Pi_\Omega \equiv \langle \Omega | \cdot \rangle : \mathcal{H} \rightarrow \mathcal{H}_{\text{open}}$ , so that a composite state  $|\Psi\rangle$  has the coherent state expansion

$$|\Psi\rangle = \int_{G/F} d\mu(\Omega) |\Omega\rangle \Pi_\Omega(|\Psi\rangle), \quad (3.70)$$

where the partial overlap  $\Pi_\Omega(|\Psi\rangle) = \langle \Omega | \Psi \rangle$  has to be intended in the same sense of the coefficients in the “isolated” case  $\psi(\Omega) = \langle \Omega | \psi \rangle$  (see eq. (3.62) and subsequent discussion): the expansion of the composite state  $|\Psi\rangle$  over the local bases  $\{|\beta\rangle\} \in \mathcal{H}_{\text{open}}$  and  $\{|n\rangle\} \in \mathcal{H}_{\text{env}}$  is implied, so that the scalar products  $\langle \Omega | n \rangle$  in  $\mathcal{H}_{\text{env}}$  are known from (3.61). Explicitly, writing  $\mathcal{H} \ni |\Psi\rangle = \sum_{\beta n} c_{\beta n} |\beta\rangle |n\rangle$ , the images  $\Pi_\Omega(|\Psi\rangle)$  comparing in eq. (3.70) read:

$$\Pi_\Omega(|\Psi\rangle) = \sum_{\beta n} g_n(\Omega) c_{\beta n} |\beta\rangle \equiv \sum_{\beta} \psi_\beta(\Omega) |\beta\rangle, \quad (3.71)$$

where we have put

$$\psi_\beta(\Omega) \equiv \sum_n g_n(\Omega) c_{\beta n} \quad (3.72)$$

in the last equality. Therefore the extension from the “isolated” case treated in paragraph 3.1.2.1 to the composite case of eq. (3.71) is quite natural in the geometrical language: instead of a single holomorphic section  $\psi(\Omega)$ , a physical state turns out to be a multicomponent holomorphic section  $\{\psi_\beta(\Omega), \beta = 1, \dots, \dim(\mathcal{H}_{\text{open}})\}$ , belonging to the tensor product between the line bundle defining coherent states and the Hilbert space of the open system.

The parametric representation of the open system induced by the coherent state is then obtained, as in 3.1.1, by factorizing the state (3.71) into a normalized, parametric state of  $|\phi(\Omega)\rangle \in \mathcal{H}_{\text{open}}$  and the corresponding amplitude  $\chi(\Omega)$ ,  $\Pi_\Omega(|\Psi\rangle) \equiv \chi(\Omega) |\phi(\Omega)\rangle$ , where

(cfr. eqs. (3.18))

$$|\phi(\Omega)\rangle \equiv e^{i\lambda(\Omega)} \frac{\Pi_{\Omega}(|\Psi\rangle)}{\|\Pi_{\Omega}(|\Psi\rangle)\|} = e^{i\lambda(\Omega)} \frac{\sum_{\beta} \psi_{\beta}(\Omega) |\beta\rangle}{\sqrt{\sum_{\beta} |\psi_{\beta}(\Omega)|^2}} \quad (3.73a)$$

$$\chi(\Omega) \equiv e^{-i\lambda(\Omega)} \|\Pi_{\Omega}(|\Psi\rangle)\| = e^{-i\lambda(\Omega)} \sqrt{\sum_{\beta} |\psi_{\beta}(\Omega)|^2}, \quad (3.73b)$$

where  $\psi_{\beta}(\Omega)$  are defined in (3.72), with the  $\Omega$ -dependent phase factor  $\exp(i\lambda(\Omega))$  left undetermined. As anticipated, to such a local phase ambiguity, the gauge freedom in defining the section  $|\Omega\rangle$  over the quotient space  $G/F$  is superimposed, with the result that the phase factors relative to  $|\phi(\Omega)\rangle$  and  $\chi(\Omega)$  actually becomes uncorrelated and, eventually, the only relevant gauge freedom is that pertaining the coherent states: in other words, we can “canonically” choose  $\chi(\Omega)$  real ( $\lambda(\Omega) \equiv 0$ ) and append the coherent state gauge freedom to the parametrized state  $|\phi(\Omega)\rangle$ .

In analogy with def. 3.1, we define **parametric representation with generalized coherent states** (of the open system related to composite state  $|\Psi\rangle \in \mathcal{H}$ ) the couple  $(|\phi(\Omega)\rangle, \chi(\Omega))$ , explicitly given by eqs. (3.70) and (3.73).

Although the continuous construction displays the very same structure of the discrete one, the former immediately results more practical than the latter, as the set of parametrized states and corresponding amplitudes becomes functions of the variable  $\Omega$  (actually, sections when considered together, see above), so that the parametric dependence is made “explicit” in a *single* state-amplitude couple. As a drawback, the physical interpretation results a little tricky: unlike, for instance, the parametric representation in molecular systems (recall this section introduction), the parameter  $\Omega \in G/F$  belongs to the *phase space* of the environment (in the sense explained in paragraph 3.1.2.1), thus it does not label a true observable of  $\mathcal{H}_{\text{env}}$ , even if the environmental coherent state  $|\Omega\rangle$  is a proper physical state since it is normalized. We shall therefore refer to  $\Omega$  as labeling an environmental *configuration*. Nevertheless, as in the discrete case, the amplitude  $\chi(\Omega)$  satisfies by construction:

$$\int d\mu(\Omega) |\chi(\Omega)|^2 = 1, \quad (3.74)$$

thus still allowing us to interpret  $\chi(\Omega)$  as a probability amplitude, and consequently  $|\chi(\Omega)|^2$  as a probability distribution, over  $G/F$ . Moreover, as can be seen by a direct calculation as in eq. (3.25), such distribution coincides with the “populations” of the diagonal elements of the environmental density matrix (in the “basis”  $|\Omega\rangle$  defining the identity resolution):

$$|\chi(\Omega)|^2 = (\rho_{\text{env}})(\Omega) \equiv \langle \Omega | \rho_{\text{env}} | \Omega \rangle \equiv \rho_{\text{env},Q}(\Omega), \quad (3.75)$$

where we have immediately pointed out that the last term  $\langle \Omega | \rho_{\text{env}} | \Omega \rangle$  is indeed the  $Q$ -representation of the environmental reduced density matrix; not surprisingly, in this case the  $Q$ -representation is a true probability distribution since it pertains a positive-definite operator (the density matrix  $\rho_{\text{env}}$ ). The identity resolution on the environment with coherent states (3.60), moreover, allows one to express the trace over the environmental degrees of freedom as

$$\text{Tr}_{\text{env}} \rho_{\text{TOT}} = \text{Tr}_{\text{env}} (\mathbb{1}_{\mathcal{H}_{\text{env}}} \rho_{\text{TOT}}) = \dots = \int d\mu(\Omega) \langle \Omega | \rho_{\text{TOT}} | \Omega \rangle \quad (3.76)$$

for any global state  $\rho_{\text{TOT}}$ <sup>14</sup>. We can therefore express the relation between the coherent state parametric representation and the reduced density matrix for the open system, mimicking the discrete case (see. eq. (3.23)), as

$$\rho_{\text{open}} \equiv \text{Tr}_{\text{env}} (|\Psi\rangle \langle \Psi|) = \int d\mu(\Omega) |\chi(\Omega)|^2 |\phi(\Omega)\rangle \langle \phi(\Omega)| . \quad (3.77)$$

Such a representation of the reduced density matrix, moreover, can be adopted to calculate the expectation values of any open system observable  $\hat{O}_{\text{open}}$ ; a straightforward calculation shows, indeed, that the cyclic property of the trace still holds, in the sense that

$$\langle \hat{O}_{\text{open}} \rangle = \text{Tr}_{\text{open}} (\rho_{\text{open}} \hat{O}_{\text{open}}) = \dots = \int d\mu(\Omega) |\chi(\Omega)|^2 \langle \phi(\Omega) | \hat{O}_{\text{open}} | \phi(\Omega) \rangle , \quad (3.78)$$

where in the last equality the quantity  $\langle \phi(\Omega) | \hat{O}_{\text{open}} | \phi(\Omega) \rangle$  has to be interpreted as a *conditional* probability distribution for the local observable  $\hat{O}_{\text{open}}$ .

To sum up, the coherent state parametric representation is a tool to describe an open system originating from a composite system in a pure state  $|\Psi\rangle$  that is made up by a normalized and parametrized state  $|\phi(\Omega)\rangle$  that functionally depends on the environmental configuration  $\Omega$ , with occurrence ruled by the probability amplitude  $\chi(\Omega)$  for the latter, while the parameter  $\Omega$  represents a point in the phase space of the environment, and the composite state  $|\Psi\rangle$  can be systematically reconstructed as

$$|\Psi\rangle = \int d\mu(\Omega) |\Omega\rangle \chi(\Omega) |\phi(\Omega)\rangle . \quad (3.79)$$

All the concepts here presented will be extensively clarified in the physical set up discussed in the next chapter 4, where the composite system will be made up by a spin- $\frac{1}{2}$  particle in the role of the open system, isotropically interacting with an environment embodied by a ring of surrounding spins. Such situation is commonly referred to as a *spin-star* model: we shall see that it naturally admits a coherent state parametric

<sup>14</sup>where the expectation value, as always, has to be taken in the same sense as before, namely by calculating the overlaps of the type  $\langle \Omega | n \rangle$  and leaving the operator part on  $\mathcal{H}_{\text{open}}$  untouched.

representation in terms of  $SU(2)$  coherent states, that are the simplest non-trivial implementation of the group-theoretic algorithm we presented throughout this chapter, with various interesting consequences.

**Example 3.2** (Bell states - coherent parametric representation). *As an immediate application of the generalized coherent state parametric representation, we come back to the Bell state example, cfr. 3.1. Let us then recall the Bell state  $|\Phi^+\rangle$  of eq. (3.26):*

$$|\Phi^+\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B) , \quad (3.80)$$

where the subsystem  $B$  is again considered as the environment for the subsystem  $A$ . Without referring to any Hamiltonian, we can still take  $G = SU(2)$  as the dynamical group for the environment since the environmental states appearing in (3.80) are those relative to the  $\text{spin-}\frac{1}{2}$  representation of  $G$ . By choosing the state  $|0\rangle_B$  as the reference state for the coherent state algorithm (the opposite choice would bring a completely identical result provided a suitable redefinition of the coordinates is performed), one can immediately see that generalized coherent states turns out to be the so-called spin coherent states; since we shall deal with the same construction in a more general framework (namely, a generic  $\text{spin-}S$  representation) in the next chapter, we don't now enter into the details and just write without proof the expansion of spin coherent states onto the  $\sigma_{z,B}$  basis  $|0\rangle_B, |1\rangle_B$  appearing in (3.80). We anticipate that spin coherent states  $|\Omega\rangle$  are in one-to-one correspondence with the two-dimensional sphere, since  $G/F = SU(2)/U(1) \simeq S^2$ , namely  $\Omega \in S^2$  (cfr. example 2.1) and can be parametrized, for instance, through the usual polar angles  $\Omega = (\theta, \varphi)$ ; moreover, the measure on  $G/F \sim \{\Omega\}$  is simply a rescaling of the euclidean measure of the spherical surface in real space, namely  $d\mu(\Omega) = \frac{1}{2\pi} d\Omega$  (the rescaling factor actually depends on the dimension of the representation). Now, according to eq. (3.70), one has to compute

$$\Pi_\Omega(\Phi^+) \equiv \langle \Omega | \Phi^+ \rangle = \frac{1}{\sqrt{2}} \sum_{i=0,1} \langle \Omega | i \rangle_B \otimes |i\rangle_A , \quad (3.81)$$

so that the two overlaps  $g_i(\Omega) \equiv \langle \Omega | i \rangle_B$ ,  $i = 0, 1$  are needed; they read[44]

$$g_0(\theta, \varphi) = \cos \frac{\theta}{2}, \quad g_1(\theta, \varphi) = \sin \frac{\theta}{2} e^{-i\varphi} . \quad (3.82)$$

Eventually, according to the general formulas (3.73), the parametric representation of (3.80) through  $\text{spin-}\frac{1}{2}$  coherent states is given by

$$|\phi(\Omega)\rangle = \cos \frac{\theta}{2} |0\rangle_A + \sin \frac{\theta}{2} e^{-i\varphi} |1\rangle_A, \quad \chi(\Omega) = \frac{1}{\sqrt{2}} . \quad (3.83)$$

By a direct calculation, one can immediately check that (3.83) exactly reconstructs the

initial Bell state (3.80) as imposed by the general expression (3.79). We just point out an interesting aspect concerning such example: the decomposition of eq. (3.81) into a normalized parametrized state  $|\phi(\Omega)\rangle$  for the subsystem  $A$  and its amplitude  $\chi(\Omega)$ , which is given by (3.83), is trivial in the sense that the amplitude is a constant factor which does not depend on  $\Omega$ . This implies that the occurrence of the parameters  $(\theta, \varphi)$  into the parametrized states of the subsystem  $A$  is uniform; since, moreover, the dependence into  $|\phi(\Omega)\rangle$  is a direct parametrization of the Bloch sphere (the usual one being obtained by putting  $\varphi \rightarrow -\varphi$ ), this implies that the open quantum system  $A$  obtained by the Bell state (3.80) is simply a qubit pointing in a generic direction with respect to the overall quantization axis “ $z$ ” (actually, with opposite longitude  $\varphi$ ).

## 3.2 Dynamics and the Parametric Representation

When considering a closed system, the main reason to introduce coherent states is related to their dynamical properties: indeed, once the dynamical group  $G$  is properly identified, coherent states define a subset of the Hilbert space  $\mathcal{H}$  that undergoes a classical-like dynamics, in the sense we are now going to explain. Subsequently, we shall sketch some possible ways to extend such idea to the composite case.

For the sake of concreteness, while presenting the general formalism[35], we also provide an immediate example in the context of field coherent states (cfr. paragraph 3.1.2.1); indeed, the first idea to introduce this class of states dates back to the very beginning of the quantum mechanics development[45]. On one hand, field coherent states are, by definition, those states that minimize the position-momentum uncertainty relation for the harmonic oscillator; on the other hand, the expectation values calculated over them of position and momentum evolves as the classical counterpart. Let us then suppose that the Hamiltonian  $H(t)$  is *linear* in the generators of the dynamical group  $G$ , and suppose moreover that the initial state  $|\psi(t_0)\rangle$  is a coherent state itself (for instance, the reference state  $|\Phi_0\rangle$ ). Introducing the *ansatz* for the state at a generic later time  $t$ , with  $\hat{\Omega}(t)$  defined by (3.46),

$$|\psi(t)\rangle \equiv \hat{\Omega}(t) |\psi(t_0)\rangle e^{i\phi(t)} , \quad (3.84)$$

it is straightforward to demonstrate that the time-dependent Schrödinger equation

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (3.85)$$

is identically satisfied if

$$\phi(t) = \int_{t_0}^t \left\langle \psi(t_0) \left| \hat{\Omega}^\dagger(t') \left( i \frac{\partial}{\partial t'} - H(t') \right) \hat{\Omega}(t') \right| \psi(t_0) \right\rangle . \quad (3.86)$$

Moreover, the time-dependence of the quotient group point  $\Omega(t)$  is obtained by the classical (Hamilton) equations (*e.g.*, in the  $\tau$  variable, *cfr.* eq. (3.49))

$$ig_{\alpha\beta} \frac{d\tau^\alpha}{dt} = \frac{\partial H_Q(\tau, \tau^*)}{\partial (\tau^\beta)^*}, \quad (3.87a)$$

$$-ig_{\alpha\beta} \frac{d(\tau^\alpha)^*}{dt} = \frac{\partial H_Q(\tau, \tau^*)}{\partial \tau^\beta}, \quad (3.87b)$$

$$(3.87c)$$

with the metrics  $g_{\alpha\beta}$  defined above eq. (3.51) and  $H_Q(\Omega)$  is the  $Q$ -representation of the Hamiltonian (again written in the  $\tau$  variable). Equations (3.86)-(3.87), together with the ansatz (3.84), define the so-called *coherent* dynamics: a coherent state of a linear Hamiltonian always remains coherent or, in other words, the dynamics generated by  $H(t)$  when acting on a coherent state is just an orbit of the dynamical group  $G$ [41]. Notice that eqs. (3.87) is the generalization of the Hamilton equations to a curved phase space, since locally one may always move to the  $(q, p)$  coordinates *via* the transformations (3.49)-(3.56) to have

$$\dot{q}^\alpha = \frac{\partial H_Q}{\partial p_\alpha}, \quad \dot{p}^\alpha = -\frac{\partial H_Q}{\partial q_\alpha}. \quad (3.88)$$

In the case of field coherent states, the underlying Hamiltonian has the general form (3.35); concentrating again on a single mode, the Hamiltonian is clearly linear in the generators:

$$H_{\text{field,sm}} = \omega \hat{a}^\dagger \hat{a} + \gamma(t) \hat{a}^\dagger + \gamma^*(t) \hat{a}, \quad (3.89)$$

so that the equations (3.84)-(3.87) can be easily applied; namely, starting from the vacuum state  $|\psi(0)\rangle = |0\rangle$ , the evolved state can be written as

$$|\psi(t)\rangle = \hat{\alpha}(t) |0\rangle e^{i\eta(t)}, \quad (3.90)$$

with

$$\hat{\alpha}(t) \equiv \hat{D}(\alpha(t)) = \exp\left(\alpha(t)a^\dagger - \alpha^*(t)a\right), \quad (3.91)$$

$$\alpha(t) = -i\omega e^{-i\omega t} \int_0^t dt' \gamma^*(t') e^{i\omega t'}, \quad (3.92a)$$

$$\eta(t) = -\frac{1}{2}\omega t - \int_0^t dt' \Re(\gamma(t')\alpha(t')). \quad (3.92b)$$

It is straightforward to check that, since  $\alpha(t) = \frac{1}{\sqrt{2}}[q(t) + ip(t)]$ ,  $\alpha(t)$  given by (3.92a) globally satisfies<sup>15</sup> the Hamilton equations (3.88) with  $H_Q(\alpha, \alpha^*) = \langle \alpha | H_{\text{field,sm}} | \alpha \rangle$ .

<sup>15</sup>the quotient space is globally flat, the metrics being identically 1 since by the unnormalized form of field coherent states it is immediately  $F(\alpha, \alpha^*) = |\alpha|^2$

From a geometrical perspective, coherent dynamics is equivalent to a parallel transport rule for sections under a suitably defined connection, together with the definition of a classical Hamiltonian that generates a flow in the homogeneous quotient space  $G/F$ : recall that the latter is the base manifold of the line bundle associated to the coherent state construction and that physical states are interpreted as the subclass of holomorphic sections (cfr. paragraphs 2.1.5.2 and 3.1.2.1). In fact, the *ansatz* (3.84) is equivalent, by taking the time derivative and using the Schrödinger equation (3.85), to the requirement:

$$i \left| \dot{\Omega} \right\rangle = H(t) |\Omega\rangle + \dot{\phi} |\Omega\rangle . \quad (3.93)$$

Now, a holomorphic section in the line bundle over  $G/F$  is defined as the overlap  $\psi(\Omega) \equiv \langle \Omega | \psi \rangle$ , see eq. (3.65), so that its time variation is given by

$$\frac{d\psi(\Omega)}{dt} = \frac{d}{dt} \langle \Omega | \psi \rangle = i \left( \langle \dot{\Omega} | \psi \rangle + \langle \Omega | \dot{\psi} \rangle \right) . \quad (3.94)$$

Using the coherent dynamics property (3.93) for the first addend and again the Schrödinger eq. (3.85) for the second one, we immediately obtain

$$i d\psi = d\phi\psi , \quad (3.95)$$

or

$$(i d - d\phi)\psi = 0 , \quad (3.96)$$

where we have omitted the understood  $\Omega$ -dependence and substituted the total “time” variation with the differential operator “d”, in analogy with the geometric picture of adiabaticity, cfr. expression (2.111) in order to emphasize that (3.96) is a rule to parallel transport a section  $\psi$ . Indeed,  $(i d - d\phi) \equiv \nabla$  is a covariant derivative in the line bundle over  $G/F$ , with connection  $d\phi$  defined as, using eq. (3.86),

$$d\phi = i \langle \Omega | d\Omega \rangle - H_Q(\Omega) \equiv \mathcal{A}(\Omega) - H_Q(\Omega) , \quad (3.97)$$

and we dubbed

$$\mathcal{A}(\Omega) \equiv i \langle \Omega | d\Omega \rangle . \quad (3.98)$$

We recognize the latter expression (3.98) as the natural local connection one-form in the principal bundle generated by coherent states, namely the connection that gives rise to the so-called *canonical geometric phase* [26, 27]. The analogy with the geometric picture of an adiabatic evolution (2.111) is therefore apparent; the substantial difference resides in the presence of the  $Q$ -representation of the Hamiltonian  $H_Q(\Omega)$  which, besides entering the explicit expression of the covariant derivative, also defines the curve in the base manifold, whereas in the adiabatic framework such a curve was described by the  $a$

*priori* given time-dependence of the external parameters.

The direct extension of the concept of coherent dynamics to the composite case requires the assumption of a restrictive additional hypothesis, despite the structure of a physical state in such case is simply given by the tensor product with the Hilbert space of the principal system; recalling eq. (3.72) a physical composite state is a multicomponent section, namely  $\psi_\beta(\Omega), \{\psi_\beta\} : G/F \rightarrow L \otimes \mathbb{C}^N, \beta = 1, \dots, N$ . Let us now suppose that there exists a local observable  $A$  for the principal system commuting with the total Hamiltonian,  $[H, A] = 0$ , and let us label by  $\{|\alpha\rangle\}$  the set of its non-degenerate eigenvectors, which we also suppose to be a basis for  $\mathcal{H}_{\text{open}} \simeq \mathbb{C}^N$ ; such assumptions implies that, when  $H$  acts on a tensor product state of the form  $|\chi\rangle \otimes |\alpha\rangle, |\chi\rangle \in \mathcal{H}_{\text{env}}$ , it is

$$H |\chi\rangle \otimes |\alpha\rangle = |\alpha\rangle \otimes H_\alpha |\chi\rangle , \quad (3.99)$$

where the operator  $H^\alpha$  only acts on the environmental Hilbert space and depends on the eigenvalue  $\alpha$  relative to  $|\alpha\rangle$ ; moreover, since  $\alpha$  is real, it is easy to convince ourselves that the  $H_\alpha$ s are self-adjoint as the original Hamiltonian  $H$  was. Let us then suppose, as before, that the total Hamiltonian  $H$  is linear in the generators  $X_i$  of the environmental dynamical group  $G$ , so that the environmental operators  $H_\alpha$  are linear, too. Our simple task, given the above assumptions, is to derive the equation of transport of a generic component  $\psi_\alpha(\Omega)$  in the tensor product bundle over  $G/F$ , see eq. (3.72), the label  $\alpha$  pertaining to the basis  $|\alpha\rangle$  introduced a few lines above, namely

$$\psi_\alpha(\Omega) \equiv \langle \alpha, \Omega | \Psi \rangle = \sum_n c_{\alpha n} g_n(\Omega) . \quad (3.100)$$

where  $|\Psi\rangle$  denotes, as usual, a generic composite state  $\in \mathcal{H}_{\text{open}} \otimes \mathcal{H}_{\text{env}}$ . Putting all together, the existence of a conserved local observable for the principal system allows us to define, component by component, a coherent dynamics even in the composite system, by using the set of environmental “effective” Hamiltonians  $H_\alpha$  of eq. (3.99) as those generating the parallel transport of each component  $\psi_\alpha$  of the multi-component section defined from  $G/F$  to the tensor product bundle  $L \otimes \mathbb{C}^N$ . Indeed, eq. (3.99) implies that, when  $|\chi\rangle$  is an environmental coherent state  $|\Omega\rangle$ , we have, on one hand,

$$H |\Omega\rangle \otimes |\alpha\rangle = |\alpha\rangle \otimes H_\alpha |\Omega\rangle , \quad (3.101)$$

on the other hand, eq. (3.93) becomes

$$i \left| \dot{\Omega} \right\rangle = H_\alpha |\Omega\rangle + \dot{\phi}_\alpha |\Omega\rangle , \quad (3.102)$$



with the obvious notation (cfr. eq. (3.86))

$$\dot{\phi}_\alpha = \left\langle \Omega(t) \left| \left( i \frac{\partial}{\partial t} - H_\alpha \right) \right| \Omega(t) \right\rangle . \quad (3.103)$$

Therefore, the equation of parallel transport (3.96) becomes

$$(\text{id} - d\phi_\alpha) \psi_\alpha = 0, \quad d\phi_\alpha \equiv \mathcal{A} - H_{\alpha,Q} , \quad (3.104)$$

where  $\mathcal{A}$  is the local connection form for coherent states defined in eq. (3.98) and  $H_{\alpha,Q} = H_{\alpha,Q}(\Omega)$  is the  $Q$ -representation of each environmental Hamiltonian  $H_\alpha$ ; notice that the complete separation of the coherent dynamics due to the presence of the local conserved quantity also implies that the Hamiltonian flow itself in the base manifold  $G/F$ , eq. (3.87), now depends on  $\alpha$ , namely the classical equations of motion describe a different curve according to  $\alpha$ , as

$$\dot{\Omega} = \{H_{\alpha,Q}(\Omega), \Omega\}_{\text{PB}} , \quad (3.105)$$

where the poisson brackets, as before, are defined in eq. (3.55) by the coherent state construction itself.

From a general perspective, the existence of a local conserved quantity is a quite restrictive requirement, and it is sufficient to find the exact solution for the composite system dynamics; nevertheless, some important physical situations possess such property. For instance, in [46] an exactly solvable model is proposed to study decoherence[47], and it indeed is characterized by the presence of such a local conserved quantity; moreover, and not surprisingly, the solution to such particular case of study is achieved by the use of field coherent states (the environment is a collection of bosonic modes), substantially being an explicit usage of the ideas sketched above and summarized in eqs. (3.104)-(3.105). On the other hand, the existence of a preferential basis for the principal system suggests a possible way to extend such ideas to a more general framework, namely by making use of the *adiabatic* approach presented in section 2.2 and, in particular, the space-adiabatic one of paragraph 2.2.4. Roughly speaking, our idea is to replace the fixed and globally conserved set of projectors  $|\alpha\rangle\langle\alpha|$  relative to the local observable  $A$  with a set of approximately conserved projectors  $P_\alpha(\Omega)$ , now depending on the point  $\Omega$  in the phase space of the environment. Indeed, the space-adiabatic machinery for the molecular case, for instance, immediately provides such decoupling by making use of the spectral projectors of the electronic adiabatic Hamiltonian  $H_e$ , which in this case is singled out at sight and canonically in the structure of the composite Hamiltonian, cfr. eq. (2.135): in other words, the principal system “almost conserved” basis is the set of electronic eigenstates  $|\phi_{\mathbf{R}}\rangle$  relative to  $H_e$ , parametrically depending on the environmental position

**R.** Generalized coherent states, on the other hand, are labeled by a point on the *phase space*, so that a globally defined and separated differential representation like eq. (2.135) is impossible in the general case we are trying to tackle. Nevertheless, the adiabatic machinery can still be pursued on the curved phase space (rather than only on a configuration space, alike the molecular case) induced by the coherent state construction, by investigating the spectral properties of the  $Q$ -representation of the total Hamiltonian of the system (see [48] and references therein). The essential feature of such approach (and of similar ones, see, *e.g.*, [39]), is the coincidence of the adiabatic parameter with that ruling the classical limit; for a spin- $S$  particle, for instance (see, again, [48] and, in a different perspective, the next chapter discussion 4.2), it is the total spin eigenvalue  $S$  that rules both expansions. However, given the adiabatic basis for the principal system,  $|\phi_\alpha(\Omega)\rangle$ , the study of the resulting effective environmental dynamics formally falls within the framework of the so-called *multicomponent WKB approximation*[49] and receive a complete formal treatment in the context of geometric quantization (see, *e.g.*, [43]).

## Chapter 4

# An application: the Spin-Star Model

The general formalism we developed in the previous chapter 3, and especially the parametric representation involving the continuous identity resolution on the environment through generalized coherent states, finds an immediate but still rich and worthwhile application in the physics of composite (open) spin systems. There exists an enormous variety of physical systems, and consequently models and formal techniques to deal with the latter, that involves interacting spins, mainly spin- $\frac{1}{2}$ ; from our point of view, composite systems made up by a central central spin- $\frac{1}{2}$  interacting with a surrounding environment, that are usually referred to as “central spin models” [50–64], are of particular interest especially in the case where the environment is made up by spins, too, essentially for two reasons.

The first reason is a physical one, as this type of systems are often characterized by a strongly *correlated* behaviour, both between the central spin and its surroundings and among the constitutive elements of the latter, so that the formal schemes usually adopted to describe the dynamics of the open system (the central spin in this case), which we briefly depicted in the introductory chapter 1, are no more available or require a sensible improvement. Indeed, it is not surprising at all that numerical methods (also involving the exact diagonalization of the total system, when implementable[51]) are often preferred to an “open system-Markovian” approach. On the other hand, those of such systems for which an exact solution is available for some reason (either analytical or numerically-exact) can become the proving ground of the quite recent question concerning the degree of non-Markovian behaviour of a system[65], confirming the fact that the assumptions underlying the Markovian approximation are usually too restrictive to capture the essential phenomenology of such spin interactions and have to be strongly

modified (see, for instance, [66, 67]) since neglecting the “backward” flow of information from the environment to the central spin is, in such cases, a too drastic simplification. A systematic way to construct a beyond-Markov reduced dynamics is well known[3], but it may still result to be not necessarily profitable. Quite interestingly, a sort of “intermediate” approach, which in the literature is usually referred to as *correlated projectors technique* has been proposed and mainly adopted for central spin models[68–70]: indeed, it is very similar to the parametric representation as it relies on a resolution of the identity on the environment but still aims at devising a system of coupled master-like equations for the resulting components of the reduced density matrix<sup>1</sup>. Following this line of reasoning, the parametric representation

- is in principle an exact formalism and
- provides an intrinsic environmental structure,

so that, in general, it offers an alternative and more refined tool to deal with strongly correlated systems. In the specific case of the *spin-star model with frustration*[71, 72] we are going to present, moreover, the generalized coherent states construction finds its immediate non-trivial implementation, as the dynamical group pertaining to the environment is the “prototypical”  $SU(2)$ , represented onto a finite-dimensional Hilbert space, so that such model is a natural application of our formalism also from a mathematical point of view.

The chapter is devoted to such a physical application of the parametric representation obtained through generalized coherent states; in the first part 4.1, we present in detail the model and how the parametric representation behaves in the fully quantum set-up, while in the second part 4.2 the most immediate consequence of the choice of coherent states is investigated, namely we exploit the coherent state “bridging” properties between the quantum and the classical world to perform a classical limit on the environment, keeping intact the quantum nature of the central spin. The result of such approach will bring to light one of the most interesting results of this thesis work: we obtain a strict relationship between the entanglement of the original composite system and the Berry’s geometric phase possibly arising in the semiclassical approach.

## 4.1 The Spin-Star Model in parametric representation

The spin-star belongs to the large family of the so-called “central-spin” models; besides our particular motivations above summarized, these kind of models are in general of

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<sup>1</sup>and, of course, it would be quite interesting to study the connections between the latter and our parametric representation in the future, especially in the continuous case.

great interest since they describe magnetic interactions that play a relevant role in the physics of candidate future nanodevices[51, 73–79]. The term “spin-star” refers to the structure of the bipartition of a global system, made up by a certain number of spin- $\frac{1}{2}$ , into a central, “privileged” spin, which we will hereafter call *qubit* for the sake of clarity, interacting with *each* of the remaining spins that, in turn, form as a whole its environment and in general may or may not interact among themselves; the different possible choices of the interactions accordingly yield very diversified phenomenologies. In paragraph 4.1.1 we present in detail the model, specifying the terminology and the main known results about our particular case of study, while in the second paragraph 4.1.2 we will show how the parametric representation using generalized coherent states provides an original insight into its physical behaviour.

### 4.1.1 The model

The particular spin-star we adopt for implementing the coherent state parametric representation is essentially characterized by the presence of *frustration*. Indeed, the central qubit interacts with the surrounding spins *via* an antiferromagnetic Heisenberg uniform coupling  $g > 0$ , thus a configuration where each of the environmental spins is counter-aligned with respect to the qubit is energetically favoured; the environmental spins, in turn, are ideally disposed along a *ring* and each of them only interact with its (two) nearest neighbours, again *via* another antiferromagnetic Heisenberg coupling  $k > 0$ , eventually inducing frustration. In order to avoid frustration with the boundary conditions, the number  $N$  of environmental spins is taken even. Let us then denote the qubit spin operators by the symbol<sup>2</sup>  $\boldsymbol{\sigma}$ , while the environmental spin operators by  $\mathbf{s}_i$ ,  $i = 1, \dots, N$ ; the Hamiltonian of the frustrated spin-star thus reads:

$$H = H_{\text{qR}} + H_{\text{R}} , \quad (4.1a)$$

$$H_{\text{qR}} = \frac{2g}{N} \frac{\boldsymbol{\sigma}}{2} \cdot \sum_{i=1}^N \mathbf{s}_i , \quad (4.1b)$$

$$H_{\text{R}} = \frac{2k}{N} \sum_{i=1}^N \mathbf{s}_i \cdot \mathbf{s}_{i+1} . \quad (4.1c)$$

Notice that the coupling strengths are chosen to depend on the number of the external ring elements as  $\sim (N/2)^{-1}$  in order to keep finite the interaction energy in the environmental classical limit. Defining the total spin of the ring  $\mathbf{S} = \sum_i \mathbf{s}_i$ , it is immediately

$$H_{\text{qR}} = \frac{2g}{N} \frac{\boldsymbol{\sigma}}{2} \cdot \mathbf{S} . \quad (4.2)$$

<sup>2</sup>more precisely, it refers to the vector of Pauli Matrices  $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$  so that the spin operators for the qubit read  $\sigma_\mu/2$ ,  $\mu = 1, 2, 3$  in our overall  $\hbar = 1$  convention

The eigenvalues and eigenvectors of such model are easily deduced from the several integrals of motion present in this case; namely, introducing the total angular momentum

$$\mathbf{J} = \mathbf{S} + \frac{\boldsymbol{\sigma}}{2}, \quad (4.3)$$

it is immediate to see that

$$[H, \mathbf{J}^2] = [H, J_3] = [H_R, \mathbf{S}^2] = [H_R, S_3] = 0, \quad (4.4)$$

which are commutation relations proper to any Heisenberg Hamiltonian, and that

$$[H, H_R] = 0, \quad (4.5)$$

which is a particular feature of (4.1) also implying  $[H, \mathbf{S}^2] = 0$  by the Jacobi identity. The commutation relations (4.4)-(4.5) mean that the integrals of motion are, besides the total Hamiltonian  $H$ , the square of the total angular momentum  $\mathbf{J}$  together with its component  $J_z$  along an undetermined quantization axis  $\equiv \hat{z}$ , the square of the spin  $\mathbf{S}$  of the external ring and its Hamiltonian  $H_R$ , whose eigenvalues  $E, J(J+1), M, S(S+1), \frac{2k}{N}E_R$  thus label, respectively, the eigensystem relative to (4.1). Obviously, such eigenvalues are not independent, since by angular momentum addition it is

$$J = S \pm \frac{1}{2} \equiv J^{(\pm)}, \quad (4.6)$$

so that the whole eigensystem structure splits into two multiples, referring to the sign in eq. (4.6); the possible energies eigenvalue, that satisfy  $E = \frac{2k}{N}E_R + E_{qR}$  due to (4.1a), are consequently classified since (4.1b) depends on  $J$  as

$$H_{qR} = \frac{g}{N} \left( \mathbf{J}^2 - \mathbf{S}^2 - \left( \frac{\boldsymbol{\sigma}}{2} \right)^2 \right) \Rightarrow E_{qR} = \frac{g}{N} \left( J(J+1) - S(S+1) - \frac{3}{4} \right), \quad (4.7)$$

hence

$$E_{qR} = E_{qR}^{\pm} = \pm \frac{g}{N} \left( \tilde{S} \mp \frac{1}{2} \right), \quad (4.8)$$

accordingly to whether  $J = J^{(+)}$  or  $J = J^{(-)}$ , and where we defined  $\tilde{S} \equiv S + \frac{1}{2}$ ; eventually, the total energies are

$$E^{\pm} = \frac{2k}{N}E_R \pm \frac{g}{N} \left( \tilde{S} \mp \frac{1}{2} \right). \quad (4.9)$$

The quantity  $\frac{g}{N} \left( \tilde{S} \mp \frac{1}{2} \right)$  is strictly positive so that, for any fixed  $S$ , the “-” multiplet has lower energy than the “+” one, apart from the case  $S = 0$  which does not contribute to the “-” multiplet, and the greater  $S$ , the smaller  $E^-$  for a given  $E_R$ . Nevertheless, in order to really identify the ground state of the system, it is also necessary to investigate

the  $S$ -dependence of the ring energies: in this sense, it is sufficient to recall the Lieb-Mattis ordering[80] relation, that pertains to the *lowest* eigenvalue in each subspace with fixed  $S$  and reads

$$E_R(S) < E_R(S + 1) . \quad (4.10)$$

Such a relation eventually implies that, as a function of  $S$ , there is a competition between the two terms  $\sim kE_R$  and  $\sim -g\tilde{S}$  appearing in  $E^-$ , that is weighted by the so-called **frustration ratio**  $\equiv k/g$ : for low  $k/g$ , the negative interaction term  $-g\tilde{S}$  dominates, so that the maximum possible value of  $S = N/2$  is that yielding the ground state energy, and this remains true for

$$0 \leq \frac{k}{g} \leq \frac{1}{4} \equiv \alpha_0. \quad (4.11)$$

As the ratio  $k/g$  increases, there exists a sequence of critical values  $\alpha_n$ ,  $n = 1, \dots, (N/2 - 1)$ , such that the ground state has  $S = N/2 - n$  for  $\alpha_{n-1} < k/g \leq \alpha_n$ , and  $S = 0$  for  $k/g > \alpha_{N/2-1} \gg 1$ , implying that in the last case the ground state belongs to the  $E^+$  multiplet. Notice that the critical values  $\alpha_n$  depend on  $N$ , with the exception of  $\alpha_0$  which equals  $1/4$  for all  $N$ .

In any case, the energy eigenvalues do not depend on the eigenvalue  $M$  relative to the total angular momentum component along the quantization axis, as the Hamiltonian is rotationally invariant. Eigenenergies are thus degenerate in  $M$ , while the eigenvectors still display such a dependence: indeed, eigenvectors are labeled by  $E_R, J, S, M$  and, once expressed as composite states in the local bases for the qubit and the ring, are of the form:

$$|\Psi(E_R, J, S, M)\rangle = a |\uparrow\rangle \left| \Phi \left( E_R, S, S_z = M - \frac{1}{2} \right) \right\rangle + b |\downarrow\rangle \left| \Phi \left( E_R, S, m = M + \frac{1}{2} \right) \right\rangle , \quad (4.12)$$

where the ring states  $|\Phi(E_R, S, m = M \mp \frac{1}{2})\rangle$  denote the simultaneous eigenvectors of the ring operators  $H_R, S$  and  $S_z$ , and  $(|\uparrow\rangle, |\downarrow\rangle)$  are the qubit eigenvectors of  $\sigma_z/2$ . The form of eq. (4.12) is again due to the angular momentum addition relation, so that  $a, b$  are Clebsch-Gordan coefficients, and the  $J$ -dependence becomes simply that of the signs “ $\pm$ ” in eq. (4.6); eventually, eq. (4.12) can be more plainly written (ignoring the “mute” dependence on  $E_R$  and  $S$  as

$$|\Psi_M^\pm\rangle = a_M^\pm |\uparrow\rangle \left| m = M - \frac{1}{2} \right\rangle + b_M^\pm |\downarrow\rangle \left| m = M + \frac{1}{2} \right\rangle , \quad (4.13)$$

where the Clebsch-Gordan coefficients are

$$a_M^\pm = \pm \sqrt{\frac{1}{2} \left( 1 \pm \frac{M}{\tilde{S}} \right)}, \quad b_M^\pm = \sqrt{\frac{1}{2} \left( 1 \mp \frac{M}{\tilde{S}} \right)}, \quad (4.14)$$

immediately satisfying  $a_M^\pm = \pm b_M^\mp$ . It is convenient to define the discretized angle  $\theta_M \in [0, \pi]$  as  $\cos \theta_M = M/\tilde{S}$ , so that eq. (4.14) is equivalently written as

$$a_M^+ = \cos \frac{\theta_M}{2}, \quad b_M^+ = \sin \frac{\theta_M}{2}, \quad (4.15a)$$

$$a_M^- = -\sin \frac{\theta_M}{2}, \quad b_M^- = \cos \frac{\theta_M}{2}. \quad (4.15b)$$

In other words, for our future purposes the spin star eigenstates are just the eigenstates of the interaction part  $\sim \boldsymbol{\sigma} \cdot \mathbf{S} \sim \mathbf{J}^2 - \mathbf{S}^2$  as we ignore the explicit dependence on  $E_R$ ; it is worth pointing out that such states already display a Schmidt-decomposed form, so that it is immediate to see that they are all entangled states (with respect to the bipartition qubit - ring) except from the extremal states of the “+” multiplet, identified by  $M = \pm \tilde{S}$  or, equivalently,  $\theta_M = 0, \pi$ ; to this respect, the angle  $\theta_M$  can be interpreted as the latitude on a sphere that parametrizes the general form of the Schmidt decomposition when it involves a two-level subsystem, since the coefficients appearing in such case are only two, positive and whose square-sum equals one<sup>3</sup>. Moreover, in our case the Schmidt bases are defined as the local components of the angular momentum along the common quantization axis “ $\hat{z}$ ”, so that the parametrization in (4.13) *via* the angle  $\theta_M$  represents a rotation on a two-dimensional Hilbert space, and such a parametrization “overlaps” with the parametrization of the Bloch sphere of the qubit. In particular, the global state with  $\theta_M = 0$  (resp.,  $\theta_M = \pi$ ) is  $|\Psi^+(\theta_M = 0)\rangle = |\uparrow\rangle |m = S\rangle$  (resp.,  $|\Psi^+(\theta_M = \pi)\rangle = |\downarrow\rangle |m = -S\rangle$ ), corresponding to a configuration where the local spins  $\boldsymbol{\sigma}$  and  $\mathbf{S}$  are parallel at the north pole (resp., south pole) of the Bloch sphere. We shall see in the subsequent paragraph that the parametric representation with coherent states immediately provides a generalization of such interpretation for the remaining, entangled eigenstates.

Since the entanglement pertains to a pure, bipartite state, plenty of entanglement measures are available (see, *e.g.*, [4]); for instance, the Von Neumann entropy[2]  $\mathcal{E}$ , defined by

$$\mathcal{E} = -\text{Tr}(\rho \log_2 \rho), \quad (4.16)$$

where  $\rho$  is the reduced density matrix of either subspace of the bipartition, in the case of the Heisenberg eigenstates (4.13) is readily computed to be independent of the multiplet and amounts to:

$$\mathcal{E}_{\text{qR}} = -h \left[ \frac{1}{2} \left( 1 - \frac{M}{\tilde{S}} \right) \right] = -h \left[ \frac{1}{2} (1 - \cos \theta_M) \right], \quad (4.17)$$

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<sup>3</sup>the longitude of the sphere represents the relative phase between the two addends and is actually set to zero



where the function  $h$  is the binary entropy

$$h[x] \equiv x \log_2 x + (1 - x) \log_2(1 - x), \quad 0 \leq x \leq 1. \quad (4.18)$$

#### 4.1.2 Parametrizing the Spin-Star: $SU(2)$ coherent states

We are now able to apply the parametric representation through generalized coherent states (cfr. paragraphs 3.1.2-3.1.2.2) to the spin-star eigenvectors (4.13).

First of all, it is necessary to identify the environmental dynamical group  $G$ ; in this case, as we can ignore the local part  $H_R$  pertaining to the ring due to the structure of the states we want to parametrize, the only relevant term in the Hamiltonian is the interaction part  $H_{qR}$  of eq. (4.1b), that contains the three  $\mathfrak{su}(2)$  elements  $S_x, S_y, S_z$  representing the total spin of the ring, eventually yielding  $G = SU(2)$ , the environmental Hilbert space being its spin- $S$  representation. The natural choice of the reference state is that of the maximal weight state of the representation: for physical convenience, we choose as in [44]  $|\Phi_0\rangle = |m = S\rangle$  (with  $m$  eigenvalue relative to  $S_z$ ), so that the natural identifications with the Cartan basis (cfr. 3.1.2) are (maintaining for the sake of clarity the indexes “ $i$ ” and “ $\alpha$ ” even if they run over only one element per type)

$$H_i = S_z, \quad E_\alpha = S^+ \equiv S_x + iS_y, \quad E_{-\alpha} = S^- \equiv S_x - iS_y, \quad (4.19)$$

where we have identified the “positive” shift generator  $E_\alpha$  with  $S^+$  since  $|\Phi_0\rangle = |m = S\rangle$ , in accordance to the convention  $E_\alpha |\Phi_0\rangle = 0$  adopted before. The maximum stability subgroup  $F$  coincides with that generated by the Cartan element  $H_i = S_z$ , as

$$e^{i\mu S_z} |m = S\rangle = e^{i\mu S} |m = S\rangle, \quad (4.20)$$

that is,  $F = U(1)$ . The quotient group is therefore  $G/F = SU(2)/U(1) \simeq S^2$ , namely the two-dimensional sphere, and is in one-to one correspondence with generalized coherent states; indeed, the generalized displacement operator assumes the form<sup>4</sup>

$$D(\Omega(\eta)) = e^{\eta S^- - \eta^* S^+}, \quad (4.21)$$

where  $\eta$  is a complex number that parametrizes the sphere, being related to the usual polar angles  $(\theta, \varphi)$  as  $\eta = \frac{\theta}{2} \exp(i\varphi)$ . Eventually applying the generalized displacement operator (4.21) to the reference state, one gets (cfr. eq. (3.46)) the so-called  $SU(2)$

<sup>4</sup>omitting the “hats” used in chapter 3

coherent states, also referred to as *Bloch coherent states*:

$$|\Omega\rangle \equiv D(\Omega(\eta)) |m = S\rangle = e^{\eta S^- - \eta^* S^+} |m = S\rangle . \quad (4.22)$$

By construction, the  $SU(2)$  coherent state  $|\Omega\rangle = |\theta, \varphi\rangle$  is nothing but a rotation in the generic direction  $(\theta, \varphi)$  of the extremal state  $|m = S\rangle$ : irrespective to  $\varphi$ , the state with  $\theta = 0$  immediately gives back the latter, while the “opposite” state  $|m = -S\rangle$  is that with  $\theta = \pi$ .

The  $S^2$  sphere is described by a single complex coordinate, like  $\eta$  appearing in eq. (4.22), and the definitions (3.48) and (3.49) immediately yield in such case

$$z = \sin \frac{\theta}{2} e^{i\varphi}, \quad \tau = \tan \frac{\theta}{2} e^{i\varphi} ; \quad (4.23)$$

in turn, this implies that Bloch coherent states (4.22), when written in terms of the  $\tau$  coordinate, assume the form

$$|\Omega\rangle = \frac{1}{(1 + |\tau|^2)^S} e^{\tau S^-} |m = S\rangle \equiv N(\tau, \tau^*)^{-\frac{1}{2}} |\tau\rangle . \quad (4.24)$$

Eq. (4.24) mimicks the form of eq.(3.52), thus by confrontation it is

$$N(\tau, \tau^*) \equiv (1 + |\tau|^2)^{2S}, \quad |\tau\rangle \equiv e^{\tau S^-} |m = S\rangle , \quad (4.25)$$

and the function  $F$  that generates the metrics becomes (cfr. expression (3.51))

$$F(\tau, \tau^*) = \ln N(\tau, \tau^*) = 2S \ln(1 + |\tau|^2) . \quad (4.26)$$

We notice that the definition of the unnormalized form  $|\tau\rangle$  of coherent states of eq. (4.25) immediately displays their holomorphic character, as the exponential expansion only involves integer powers of the base manifold coordinates  $\sim \tau^k$ <sup>5</sup>. A straightforward calculation eventually shows that the identity resolution on the environmental Hilbert space (cfr. eqs.(3.53) and (3.60)) reads:

$$\mathbb{1}_{\mathcal{H}_S} = \int_{S^2} d\mu(\Omega) |\Omega\rangle \langle\Omega| = \frac{\tilde{S}}{2\pi} \int_{S^2} d\Omega |\Omega\rangle \langle\Omega| , \quad (4.27)$$

where  $d\Omega \equiv \sin \theta d\theta d\varphi$  is just the euclidean measure on  $S^2$ .

As a last step, in order to proceed with the parametric representation, the overlaps  $\langle\Omega|m\rangle$  with the environmental basis employed in the decomposition of the original state are needed; in the case of the states (4.13), such basis is that corresponding to  $S_z$ ,

<sup>5</sup>and in the transition functions of the associated line bundle the normalization factors cancels out, so that the holomorphic property is satisfied

that is the total environmental spin along the quantization axis, therefore also including the reference state  $|m = S\rangle$ . Thus, the overlaps are readily obtained by expanding the exponential in the initial definition of coherent states (4.22)

$$|\Omega\rangle = \sum_{m=-S}^S g_m^*(\Omega) |m\rangle, \quad (4.28)$$

where the coefficients  $g_m^*(\Omega)$  are expressed, for example as functions of  $(\theta, \varphi)$ , as

$$g_m^*(\Omega) = \sqrt{\binom{2S}{m+S}} \left(\cos \frac{\theta}{2}\right)^{S+m} \left(\sin \frac{\theta}{2}\right)^{S-m} e^{i(S-m)\varphi} \equiv \tilde{g}_m(\theta) e^{i(S-m)\varphi}, \quad (4.29)$$

where we singled-out the  $\theta$ -dependent part (which is real)

$$\tilde{g}_m(\theta) \equiv \sqrt{\binom{2S}{m+S}} \left(\cos \frac{\theta}{2}\right)^{S+m} \left(\sin \frac{\theta}{2}\right)^{S-m}. \quad (4.30)$$

Therefore,

$$\langle \Omega | m \rangle = g_m(\Omega) = \tilde{g}_m(\theta) e^{-i(S-m)\varphi} \quad (4.31)$$

Finally, applying the general formulas (3.73) and (3.79) with the identity resolution (4.27) and the overlaps given by (4.31), we obtain for the spin-star eigenstates (4.13):

$$|\Psi_M^\pm\rangle = \frac{\tilde{S}}{2\pi} \int d\Omega |\Omega\rangle \chi_M^\pm(\Omega) |\phi_M^\pm(\Omega)\rangle, \quad (4.32)$$

where

$$|\phi_M^\pm(\Omega)\rangle = \frac{a_M^\pm \tilde{g}_{M-\frac{1}{2}}(\theta) |\uparrow\rangle + b_M^\pm \tilde{g}_{M+\frac{1}{2}}(\theta) e^{i\varphi} |\uparrow\rangle}{\sqrt{\left(a_M^\pm \tilde{g}_{M-\frac{1}{2}}(\theta)\right)^2 + \left(b_M^\pm \tilde{g}_{M+\frac{1}{2}}(\theta)\right)^2}}, \quad (4.33a)$$

$$\chi_M^\pm(\Omega) = e^{-i(\tilde{S}-M)\varphi} \sqrt{\left(a_M^\pm \tilde{g}_{M-\frac{1}{2}}(\theta)\right)^2 + \left(b_M^\pm \tilde{g}_{M+\frac{1}{2}}(\theta)\right)^2}, \quad (4.33b)$$

and the coefficients  $a_M^\pm, b_M^\pm$  are defined in eqs. (4.14) or (4.15); notice that we decided to append the phase factor  $\exp(-i(\tilde{S}-M)\varphi)$  in the amplitude part (4.33b) by making real in all cases the coefficient relative to the  $|\uparrow\rangle$  component of the qubit parametrized states (4.33a). We remark that such a phase factor is inherited from the explicit definition of the coherent states  $|\Omega\rangle$  (4.28); since coherent states are, in turn, only sections over the sphere  $S^2$  (as discussed in general in paragraph 3.1.2.1), they are locally defined up a  $\Omega$ -dependent phase factor  $\exp(i\mu(\Omega))$ . This means that, in principle, the  $\varphi$ -dependence can be made vanish even in the amplitude  $\chi_M^\pm$  (while it is obviously absent in its square modulus) by choosing, for each global state,  $\mu(\Omega) = -(\tilde{S}-M)\varphi$ ; on the other hand, such a gauge redefinition is possible only locally in the base manifold coordinates, as

extensively discussed in the paragraph 2.2.3 about the emergence of Berry's phase.

The expressions (4.33) can be further simplified by making explicit use of eq. (4.30):

$$|\phi_M^\pm(\Omega)\rangle = \frac{1}{v_M^\pm(\theta)} \left( \frac{a_M^\pm}{b_M^+} \sin \frac{\theta}{2} |\uparrow\rangle + \frac{b_M^\pm}{a_M^+} \cos \frac{\theta}{2} e^{i\varphi} |\downarrow\rangle \right), \quad (4.34a)$$

$$\chi_M^\pm(\Omega) = v_M^\pm(\theta) \zeta_M(\theta) e^{-i(\tilde{S}-M)\varphi}, \quad (4.34b)$$

where we defined the functions

$$v_M^\pm(\theta) \equiv \sqrt{\left(\frac{a_M^\pm}{b_M^+} \sin \frac{\theta}{2}\right)^2 + \left(\frac{b_M^\pm}{a_M^+} \cos \frac{\theta}{2}\right)^2}, \quad (4.35a)$$

$$\zeta_M(\theta) \equiv b_M^+ \sqrt{\binom{2S}{S+M-\frac{1}{2}}} \left(\cos \frac{\theta}{2}\right)^{S+M-\frac{1}{2}} \left(\sin \frac{\theta}{2}\right)^{S-M-\frac{1}{2}}. \quad (4.35b)$$

Such a great simplification is essentially due to the fact that the open system considered is a qubit, so that in the local angular momentum bases the environmental states appearing in eq. (4.13) are labeled by only two  $S_z$  eigenvalues,  $m = M - \frac{1}{2}, M + \frac{1}{2}$ , that differ by one, also affecting the relative phase  $\exp(i\varphi)$  between the  $|\uparrow\rangle$  and  $|\downarrow\rangle$  in the qubit parametrized states (4.34). Moreover, by considering only the ground state multiplet, it is  $a_M^- = -b_M^+$  and  $b_M^- = a_M^+$  so that

$$v_M^-(\theta) = 1 \quad (4.36)$$

and, consequently,

$$|\phi^-(\Omega)\rangle = -\sin \frac{\theta}{2} |\uparrow\rangle + \cos \frac{\theta}{2} e^{i\varphi} |\downarrow\rangle \quad (4.37a)$$

$$\chi_M^-(\Omega) = \zeta_M(\theta) e^{-i(\tilde{S}-M)\varphi}, \quad (4.37b)$$

that is, the qubit parametrized states for the ground state multiplet do *not* depend on the total angular momentum  $z$ -component  $M$ . In order to better understand the physical picture emerging from the results (4.34) and, in particular, (4.37), let us recover the general interpretation of the parametric representation presented in paragraphs 3.1.1 and 3.1.2.2: a parametric representation of an open system (the qubit), given the pure state of the composite system is in (the spin-star eigenstate  $|\Psi_M^\pm\rangle$ , eq. (4.13)), provides a set of pure, normalized states  $|\phi_M^\pm(\Omega)\rangle$ , describing the open system, that depend on some environmental parameter (the point  $\Omega$  labelling the coherent state  $|\Omega\rangle$  the environment is in), whose occurrence is ruled by the probability amplitude  $\chi_M^\pm(\Omega)$ ,  $\int d\mu(\Omega) |\chi_M^\pm(\Omega)|^2 = 1$ . We want to remark that the dependence on the labels  $\pm, M$  has nothing to do with that characterizing the parametric representation, as they are quantities defining the specific, initial composite state; nevertheless, they deeply affect the qualitative behaviour of the description, as we shall see shortly after. The probability distribution  $\sim |\chi_M^\pm(\Omega)|^2$ ,

moreover, coincides with the  $Q$ -representation of the environmental reduced matrix or, in other words, gives a probability distribution for the environmental configuration  $\Omega$  which is correctly normalized *irrespective* to the open system state. On the other hand, an “indirect” effect of the qubit is still present: indeed, as testified by the very definition (3.73), the probability distribution  $\sim |\chi_M^\pm(\Omega)|^2$  depends on the same coefficients  $c_{\beta n}$  that pertain to the qubit; conversely if the ring were alone, the sum over  $\beta$  in (3.73) would have been absent, and the distribution  $|\chi(\Omega)|^2$  would have only depended on the coefficients describing the ring pure state.

In the specific case we are considering, the probability distribution does not depend on  $\varphi$ , namely  $|\chi_M^\pm(\Omega)|^2 = (v_M^\pm(\theta)\zeta_M(\theta))^2$ , cfr. eq. (4.34b); moreover, as the normalization condition does contain the measure  $d\mu(\Omega) = \frac{\tilde{S}}{2\pi} \sin\theta d\theta d\varphi$ , it is convenient to define the “latitude” probability distribution over  $\theta \in [0, \pi]$

$$p_M^\pm(\theta) = \tilde{S} \sin\theta (v_M^\pm(\theta)\zeta_M(\theta))^2, \quad \text{s.t.} \quad \int_0^\pi d\theta p_M^\pm(\theta) = 1. \quad (4.38)$$

We report in Fig. 4.1(a) the ground state environmental distributions  $p_M^-(\theta)$  for different values of  $M$  and  $S$ ; for each  $S$ , the values of  $M$  are chosen in order to always produce the four ratios  $\cos\theta_M = \frac{M}{S} = \frac{9}{11}, \frac{3}{11}, -\frac{3}{11}, -\frac{9}{11}$  that are in one-to-one correspondence with the angle  $\theta_M = \arccos \frac{M}{S}$ . The distributions are grouped according to the value  $\theta_M$ , each group being denoted by a different colour; notice that  $\theta_M$ , plotted as a vertical dashed line, approximately represents the center of each group of distributions. When the quantum character of the environment is reduced by increasing  $S$  and keeping the ratio  $\cos\theta_M$  fixed, it is immediately seen that the distributions become more peaked around  $\theta_M$ , resulting in turn narrower to preserve their integral over  $\theta$  (cfr. the next section 4.2). Moreover, we notice a shift of the maxima of the distributions with respect to  $\theta_M$  that become more evident for small  $S$  irrespective to  $M$  and for  $\left|\frac{M}{S}\right| \lesssim 1$ ; such shifts are the above mentioned indirect signature of the existence of the qubit, since on its own the function  $\tilde{g}_m(\theta)$  would be peaked around  $\theta = \arccos \frac{m}{S}$ ; in particular, by direct inspection of the initial expression (4.33b), in the ground state  $\tilde{g}_{M-\frac{1}{2}}$  and  $\tilde{g}_{M+\frac{1}{2}}$  are respectively weighted by  $\sin \frac{\theta_M}{2}$  and  $\cos \frac{\theta_M}{2}$ , so that for  $\theta_M \gtrsim 0$  the dominant function is  $\tilde{g}_{M+\frac{1}{2}}$ , while for  $\theta_M \lesssim \pi$  is  $\tilde{g}_{M-\frac{1}{2}}$ . Such effect in the excited multiplet is reversed, while the general  $S$ -behaviour (the smaller  $S$ , the greater the shift) is clearly maintained, as can be directly seen in Fig. 4.2.

The environmental probability distribution  $\sim |\chi_M^\pm(\Omega)|^2$  rules the occurrence of the qubit parameters appearing in eq. (4.33a) and also weight the local observables distribution as

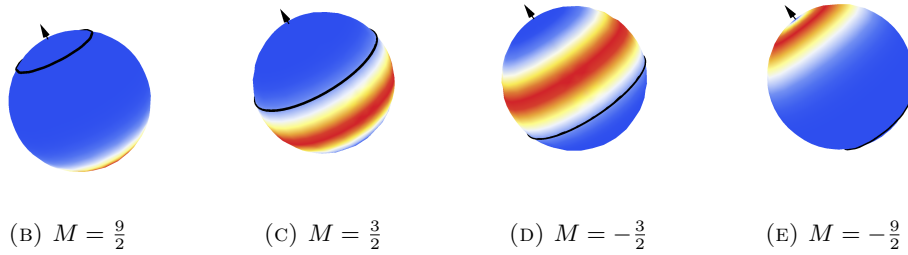
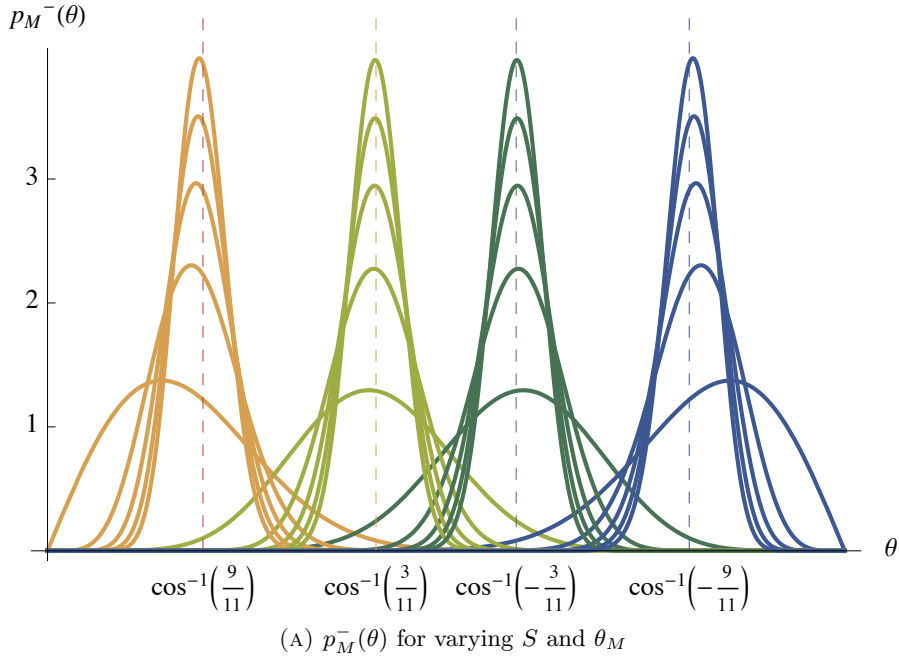


FIGURE 4.1: Environmental probability distributions for the ground state. Upper panel: latitude environmental distribution for the ground state multiplet  $p_M^-(\theta)$  for  $\frac{M}{S} = \frac{9}{11}, \frac{3}{11}, -\frac{3}{11}, -\frac{9}{11}$  (from left to right) and  $S=5,16,27,38,49$  (from below); the vertical dashed lines mark the corresponding values of  $\theta_M$ , each identified by a given color. Lower panel: qubit-states distributions,  $\pi_M^-(\pi - \theta, \varphi)$ , on the Bloch sphere for  $S = 5$  and  $\theta_M$  as in the upper panel. A black line of latitude marks  $\theta_M$  on each sphere, and the corresponding value of  $M$  is reported below.

in eq. (3.78). On the other hand, a generic two-level system pure state (ignoring its overall phase factor) can be represented as a point on the Bloch sphere, *via* the parametrization

$$|\phi(\Theta, \Phi)\rangle = \cos \frac{\Theta}{2} |\uparrow\rangle + \sin \frac{\Theta}{2} e^{i\Phi} |\downarrow\rangle \quad (4.39)$$

implying that the  $\sigma_z$  eigenstates correspond to  $\Theta = 0, \pi$ <sup>6</sup>; since in the case we are considering there is a single quantization axis  $z$ , so that all the polar angles so far introduced are defined with respect to such a physical direction, we can directly address the question of the relationship between the coordinates relative to the generic parametrization (4.39) and the parametrized states (4.34a) obtained from a specific composite state

<sup>6</sup>Again, the parametrization is only local as the coordinates  $(\Theta, \Phi)$  of the Bloch sphere are local.

$|\Psi_M^\pm\rangle$ . In the context of the parametric representation, such a relationship is an example of local observable probability distribution in the sense of the definition (3.78), with  $\hat{O} = |\phi(\Theta, \Phi)\rangle\langle\phi(\Theta, \Phi)|$ , with  $|\phi(\Theta, \Phi)\rangle$  given by eq. (4.39), and simply amounts to evaluate  $|\chi(\Omega)|^2 \sim p(\theta)$  in the Bloch sphere variables  $(\Theta, \Phi)$ . To this end, it is convenient to cast the parametrized states (4.34a) into the form (4.39) as

$$|\phi(\Theta_M^\pm, \Phi^\pm)\rangle = \cos \frac{\Theta_M^\pm(\theta)}{2} |\uparrow\rangle + \sin \frac{\Theta_M^\pm(\theta)}{2} e^{i\Phi^\pm(\varphi)} |\downarrow\rangle, \quad (4.40)$$

where we also admitted the two different identifications (the sign being again relative to the multiplet) between the longitudes

$$\Phi^+(\varphi) = \varphi, \quad \Phi^-(\varphi) = \varphi + \pi. \quad (4.41)$$

Thanks to such a choice, eq. (4.40) becomes for the ground state multiplet

$$e^{i\pi} \left( -\cos \frac{\Theta_M^-(\theta)}{2} |\uparrow\rangle + \sin \frac{\Theta_M^-(\theta)}{2} e^{i\varphi} |\downarrow\rangle \right) \quad (4.42)$$

and for the subsequent the overall “-” sign can be ignored. In this way, the Bloch sphere latitudes  $\Theta_M^\pm(\theta)$  are related to that of the coherent state  $\theta$  by

$$\tan \frac{\Theta_M^\pm(\theta)}{2} = \left( \tan \frac{\theta_M}{2} \right)^{\pm 1} \tan \frac{\theta_M}{2} \cot \frac{\theta}{2}. \quad (4.43)$$

Therefore, the environmental probability distribution  $p_M^\pm(\theta)$  can be represented over the Bloch sphere by solving eq. (4.43) with respect to  $\theta$ , and evaluating

$$\pi_M^\pm(\Theta) \equiv p_M^\pm(\theta(\Theta)) \quad (4.44)$$

In the ground state multiplet, eq. (4.43) immediately yields  $\theta = \pi - \Theta$  *irrespective* to  $M$ , and the Bloch sphere latitude distributions are simply  $\pi_M^-(\Theta) = p_M^-(\pi - \Theta)$ , namely they are symmetric to the original  $p_M^-$  with respect to the equator of the sphere<sup>7</sup>. They are reported as a color-gradient plot on the Bloch sphere  $(\Theta, \Phi)$  in Fig 4.1(b)-(e) below the corresponding  $p_M^-$  distribution (only for  $S = 5$ ), together with the corresponding parallel  $\theta_M$ .

Another interesting example of local distribution is that of a given  $\frac{\sigma_z}{2}$  eigenvalue; for example, the probability distribution to have  $\frac{\sigma_z}{2} = \frac{1}{2}$  is obtained by applying eq. (3.78)

<sup>7</sup>notice that, since that the probability  $p$  does not depend on  $\varphi$ , the longitudes identifications (4.41) are completely irrelevant. On the other hand, if one had simply put  $\Phi = \varphi$  also in the ground state multiplet, it would have been  $\Theta^- = \theta + \pi$ , making no sense as we want both  $\Theta$  and  $\theta$  lying in  $[0, \pi]$ .

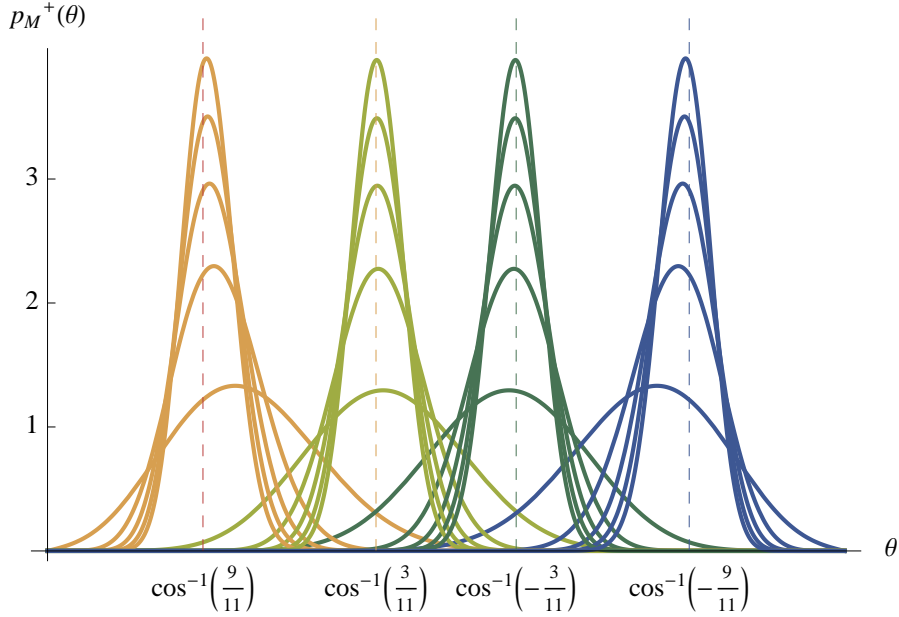


FIGURE 4.2: Environmental probability distributions for the excited state Latitude environmental distribution for the excited state multiplet  $p_M^+(\theta)$  with the same values of  $M$  and  $\tilde{S}$  as in Fig. 4.1

with  $\hat{O} = |\uparrow\rangle\langle\uparrow|$ , yielding

$$d\mu(\Omega) |\chi_M^\pm(\Omega) \langle \phi_M^\pm(\Omega) | \uparrow \rangle|^2 \sim d\theta p_M^\pm(\theta) \cos^2 \frac{\Theta_M^\pm(\theta)}{2} \equiv d\theta y_M^\pm(\theta; \uparrow), \quad (4.45)$$

where, the functions  $\Theta_M^\pm(\theta)$  are again given by (4.43), and we defined

$$y_M^\pm(\theta; \uparrow) \equiv p_M^\pm(\theta) \cos^2 \frac{\Theta_M^\pm(\theta)}{2}. \quad (4.46)$$

The  $\theta$ -integrated probability  $Y$  of measuring  $\frac{\sigma_z}{2} = \frac{1}{2}$ <sup>8</sup> is given by

$$(a_M^\pm)^2 = \text{Tr}(|\uparrow\rangle\langle\uparrow| \rho_q) \equiv Y \left( \frac{\sigma_z}{2} = \frac{1}{2} \right) = \int_0^\pi d\theta y_M^\pm(\theta; \uparrow) \quad (4.47)$$

with  $\rho_q$  being by construction the reduced density matrix of the qubit obtained from the global state  $|\Psi_M^\pm\rangle$ . In Fig. 4.3 we report the ground state distributions  $y_M^-(\theta; \uparrow)$  with  $M$  and  $S$  chosen as in Fig. 4.1(a); clearly, the distributions are not normalized and their integral consistently varies with  $M$  and  $S$  as  $(a_M^-)^2 = \sin^2 \frac{\theta_M}{2}$ . The behaviour of  $y_M^-(\theta; \uparrow)$  is easily understood as the result of the antiferromagnetic interaction that in the ground state tends to counter-align the qubit and the environmental spin: for small  $\theta_M$  the qubit has small probabilities of being directed towards the positive  $z$  axis since it tends to stay counter-aligned with respect to the environmental spin, which is in turn approximately peaked around  $\theta_M$ .

<sup>8</sup>namely, the usual quantum mechanical probability for a local observable



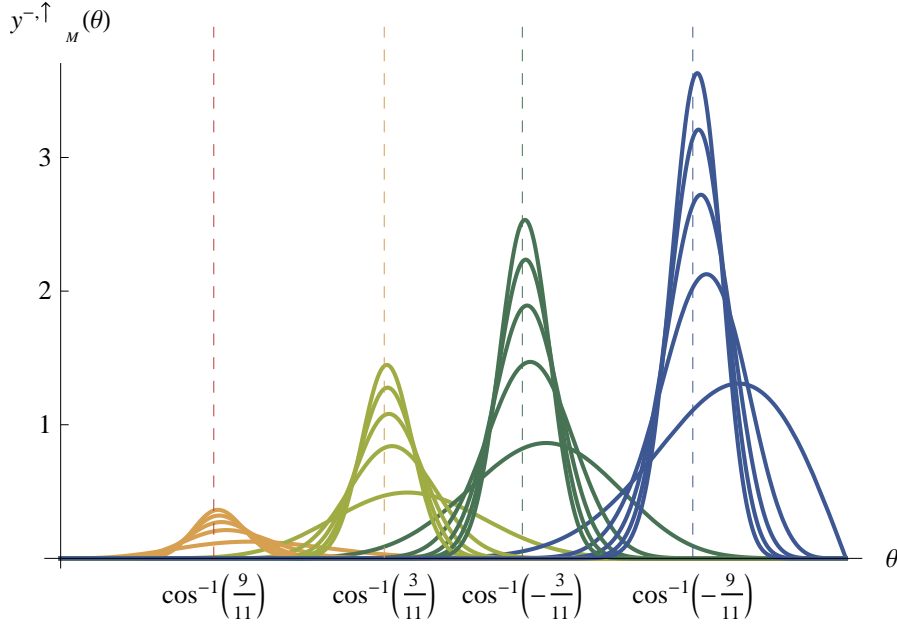


FIGURE 4.3: Local conditional probability distribution  
 Conditional probability distributions for the qubit to be in the  $|\uparrow\rangle$  state when the total system is in its ground state. Values of  $S$  and  $M/\tilde{S}$ , as well as dashed lines, as in Fig. 4.1.

Qubit parametrized states (4.34a) or (4.40) can always be viewed as eigenstates of an appropriately defined Zeeman Hamiltonian, of the form

$$H_Z(\hat{\mathbf{n}}) \sim \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}, \quad (4.48)$$

where  $\hat{\mathbf{n}}$  is the unit vector in real space relative to the direction of the Zeeman field. For each field direction, there is a positive and a negative energy eigenvalue (with the corresponding eigenstate) that only depend on the modulus of the interaction, while the eigenstates have angular dependence and are indeed opposite parametrization of the Bloch sphere (cfr. example 2.5); for instance, the state  $|\phi^-(\Omega)\rangle$  (4.37a) is exactly the negative energy eigenstate of  $H_Z(\theta, \varphi)$ , the field being embodied by the environmental coherent state direction  $(\theta, \varphi)$ , and is derived from the original negative energy multiplet. On the other hand, such a plain picture cannot be given for the excited multiplet states  $|\phi_M^+(\Omega)\rangle$ , since a further  $\theta_M$  dependence is present, preventing one to consider the “+” qubit parametrized states as the positive energy eigenstate of a single Zeeman term. Moreover, the positive and negative interaction energies (4.8) slightly differ in modulus. Nevertheless, we can always define a set of effectively local Zeeman Hamiltonians  $H_{Z,M}^\pm(\Omega)$  whose eigenvalues equal that of the global system and the corresponding eigenvectors be parametrized states originating from the appropriate multiplet by requiring

$$E_{\text{qR}}^\pm \equiv \left\langle \phi_M^\pm(\Omega) \left| H_{Z,M}^\pm(\Omega) \right| \phi_M^\pm(\Omega) \right\rangle \quad (4.49)$$

As for the ground state multiplet, we have just noticed that

$$H_{Z,M}^-(\Omega) = H_Z^-(\Omega) = |E_{\text{qR}}^-| \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}(\theta, \varphi) , \quad (4.50)$$

with  $\hat{\mathbf{n}}(\theta, \varphi) \equiv (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ , has  $|\phi^-(\Omega)\rangle$  as its negative energy eigenstate. For the excited multiplet, instead, we can exploit the parametrization (4.40) which is at sight the parametrization of a positive energy eigenstate for a field directed towards  $(\Theta_M, \varphi)$  to obtain

$$H_{Z,M}^+ = E_{\text{qR}}^+ \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}(\Theta_M, \varphi) . \quad (4.51)$$

In other words, since in general  $\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}(\Theta, \Phi) |\phi(\Theta, \Phi)\rangle = |\phi(\Theta, \Phi)\rangle$  (with  $|\phi(\Theta, \Phi)\rangle$  given by (4.39)), eq. (4.49) is satisfied by putting

$$H_{Z,M}^\pm(\Omega) = E_{\text{qR}}^\pm \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}(\Theta_M^\pm, \Phi^\pm) , \quad (4.52)$$

where the angles are those relative to the Bloch sphere parametrization (4.40) so that the relations with the coherent state variables are given by (4.41)-(4.43). The physical picture associated to eqs. (4.49)-(4.52) is, therefore, that when the star is in one of its eigenstates  $|\Psi_M^\pm\rangle$ , the central qubit behaves as if it were a *closed* system in a positive (or negative) eigenstate of a parametrically dependent Zeeman Hamiltonian, whose field direction is picked up by the coherent state configuration  $\Omega = (\theta, \varphi)$  through the function  $\hat{\mathbf{n}}(\Theta_M^\pm(\theta), \Phi^\pm(\varphi))$ ; the  $\Omega$  dependence, in turn, is weighted by the environmental probability distribution  $|\chi_M^\pm(\Omega)|^2$ . Moreover, eq. (4.49) provides a hint to extend the definition (3.78) from “genuine” local observables to *effectively local* ones. Namely, since the l.h.s. of eq. (4.49) does not depend on  $\Omega$ , nor should the r.h.s., so that one can safely multiply the latter by  $1 = \int d\mu(\Omega) |\chi(\Omega)|^2$ , obtaining

$$E_{\text{qR}}^\pm = \int d\mu(\Omega) |\chi(\Omega)|^2 \left\langle \phi_M^\pm(\Omega) \left| H_{Z,M}^\pm(\Omega) \right| \phi_M^\pm(\Omega) \right\rangle \quad (4.53)$$

which is exactly of the form (3.78), with  $\hat{O}_{\text{open}} = \hat{O}_{\text{open,eff}}(\Omega) = H_{Z,M}^\pm(\Omega)$ . In other words, all the interaction energy of the star is appended to the central qubit, provided that the effectively local Hamiltonians  $H_{Z,M}^\pm(\Omega)$  governing the qubit parametrically depend on the ring coherent state configuration  $\Omega$  and the star state labels  $(J, M)$  as in (4.52). In such effective description, the roles of the global configuration and that of the environment are not well separated, since in (4.52) both the functional form of the dependence on  $\Omega$  and the latter occurrence probability  $|\chi_M^\pm(\Omega)|^2$  do depend on the labels  $(\pm, M)$  identifying the star eigenstate  $|\Psi_M^\pm\rangle$ . In the next paragraph, however, we shall see that taking the classical limit for the environment implies a sharp simplification in the local effective picture but still keeping trace of the original quantum configuration.

## 4.2 The environmental classical limit: from entanglement to Berry's Phase

As anticipated, generalized coherent states provide a straightforward manner to perform the classical limit of the quantum system where they are defined. More precisely, the usual classical limit  $\hbar \rightarrow 0$  can be replaced in the treatment by rescaling the generators  $X_i$  of the dynamical group as  $X_i \rightarrow X_i/N$ , letting  $N \rightarrow \infty$ , where  $N$  is the “particle” number[81] (that is actually proportional to the dimension of the representation of the dynamical group  $G$ ), and expressing the operators of interest as a distribution over the phase space, for instance, the  $Q$  representation (the other representations differ by an ordering term that disappears in the classical limit). This is because, on one hand, the  $Q$  representation of an observable of the form  $\hat{O}(X_i/N)$  is generically expanded as a power series in  $1/N$

$$\left\langle \Omega \left| \hat{O} \left( \frac{X_i}{N} \right) \right| \Omega \right\rangle \equiv O_Q(\Omega) = O^{(0)}(\Omega) + \frac{1}{N}O^{(1)}(\Omega) + \dots \quad (4.54)$$

and the map  $\hat{O} \rightarrow O_Q$  is injective, so that the  $Q$  symbol characterizes entirely the operator[82]. On the other hand (when the generators are rescaled as above) the  $Q$  expansion (4.54) of the commutator of two observables  $A$  and  $B$  is related to the  $Q$  expansions  $A_Q$  and  $B_Q$  by (see, for instance, [49])

$$[A, B]_Q = i\{A_Q, B_Q\} + \mathcal{O}\left(\frac{1}{N}\right), \quad (4.55)$$

where the symbol  $\{\cdot, \cdot\}$  represents the Poisson brackets as defined in eq. (3.55), so that the classical observable algebra is achieved by  $N \rightarrow \infty$ . Therefore, by taking the limit  $N \rightarrow \infty$  in eq. (4.54) one has

$$O_{\text{cl}}(\Omega) \equiv \lim_{N \rightarrow \infty} \left\langle \Omega \left| \hat{O} \left( \frac{X_i}{N} \right) \right| \Omega \right\rangle = O^{(0)}(\Omega), \quad (4.56)$$

implying that the classical limit  $O_{\text{cl}}(\Omega)$  coincides with the first term  $O^{(0)}(\Omega)$ , called *principal symbol* of  $\hat{O}$ . In general, the  $Q$  representation (4.54) is evaluated by taking the  $Q$  representations of the various powers  $\sim (X_i/N)^k$  appearing in  $\hat{O}$ , and the principal symbol  $O^{(0)}(\Omega)$  is the only term containing the linear ones  $\sim X_i/N$ <sup>9</sup>, which are, in turn, the classical limits of the generators themselves. In the  $SU(2)$  case, for instance, the rescaled generators are

$$\left\langle (\theta, \varphi) \left| \frac{S_i}{S} \right| (\theta, \varphi) \right\rangle = \hat{n}_i(\theta, \varphi), \quad i = x, y, z \quad (4.57)$$

<sup>9</sup>while other powers  $\sim (X_i/N)^k$ ,  $k > 1$  contribute both to the principal symbol and subsequent terms.

where  $\hat{n}_i(\theta, \varphi)$  is, as usual, the  $i$  component of the unit vector pointing at  $(\theta, \varphi)$ .

As for the spin star (recall the Hamiltonian (4.1)), the classical limit for the environment is achieved by letting  $S \rightarrow \infty$ ; to this end, the number  $N$  of environmental spins has to go to infinity together with  $S$  with a fixed ratio  $S/N = 1/2$ . From a more physical perspective, the number of spins  $N$  is fixed; if it is also very large, the prescription of the limit is practically obtained by varying the frustration ratio  $k/g$ : in fact, as  $k/g$  decreases, the quantum character  $1/S$  of the system continuously lessens and eventually, for  $\frac{k}{g} \rightarrow \alpha_0 = \frac{1}{4}$ , the ground state of the system has the desired  $S = N/2$ . Notice that in the definition (4.1) the rescaling factor  $1/S = 2/N$  is already present, so that no further rescaling is needed. Before proceeding, it is worth to point out that in the formal construction recalled at the beginning of this paragraph (see eqs.(4.54)-(4.56)) the system undergoing the limit is isolated and the coordinates  $\Omega$  appearing in the classical description are phase space points, in principle undetermined; however, when the system is composite the situation dramatically changes since, for each given composite state, the  $\Omega$  occurrence is completely determined by the  $Q$  representation of the environmental density matrix: we already mentioned that  $\rho_{Q,\text{env}}(\Omega) = |\chi^2(\Omega)|$ , the explicit form in principle depending on  $M$ ,  $S$  and on the multiplet  $\pm$  that the original state  $|\Psi_M^\pm\rangle$  belonged to. In addition, recall that  $\int d\mu(\Omega)|\chi^2(\Omega)| = 1$  irrespective to the parameters  $M, S$ ; we are now going to show that

$$p_M^\pm(\theta) \xrightarrow{S \rightarrow \infty} \delta(\theta - \theta_M), \quad (4.58)$$

as already suggested by the shapes reported in Fig 4.1<sup>10</sup>. Before proceeding, it is worth to point out that the result (4.58) implies that in taking the limit we also admit that the quantum number  $M$ , since it is defined in the range  $[-S, S]$ , varies with  $S$ , and that we consider the ratio  $\cos \theta_M = \frac{M}{S}$  fixed. We shall return to this point later. Let us then recall that  $p_M^\pm(\theta) = \tilde{S} \sin \theta (v_M^\pm(\theta) \zeta_M(\theta))^2$ , with  $v_M^\pm$  and  $\zeta_M(\theta)$  defined in eq. (4.35); recall moreover, that  $v_M^- = 1$ . As for  $v_M^+$ , in the limit it will be  $v_M^+(\theta) = 1$ , as well, so that it is sufficient to concentrate on  $\zeta_M^2(\theta)$ : considering it as a function of  $x \equiv \cos \theta$  and proving that  $\mathcal{D}_{\tilde{S}}(x; \cos \theta_M) \equiv \tilde{S} \zeta_M^2(x) \rightarrow \delta(x - \cos \theta_M)$  will eventually imply the claim (4.58). Explicitly (we also dub  $\cos \theta_M \equiv x_0$ ), we have

$$\begin{aligned} \mathcal{D}_{\tilde{S}}(x; x_0) &= \frac{\tilde{S}}{2} (1-x_0) \binom{2\tilde{S}-1}{\tilde{S}(1+x_0)-1} \left[ \frac{1}{2}(1+x) \right]^{\tilde{S}(1+x_0)-1} \left[ \frac{1}{2}(1-x) \right]^{\tilde{S}(1-x_0)-1} = \\ &= \mathcal{C}(x; x_0) \tilde{S} \frac{(2\tilde{S})!}{[\tilde{S}(1+x_0)]! [\tilde{S}(1-x_0)]!} \left[ \frac{1}{2}(1+x) \right]^{\tilde{S}(1+x_0)} \left[ \frac{1}{2}(1-x) \right]^{\tilde{S}(1-x_0)} \end{aligned} \quad (4.59)$$

<sup>10</sup>only for the ground state, but the result (4.58) is valid also for the “+” one

where we defined

$$\mathcal{C}(x; x_0) \equiv \frac{1 - x_0^2}{1 - x^2} . \quad (4.60)$$

Using the Stirling formula to evaluate the factorials in eq. (4.59), we get

$$\mathcal{D}_{\tilde{S}}(x; x_0) = \mathcal{C}(x; x_0) \sqrt{\frac{\tilde{S}}{\pi(1 - x_0^2)}} \left[ \left( \frac{1+x}{1+x_0} \right)^{(1+x_0)} \left( \frac{1-x}{1-x_0} \right)^{(1-x_0)} \right]^{\tilde{S}} . \quad (4.61)$$

Now, the distributional definition of a Dirac delta is obtained as follows; let us put for convenience  $\varepsilon \equiv 1/\sqrt{\tilde{S}}$ , so that the classical limit is given by letting  $\varepsilon \rightarrow 0^+$ , and dub the divergent part  $\mathcal{I}_\varepsilon(x; x_0)$  in such a way that

$$\mathcal{D}_\varepsilon(x; x_0) = \mathcal{C}(x; x_0) \sqrt{\frac{1}{\pi(1 - x_0^2)}} \mathcal{I}_\varepsilon(x; x_0) , \quad (4.62)$$

that is

$$\begin{aligned} \mathcal{I}_\varepsilon(x; x_0) &\equiv \frac{1}{\varepsilon} \left[ \left( \frac{1+x}{1+x_0} \right)^{(1+x_0)} \left( \frac{1-x}{1-x_0} \right)^{(1-x_0)} \right]^{\frac{1}{\varepsilon^2}} = \\ &= \frac{1}{\varepsilon} \exp \left\{ \frac{1}{\varepsilon^2} \left[ (1+x_0) \log \frac{1+x}{1+x_0} + (1-x_0) \log \frac{1-x}{1-x_0} \right] \right\} . \end{aligned} \quad (4.63)$$

Expressing the last equality as a power series in  $x - x_0$ , the divergent part becomes

$$\mathcal{I}_\varepsilon(x; x_0) = \frac{1}{\varepsilon} \exp \left\{ -\frac{1}{\varepsilon^2} \frac{(x - x_0)^2}{1 - x_0^2} + \frac{1}{\varepsilon^2} \mathcal{O}(x - x_0)^4 \right\} . \quad (4.64)$$

The convolution of  $\mathcal{D}_\varepsilon$  with a generic test function  $f$  with support in  $[-1, 1]$  is therefore, in the classical limit  $\varepsilon \rightarrow 0^+$

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0^+} \int_{-1}^1 dx \mathcal{D}_\varepsilon(x; x_0) f(x) &= \lim_{\varepsilon \rightarrow 0} \int_{-1}^1 dx \frac{1}{\sqrt{\pi(1 - x_0^2)}} \mathcal{I}_\varepsilon(x; x_0) \mathcal{C}(x; x_0) f(x) = \\ &= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{\sqrt{\pi}} \int_{-\frac{1}{\varepsilon} \sqrt{\frac{1-x_0}{1+x_0}}}^{\frac{1}{\varepsilon} \sqrt{\frac{1+x_0}{1-x_0}}} dy \exp \{ -y^2 - \mathcal{O}(\varepsilon^2 y^2) \} \mathcal{C} \left( \varepsilon \sqrt{1 - x_0^2} y + x_0; x_0 \right) f \left( \varepsilon \sqrt{1 - x_0^2} y + x_0 \right) = \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} dy e^{-y^2} \mathcal{C}(x_0, x_0) f(x_0) = f(x_0) , \end{aligned} \quad (4.65)$$

where in the second equality we switched to the variable  $y \equiv \frac{1}{\varepsilon} \frac{x - x_0}{\sqrt{1 - x_0^2}}$ , and in the last one we used the definition (4.60) that gives  $\mathcal{C}(x_0, x_0) = 1$ , eventually proving the initial claim (4.58) since  $x_0 \equiv \cos \theta_M$ , and  $v_M^+(\theta = \theta_M) = 1$ .  $\square$

The nice result (4.58) means that, considering the spin-star composite system, the probability distribution ruling the coherent state latitude  $\theta$  collapse into a Dirac-delta that

sets its value to  $\theta_M$ , which in the limit is the latitude of the total angular momentum  $J$ , as there is no more distinction between  $J^{(+)} = S + \frac{1}{2}$  and  $J^{(-)} = S - \frac{1}{2}$ . In other words, the requirement  $\frac{M}{S} = \cos \theta_M = \text{const}$  coincides with the requirement that the total angular momentum  $z$ -component is finite in the classical limit.

As for this last issue, we still have to remark an important point: in our formal treatment, we set  $\hbar = 1$  and consistently rescaled the generators of the environmental dynamical group in order to obtain finite observables, instead of simultaneously letting  $S \rightarrow \infty$  and  $\hbar \rightarrow 0$  with  $S\hbar = \text{const}$ ; the reason of such choice is easily understood, as we want to perform the classical limit *only* on the environment keeping finite both the values of global and local observables; letting  $\hbar \rightarrow 0$  would have also implied to lose the quantum nature of the principal system. In this sense, the coherent state formalism allows us in this situation to have  $\hbar = 1$  but still define a consistent environmental classical limit. Indeed, let us now consider how the interaction Hamiltonians, both global and effectively local, are affected by such limit; the prescription (4.56) implies for (4.1b), on one hand (recall  $\frac{S}{N} = \frac{1}{2}$ ):

$$H_{\text{qR}} = \frac{2g}{N} \boldsymbol{\sigma} \cdot \mathbf{S} \xrightarrow{S \rightarrow \infty} H_{\text{lim}}(\theta, \varphi) = g \frac{\boldsymbol{\sigma}}{2} \cdot \hat{\mathbf{n}}(\theta, \varphi) , \quad (4.66)$$

its two eigenvalues consistently collapsing into

$$E_{\text{qR}}^{\pm} = \pm \frac{g}{N} \left( \tilde{S} \mp \frac{1}{2} \right) \xrightarrow{S \rightarrow \infty} \pm \frac{g}{2} \equiv E_{\text{lim}}^{\pm} . \quad (4.67)$$

On the other hand, the effectively local Hamiltonians (4.52), thanks to the relation (4.58) which sets  $\theta = \theta_M$ , becomes the *same* limit Hamiltonian

$$H_{Z,M}^{\pm}(\Omega) \xrightarrow{S \rightarrow \infty} H_{\text{lim}}(\theta_M, \varphi) = H_{\text{lim}}(\theta, \varphi) , \quad (4.68)$$

and the qubit parametrized states (4.34a) (starting from which the effectively local Hamiltonians were constructed), consistently collapse into the eigenstates of  $H_{\text{lim}}(\theta_M, \varphi)$ , the ones belonging to the “+” multiplet becoming its positive energy eigenstate, and *mutatis mutandis* the “-” one (and the same for the energies, again by construction):

$$|\phi^-(\Omega)\rangle \xrightarrow{S \rightarrow \infty} -\sin \frac{\theta_M}{2} |\uparrow\rangle + \cos \frac{\theta_M}{2} e^{i\varphi} |\downarrow\rangle , \quad (4.69a)$$

$$|\phi_M^+(\Omega)\rangle \xrightarrow{S \rightarrow \infty} \cos \frac{\theta_M}{2} |\uparrow\rangle + \sin \frac{\theta_M}{2} e^{i\varphi} |\downarrow\rangle . \quad (4.69b)$$

Let us now comment about the physical picture emerging from the results (4.66)-(4.69), recalling the assumptions we adopted to derive them; the global system in the fully quantum description (the spin-star) is in a given energy eigenstate  $|\Psi_M^{\pm}\rangle$ , characterized

by the quantum numbers  $M$  (or  $\theta_M$ ),  $S$  and  $J = J^{(+)}, J^{(-)}$ . The parametric representation of such composite state makes the central qubit to be still in an eigenstate of the effectively local Hamiltonians  $H_{Z,M}^{\pm}(\Omega)$ , eq. (4.52), in general depending on the global quantum numbers and on the environmental configuration  $\Omega$  in a non-trivial way. The occurrence of the configuration  $\Omega$  and of the corresponding qubit parametrized state are ruled by a probability distribution that contains the information about the reduced environmental density matrix through its  $Q$ -representation. The classical limit for the environment makes the latter collapse into a Dirac-delta centered on the angle  $\theta_M$  defining the initial eigenstate  $z$ -component of the total angular momentum, while the longitude  $\varphi$  is not affected as it does not enter the environmental probability distribution at all; the limit implies for the qubit parametrized states to be subjected to a “unique” Zeeman term whose spatial parameters  $(\theta, \varphi)$  are those of the environmental coherent state, but where only the latitude of the field is fixed by the global state configuration as  $\theta = \theta_M$ , whereas the longitude still remains arbitrary. Notice that starting from a *given* composite state  $|\Psi_M^{\pm}\rangle$  implies the choice of the quantization axis  $z$  in physical space, with respect to which the angle  $\theta$  is defined; consistently such a choice is still present in the description even after the environmental classical limit is taken, as the quantum nature of the qubit is preserved: in other words,  $\theta$  now represents the direction of the field with respect to the quantization axis of the qubit.

The content of the above discussion allows us to take our last step forward and relate the entanglement of  $|\Psi_M^{\pm}\rangle$  to the Berry’s phase emerging in the corresponding effectively-local model<sup>11</sup>. In particular, the fact that the field longitude is left undetermined in the local description implies that the qubit state may still change with  $\varphi$ , while the original global system state remains unchanged. These possible internal variations include the adiabatic precession of the field  $\hat{\mathbf{n}}(\theta_M, \varphi)$  (see eq. (4.66)) around the  $z$  axis, which gives rise, when closed paths are considered, to a Berry’s geometric phase that reads

$$\gamma_{\pm} = \mp\pi(1 - \cos\theta_M) , \quad (4.70)$$

where the  $\pm$  sign refers to the qubit that adiabatically follows the field being in the ground or excited state of  $H_{\text{lim}}(\hat{\mathbf{n}})$ . By a direct confrontation, the entanglement between the qubit and the ring when the star is in any of the states  $|\Psi_M^{\pm}\rangle$  is, from Eq. (4.17),

$$\mathcal{E}_{\text{qR}} = -h \left[ \frac{\gamma_{\pm}}{2\pi} \right] , \quad (4.71)$$

*i.e.* the binary entropy of the  $2\pi$  normalized Berry’ phase. Notice that, being  $h[x] = h[1 - x]$ , the dependence of the phase on  $\pm$  is not transferred into the entanglement, as it must be the case, according to eq. (4.17). Therefore, Berry’s phase appearing

<sup>11</sup>Recall paragraphs 2.2.2 and 2.2.3

in the effectively local model of a qubit in a field is a measure of the entanglement characterizing the eigenstates  $|\Psi_M^\pm\rangle$  from which it is derived through the environmental classical limit.

Let us further comment about the result (4.71): when we describe the physical scenario in terms of only one quantum system (the qubit), effectively reducing the environment to an external field which is treated at a classical level, we can no longer speak about entanglement (there cannot be entanglement if a system is not composite). However, thanks to the use of the parametric representation, the entangled structure of  $|\Psi_M^\pm\rangle$  causes the dependence on  $\varphi$  appearing at the fully-quantum level to be conveyed from the environment to the qubit, such a parametric dependence (that leads to the emergence of the Berry's phase) also surviving in the large- $S$  limit. To this respect, notice that  $\varphi$ -paths in the parameters space that give rise to no Berry's phase (the trivial ones  $\theta_M = 0, \pi$ ) derive from *separable* states in the original fully-quantum mechanical description. Generally speaking, the result embodied by eq.(4.71) pertains to the analysis of the relation between geometrical properties of quantum systems and the structure of their states[83, 84]. In order to accurately collocate this result in the overall picture, let us further comment upon its meaning. Evidently, geometrical effects may characterize the behaviour of a physical system when there is a space to be explored. So far, this was thought possible in two distinct physical setups:

1. a closed system, *i.e.* a system with a local parametric Hamiltonian, in which case the geometrical space is that of the Hamiltonian parameters;
2. an isolated system in a pure state that is not an eigenstate of its Hamiltonian; the state unitarily evolves accordingly and makes cyclic paths in the Hilbert space itself (the phase being called projective, or Aharonov-Anandan phase, see[85]).

Notice that the adiabatic motion of the external parameters induces a path in the Hilbert space of the closed system, so that the situation 2 formally includes 1. However, as for the results about the relationship between the entanglement of some bipartition and the geometric effects considered in the case 2[86–89], the explored Hilbert space is that of the *overall*, evolving system, and the geometric phase is the projective one pertaining to it. Such a “dynamical” setup is also adopted for obtaining non-Abelian generalizations of geometric phase[90], which have been applied to the case of mixed states undergoing both unitary and non-unitary evolutions [91, 92]. Moreover, from a more conceptual perspective, notice that in order for a system to be in a pure but not stationary state, it must have interacted, at some time, with another physical system, usually represented as an external apparatus. In such early stage of its dynamics the system cannot be modeled as isolated but, as we want it left in a pure state, we can describe it as closed,



which bring us back to the setup 1. From the above analysis, a somehow puzzling picture emerges when we consider an open quantum system which is part of an isolated system in a stationary state: studying the open quantum system by the effectively-local approach allows one to highlight possible geometrical effects which, on the other hand, appear to have no place in the description based on the reduced density matrix, as there is no geometrical space to be explored when the composite system from which it is derived is in a stationary state. At the same time, studying the open quantum system in terms of its density matrix allows one to highlight entanglement properties which, on the other hand, lose their meaning when the effectively-local approach is adopted, as there can be no entanglement with a classical environment. Therefore, neither of the above schemes can relate the entanglement between parts of an isolated system in a stationary state, with the geometrical effects arising in any of its parts. In the parametric representation, which is exact and still provides an interpolation between the two approaches, such a relating procedure becomes available as a crossover from a quantum to a classical environment, as embodied by eq. (4.71), thanks to the fact that the geometrical space for the open system is immediately provided by the environment itself, and that the environmental classical limit of a stationary global situation still allows for an internal effective variation of the parameters (no matter how the latter is achieved), weighted in addition by the entanglement of the initial composite state. Put in the converse way, the parametric representation offers a method to bring the entanglement into the effectively local description, at least whenever strict relations as (4.58) are obtained when performing the environmental classical limit.

As a final remark, we notice that, not surprisingly, the physical setup we consider for the emergence of Berry's phase is similar to that introduced in paragraph 2.2.4, see eq. (2.144), as the external parameters are also in that case quantum degrees of freedom for the environment, but some important differences have to be pointed out. In the molecular parametric representation, the environmental parameter space coincides with that of the nuclear coordinates  $\mathbf{R}$ , while in the generalized coherent states construction  $\Omega$  is a point of the phase space; therefore, in the former case there is a neat separation between the coordinates and the conjugated momenta, which are globally represented as the gradient  $\nabla_{\mathbf{R}}$ , while in the latter such separation is absent. As a consequence, the molecular setup allows the global Hamiltonian to be written in the separated form (2.135), where the electronic part  $H_e(\mathbf{R})$  induces the parametrization of the adiabatic eigenstates  $|\phi(\mathbf{R})\rangle$ , and the kinetic energy term is that responsible for the emergence of Berry's phase in the nuclear effective Hamiltonian; this is not possible for the spin Hamiltonian (4.1b), as a differential representation of the generators (see again [35]) is only locally defined in  $G/H$  and still not provides a separated form like (2.135). The analogy with the molecular case comes out back when considering the environmental

classical limit, since the explorable parameter space is again a one dimensional space (the circle), thanks to  $\theta = \theta_M$ , embedded into the two-dimensional phase space (the  $S^2$  sphere), so that the former can be considered as a “coordinate” space<sup>12</sup>.

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<sup>12</sup>notice, however, that we do not define an environmental effective Hamiltonian, nor the Berry’s potential, since it is not necessary in order to evaluate the Berry’s phase in the limit closed model, and that it is Berry’s phase the quantity entering (4.71)

## Chapter 5

# Conclusions and future perspectives

In this thesis work we propose a method to study the behaviour of an open quantum system, called *parametric representation*. The parametric representation provides a formalism to describe the state of the open quantum system under investigation taking into account the structure of the surrounding quantum environment if the state of the composite system “open quantum system+environment” is known. The description is axiomatically exact and associates to the principal system a set of pure states, parametrized by the environmental degrees of freedom, each of the pure states occurring together with an amplitude that is related to the probability for the open system to be actually described by that given pure state. Such set of amplitudes, on the other hand, also describes the occurrence of the environmental state associated to the actual value of the parameter contemporarily describing the environment and appearing in the principal system state, irrespective to the latter configuration. The parametric representation, moreover, provides an extension of the usual reduced density matrix formalism as, firstly, it can naturally reproduce the correct set of expectation values for any local observable and, secondly, allows one to associate to the latter a local probability distribution in the variable representing the environment, the expectation values resulting to be an integrated version of such distribution, in the same way the reduced density matrix proves to be an integrated version of the parametric representation of the open system. The formalism is completely general, as it can deal with any state of an isolated composite system, and its actual implementation displays a diversified behaviour according to the choice of the parametric structure of the environment; a surplus value in the description is achieved once the variable embodying the environmental degrees of freedom is continuous, and in particular when coherent states are adopted. Indeed, without spoiling the applicability of the formalism to whatever physical situation pertaining to the open

quantum system scenario thanks to a construction of general validity based on group-theoretic arguments, the usage of coherent states provides a canonical parametrization which is particularly useful in the understanding of the quantum-to-classical crossover of the environment. Moreover, the formal character of the coherent state construction immediately provides a natural geometric framework for the overall description.

As a first direct outcome, this thesis work clarifies why modelling a quantum system with a parametric Hamiltonian implies the existence of an environment ("the rest of the Universe" to use Berry's words[19]) which in principle must be derived as a proper classical limit of some underlying fully quantum theory, and it shows that a non-trivial parametric dependence can arise if and only if such environment is entangled with the system itself. One of the most relevant consequences of the above statement is that the emergence of observable (*i.e.* gauge-invariant) quantities which are not eigenvalues of Hermitian operators of the system under analysis, such as the Berry's phase, turns out to be related not only to the fact that an environment exists [93], but specifically to the condition that the system be entangled with its environment. Considering the paradigmatic case of the Heisenberg spin-star model as our first application of the parametric representation with generalized coherent states, the above stated claims manifest themselves in a natural and deep fashion. In fact, an explicit and strict relation between the entanglement characterizing the composite state of the fully quantum mechanical setup and the Berry's phase possibly arising in the local model obtained from the environmental classical limit of the former is established: the entanglement results to be the binary entropy of the  $2\pi$ -normalized Berry's phase, which suggests a possible way to experimentally access the entanglement properties *via* the observation of gauge-invariant phases.

Regarding the future perspectives the parametric representation opens, the general applicability of the formalism allows one to deal with phenomena that manifest themselves and can be interpreted very differently depending on the way the environment is modelled, not only in physical (see for instance Refs.[46, 94, 95]) but also in chemical and biological processes[96–98], especially in the context of the study of quantum correlations and decoherence. In particular, the large amount of physical situations whose description belongs to the spin-boson model family is immediately amenable of such a formal treatment as the generalized coherent states for the environment would actually coincide, in such case, with the usual and well-known field coherent states.

In the considered example of the spin- $\frac{1}{2}$  star with frustration, the quantum-to-classical crossover of the environment can be achieved by varying the frustration ratio between the couplings, paving the way to an experimental analysis of our results; indeed, it is worth mentioning in such context that the capability of tuning the interaction parameters

is recognized as one of the key features of quantum simulators (see e.g. Ref.[99] and references therein, and Refs.[100, 101]), so that we think that an experimental control on the value  $S$  ruling such a crossover could be possible. Moreover, different types of interaction between the environmental spins still define exactly solvable models[102] that can be treated in the same framework here proposed, in particular the antiferromagnetic Lieb-Mattis and Heisenberg-on-a-square-lattice ones, thus expanding the set of real (or simulated) physical systems where to look for a possible experimental analysis of our results.

Finally, it would be interesting to examine in depth all the dynamical aspects regarding the parametric representation; in particular, the adoption of generalized coherent states, besides opening the possibility of using established approaches for dealing with quantum dynamics in phase space, such as the the path-integral formalism, the adiabatic perturbation theory, the Born-Oppenheimer approximation, and generalizations to curved phase spaces of multi-configurational Eherenfest methods[15, 16, 26–28, 55, 103], puts the description of any open quantum system in a definite geometrical framework. Thus, non-local aspects of open quantum system dynamics, such as, for instance, the problems related to the non-Markovianity[65] of the dynamical map, may acquire in the geometric setting provided by the coherent states parametric representation a more natural and deeper interpretation.



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